Modelling CO_2 Transport and the Effect of Impurities: A New Equation of State for CCS Pipeline Transport

A thesis submitted to the University of Nottingham
for the degree of Doctor of Engineering

Thomas Alexander Demetriades

Supervisors: Prof. Trevor Drage, Dr. Richard Graham

June 2014

"If you want to get from A to B
I'll give you this advice for free:
You'll find that cycling in the snow
Is not the quickest way to go!"

— Colin McNaughton

Acknowledgement

I am fortunate to have enjoyed a multitude of fantastic experiences whilst working on this EngD, having spoken with many interesting people, having had the opportunity to travel far–and–wide, and having found a niche for my skills. There have been good times that I shall remember with fondness, and tough times that I will try to use to make myself better. My journey has been an enjoyable one, and I cannot believe this part of my life is over already.

I am particularly indebted to RWE nPower and RCUK, whose funding provided the opportunity for me to conduct this research, and to my supervisors Dr. Richard Graham and Prof. Trevor Drage, whose scholarly input and gentle guidance over the course of four years have permitted me to produce this thesis. I am truly grateful for having been allowed to draw on your extensive experience and expertise, from which I have learned many valuable lessons that were applied in this EngD, and hopefully which I will be able to take with me beyond its conclusion. I can only imagine the turmoil you two must have gone through during this time in trying to keep me focussed and on track! This thesis is an unfair reflection of your constant patience and kindness in dealing with me, and anything good about it is undoubtedly down to your calm and thoughtful input, whilst anything that is found to be lacking wholly down to me.

To my parents Elaine and Drosos, who always ensured I had everything I needed to allow me to reach this point. You have given me the foundation to jump into the rest of my life having enjoyed the most wonderful start. I only hope I can do you two justice.

Finally, I add my deepest thanks of all to my best friend; my constant companion; my soul–mate; and my most worthy adversary; Emma, soon to become my wife. Your love and support, the inspiration I get from you every day, and your help in reminding me what I was trying to achieve when I occasionally lost sight of my aims, have in no small part contributed towards me completing this work.

My acknowledgement is a very poor tribute to all of you, so difficult is it for me to adequately express what you have given me every day for so many years. But please know that throughout my journey, I have always felt your constant love and support, and I have never allowed myself to take for granted the sacrifices you have made for me. For allowing me to reach this pinnacle, I shall always remember these things with a profound sense of gratitude.

Abstract

In this EngD project I developed a new, analytic equation of state for use in the area of CCS pipeline transport. It was my aim to design a model which would exhibit a high degree of accuracy within the anticipated window of operation of CCS pipelines; from 260 to 335K and 1 to 200bar, whilst simultaneously retaining a simplicity and ease–of–use, a lack of which made some other available equations particularly unwieldy. Having conducted a comprehensive literature review and attended many academic and industrial conferences throughout this project, I felt that there was a need for an equation of state which could perform both these functions. This was the key motivation for my work, and the model presented in this thesis was developed in order that it might contribute towards negating the many concerns that currently surround the pipeline transport stage of CCS.

I aimed for the proposed model to display a complexity approaching that of some of the simpler equations currently available, whilst incorporating sufficient flexibility to give thermodynamic predictions to a standard approaching that of those which are more complicated. I defined criteria by which the proposed model could be judged, so that it could be applied with confidence in the determination of the physical properties of carbon dioxide mixtures during CCS pipeline transport.

Work was carried out by fitting the parameters of the proposed model to experimental data gathered from the literature, so that it would be able to determine the homogeneous phase pressure and vapour–liquid equilibrium behaviour of carbon dioxide and other relevant gas mixtures. The project yielded a number of excellent outputs, not least the satisfaction of the primary aim which was the proposal of a model, which through this EngD, I demonstrated had the ability to meet the demands that were set. In carrying out this work, I also developed several highly useful auxiliary mathematical methods which helped in ensuring the proposed model was as accurate as possible.

For the case of modelling pure carbon dioxide, the proposed equation worked exceptionally well, providing highly accurate predictions for homogeneous density and vapour liquid equilibrium, which were well within the targets set. A paper on this was published in May 2013. In extending the model to incorporate some binary mixtures I again found that it demonstrated a clear ability to capture the necessary physical behaviours within the target range. I concluded with suggestions as to ways in which the work presented here could be developed further, as well as the many avenues for future work in other areas that this EngD project had opened up.

List of Figures

List of Tables

List of Mathematical Nomenclature

a	Model parameter for the proposed equation of state
b	Model parameter for the proposed equation of state
c	Model parameter for the proposed equation of state
d	Model parameter for the proposed equation of state
e	Model parameter for the proposed equation of state
f	Model parameter for the proposed equation of state
f	Fugacity
g	Model parameter for the proposed equation of state
G	Gibbs free energy
m	Total mass of a system
M_{r}	Molecular mass
N	Total number of moles in a system
N_i	Total number of moles of substance i
N_{rest}	Total number of moles of all substances other than i
P	Pressure
P_{c}	Critical pressure of carbon dioxide unless otherwise specified
P_{vap}	Vapour pressure; that at which the bubble and dew points occur
R	The universal gas constant
S	Entropy
T	Temperature
T_{c}	Critical temperature of carbon dioxide unless otherwise specified
u_i	Bubble point molar volume for substance i
U	Internal energy
v	Molar volume
v_{BP}	The volume at which the bubble point occurs
v_{c}	Critical molar volume of carbon dioxide unless otherwise specified
v_{DP}	The volume at which the dew point occurs
v_{t}	Typical molar volume of carbon dioxide unless otherwise specified
V	Total volume of a thermodynamic system
w_i	Dew point molar volume for substance i
W	Weighting constant
x	Concentration in the liquid phase
y	Concentration in the vapour phase
Z	Compressibility factor
Z_c	Critical compressibility factor of carbon dioxide unless otherwise specified
Γ	Coexistence constraint
μ	Chemical potential
ξ_{BP}	Bubble constant
ξ_{DP}	Dew constant
ρ	Density
Υ	Dew ratio
ϕ	Fugacity coefficient
χ_{DP}	Critical constant
ω	Acentric factor
*	Used to denote a dimensionless quantity
$\tilde{}$	Used to denote an estimated quantity

Acronyms and Abbreviations

Ar	Argon
BP	Bubble Point
CAT	Carbon Abatement Technology
CCS	Carbon Capture and Storage
CH_4	Methane
CO	Carbon Monoxide
CO_2	Carbon Dioxide
DP	Dew Point
EOR	Enhanced Oil Recovery
EoS	Equation of State
GHG	Greenhouse Gas
H_2	Hydrogen
H_2S	Hydrogen Sulfide
Hg	Mercury
IEA	International Energy Agency
IGCC	Integrated Gasification Combined Cycle
IGL	Ideal Gas Law
LCO_2	Liquefied Carbon Dioxide
LIN	Liquefied Nitrogen
LNG	Liquefied Natural Gas
N_2	Nitrogen
NIST	National Institute of Standards and Technology
NO_x	Nitrogen Oxide
O_2	Oxygen
ppb	parts per billion
ppm	parts per million
PR	Peng–Robinson (Equation of State)
RK	Redlich–Kwong (Equation of State)
SATP	Standard Ambient Temperature and Pressure
SO_x	Sulphur Oxide
SRK	Soave–Redlich–Kwong (Equation of State)
SW	Span–Wagner (Equation of State)
VdW	Van der Waals (Equation of State)
VLE	Vapour–Liquid Equilibrium

Contents

Chapter 1

Establishing the Need for a New Equation of State

1.1 Environmental Concerns

"'Business as usual' emissions will take greenhouse gas concentrations and global temperatures way beyond the range of human experience. In the absence of action, the stock of greenhouse gases in the atmosphere could more than treble by the end of the century" [1].

The acceleration in industrialisation of the world's major economies since the middle of the twentieth century has been facilitated by energy from coal–fired power stations and other heavy industry. Until very recently, energy extraction from fossil fuels was neither a clean, nor particularly efficient process, and the damage being done to the environment, encompassing all manner of habitable locations and natural resources needed for the sustenance of life and biodiversity, through the emission of greenhouse gases from large–scale power generation and other heavy industry has begun to be more fully understood [2]. In particular, a strong link between global warming and the release of carbon dioxide (CO_2) during power generation has been identified [3]:

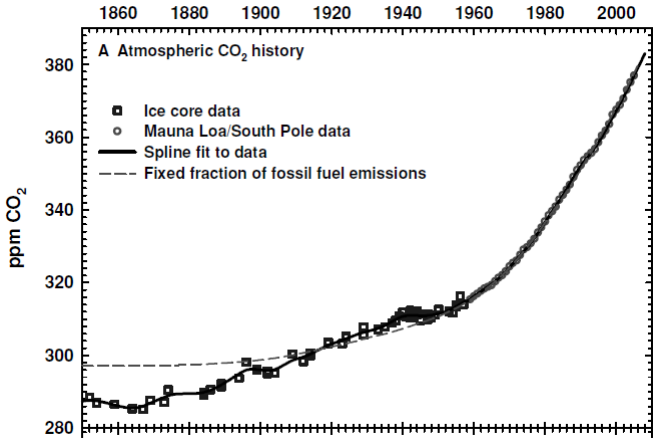

Figure 1.1: Rising levels of atmospheric carbon dioxide

In recent times the first readings of 400ppm atmospheric carbon dioxide have been recorded [4] (see Figure 1.1), signifying that we are now at a watershed moment in terms of the well–being of our atmosphere, and consequently, that a change is urgently needed. Targets of keeping global temperature rises to less than 2°C above 1990 levels by 2050 [5] necessitate that abatement of emissions of all greenhouse gases, of which carbon dioxide is the most abundantly emitted, should become a priority [6].

1.1.1 A Problem Needing A Solution

It is widely agreed that the situation with regard to greenhouse gas emissions from power generation is not sustainable [7]. Targets for an 80% reduction of carbon dioxide emissions by 2050 [6] have resulted in an impetus for investigation into new power generation techniques [5, 6]. It has also partly been due to an awareness that there is an ever–increasing gap between the demand for energy and the capacity of existing power generation facilities. Questions have been raised about the sustainability of previous fossil–fuel power generation methods [8], in terms of their economic viability [1, 9], in terms of preserving resources [10], and in terms of environmental sustainability [8].

In particular, it has become clear that the problem of combating the climate change brought about by industrial–scale power generation and heavy industry such as steel manufacture and cement works is no longer simply a technological one [11]. It incorporates very important considerations including regulatory implementation, economic and financial management, and sociological responsibility. The difficulty of finding a simultaneous solution to the apparently contradictory targets of en-

suring energy security [8], keeping costs low [1], and maintaining carbon emissions reductions [12, 4] forms the basis of this 21st–century energy concern.

The problem stems from the fact that we find ourselves committed to gaining a large proportion of our energy from fossil fuels [11]. Using the combustion of coal, oil and natural gas is such a well–established method of energy extraction that it poses an immense challenge in order to radically alter our habits and obtain energy from a different source. One problem is that although more environmentally friendly and sustainable methods of energy extraction such as wind, tidal and solar power have potentially huge capacity, they are currently nowhere near as dependable as fossil–fuels [13]. Additionally, hopes pinned on the long–term viability of nuclear power have yet to be proven [14], especially in the wake of the Fukushima disaster in March 2011 [15]. As such, relying entirely on any of these alternative technologies could leave massive energy shortfalls. As things stand therefore, these methods are, despite extensive research and development programmes, unsuitable for anything other than contributing small amounts to the overall generation of power.

Of course, it is inevitable that one day, any dependence on fossil fuels will have to cease, as the stock of resources starts to dwindle [11]. On the other hand, it is a reality that for the foreseeable future, while the alternative technologies which one day will provide the entirety of our energy are developed; a process expected to take decades, that the majority of our energy will have to continue to come from fossil fuel sources [10]. It is imperative therefore that during this time, far better use of what is available will have to be made, in terms of efficiency of generation, in terms of reduction of use, and by the minimisation of the environmental impacts associated with its continued and widespread use. These aims appear contradictory, as it would seem to be self–evident that the ability to reduce the environmental impact of power–generation should come at the cost of either reduced efficiency of the overall energy production process, or increased cost to the end user [16].

The reconciliation of the many differences in the necessary requirements of on–going and new generation methods will have to be implemented in such a way as to ensure a long–term viability. Specifically, any medium–to–long term solution which could allow for continued energy extraction from our most abundant energy sources, without the dogmatic long–term disintegration of the Earth's ability to support life, would be of tremendous value.

1.1.2 Carbon Capture and Storage

Carbon Capture and Storage (CCS) is one of the key strategies whose aim is reducing the emissions of Green House Gases (GHG). It is seen in particular as a key carbon abatement technology (CAT), by which it is hoped that the rising levels of carbon dioxide emissions with which we associate environmental destruction can be mitigated [17]. Its place as a one of the main strategies for carbon abatement is highlighted by the International Energy Agency (IEA) Blue map, and its importance is highlighted by being mentioned alongside technologies such as nuclear power and biomass, or strategies such as efficiency improvements [17]. Broadly speaking, CCS aims to do this by taking the emitted carbon dioxide and storing it underground. In its most simple form, CCS may be considered a five stage process (see Figure 1.2) whereby these damaging emissions are captured and isolated from the environment [2].

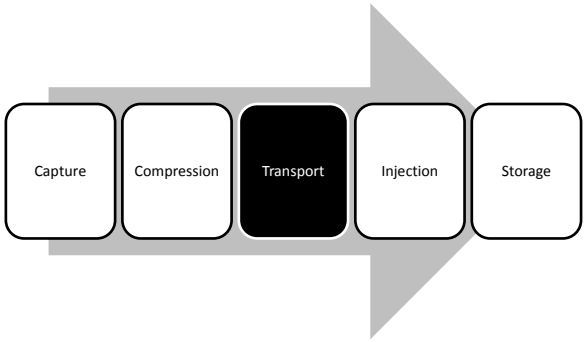

Figure 1.2: The CCS Chain with the transport stage, which is the technical focus of this research project, highlighted

With much development of the underlying technical understanding and of the contextual issues to do with this new technology still required however, CCS is still envisaged to be some way off from being deployed on the scale required to affect a meaningful reduction in carbon emissions.

Capture

The capture phase is where the carbon dioxide is removed from the exhaust stream of the power plant or other industrial process. There are three main ways in which this can be done [8]:

- Post–combustion carbon capture sequesters the carbon dioxide after combustion of the fossil fuel, separating it from the exhaust stream using a chemical

solvent or a physical absorbent.

- Pre–combustion carbon capture, or Integrated Gasification Combined Cycle (IGCC), prevents a release of carbon dioxide into the atmosphere by separating the carbon from the hydrogen in the fuel through a gasification process. From here the hydrogen is used for further power generation after being separated from the carbon dioxide.

- Oxy–fuel combustion involves burning the fuel in an oxygen–rich mixture containing carbon dioxide instead of in air, before some carbon dioxide is removed and some retained to help burn more fuel.

The current state of technological development would suggest that post–combustion capture is the favoured option as it can retrofit onto pre–existing plant and be turned off without affecting generation. It is anticipated however that IGCC will become the favoured option eventually due to cost effectiveness [2]. Either way, the understanding needed to carry out CCS capture is in place, and has been repeatedly demonstrated on different scales (from small to large).

Compression

A conservative estimate of the amount of carbon dioxide released globally from power generation sources in 2000 is 9Gt [5]. Assuming Standard Ambient Temperature and Pressure (SATP); 25°C and 1bar, this equates roughly to $4.581 \times 10^{12}\text{m}^3$. Given that CCS aims eventually to capture 100% of carbon emissions from power plants [18], there is simply no way this volume could be handled unless it could be compressed to a much smaller volume. More importantly, if geological storage is to be used then compression is essential to overcome the reservoir pressures found at depths intended for CCS of around 2km, which in some cases could be as high as 200bar [18]. At its critical point, carbon dioxide is approximately 65 times less voluminous than at SATP, suggesting that CCS must by necessity contain a stage for compression of the captive gases so as to allow a higher quantity to be processed and ultimately isolated from the environment. It is anticipated that compression would usually occur at the same facility as the capture stage. Much research on different compression technologies has been carried out, and it is also likely [19] that CCS–scale compression could be implemented whenever CCS is needed. Yet, it is important to remember that compression is an energy intensive process, requiring in the case of post–combustion capture, as much as 4% of the total energy output

of the power plant [19]. As far the interaction between the compression and transport stages is concerned, compression facilities must be able to meet the pressure requirements of the subsequent stages. It is also important for the operation of CCS systems, particularly when it comes to contingency planning and dispersion modelling in the case of pipeline failure, to be able to understand the compression and depressurisation requirements and behaviour which occurs in CCS. This requirement is explored in more depth later in this thesis.

Transport

Since sources of carbon dioxide are, generally speaking, not in the proximity of the location of the storage sites, some sort of mass transport infrastructure is required to deliver the captured, compressed carbon dioxide gas mixtures to the storage site. Two options for transport are usually considered; pipeline [20, 21, 22, 23] which can be further sub–categorised into on–shore and off–shore pipes, and ship or tanker [21, 24, 25, 26], with each method being employed as determined by locally occurring conditions. Given the geographically disperse nature of sites used for power generation and those which are suitable for the latter stages of CCS, transport infrastructure, particularly pipelines, will be immense structures, for which cost–minimal installation and guaranteed safe operation will be profoundly important. As a direct result of these requirements as well as the fact that transport infrastructure is almost inevitably going to have to be routed close to inhabited areas, the issue of CCS transport is one which is subject to particular scrutiny. With pipelines being the favoured option for transport due to a lower average operating cost for anything other than very long distances (see Figure 1.3), the potentially convoluted planning and construction process, and a perceived lack of ability to guarantee safe operation (for example, as seen in the Barendrecht case, see Figure 1.16 [27]) could inhibit the installation of pipeline infrastructure during the early days of CCS, until this technology has been proven.
As can be seen from Figures 1.3 and 1.4, with the anticipated costs of pipeline transport comparing favourably to those of shipping costs over shorter distances, it is expected to be the favoured option in satisfying the majority of demand for CCS transport.

Injection

The most economically favourable and high capacity sites which have been earmarked for CCS storage are located under ground in geological structures such as

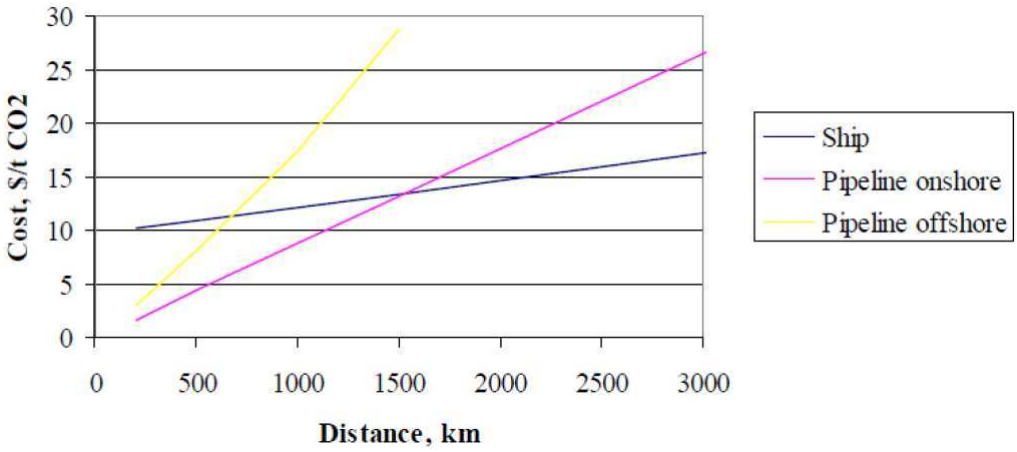

Figure 1.3: Comparison of the anticipated operation costs for different transport methods for a specific volume (6MT) of carbon dioxide [28]

reservoirs or disused oil fields. In order to get the captured carbon dioxide from the transport vessel into the final storage location, it must be injected into the storage site back down the tubing at a high enough pressure to allow the carbon dioxide to overcome the significant pressures found within these formations, and be driven down into the structure. Storage sites must undergo rigorous testing before being allowed to have CO_2 injected. Criteria for storage sites include having a structure that will ensure both minimal migration of the carbon dioxide, and minimal release during seismic activity [8].

Storage and Monitoring

This is the only stage of CCS which requires no active input. After injection, the carbon dioxide remains in place indefinitely and must be monitored to ensure migration to neighbouring geologic formations or potential releases do not occur. In this way, the carbon dioxide is sequestered from the atmosphere and the associated environmental impacts mitigated.

This is a vast simplification of the overall CCS process and the piecemeal presentation given here does not do justice to the overall complexity of the system. In reality the five stages are highly inter–dependent and the interactions between consecutive stages are significant enough that they need to be carefully accounted for [29, 30] in the design of the overall process.

A significant added complexity to the operation of CCS arises from the fact that impure carbon dioxide will have to be processed. In particular, given the range of chemical components found in fossil fuels, for example the different hydrocarbons involved, and specifically the non–hydrocarbon impurities originating from the formation of fossil fuels over many millions of years, as well as different combustion and capture technologies which vary from generator to generator, it is to be expected that CCS capture modules will not produce a pure stream of carbon dioxide. Instead, they will include various chemical impurities which would then be present for the rest of the CCS chain. The thermodynamic effect of these impurities on the overall physical properties of carbon dioxide is profound [31], and there must be scope to understand the effect these have within all the CCS processes. In particular, significant amounts of nitrogen, hydrogen, oxygen, and water could all be found in an untreated fossil exhaust stream. These impurities all affect the physical properties of the carbon dioxide in such a way as to significantly alter the operating parameters of a CCS pipeline, such as wall thickness, diameter, phase behaviour, and pressurisation. A rigorous understanding of the effect of these impurities is essential therefore.

1.2 The Need for An Accurate and Simple–to–Use Equation of State in CCS Pipeline Transport

Many of the most pressing requirements for a timely deployment of CCS seem to be heavily related to the transport stage [32]. Of these, one of the main barriers to overcoming the many political, social and regulatory issues surrounding CCS transport is our lack of ability to accurately predict how the physical properties of carbon dioxide change as the type and amount of chemical impurity varies [31].

Typically, properties such as pressure, density and phase behaviour are calculated using an Equation of State (EoS). This is a formulation relating the important thermodynamic quantities which determine the nature and key characteristics of the system. Presently, there are several available equations of state which could be utilised [33, 34, 35], but all have their relative drawbacks: namely, those which are more accurate are agreed to be also more cumbersome in their implementation, whilst those which exhibit the property of being easier to use fall significantly short of the level of accuracy needed to be of use in CCS.

In particular, there is a clear need at this moment [36], so far as the pipeline transport stage of CCS is concerned, for an equation of state which can accurately depict the key physical behaviours of carbon dioxide–rich gas mixtures in a simple and effective way, without excessive functional complexity or a requirement on high computing power. If such an equation was developed, it would allow safe design and operation of pipelines because it would describe in a quantitative way the variation of pressure, density and phase behaviour as a function of impurity content. This in turn would allow the thermodynamic properties of the system to be evaluated both with increased ease and reduced uncertainty.

As an example, one major area in which there is a direct application of an equation of state in CCS pipeline is in understanding methods of fracture propagation [37, 38]. If CCS pipelines are to be routed through or close to populated areas, the possibility of external influence (for example, diggers or other such heavy machinery) on the pipe resulting in damage cannot be discounted, and so a detailed knowledge of the thermodynamic behaviour before, during, and after failure of pipe is essential. The field of fracture mechanics is particularly dependent on accurate equations of state being available, and deals with how the pipe structure can cope with such external influences [37]. Clearly there is an important safety implication here, and one very clear reason why accurate equations are necessary.

The need for accuracy also pervades cost considerations. Being able to accurately predict the pressures a pipeline will need to undergo given an anticipated impurity stream could save excessive pipe wall thickness being implemented, and in doing so save considerably on the significant capital requirement for CCS pipelines.

As we have identified, there is much that needs to be understood before safe, socially acceptable and cost effective CCS transport networks can be constructed, especially in the prediction of key physical behaviours such as density, pressure and phase behaviour. In light of the pressing need for quick deployment of all the CCS stages, it would seem to be pertinent to ensure that arguments relating to the safe operation of CCS pipelines be neutralised now with the development of a new equation of state which could perform in the ways described here so as to facilitate the high standards of operation required.

1.3 A Contextual Literature Review

1.3.1 Overview of the Literature Surrounding CCS Pipeline Transport

The main aim of this contextual literature review is to establish scope for this EngD research project and to help define our aims. We thus seek to determine the ways that existing equations of state are understood to be lacking, and also to look for the anticipated optimum operating conditions for the pipeline transportation of carbon dioxide so that we can focus our work and ensure its relevance. As established in Section 1.1.2, the principal methods which are likely to possess the required scale for CCS transport are pipelines and ship [26] (see both illustrations in Figure 1.4), with almost no consideration or mention of any other method throughout the entire literature, except for one brief mention of road or rail transport [32], where it also mentions how unsuitable these methods are for large scale transportation. Thus, for the purpose of this project and the current literature review, it will be assumed that there are just these two choices, and that of these, pipeline transport will be the favoured option in the majority of (but not all) cases.

Figure 1.4: The two methods of transport in the CCS process: pipelines (left, [39]), and shipping (right, [26]). Note that most CCS pipelines will be buried below ground. Given the relative lack of CCS pipelines currently, the picture on the left is actually an illustration of an oil pipeline.

Crucially, within the literature, there is a broad consensus that there is currently a lack of any suitable equation of state for specific application to CCS pipeline transport [40, 41]. Also mentioned in the literature is the lack of reliable thermodynamic data for the determination of optimum CCS pipeline transport conditions [29, 30]. The literature also notes that there has been far more study of the other processes

in CCS, notably capture and storage. We are reminded [42] that transport has, in the past, been assumed a problem of inferior difficulty and technical importance, yet we are now facing the very real possibility that the deployment of CCS could be limited to how quickly we can understand the thermodynamics underlying the transport of carbon dioxide [40] and overcome the political hurdles directly arising from this lack of certainty. In the literature, some simulations of the transport process are reported [29], in which particular attention to the upstream interface between capture and transport, including compression, is given, as opposed to the downstream interface of transportation with injection and storage, finding that if energy usage for transport is to be minimised, then the important factors are inlet pressure, amount of impurities in the carbon dioxide, temperature and compressor efficiency.

One of the main issues surrounding CO_2 transport is the need for onshore pipelines. Whichever option is chosen for offshore transportation, routing of pipelines onshore is almost certainly going to cause problems, especially in regions where population density is high, such as in the Humber region of the UK where large–scale CCS projects are expected to be based [43]. One major reason for this is the likelihood with which external influence such as tractors or diggers could cause a pipeline failure; an eventuality whose probability far outweighs that of a failure arising from an internal failure in the pipeline such as corrosion or pressure surge. There are significant problems [44] with how to route the pipeline in such situations, such as social resistances in the form of people not wanting high pressure carbon dioxide pipelines running close to their place of residence, for obvious reasons when considering the possible health effects of exposure to CO_2 (see Section 1.3.2). Such discussions and the reservations of those who live close to the planned route of CCS pipelines are exacerbated in light of the fact that corrosion is a reasonably likely consequence of transportation of supercritical carbon dioxide with water impurity in it [45, 46]. The extent to which it is important to avoid excessive corrosion of the transport vessel ensures that water levels must be kept to a minimum [31], this is to be enforced with strict drying regimes before the carbon dioxide is allowed to enter the pipeline network. The tolerance of water level in the fluid depends on the other chemical components present in the mixture, so it is understood that the quantity of water allowed is likely to be negligibly small. This highlights the requirement for a rigorous and safe pipeline operating procedure with minimal pipeline failure probability. Again, this points back to the requirement for an accurate and easy to use equation of state for use in this area.

Clearly, safety and value for money are considerable issues when it comes to any

of the CCS processes. Given that pipelines will, by their very nature, have to pass through populated areas, a leak from a high pressure carbon dioxide pipeline is likely to cause many problems. The literature notes that since carbon dioxide is heavier than air, if there is a leak it is likely that it will gather in pockets near the ground [47], rather than rise away as might be the case with a natural gas leak. This is particularly problematic for onshore pipelines, with carbon dioxide being an asphyxiant, exposure to anything other than minimal concentrations of which for anything other than very short periods of time can have extremely detrimental health effects [31].

Because of this, it is most important to the safe operation of transportation mechanisms that the pressure, density and phase behaviour of the fluid mixture can be understood. In this way, these characteristics could be accounted for and controlled in order to ensure the pipeline infrastructure does not fail and cause a leak. This eventuality could be brought about in two different ways: Firstly, if the pressure was allowed to become too high this could cause a rupture in the pipeline wall, with the carbon dioxide then being allowed to escape. This suggests that it is important to be able to predict how pressure will vary depending on impurity content and other factors. Secondly, if multi–phase flow is allowed to occur, the difference in viscosity and density of the two phases could weaken the pipeline integrity at valves, pumps, and compressors, situations which again could lead to failure of the pipeline structure. For this reason, it is vitally important that the location of any two–phase region in which both liquid and vapour would coexist should be avoided. It is particularly important to be able to accurately identify where such a two–phase region might occur, given the particular composition of the fluid mixture contained within the pipe. This is because two different phases means two different densities, and therefore two different flow speeds and two different flow regimes, causing damage to the pipeline. Figure 1.5 shows how and where the introduction of a small amount of impurity can create a two–phase region [48].

The literature also lists other key considerations for pipeline operation. For example, it is necessary to avoid formation of solid hydrates or other waxy substances which could disturb the flow rate or cause blockages within the pipe interior [49]. An EoS is again needed for these predictions.

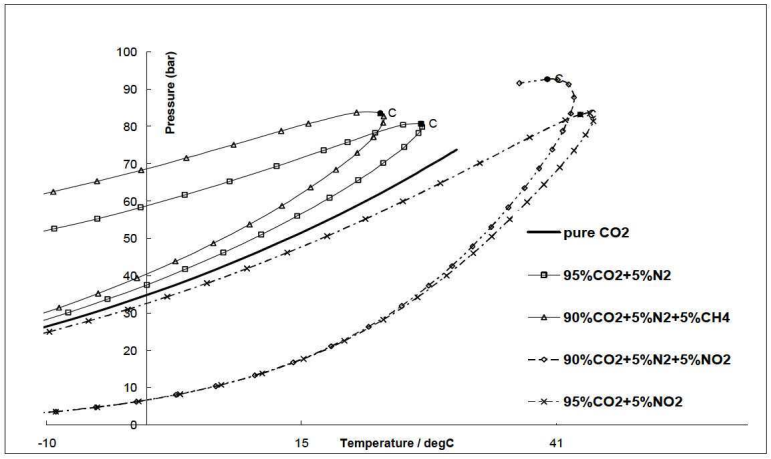

Figure 1.5: Location of the two phase region depending on impurity [48]

1.3.2 Health Impacts of High Concentration Carbon Dioxide

Carbon dioxide is classed as a GHG and its contributions towards global warming are well documented [1, 3]. CCS is a key CAT and it is hoped that in years to come it will help to stop the current pattern of global increases in atmospheric temperature that have been seen in recent decades. There are some other industrial uses for CO_2 which could be utilised in order to help prevent its release into the atmosphere, such as in EOR (enhanced oil recovery) or the food industry [26, 50]. Generally, the amount of CO_2 demanded for these are nowhere near the amount of CO_2 emitted by power plants and other heavy industry, although the lessons learned from EOR in the USA are invaluable for pipeline transportation of CO_2 in CCS as there are several areas of technical knowledge which overlap.

Pure carbon dioxide is a gas at SATP. Despite the fact that it is a key component of our atmosphere, without which life could not exist, in high concentrations it is toxic. The characteristic of carbon dioxide which makes it particularly dangerous to humans, aside from the threat to our atmosphere, is that it is an asphyxiant, restricting the ability of the haemoglobin in blood to transport oxygen round the body. Table 1.1 summarises the health effects of increasing concentrations of carbon dioxide:

From this table we can see why it is vital to prevent a release of CO_2 from pipelines where the quality would be above 90%. This reasoning also determines indirectly

Concentration	Effects [51]
< 1%	quite harmless
1—5 %	moderate symptoms such as drowsiness and headache will take effect
5—10 %	effects will become more severe, with dimmed vision, reduced hearing and shortness of breath all possible
10%	symptoms of prolonged exposure become very serious; muscular tremor, increased blood pressure and even unconsciousness
> 10%	death within a few minutes

Table 1.1: Effects on health of increasing carbon dioxide concentration

how far away carbon dioxide pipelines will need to be positioned from inhabited areas. The study of the dispersion of carbon dioxide [37], coupled with the information in Table 1.1 makes for a very important consideration in this way. Dispersion modelling is another area where accurate equations of state could be deployed with great benefit therefore.

Transportation of carbon dioxide for CCS occurs at high pressures so that more can be transported in a given space of time, and for a lower average cost. It is also the intention that CCS should process only mixtures with the highest possible level of CO_2, again for financial reasons. If there is to be a leak from the transport vessel therefore, it is probable that high concentration carbon dioxide will be dispersed outwards into a very wide area with very high velocity [47]. A further property of CO_2 is that it is colourless, tasteless and odourless, meaning that it would be very hard to discern whether such a leakage of CO_2 had occurred until the symptoms mentioned above started to set in, by which point it could already be too late. This is especially worrying as carbon dioxide could potentially be leaking for a long time before being noticed and tracked down. Furthermore, with a molecular weight of 44, carbon dioxide is heavier than air, which has an average molecular weight of around 29, and so any such leakage would accumulate at ground level (as opposed to hydrogen or natural gas leakages which would rise away from the ground). The clear safety implication of this is that if there is a carbon dioxide leak from a CCS pipeline close to a populated area, then the humanitarian effect could be disastrous, as it would not disperse from where people are situated, whilst the presence of the carbon dioxide would not be discernible until it was doing harm.

1.3.3 Properties of Carbon Dioxide and its Mixtures

In conducting this literature review, we are frequently reminded of the importance of being able to accurately model the behaviour of CO_2, both on its own and as part of a mixture. One of the areas of knowledge that is currently lacking, as is evident from the available literature data, is that of thermodynamic pressure–volume–temperature–composition (P–v–T–x) data. This is key in in being able to identify the important features and physical behaviours which need to be accounted

for. Another important consideration for physical behaviour of carbon dioxide is the phase diagram [52], which can be seen in Figure 1.6

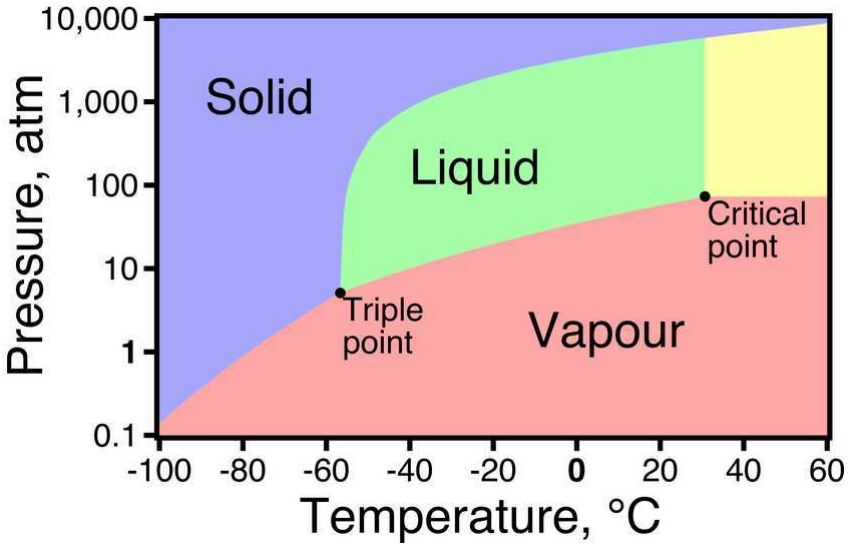

Figure 1.6: Phase diagram for pure carbon dioxide [52]

Both pressure and phase behaviour are important considerations for modelling how carbon dioxide behaves when being transported because the interaction between the liquid and vapour phase determines where the two–phase region lies. There are some density and phase behaviour measurements of carbon dioxide and its mixtures available in the literature, for example [53, 54], although the overall impression gained from such sources is that the data which is available represents a very small amount of that which is needed in order to more fully understand this area [55].

Another important consideration in the modelling of carbon dioxide is its viscosity (see Figure 1.7), which is also calculated by use of an equation of state. Viscosity is the resistance of a fluid to being deformed by a force. Since the carbon dioxide is driven in the pipeline by the high pressure, viscosity is an important consideration as is affects the ability of the mixture to flow more easily, and in turn the energy requirement to drive that mixture. The viscosity of a gas is usually lower than for a liquid of the same chemical species [56].

Also important is the compressibility. Since the carbon dioxide is to be compressed before transportation and subsequent injection and storage, it is advantageous to

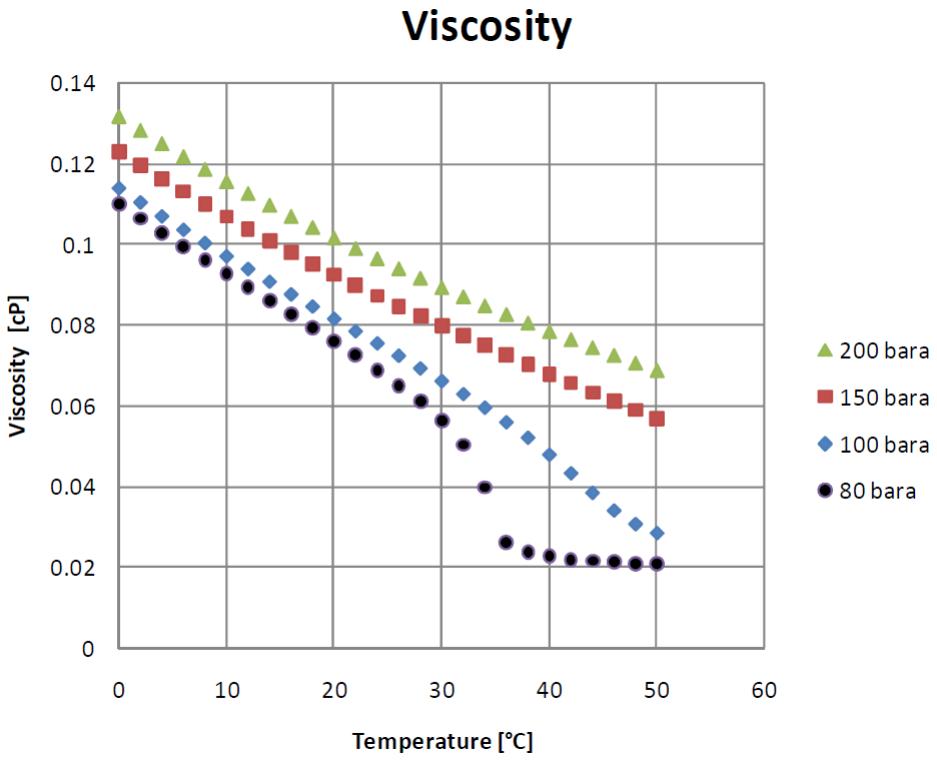

Figure 1.7: Viscosity of pure carbon dioxide as a function of temperature and pressure [56]

be able to do so with the minimum energy penalty, for which an understanding of the pressure behaviour is needed. The compressibility factor Z, defined by

$$Z = \frac{Pv}{RT}, \tag{1.1}$$

where P is the pressure, v is the molar volume, R is the Universal Gas Constant, and T is the absolute temperature. Ideal gases exhibit the property that $Z = 1$, and indeed, setting this in equation (1.1) yields the ideal gas law (IGL). Gases do not usually have this property however, and $Z < 1$ means that the particles can move easily, brought about either by a higher temperature, where the molecules have higher kinetic energy, or by low pressure, in which case they have more freedom to move. In this situation, they can easily be compressed. Conversely, $Z > 1$ means that the molecules have a low mobility, brought about either by low kinetic energy from low temperature, or high pressure. Again, this means that they cannot so easily be compressed. In equation (1.1), the variation of Z with changes in P or T is an interesting problem which gives us some amount of insight to the properties of the substance under consideration [56].

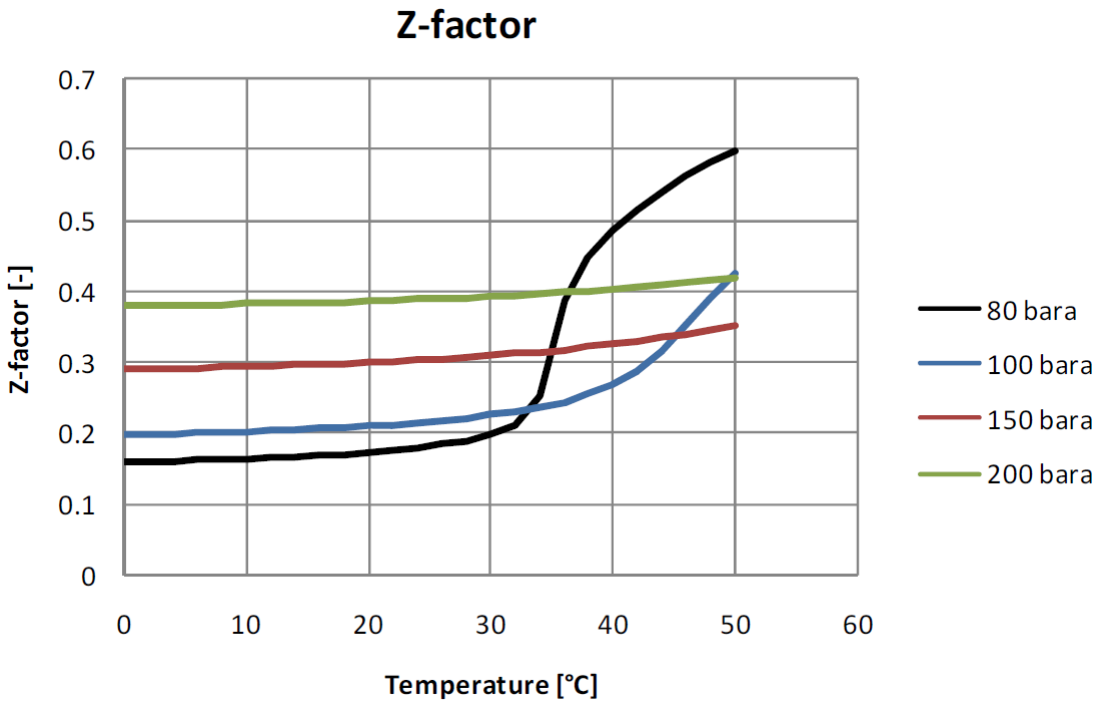

Figure 1.8: Compressibility of pure carbon dioxide as a function of temperature and pressure [56]

Density ρ is also an important consideration:

$$\rho = \frac{m}{V} = \frac{m}{Nv}, \tag{1.2}$$

where m is the total mass of substance being considered, V is the total volume, v the molar volume, and N the number of moles. We note that the the quantity m/N represents the molar mass, so by using Equation (1.2) we have a very convenient formulation for relating density and volume. The variation of density with temperature and pressure is also an important consideration when it comes to understanding the behaviour of a fluid [56].

The existence of impurities in the carbon dioxide affects its overall transportability. This is because these impurities affect the physical characteristics such as viscosity, compressibility, density and phase behaviour, as demonstrated in Figures 1.8 and 1.9 [56]. The same qualitative behaviour in changes to viscosity, compressibility and density after the introduction of an amount of impurity are also reported [56], at which point the difference between experimental data and predictions made by an

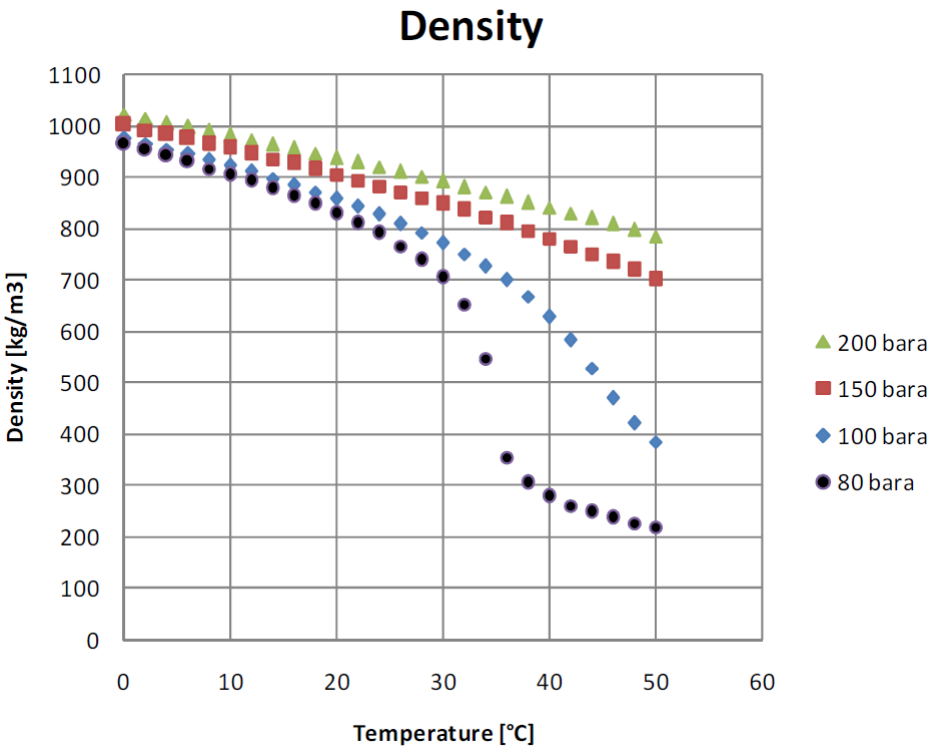

Figure 1.9: Density of pure carbon dioxide as a function of temperature and pressure [56]

equation of state is highlighted. The literature draws on differences between data obtained from ideal theoretical cases and the real practical case [57]. The major disadvantage of depending on experimental measurements of behaviour as opposed to using an equation of state is that these are only valid at the points measured, and cannot usually be interpolated between or extrapolated beyond to give a meaningful insight for any situation not explicitly described. In the field of carbon dioxide transportation, it is hoped that predictive models and equations of state can be backed up by, and used to explain the experimental data, although in some places [57] the literature warns that inefficiencies or inaccuracies of the measuring process could translate into a reliance on poor thermodynamic data.

Because of this, it is not enough to describe a system solely based on experimental measurements. It would seem to be advantageous therefore to incorporate an equation of state when calculating the physical properties, such as the pressure, of a system. Ideally, in order to minimise uncertainty in the description of behaviour of a system, experimental measurements would be validated with an equation. In an area of such uncertainty as CCS transportation, this will be the only way to provide acceptable data, but given there exists such an insufficiency of thermodynamic data

in this area, obtaining a good fit of the relatively few data points which are available by use of an accurate equation of state is highly important.

As has been mentioned in this literature review, it is not expected that CCS pipeline transport will have to deal with a pure stream of carbon dioxide, due to the capture technology used (see Section 1.1.2) and due to the presence of impurities in the fuel itself even before combustion has taken place. In fact, depending on the capture technology used, the amount of chemical impurities can vary, as shown in Table 1.2 [8].

Capture Technology	**N_2 (% mol)**	**H_2 (% mol)**	**O_2 (% mol)**	**SO_2 (% mol)**	**NO (% mol)**	**H_2S (% mol)**	**CO (% mol)**	**CH_4 (% mol)**
Post–Combustion	Tr.	Tr.	0.01	0.01	0.01	Tr.	Tr.	Tr.
Pre–combustion	0.5	1.0	0.05	Tr.	Tr.	0.05	0.05	1.0
Oxy–fuel	2.0	Tr.	2.0	0.1	0.01	Tr.	Tr.	Tr.

Table 1.2: Typical dried, treated CCS mixture impurities for different capture technologies

Of course, impurity species are not limited to the most commonly occurring such as N_2, H_2, and O_2, as smaller amounts (on a ppm or ppb scale) of SO_x, NO_x, H_2S, CO, CH_4, and even Hg and Ar, and others can all be present. All of the different impurities can have different effects on the transportability of the carbon dioxide, for example their effects on corrosion or toxicity, which is why it is important to know how much of them is present so that their effect on the physical properties of the carbon dioxide mixture can be calculated by use of an equation of state. It is noted that an ability to factor in the effects of different components on the behaviour of the exhaust stream would be beneficial, and in a way, if such a method that could incorporate any one of the many impurities mentioned here existed, then it wouldn't matter which components were considered in developing this model, as the method would then have scope to incorporate any other compositions at a later date.

Water is usually to be found in significant concentrations in untreated exhaust streams [8], but in light of the fact that this could cause significant corrosion issues, the literature suggests [45, 46] that an extensive drying regime be in place before the transport stage of CCS, bringing this amount down as low as 10ppm, at which point corrosion is no longer an issue. As such, H_2O is not factored into our considerations and figures in Table 1.2 are given for dried mixtures.

A second problem arises from the fact that transportation of the captured CO_2

needs to take place entirely within a single phase, as has been mentioned. When transporting the captured substance (be it in the liquid, vapour or supercritical phase), the pressure drop in the pipeline with distance can be significant (and varies depending on impurity content) [20]. As such, compression pumps are needed at regular intervals: firstly to revive the pressure which drives the fluid down the pipe, and secondly so that the carbon dioxide can be delivered to the injection site at a pressure which is appropriate for that in the storage site. These pumps are highly necessary to the process of CO_2 transportation, and cannot deal with multiple phase mixtures as they need to be set up either to admit a gas, or to admit a liquid, but cannot be utilised to allow both simultaneously. This is due to the differences in viscosities and densities between a gas and a liquid [56] (see Figures 1.7 and 1.9), and is further reason why a clear and accurate identification of the phase boundary is vital. Related to this is the important consideration for how changing pressure can bring about a phase change during pipeline transport. Figure 1.10 shows how different impurities present in carbon dioxide can cause a different pressure drop [20]. The impacts of such a drop are that it affects how often pipe repressurisation is needed, and it could lead to a situation of multi–phase flow if this pressure drop represents a trajectory that would enter the two-phase region.

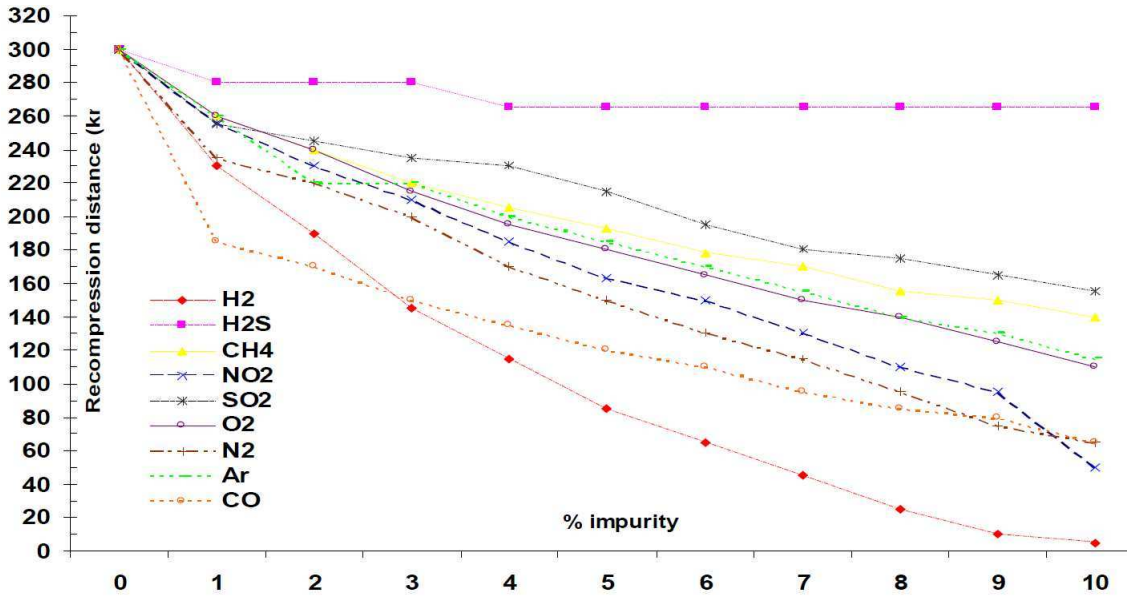

Figure 1.10: Effect of impurity on pressure drop with distance along a pipeline [20]

We can clearly see that the pressure drop with distance is more in the presence of some impurities than others. Also important is how temperature changes with dis-

tance along the pipe, as the evolution of these two variables could determine whether the phase plane trajectory enters the two–phase region mentioned previously. In reality, pipeline transport of carbon dioxide will operate close to the critical point or in the supercritical phase in order to increase density and compressibility and to reduce viscosity, so as to maximise cost–effectiveness. A small fluctuation from the intended operation conditions at this location of the phase diagram could see the mixture enter the multi–phase region. Yet again, this is a clear promotion of the need for an equation of state which is accurate in predicting the phase behaviour of CCS–relevant mixtures.

1.3.4 Pipe Transport of Carbon Dioxide

For the pipeline transportation of carbon dioxide, may lessons may be learned and transferred from the many years of experience in using pipelines to transport natural gas. For CCS, pipe transport is expected to occur mainly in the supercritical region as shown in Figure 1.11 or dense phase region. Here, carbon dioxide exhibits the viscosity of a gas, which is advantageous as this will allow for an easier flow, requiring less of a pressure gradient to drive it, with the density of a liquid, which is again advantageous as it allows a higher mass of carbon dioxide to be transported in any given time. The below diagram shows the location of this ideal operating condition in the phase diagram [52].

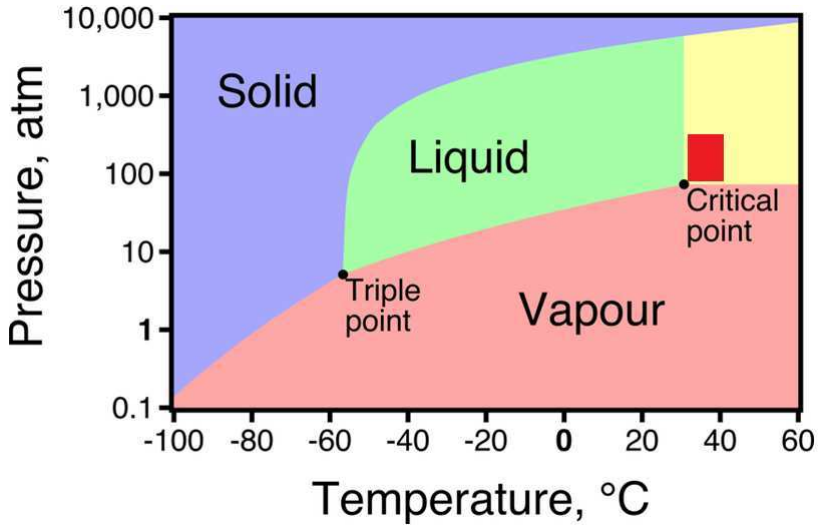

Figure 1.11: Anticipated region of the carbon dioxide phase diagram for pipe transport [52]

The main feature of transportation in this area is not so much the moderately high temperature upto 40°C, but the very high pressure of upto 200bar; or 20MPa. This is important for many reasons, not least because the safety considerations for such high pressure carbon dioxide are significant. The pipeline structure must be capable of withstanding this pressure, as failure at this pressure is likely to cause the dispersion of toxic levels of carbon dioxide over a large area, with the implications as discussed in Section 1.3.2. The necessity of mitigating these risks results in the mandate that pipelines must be very well designed and tested; a process requiring considerable investment. It is estimated that high pressure carbon dioxide pipelines for carbon dioxide transportation will have an installation cost of £1M to 2M per km [51]. With a potential instalment of tens of thousands of km of CCS pipelines by 2050, if CCS is to be successful, this gives a total cost just for the building and installation of these running to tens of billions of pounds, not even accounting for the other four main stages of CCS (see Figure 1.2). This is a massive investment and so the ability to operate safely is even more important. One mitigation strategy for this cost is to have the pipelines running at lower pressures. This causes two problems of its own however, in so far as the final pressure must be consistent with that which is required at the injection site [18], and also that if a lower pressure is permitted in the pipe, then more regular re–pressurisation stations along the length of the pipe will be needed (it may be possible to have CCS pipelines operating wholly in the gas phase). In this scenario, any savings made by running at lower pressure could be countered by the need for a greater number of re–pressurisation stations. The corrosion and hydrate formation considerations mentioned are also important for pipeline transportation. Corrosion must be avoided so as to prevent failure of the pipeline and subsequent dispersion of toxic levels of carbon dioxide. Hydrate formation must be avoided so as to prevent narrowing and blockage of the pipeline which could lead to pressure build–up, culminating in the worst case scenario in a more catastrophic failure. Again, this would lead to dispersion of toxic levels of carbon dioxide. One parameter that can be manipulated to alter the flow rate and thus reduce the likelihood of pipeline blockages is pipeline diameter [58], which also has a profound impact on the running costs of the pipeline. This is something that designers of pipelines could factor into their considerations with the help of a suitably accurate EoS.

As has been mentioned earlier in this literature review, it seems that the preferred option for most of the needs of the CCS transport stage will be pipelines.

1.3.5 Ship Transport of Carbon Dioxide

Ship transportation of carbon dioxide occurs at much lower pressures than in pipelines, close to the triple point of carbon dioxide, for the simple reason that ship hulls are less able to withstand such high pressures. Transportation in the solid phase is impossible due to the lack of fluid properties, and as it would require more energy to get the carbon dioxide onto and off the ship. In order to maximise density (see Figure 1.9), transportation by ship is expected to occur at lower temperature, in the liquid phase close to the triple point [52] (see Figure 1.12).

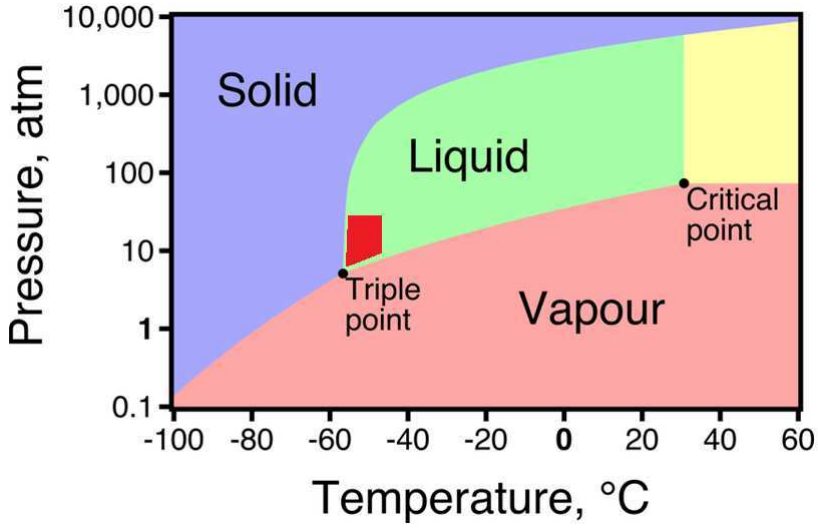

Figure 1.12: Anticipated region of the carbon dioxide phase diagram for ship transport [52]

To be consistent with the aim of keeping transportation costs as low as possible, much of the literature suggests that just as the CCS pipeline transport can take lessons from the EOR industry, CCS ship transport can utilise current knowledge gained from the operation of Liquefied Natural Gas (LNG) transport ships, in terms of dealing with both the pressure and the expected temperature variations. As an example, since carbon dioxide would be transported at around $-50°C$ in ship transport, which is colder than most places on Earth, it is expected that it would heat up during the transportation process. As well as the technical expertise to be gained from LNG transport, it is suggested that combining usage of LNG ships with usage of carbon dioxide ships, by carrying the LNG from ocean to shore in one direction, and both Liquefied Carbon Dioxide (LCO_2) and Liquefied Nitrogen (LIN) from shore to the ocean in the opposite direction as shown in Figure 1.13 [24] would

be an excellent way to minimise the capital costs associated with ship transport [24].

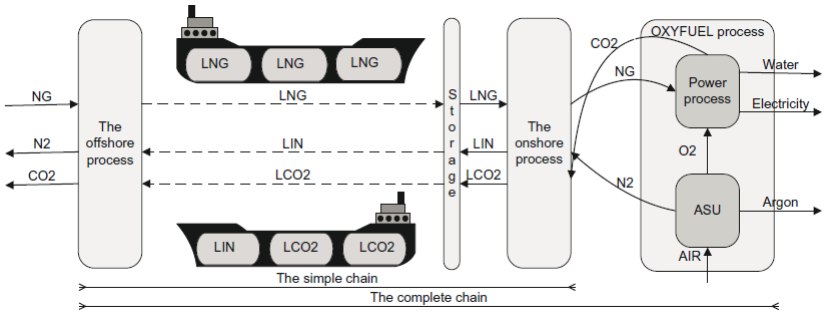

Figure 1.13: Multiple uses of ships to minimise operating costs [24]

One of the main considerations for ship transport that does not apply to pipeline transportation is that the carbon dioxide must be stored prior to loading onto the ship. This causes two problems: if this intermediate storage is at ship pressure, then the storage container must be capable of withstanding this increased pressure, and if not, then there must be enough volumetric capacity to store all the carbon dioxide. As with other factors, this increases both the fixed and variable cost requirements. Despite this, most of the literature [59, 24, 28] seems to be in agreement that over long distances, ship transport offers better cost–effectiveness than pipeline transportation, although this must be offset by the costs of liquefaction, and for shorter distances, pipe transport has the edge.

1.3.6 Compression of Carbon Dioxide

Compression is the stage which comes before transportation in the CCS chain (see Figure 1.2), and the two processes, although technically separate, are inextricably inter–dependent. This is because the pressurisation and the ability to control the pressure at all stages of the transport process is of vital importance. We highlight how important it is to integrate considerations about the operations and limitations of the compression within the transport stage, as well as to highlight how compression, like transportation, has as one of its main aims, the minimisation of its energy requirement, and maximisation of the throughput of carbon dioxide. This brief section is included in this literature review in order to establish the key considerations for this stage of CCS from the point of view of the neighbouring transport stage.

As mentioned, carbon dioxide in CCS must necessarily be compressed in order to

create a driving force within the pipeline and because of the vast amount of it that power generation produces. The extent to which this pressurisation must take place is not without its problems.

All the relevant literature makes some reference to the fact that compression of carbon dioxide is an energy intensive process. We are reminded [19] that in a coal–fired IGCC power plant, compression of carbon dioxide for subsequent transportation can take up more 4% of the gross output of that plant. This represents a large energy penalty. It is also noted [18] that in CCS, there is a target pressure at which the carbon dioxide mixture must be delivered to the injection site. It is mentioned that for most geological sequestration sites, an inlet pressure of around 150bar would be needed [18]. Working backwards along the CCS chain from this, and bearing in mind the expected depressurisation that occurs in the pipeline with distance (see, for example, Figure 1.10), there is a target pressure for the interface between the compression and pipeline transport processes. This cannot be too low as this would result in a lack of drive at the injection site, and it cannot be too high as this would incur unnecessary costs through extra pipe wall thickness, and energy penalties.

Compression systems operate in a multi–stage format, each stage compressing the carbon dioxide a little bit more than the previous, but there are also high–efficiency, single stage compressors [60] currently being developed. These operate by a combination of shock compressors, similar to those used in supersonic flight engines, and the more conventional centrifugal compressor designs. The phase plane trajectory; that is the path taken as temperature and pressure vary is most important during the compression process, just as in the transport process: Depending on the impurities in the carbon dioxide mixture, this can create the scenario of a two–phase region in the phase diagram which must be avoided during compression just as in transport. There are different strategies which can be employed to compress the carbon dioxide from low pressure to high in such a way as to avoid a multi–phase situation, either via a series of small pressurisation and cooling stages, or by one large pressurisation stage followed by one large cooling stage (such as with the shock compressor mentioned above). Yet again, for this task there is a clear need to be able to positively identify both the location of the two phase region and the pressure behaviour depending on impurity [61].

Another important consideration is the quality of the carbon dioxide to be compressed, and for this, it is mentioned that for compression in EOR, a 95% + purity is recommended. For CCS, the required purity will be dependent on the costs as-

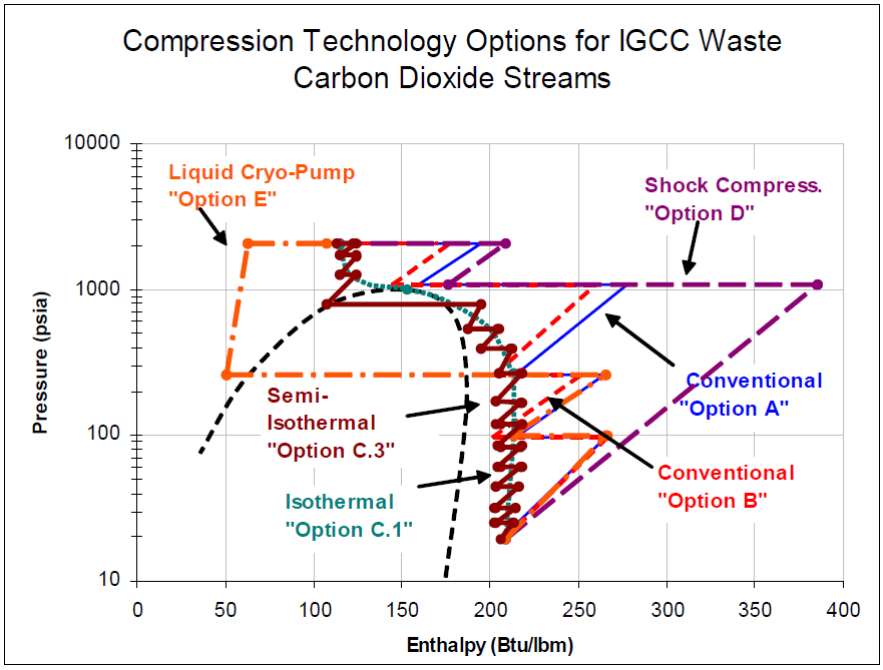

Figure 1.14: Example phase plane trajectories for compression [61]

sociated with transport and injection to the final storage site, but is likely to be higher than this [18, 31]. The fact that the presence of different impurities in differing amounts affects the location of the two–phase region (as is shown in Figure 1.15) causes further issues in this way [62]. Again, this calls out for an equation of state which can accurately predict the exact location of the multi–phase region, depending on the impurities present. In conducting this literature review we found it difficult to find a wide range of data or examples detailing this sort of behaviour other than a few repeated and well–documented cases [62].

As for the energy penalty, once an acceptable compression trajectory has been identified, it is the case that interstage cooling reduces the overall power requirement for CO_2 compression [63]. As for compression methods, there seem to be two main conventional methods which are currently in use; intercooled compression and adiabatic compression with heat recovery [18], as seen in Figure 1.14. Either way, it is noted that the energy penalty in a plant whose output is, for example, 383MW would be around 20MW [18], which is in good agreement with the 4% energy penalty value quoted previously [19]. Traditionally, high–speed reciprocating compressors have been used for CO_2 compression for EOR [64]. This method is more flexible, takes less time, and since the machinery is lighter, can be relocated to a new compression site relatively easily. Some of the literature [64] suggests that in the near future,

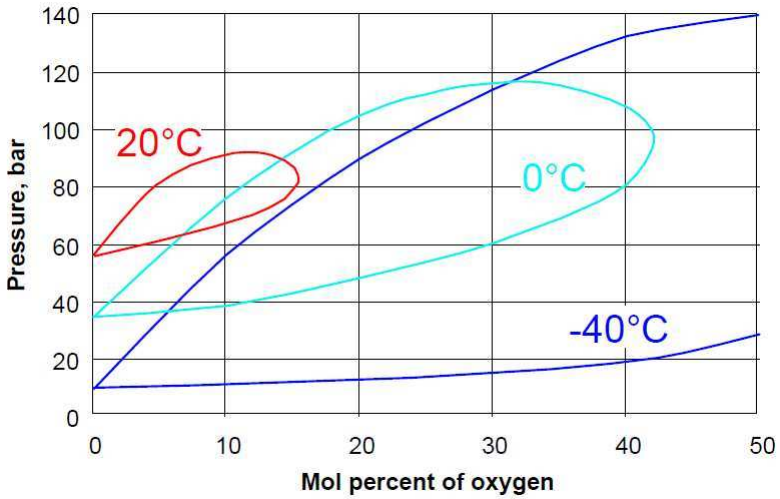

Figure 1.15: Existence of the two–phase region in a carbon dioxide–oxygen mix [62]

centrifugal compressors are likely to be favoured since the capacity of reciprocating compressors would not be large enough to meet the demand for CO_2 compression in CCS. Furthermore, reciprocating compressors are maintenance intensive, and are very expensive to operate. Thus, centrifugal compressors seem to offer many advantages.

The main drawback for centrifugal compressors so far as considerations for the CCS interface with pipeline transport are concerned is that the maximum compression is lower than for reciprocating compressors (see Table 1.3). Nevertheless, since the maximum anticipated operating pressure for CCS pipelines is expected to be around 150–200bar, centrifugal compressors still have the ability to compress the carbon dioxide directly to the required level. There are two main strategies when it comes to CCS compression in anticipation of the subsequent transportation process. Nominally, these are referred to as compression and compression and pumping [18]. Compression and pumping takes into consideration the expected pressure drop during transport. This is an extremely important consideration as the carbon dioxide undergoes significant depressurisation when in the pipeline as shown in Figure 1.10, and so if the injection pressure is to be met whilst also allowing for depressurisation during transit, then either an initial pressurisation to a level far above this is needed, and the CCS pipes must be able to cope with this elevated level, or regular repressurisation whilst the carbon dioxide is in transit is needed. Each option has advantages and disadvantages.

The effect of impurities on the maximum pressure of the pipeline in the case of compression (see Figure 1.10) must therefore be taken into account when determining the pressurisation target for the carbon dioxide, so that it arrives at the storage site at the correct pressure. Again, this demonstrates another application of accurate equations of state. Data, whether empirically or experimentally determined, for the exact depressurisation with distance, depending on a single impurity content has been difficult to find. By way of a summary, we include Table 1.3, extracted from the literature, on the main technologies and performance indicators of existing compression technologies which can be used on carbon dioxide, as a way of highlighting the anticipated pressure ranges equations of state must be applicable to.

Compression Technology	Maximum Pressurisation (bar)	Maximum Flow Rate (m^3/hr)	Maximum Power (kW)	Source
Centrifugal	178	82'100	11'640	[63]
Reciprocating	414	4'600	5'968	[63]
Supersonic	—	2'621	—	[60]

Table 1.3: Existing compression technologies, as summarised from the literature. — means data not available

1.3.7 Regulation, Politics, and Economics

The prospect of transporting high temperature, high pressure carbon dioxide in concentrations which would have toxic effects and could be lethal if leaked, in a vessel constructed of a material which the carbon dioxide mixture could degrade and corrode is understandably unpopular with many people. Moreover, the possibility of external influence on CCS pipelines causing failure and leakage, and the subsequent need for a deep understanding of fracture and dispersion modelling enhances this opinion. The literature goes in to great depth about the many safety requirements that will have to be met to ensure that those who find themselves close to (perhaps within 100m) such transportation networks are sufficiently protected, whilst also avoiding the scenario whereby ensuring this level of safety does not result in such high costs being incurred as to make CCS prohibitively expensive. Of the many important obstacles which must be overcome if carbon dioxide transportation is to be possible, deciding where to place, and how to route the onshore pipelines will prove to be particularly difficult [65, 66], as will trying to convince stakeholders, particularly those who live nearby, of the benefits of placing carbon dioxide pipelines there. To add to the difficulty, obtaining permission from relevant local or national Governments will also be a time consuming and costly process. As an example, since beaches are considered to be areas of natural beauty or of importance to local wildlife, the installation and maintenance of CCS transport infrastructure at coastal

locations is potentially problematic. Listed in the literature are the key stages of proposing a route, assessing the environmental impacts along this route, considering alternative routes and finally obtaining any rights of way for the chosen route [8]. Again, guarantees of safe operation are required.

There are likely to be high levels of inflexibility for the onshore section of the pipeline route as a result: Clearly there is little choice in infrastructure location at either end of the transport process; close to the on–land power plant, and close to the oceanic storage site, but one more also where land becomes sea (this is as true of ship transportation as offshore pipe transportation as there will be similar levels of social resistance to shipping terminals as for pipelines traversing beaches and other sea–side resorts). Of course there may be other points of inflexibility wherever there are areas of dense population, for example in the previously mentioned Humber region of the UK [43]. Furthermore, there will have to be strict regulatory frameworks in place for the injection and storage phases of CCS to ensure that there is no chance of a leak [65]. This highlights another use for accurate equations of state in helping to define pipeline transport purity standards.

Public acceptance of the infrastructure requirements for CCS pipeline transport is key, as it may in some cases be reliant on some fairly irrational fears having to be quelled [8]. The Barendrecht example is important in this regard, as it shows that popular resistance to the idea of CCS–related activities can be enough to stall such projects [67, 27], as demonstrated in Figure 1.16.

Figure 1.16: Popular resistance to the Barendrecht carbon dioxide storage proposals, which eventually derailed the project, including demonstrations (left, [67]) and media hype (right, [27])

As well as resistance from those without technical understanding, a significant amount of resistance can come from those who do understand the technologies and want to raise their own concerns about it through this understanding. As has been

established by this literature review, the pipeline transport of carbon dioxide can be a risky business. A particular issue is energy penalties for the compression and transport processes [68]. Concerns over safety and energy penalties can, in the short–term, only be satisfied by increasing spending, but since CCS is expensive enough already, there will have to be mechanisms in place to ensure that spending on transportation does not get too high. It is the opinion of a selection of CCS experts that the main ways to keep costs low during transportation will be to employ economies of scale and to have fully researched the likely consequences of transport [69].

It is a dangerous position for the implementation of transportation to be in that all three of regulatory, political and economic considerations act as considerable barriers to this being done successfully. This threatens to derail the progress which is being made and so, whereas the implementation of the CCS pipelines is a technical project at heart, it is vital that these considerations are not neglected.

The compression of carbon dioxide to the level required so that it may be transported with the minimum energy penalty through viscosity minimisation and density maximisation requires a very precise knowledge of how the mixture quality affects the thermodynamics of the overall process. This can again be helped by a good equation of state. One of the main criticisms of CCS is that it poses such a large financial cost and energy penalty from capture to storage that left to their own devices, many privately–owned firms would never choose to implement it. This is because the financial penalty brought about by the loss of revenues from power used in CCS instead of being sold to consumers would be too much of a liability.

Very careful management of the operation of capture and transport is needed to minimise the cost burden [70] and the need for Government intervention. The question of how best to minimise the energy requirement to carry out CCS is at the centre of how to implement this process, and herein lies one of the main challenges to be considered; not just in this research project, but by the global energy industry as a whole. Again, equations of state are central to this theme as they will help to define purity standards and develop fracture and propagation models.

The most important fact to remember about transport in CCS is that however large the hurdles to be overcome are, be they social and regulatory [27, 43], financial and economic [69] or technical [68], it is absolutely vital that pipeline transport plays its part or CCS cannot happen. Put simply, this is because if there is no ability to transport the millions of tonnes of carbon dioxide released every year from the

power plants to the geological sequestration sites, and since there is nowhere else to store it, those emissions of carbon dioxide would simply have to be released back into the atmosphere, bringing back into play the environmental concerns raised at the start of Chapter 1.

1.3.8 General Issues Surrounding CCS

As with any technology which promises to radically change established methods of operation, comprehensive risk analyses need to be conducted and safety testing needs to be done, the claims need to be substantiated and economic and financial viability need to be assessed. The first potential problem that arises when one looks at the CCS process from start to finish is that of transporting gas or liquid at high pressure, which has clear safety implications. The materials used to transport matter at such high pressure must have been rigorously tested to ensure that they are up to the task, and contingency plans must be in place, should they fail.

One option likely to be chosen by industry to avoid failures caused by transgressions of small safety margins, is that large safety margins will be put in place for aspects such as the pressures pipes can withstand. This would negate the fact that the exact carbon dioxide mixture behaviour is unknown, but would also constitute potentially unnecessary safety arrangements raising costs even higher. In the scenario of a lack of suitable thermodynamic models, such actions are a likely requirement of government legislation ensuring the new technologies err on the side of caution [48]. As discussed in this literature review, the social implications of placing, for example, a pipeline transporting gas at high pressure through a residential area are unthinkable if the pipe fails (although due to localised social resistances to such a scenario such as seen at Barendrecht, pipeline transportation will generally not be allowed to occur in densely populated areas). A further problem with CCS which is emerging is its interaction with the world of politics and its use as a political tool. The divorce of knowledge and power between engineers and politicians with regard to CCS could result in politically–motivated claims about CCS being made and unobtainable targets for it being set, perhaps resulting in lost confidence in CCS.

For example, the UK Government has pledged an 80% reduction in CO_2 emissions by 2050 [5, 6]. This still seems a very long way off given current trends, and even in the short run, it seems that promises made at the Copenhagen Climate Conference in December 2009 are inconsistent with the aim of global temperature stabilisation [12]. In the long run, this sort of action could lead to a perceived failure of CCS, which could undermine its political viability and subsequent social accep-

tance, including, notably, acceptance for the pipeline transport networks which are so necessary to make CCS happen. The capabilities of CCS therefore need to be clearly defined to avoid this type of misunderstanding. On the theme of political uncertainty regarding CCS, there is also the problem of how all new power plants in the UK are required to be "capture ready" [65]. Although this is so that CCS may be implemented more quickly and easily, the clear problem is that there is no clear definition of what this phrase means, and the potential for ambiguity could lead to a slowdown in deployment of CCS. Indeed, the UK Government has recognised the need to have a definition for what this particular phrase means, and while this definition is likely to take time to be agreed upon, the wider problem of implementing successful capture and transport systems goes on. This, in a sense, encapsulates the regulatory and political problem for CCS, in that it is a time–consuming and bureaucratic process, potentially rife with llitigation and delay, whereas the idea of CCS was created because of a lack of available time within which carbon emissions must be reduced.

There are further general problems with CCS. Of these, the organisational commitment required to implement such a large–scale operation, whilst keeping the cost (in both financial and energy terms) as low as possible is particularly prominent. Failure to do so could result in power generation companies concluding that CCS is not financially viable, in which case they could, under a free market system, cease to operate it altogether. This again highlights that economically acceptable operation of CCS is vital, and further promotes the need for an accurate equation of state underlying all considerations for the operation of CCS pipelines.

1.4 A Technical Literature Review

1.4.1 Overview of the Literature Surrounding CCS Pipeline Transport

Having conducted the contextual literature review, we acknowledge the pressing need for an equation of state for application to CCS pipeline transport which is more accurate and more user–friendly than those which are currently available. The main aim of this technical literature review is to advance the ideas set out in the contextual literature review, and to highlight those sources that will be of use to us as we proceed with the technical element of this project.

1.4.2 Physical Constants Used Throughout this Project

We begin by noting some physical constants which will appear repeatedly throughout this work, their numerical values, dimensions, and nomenclature [71].

Chemical Component	Molecular Mass, M_r (kg.mol^{-1})	Critical Temperature, T_c (K)	Critical Pressure, P_c (MPa)	Critical Molar Volume, v_c (m^3.mol^{-1})	Critical Compressibility Factor, Z_c (1)	Acentric Factor, ω (1)	Universal Gas Constant, R (J.mol^{-1}.K^{-1})
Carbon Dioxide	0.04400964	304.1282	7.3773	9.41185×10^{-5}	0.274588	0.228	8.3144621
Nitrogen	0.02801344	126.19	3.3978	9.01×10^{-5}	0.291785	0.040	
Hydrogen	0.002015894	32.97	1.293	6.415×10^{-5}	0.311073	-0.220	
Oxygen	0.03199886	154.59	5.043	7.34×10^{-5}	0.287985	0.022	

Table 1.4: Values for physical quantities used in this research project. (1) means a dimensionless quantity

1.4.3 The Thermodynamic Basics of Modelling Vapour–Liquid Equilibrium

We note the importance of modelling the interaction between the liquid and vapour phases of a given system within the context of CCS pipelines. In modelling the equilibrium between the vapour and liquid phases within a system, we need to impose [72]:

- Thermal Equilibrium: That the temperature within the different phases for each chemical component of the mixture, and between the different components themselves are all the same. We can impose this condition during the modelling of Vapour–Liquid Equilibrium (VLE) by ensuring the same value for the temperature T is used throughout all calculations.

- Mechanical Equilibrium: In a similar way to the requirement for constant temperature, we require that the pressure within each phase of each component is matched. We similarly impose this by assuming that the same value of pressure P occurs throughout the system.

- Equilibrium of Chemical Potential: That the number of molecules between each phase in each component is not changing, and thus that there are no phase transitions occurring. We do this by matching the fugacity of each phase (vapour and liquid) for each chemical component in the mixture.

If our proposed model is to retain a degree of physical truth, it must be able to compute vapour–liquid equilibrium as well as to give a true relation between volume and pressure. In thermodynamics, generally speaking, an equilibrium can be said to have been reached when the temperature, pressure and chemical potential are all

steady (no time–variation), such as is described in the above list, and that these quantities are matched between distinct phases of a system. For our consideration, this should mean that the numerical value for all of these quantities is the same in both the liquid and the vapour phase for all components in the mixture.

In the case of determining phase equilibrium, an important consideration is the minimisation of the Gibbs Free Energy G. In order to achieve thermodynamic equilibrium, the second law of thermodynamics gives the Gibbs Free Energy G as

$$G = U + VP - TS, \tag{1.3}$$

where U is the system internal energy, V is the total volume, P the pressure, T temperature, and S entropy. Dividing both sides by the number of moles N in the system;

$$\frac{G}{N} = \frac{U}{N} + \frac{VP}{N} - \frac{TS}{N}, \tag{1.4}$$

whence, since the molar Gibbs Free Energy G/N is precisely the chemical potential μ, we have

$$\mu = \frac{U}{N} + \frac{VP}{N} - \frac{TS}{N}. \tag{1.5}$$

In establishing vapour liquid equilibirum, we require that the chemical potential is steady [73], so taking the derivative of both sides of equation (1.5) gives

$$\partial\mu = \frac{1}{N}\partial U + \frac{P}{N}\partial V + \frac{V}{N}\partial P - \frac{T}{N}\partial S - \frac{S}{N}\partial T. \tag{1.6}$$

Since we are seeking the conditions necessary for equilibrium, we may assume that U, P, S and T are fixed (but not V as the volume can change across a phase transition at equilibrium). This leaves

$$\partial\mu = \frac{P}{N}\partial V. \tag{1.7}$$

1.4.4 Fugacity

The Gibbs–Helmholz Equation gives

$$\mu = \mu_0 - RT\log\left(\frac{f(V)}{P(V)}\right), \tag{1.8}$$

where μ_0 is a fixed reference value for the chemical potential and $f(V)$ is the volume–dependent fugacity, with the same units as pressure, exhibiting the property that

$$\lim_{V\to\infty} f(V) = 0, \tag{1.9}$$

and

$$f(V) = \phi(V)P(V), \tag{1.10}$$

where the dimensionless quantity $\phi(V)$ is called the fugacity coefficient. The concept of fugacity is crucial to modelling vapour liquid equilibrium. It is a quantity which describes a particle's tendency to swap between the vapour and the liquid phases, and so given the original aims for achieving VLE, we note that we should want to arrive in a situation where the values for fugacity at the coexisting points are the same. Differentiating Equation (1.8) gives

$$\partial\mu = -RT\partial\bigg(\log\left(\frac{f(v)}{P(v)}\right)\bigg). \tag{1.11}$$

Upon equating the two expressions for $\partial\mu$ in Equations (1.7) and (1.11), we get

$$-RT\partial\bigg(\log\left(\frac{f(V)}{P(V)}\right)\bigg) = \frac{P}{N}\partial V, \tag{1.12}$$

whence

$$\begin{aligned}
\partial\bigg(\log\left(\frac{f(v)}{P(v)}\right)\bigg) &= -\frac{1}{RT}\frac{P}{N}\partial V && (1.13)\\
&= -\frac{1}{RT}\frac{P}{N}\partial V + \left(\frac{\partial V}{V} - \frac{\partial V}{V}\right) && (1.14)\\
&= \frac{1}{RT}\left(\frac{RT}{V} - \frac{P}{N}\right)\partial V - \frac{\partial V}{V}. && (1.15)
\end{aligned}$$

Integrating this over V from V_1 to V_2 and allowing $V_1 \to \infty$ whilst also setting $V_2 = V$ gives

$$\begin{aligned}
\log(\phi(V)) &= \frac{1}{RT}\int_{\hat{V}=\infty}^{\hat{V}=V}\left(\frac{RT}{\hat{V}} - \frac{P}{N}\right)\mathrm{d}\hat{V} - \log(V) + \lim_{V\to\infty}\log(V) && (1.16)\\
&= \frac{1}{RT}\int_{\hat{V}=\infty}^{\hat{V}=V}\left(\frac{RT}{\hat{V}} - \frac{P}{N}\right)\mathrm{d}\hat{V} - \log(V) - \log\left(\frac{P}{RT}\right) + \\
&\quad + \log\left(\frac{P}{RT}\right) + \lim_{V\to\infty}\log(V) && (1.17)\\
&= \frac{1}{RT}\int_{\hat{V}=\infty}^{\hat{V}=V}\left(\frac{RT}{\hat{V}} - \frac{P}{N}\right)\mathrm{d}\hat{V} - \log(Z) + Z - 1 && (1.18)
\end{aligned}$$

where the final terms of the last equality are imposed in order to ensure correct asymptotic behaviour at very low pressures, and where Z is as defined in Equation (1.1). This equation is exactly as given in Equation (2.3.9) of [72] for the fucacity of a pure substance. The implication of the condition that each of temperature, pressure and chemical potential be in equilibrium for substance "i" in order for us to determine the VLE is that the value of the quantity $\log(\phi_i(V))$ (with the subscript i denoting the substance) as given in Equation (1.19) be the same at each of the coexisting volumes; the bubble point volume V_{BP} and the dew point volume V_{DP}.

Equation (2.3.1) of [72] also gives the fugacity expression for substance i occurring in a mixture

$$\log(\phi_i(V)) = \frac{1}{RT}\int_{\hat{V}=\infty}^{\hat{V}=V}\left(\frac{RT}{\hat{V}} - \left(\frac{\partial P}{\partial N_i}\right)\right)\mathrm{d}\hat{V} - \log(Z), \tag{1.19}$$

which we will also be required to implement in order to impose the correct VLE behaviour of mixtures. We relate Equations (1.18) and (1.19) later.

1.4.5 The Relation Between Volume and Density

We expand Equation (1.2) and note the relation between total volume V with units m^3, molar volume v with units $\mathrm{m}^3\mathrm{mol}^{-1}$, and density ρ with units $\mathrm{kg.m}^{-3}$:

$$\rho = \frac{m}{V} = \frac{m}{Nv} = \frac{m/N}{v}, \tag{1.20}$$

where N is the number of moles and m is the total mass in kg. We can immediately identify the quantity m/N in (1.20) as being the molar mass of the substance, values for some substances of which are given in Table 1.4. This convenient relation between molar volume and density means that being able to relate pressure with volume is equivalent to being able to relate pressure with density.

1.4.6 A Summary of Equations of State

As discussed in the contextual literature review, we can see the benefits that might arise if there existed an equation of state which could accurately describe the key physical behaviours of carbon dioxide and CCS–relevant carbon dioxide mixtures. Here we summarise some of the most significant equations of state (judged as such by their overall usage, or contribution to the evolution of equations of state over time). There are many such equations of state available for use in the different stages of CCS. A review of the literature has highlighted the following as being those which

are discussed most often. Here, we discuss the merits and drawbacks of each.

Ideal Gas Law (IGL), 1834

The most basic equation of state combines the general qualitative observations that as the pressure acting on a fluid increases, its volume will decrease, temperature being held constant (Boyle's Law), and that as the temperature of a fluid increases, its volume will increase, the pressure being held constant (Charles' Law):

$$P = \frac{RT}{v}, \tag{1.21}$$

where P is the pressure in Pa, T the temperature in K, and $v = V/n$ the molar volume in $\mathrm{m^3mol^{-1}}$. Here, R is the universal gas constant and has the value as given in Table 1.4. Notice that setting $Z = 1$ in Equation (1.1) yields the IGL (1.21).

The ideal gas law makes a good approximation of the behaviour of many gases in certain circumstances, notably when under low–pressure and the particles are allowed to occupy a large volume, interacting very infrequently. As the pressure is increased however, and these molecular interactions increase, the scope of the IGL to describe how these effect the pressure becomes severely limited.

Van der Waals Equation (VdW), 1873

In order to combat the limitations of the IGL in describing gas behaviour as pressure is increased, the Van der Waals equation was introduced to account for non–ideal behaviour:

$$P = \frac{RT}{v - b} - \frac{a}{v^2}, \tag{1.22}$$

where P, T, v and R have the same units as before, and the quantities a, with units $\mathrm{m^6mol^{-2}}$, and b, with units $\mathrm{m^3mol^{-1}}$ are parameters of the equation allowing for an improved flexibility and description of the physical behaviour. The rationale behind this formulation was based on two important theories:

- as the pressure increases and particles move closer together, they are not, in reality, able to get arbitrarily close, as the IGL would suggest. The contemporary understanding of the structure of the atom in the 19^{th} century was such that it was believed that atoms were "hard spheres" (rather like snooker balls), and that they could not be deformed or compressed beyond the limits of their boundaries. Thus, upon increasing the pressure to arbitrarily high values, it would not be the case that atoms could get infinitely close together,

but instead could never approach closer to each other than the diameter of one of these hard spheres (using the snooker balls analogy again, this would be equivalent to noticing that you could only ever fit n balls into a box designed to accommodate n balls, no matter how hard you try). This therefore excluded an amount of volume from the consideration, so the term containing b in the VdWEoS is often referred to as the volume exclusion term. Whereas the hard spheres interpretation of atomic structure is now known to be invalid, the volume exclusion term still retains a significant amount of physical relevance at all but the most extreme of pressures.

- there are other important physical interactions that exist between particles, notably that forces created by charge come into play at small distances. In the 19^{th} century it had been understood for some time that protons and electrons carried opposing charges (neutrons had not been identified yet). Under the hard spheres interpretation of the atom, it was believed that the negatively charged electrons sat on the surface of the sphere, which contained the positively charged protons. As atoms came into close proximity, the opposing charges caused an attractive force. This effect is described by the parameter a, and the term containing this parameter is referred to as the attractive potential term.

The Van der Waals equation represented a step forward in thinking about describing physical behaviour of fluids, but ultimately it still falls some way short in accurately describing this.

Redlich–Kwong Equation (RK), 1948

The Redlich–Kwong EoS [33] extended this thinking by elaborating on the VdWEoS. They suggested

$$P = \frac{RT}{v-b} - \frac{a}{\sqrt{T}v(v+b)}, \tag{1.23}$$

with all quantities having the same dimensions as before. By doing so, the aim was to give the model more flexibility in describing complicated physical behaviour. The parameters a and b were defined:

$$a = 0.4278\frac{R^2T_c^{5/2}}{P_c} \tag{1.24}$$

$$b = 0.0867\frac{RT_c}{P_c} \tag{1.25}$$

In the paper in which Redlich and Kwong proposed this equation, the importance of calculating fugacities was also acknowledged. As we have seen from Equation (1.19), fugacity is a vital concept in modelling VLE.

Soave–Redlich–Kwong Equation (SRK), 1972

The Soave–Redlich–Kwong EoS is another cubic equation state, further developing the previous models.

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)}, \tag{1.26}$$

with all quantities having the same dimensions as previously, but with parameter definitions altered slightly:

$$a = 0.42748[1 + (0.48 + 1.574\omega - 0.176\omega^2)(1 - \sqrt{\frac{T}{Tc}})]^2 \frac{R^2 T_c^2}{P_c}, \tag{1.27}$$

$$b = 0.08664 \frac{RT_c}{P_c}. \tag{1.28}$$

The Soave–Redlich–Kwong was a modification to the previous version of the model, incorporating for the first time a consideration for the effects of the relative distribution of mass and charge in different chemical species which would have an effect on physical behaviour, the parameter describing this being ω, and being referred to as the acentric factor.

Peng–Robinson Equation (PR), 1976

The Peng–Robinson equation [34] of state also incorporated use of the acentric factor:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b) + b(v-b)}, \tag{1.29}$$

where the quantities again have the same dimensions as before, and parameters this time being defined as

$$a = 0.45724[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - \sqrt{\frac{T}{Tc}})]^2 \frac{R^2 T_c^2}{P_c}, \tag{1.30}$$

$$b = 0.07780 \frac{RT_c}{P_c}. \tag{1.31}$$

It is noticeable that the PREoS took an almost identical form to that of the SRKEoS, suggesting that it had been the intentions of the creators not to generate a new form

of equation, but to seek an improvement to an existing equation through numerical optimisation. This is a key concept in the evolution of Equations of State.

Span–Wagner Equation (SW), 1996

Whereas the above equations of state all belong to the family of cubic equations, the Span–Wagner equation of state is a completely different type. It is of far higher order, and is calibrated with a high number of parameters, thus giving it exceptional performance. Typically this is less than 1% out [74] from established experimental data, but the usual accuracy of the Span–Wagner equation in describing the key physical behaviour of pure carbon dioxide makes it a good substitute for having the experimental data, and often this equation is taken to be the authority on describing pure CO_2. The major drawback of the SWEoS which precludes it from being of any value in CCS despite its tremendous accuracy is its inability to describe anything other than pure carbon dioxide.

Wide–Range Equation of State for Natural Gases and Other Mixtures (GERG), 2008

The GERG is similar to the SWEoS in that it is highly parametrised and of high order, exhibiting a high degree of accuracy in most cases, and for most CCS–relevant chemical species including hydrogen. It is very often referred to in CCS documentation as giving excellent descriptions of the physical behaviour of many CO_2–rich mixtures, except notably in the case of binary mixtures of carbon dioxide and hydrogen. The major limitation of the GERG is its computational complexity, which in a similar way to the SWEoS may prohibit it from a wider deployment in helping to understand CCS pipeline transport. In the case of pure CO_2 the GERG equation is the same as SWEoS. There is a previous version of the GERG, from 2004.

Relative Performance of Existing Equations of State

The literature makes reference to all these equations to varying degrees. We found the model referred to most often in the literature and discussed at conferences was the PREoS, for its relative ease of use and computational simplicity. This is in spite of its disability in describing certain behaviours which are key to the understanding of CCS pipeline transport, most notably the trouble it has in dealing with liquid–incompressibility and mixtures, where its errors can reach 40% (see Table 4.2), even in the pure case. We felt, as is echoed by many in the CCS industry, that this sort of performance will not be suitable for use in helping to accurately predict the behaviour of the gas in the pipelines, due to the implications discussed in Section

1.3 of this thesis.

The next most commonly mentioned model was the GERG, often cited as being of great use in describing the VLE of CO_2–rich mixtures for all CCS relevant chemical impurities apart from hydrogen. Typically errors were around the 1-3% mark, which we suggest would be acceptable for use in CCS.

The SWEoS is often held up as an example of what CO_2 equations of state could achieve if it could be generalised to other chemical components, but ultimately, this drawback is its downfall, and is why it too is unsuitable for use in CCS. Despite this, it does highlight that tremendous accuracy can be achieved in an EoS by utilising a very high number of parameters (188 in all in the case of the SWEoS), whereas we should not be surprised to find that the PREoS with only two fitting parameters can struggle to explain the data. We also note however that the size of the window of relevance also plays a role in the trade–off between simplicity and accuracy, and that an equation which aims to describe physical behaviour over a very wide range is bound to suffer from lower accuracy or the need for increased complexity. An equation which was specifically focussed on the temperature and pressure window of operation for CCS pipelines could potentially exhibit a level of accuracy as needed for application to CCS pipelines without a requirement for extra terms or model parameters.

1.4.7 A Summary of Literature Thermodynamic Data Used for Fitting

As part of the technical literature review, we conducted an extensive review of the available thermodynamic data from various literature going back as far as 1930. This was because we would need to fit any proposed equation to the physical data. We summarised this data from the literature in the Appendices either into the form P–v_{BP}–v_{DP}–T–x–y if being used for for VLE descriptions, or P–v–T–x–y (we use x to denote the concentration in a liquid and y to denote the concentration in a vapour) if being used for density–pressure descriptions. It was further sub–categorised into sections pertaining to the particular binary mixture which was being described.

As was highlighted by Table 1.2, we determined that the most commonly occurring impurities to be found in CCS pipelines were nitrogen, hydrogen, and oxygen, after water had been removed due to its role in causing corrosion. We thus summarised data for binary mixtures CO_2–N_2, CO_2–H_2, and CO_2–O_2. We note at this point the almost total lack of ternary data for any of the derivative systems of these

mixtures which contained mostly carbon dioxide. Where the literature data had been given in units other than S.I. (MPa for pressure, $m^3.mol^{-1}$ for molar volume, K for temperature), we manipulated it from its published form into these standard units in order to make for an easy application to our method.

As was to be expected, the literature data was presented in a very wide variety of formats (isothermal, isobaric, isochoric), and so had either to be analysed and converted into a form we could use, or discarded. Since many equations of state such as PREoS give a formulation for the pressure in terms of volume and temperature $P(v, T)$, and given the volume–dependent nature of the necessary fugacity constraints (1.19) and (1.16) which we would have to impose during model development, we highlight here the necessary criteria for the data to be of use to us in our fitting:

- The data must contain the full array of thermodynamic information. That is pressure, molar volume, temperature, and composition (such data being henceforth referred to as P–v–T–x data), or information allowing us to formulate this array. For example we could calculate molar volume v from the compressibility factor Z (see Equation (1.1)) or from density ρ (see Equation (1.2)).
- The data must be isothermal.
- For VLE data, this must be given at coexisting pressure and not coexisting composition.
- Since an equation of state should be able to give predictions for both density–pressure and VLE behaviour, it will be useful if we could find both these types of data at each temperature, although not essential, because to a certain degree the density behaviour can be inferred from VLE data.

The data we collected from the literature is summarised in the Appendices. We also acknowledge the National Institute of Standards and Technology database [74], from which we could take the required thermodynamic data for pure substances.

1.5 Project Aims

1.5.1 Motivation for this EngD Research Project

CCS is one of the main medium–to–long term strategies by which it is hoped the environmental impact of power generation and other heavy industry can be minimised.

It is evident from this literature review that the role of transport in CCS is vital. Furthermore, the ability to safely carry out the transportation of carbon dioxide for CCS is highly dependent on both the impurities that reside within it from the fuel that was used in combustion, and the capture process itself. This necessitates an equation of state which is specific to this particular cause.

A crucial and often overlooked aspect of the CCS chain is CO_2 transportation, for which technological and legislative issues on how to transport large volumes of CO_2 in a safe and energy efficient manner remain. Whilst CO_2 pipelines have been operational for over 30 years, mainly in the United States for EOR, transportation of anthropogenic CO_2 on the scale required for CCS has not been attempted before [41]. Again, a suitable equation of state would help to implement this with increased certainty of safety and success.

Following on from our analysis of the various equations of state available at present, and in light of this need, we feel therefore that there is a pressing need for a new equation of state for a specific application to the design and operation of CCS pipelines, which is simultaneously both sufficiently user–friendly and accurate.

1.5.2 Formalisation of Aims

This main aim of this EngD project shall therefore be to propose a new equation of state which is particularly relevant to CCS pipeline transportation. Specifically, we will aim for it to be highly accurate within the expected window of mechanical and thermal operation of CCS pipelines; upto 200 bar and between approximately 0 and 40°C. It would also be useful for dispersion modelling if the accuracy of the model could last down as low as approximately -10°

We will aim to define the new equation of state in the form $P(v, T)$, so that it can easily be used for describing the key physical behaviours of CO_2 such as density–pressure relations, as well as phase behaviour during the pipeline transport stage of CCS. It is our intention that this equation should simultaneously be more user–friendly than some other EoSs, which can be very complicated, and which do not generalise to the case of mixtures, whilst also being more accurate than those which are currently widely used.

Taking as inspiration the performance of currently available equations, we feel that if we could demonstrate that our equation can have an inaccuracy level of under 2% for descriptions of pure carbon dioxide, and under 5% for mixtures in both VLE

and density predictions, whilst also retaining a suitable level of simplicity, this would represent a significant improvement over the currently widely used models. In order to position our equation thus, we observe the evolution in the form of these currently used equations of state from the simple, such as the IGL, VdWEoS, RKEoS, SRKEoS and PREoS through to the more complicated such as the SWEoS and GERG, and note that although the PREoS is widely used due to its simplicity, it is unsuitable for describing CO_2 behaviour in CCS transport due to its consistent lack of accuracy throughout the region of interest, exhibiting errors as high as 40% in some places, and that whereas the SWEoS is highly accurate, this comes at the cost of a very high degree of functional complexity and a reliance on a large number of parameters, making it very difficult to work with and generalise to the case of mixtures. This suggests we should look for something between the PREoS and the SWEoS in terms of both complexity and accuracy.

To bring about this aim, we will thus seek an equation that would match the literature experimental data or data taken from NIST significantly more accurately than the PREoS, but without the need for high functional complexity, or the requirement for a large number of parameters predominant in more complicated equations of state, although we do note that for descriptions of pure CO_2, NIST uses the SWEoS due to its superior accuracy in this case. This data is generally not more than 0.05% out from peer–reviewed experimental data, making it ideal for our purpose of being highly accurate data to which we will fit our equation in the case of pure carbon dioxide.

1.5.3 Scope for Application of this Project

One of the main barriers to overcoming the many political, social and regulatory issues surrounding CCS transport is our current lack of ability to predict how the physical properties of carbon dioxide change as the type and amount of constituent chemical impurities vary. Presently, there are several equations of state which could be utilised, but all have their relative drawbacks. Bearing in mind there is a balance to be struck between faster equations and those which are more accurate, then in particular, there is a clear need at this moment for the development of an equation of state which can accurately depict the physical behaviour of carbon dioxide and impurities during the transport stage of CCS in a simple, effective way without excessive computational cost.

There is also much that needs to be better understood before safe, socially acceptable and cost effective transport networks can be constructed, especially in the

prediction of key physical behaviour such as density–pressure or volume–pressure and phase behaviour. We feel that if we are able to formulate the model specified within our aims in Section 1.5.2, this will be of tremendous value in the design and subsequent operation of CCS pipelines, and in this way will have a very clear application and hopefully, a large demand.

Chapter 2

Methodologies and Mathematical Techniques to be Used in this Project

2.1 Outline of Method

Following on from the literature review and project aims set out in Chapter 1, we will proceed by proposing a physically relevant formulation for our equation of state. Based upon our observations made in the literature review of the natural trade–off between the complexity and performance of an equation, we will be required to ensure that our proposed model has sufficient flexibility to obtain the target level of accuracy outlined for the proposed model. If this target can be achieved in the majority of cases, we will deem the project to be a success, as we will feel a very good compromise between the the simpler, less accurate equations, and those which are more complex but also more accurate would have been found. In doing this, we feel we will have offered a very tangible solution to many of the design and operation problems CCS pipeline transport faces due to a lack of certainty in the prediction of physical behaviours.

Like those equations such as the PREoS at the simpler end of the spectrum, we will make ours pressure–explicit, and it will be given as a function of the temperature T and the molar volume v, as is also the case for the PREoS; one of its features which makes it particularly user–friendly. It will also depend explicitly on

a number of parameters; quantities which we will be required to give temperature dependent definitions for in order to allow our model to render full thermodynamic descriptions of density and phase behaviour. Thus, the equation will be of the form $P(v, T; a, b, c, \ldots)$, where a, b, and so on are the parameters of the equation, and the "..." is used to denote that the pressure depends on as many such parameters as we feel is necessary to give the model a good chance of being suitably accurate. This will be a two–stage process:

Firstly, we will fit the equation to the pure CO_2 data taken from the NIST database [74] in order to give temperature–dependent expressions $a(T)$, $b(T)$, ... for each of the model parameters. The temperature range of these expressions will be the same as the CCS–relevant window of temperatures, which the literature review and attendance at many conferences suggested as being similar to atmospheric temperatures for the majority of planet Earth, around 0 to 40°C. The pressure range will be from atmospheric pressure up to 200bar, which we understand to be approximately the necessary maximum in order to maximise throughput whilst limiting the financial burden, as noted in Table 1.3. In the first instance, this will have created an equation of state which is valid in the case of pure carbon dioxide only, in the region of interest of CCS transport, and this will then form the foundation of the rest of the model.

We will subsequently consider binary mixtures, and for each distinct mixture highlighted as being of particular relevance to CCS in Table 1.2, we will propose mixing rules for each of the parameters from the original equation to allow this generalisation. At this early stage, we acknowledge, based the role played by parameter a in the PREoS, that linear mixing rules may not be sufficient to allow a suitable degree of flexibility in the fitting, and we are prepared to have to try quadratic mixing rules as necessary. The literature review revealed that the most consistently occurring chemical impurities likely to have a major impact on the pipeline transport of CCS are nitrogen, due to its abundance in the atmosphere and subsequently in CCS mixtures, hydrogen, emanating from combustion of the fossil fuel, for which an interesting point is that even the GERG is acknowledged to have some shortcomings, and oxygen, also naturally occurring in the air and used for the combustion of the fossil fuel, occurring in significant quantities in CCS. Since drying regimes will be very strict in order to minimise pipeline corrosion, we do not incorporate water into our consideration for the model.

An important realisation is that the mixing rules for each parameter will themselves be dependent on sub–parameters, which we will also need to find temperature–dependent expressions for. This will be done following on from our extensive har-

vesting of data from the literature, we will use that which we deem appropriate to calibrate the proposed system; which incorporates both the original equation, and the mixing rules. For nitrogen, hydrogen and oxygen in turn, we will load the literature and NIST data, formatted into ".txt" files, either sub–categorised into density or VLE data, to our chosen modelling software package "Mathematica 9 for Students", by Wolfram. From here, we will write code and algorithms to utilise the software in minimising an error function for the sub–parameters, ensuring both density and phase behaviour is adhered to, and in doing so, we will be able to determine the numerical value of each parameter at the temperature we fitted to the data at.

This will be repeated at each temperature point within the CCS–relevant temperature range we have been able to collect data for until we are able to specify the value of each parameter at a variety of temperature points throughout this range. We will subsequently give a temperature–dependent form for each of the sub–parameters, thus closing off the system and allowing us to give a formulation for P solely in terms of v and T for each binary mixture..

2.2 Selection of Data

Before proceeding to fitting the proposed equation to the various NIST and experimental data we collected, a thorough survey of available density and coexistence data sets was conducted. This utilised various other literature reviews done previously [55, 75] as well as other data sets found manually by searching through on–line journals.

As mentioned in the introductory chapter, in order for our method to be able to utilise a particular data set, we required the following:

1. In the case of homogeneous density data, the set should contain the full array of thermodynamic information: the pressure P, the molar volume v, the temperature T, and the composition of the mixture x. Alternatively, it could give values that would allow a direct calculation of these four variables, for example, v could be calculated from Z by use of equation (1.1), or from ρ by use of equation (1.20).

2. In the case of coexistence data, that coexisting dew and bubble points be given at constant pressure as opposed to constant composition. Thus, we need each data point in the form P–v_{BP}–v_{DP}–T–x–y, where v_{BP} is the bubble point molar volume and v_{DP} is the dew point molar volume.

3. Ideally, that the data be precisely isothermal, or alternatively not more than a few thousandths of a Kelvin out from each other at each data point, in which case the data would be considered isothermal.

Based on the accumulation and subsequent analysis of the literature thermodynamic data, we made the following observations:

1. A lot of the data was incomplete in respect of either point 1 or 2 above. In our reproduction of thermodynamic data from the literature in the Appendices, we used " — " to denote a piece of data which was not available. It can be seen that this occurred very regularly within the literature.

2. Specifically, the majority of the surveyed VLE literature contained neither any reference to the molar volumes, nor any data allowing us to calculate these (compressibilities or densities). Our initial approach had been to abandon such data and only consider using the data which gave all values P–v–T–x, but upon a holistic analysis of the data we concluded that this would have resulted in us discarding the vast majority of the VLE data, to the extent that we would not have been able to carry out a fitting with the data that was left. As a direct result, after considering estimating these through either Maximum Likelihood Estimation or as part of the numerical search algorithm, we produced a novel non–probabilistic estimative method for reconstructing these missing volumes, so that the majority of the data could be salvaged and utilised in the fitting.

3. Some sources [76, 77, 78] listed their measurements in ways other than isothermally. Where such data could be reconfigured into such a form that rendered it isothermal, we did this, otherwise we discarded it.

4. At some points the compositions were not reported. In this case we had to discard that particular data point.

5. Occasionally [79] some sources plotted the data in graphical form but did not seem to include the tabulated data. In this scenario we also had to neglect that data.

6. Some of the data we summarised was at a temperature far outside the range of relevance for CCS pipeline operation. This was discarded. For example, in [80], the temperatures (543–704K) were too high. Similarly for [81] (673.15K).

7. Occasionally, published data was not isothermal, in this case usually being isochoric [82], or occasionally at constant composition [75]. In particular,

some of the data presented in [82] was isochoric, and some approximately isothermal. The isochoric data was discarded.

8. We found some contradictory data, as is to be expected in a data survey as comprehensive as that which was undertaken here. This is even less surprising, given the data was measured across a period of many years, different institutions, and using a wide variety of methods, for example by use of a Pycnometer or Burnett Apparatus for density measurements.

9. A lot of sources listed virial or calculated/optimised binary interaction coefficients [83, 75, 84, 85] based on work they had done. We did not concern ourselves with those as our aim was to fit a completely new equation of state rather than to optimise existing equations.

10. The given values for critical properties seemed to be inconsistent between sources, e.g. in [75] where a value for the critical pressure of carbon dioxide of 7.3752MPa was taken; a slight disagreement from the figure we used based on the majority of other sources, as detailed in Table 1.4.

11. Some data appears to have been duplicated within the literature [83, 86]. In this case several of the authors of both papers were the same.

12. Some sources gave measurements for pure components, for example for pure carbon dioxide [87, 88] or pure nitrogen [89]. The conclusions drawn in these sources suggested that the methods they had used to generate their data were consistent with the Span–Wagner equation in the case of pure carbon dioxide. Thus, owing to the superior availability of data and similar accuracy, we opted to take all our pure data from the NIST database.

13. There was an abundance of density measurements for the binary system CO_2–CH_4 [53], but very little by way of VLE data, and that which was available was very fragmented, meaning it would have been difficult to include considerations for CH_4 at this stage.

14. The VLE data reported in [53] was not given at constant vapour pressure, as required by our method, rather it was given at coexisting compositions. We thus used a smoothed linear interpolation on their reported pressures to allow us to use this data as the lack of any other sources for this composition coupled with the comprehensive nature of this particular data set required us to do so.

15. Very infrequently [90, 91] some data was found to be extremely lacking in quality. In such cases, the lack of internal consistency was exposed by our equation

when we tried to fit using it. In this case we neglected the volume element of these measurements and employed our own volume estimation method.

2.3 Availability and Coherence of Data

Generally, we found the availability of data detailing both homogeneous density and VLE behaviour at the same temperature to be low. Furthermore, that which was presented was done so in a wide variety of formats, in different units, and with some elements missing. In the literature review, much was made of the lack of high–quality thermodynamic measurements which are of relevance to the CCS pipeline transport industry, and given that the calibration of any relevant equation of state, including our own, is dependent on the availability of such data, we include in our conclusions suggestions for which measurements can be taken next in order to allow for this to be done.

We carried out a brief analysis of the state of the literature data in its current form, and found that all the given pressure–density measurements could be used, as these always contained the information we required. For the VLE data it was a different story however and much of it would have had to have been discarded unless we could incorporate a good estimate for the volume values it was missing. the extent to which we would have had to discard large amounts of data without this estimation method is shown in Table 2.1.

Mixture	Usability of data?			Total
	Yes	With Volume Estimation	No	
CO_2–N_2	40	239	123	402
CO_2–H_2	0	185	131	316
CO_2–O_2	26	109	134	269
TOTAL	66 (6.7%)	533 (54.0%)	388 (39.3%)	987

Table 2.1: A summary of the number of literature VLE data points needing to undergo volume estimation in order to be used in fitting

Without a method for utilising the data where volumes are missing, we would only have been able to use 6.7% of the literature data. With volume estimation, we were in a position to use up to 60.7% of that data, thus giving the equation more physical relevance.

2.4 Estimation of Coexisting Molar Volumes

As noted previously, we observed that a lot of the VLE data, especially that describing the binary systems CO_2–H_2 and CO_2–O_2, found in the literature was lacking a volumetric element. Such data points are noted in the Appendices under the "Vol. Est." column, by which we meant that even though the data point did not contain the volumetric information, it might be still be usable if we could somehow introduce a suitable method of volume estimation. We thus developed from scratch a novel process to estimate both the bubble and dew coexistence volumes in compensation for those data missing in the literature. This was primarily down to the fact that our method of fitting the parameters to the chosen form of the equation required all elements of the thermodynamic description (temperature, pressure, volumes and compositions) to be present, but owing to the relative sparsity of VLE data containing all this necessary information (see analysis in Table 2.1), we felt some way of incorporating that which was available would be better than discarding it altogether. We do, of course, acknowledge that experimental measurements of a quality high enough to be published in peer–reviewed journals would have been preferable to having to estimate volumes.

2.4.1 Mixture Bubble Point Volume Estimation

In the following two Sections we denote a bubble point volume by u and a dew volume with w for notational convenience.

We estimated the mixture bubble volume $\tilde{u}_{\mathrm{MIX}}$ by taking a weighted average of the pure carbon dioxide bubble volume and the pure nitrogen (respectively, hydrogen, oxygen) volume at the same pressure, with the weighting given by the concentration of nitrogen (respectively, hydrogen, oxygen), adjusted by an empirical constant ξ_{BP}. The pure data was available in all cases from NIST, and the compositions were reported as part of the literature data. This definition was given for each temperature and pressure by:

$$\tilde{u}_{\mathrm{MIX}} := (1 - x_{\mathrm{N_2}}^{\xi_{\mathrm{BP}}})v_{\mathrm{CO_2}} + x_{\mathrm{N_2}}^{\xi_{\mathrm{BP}}} v_{\mathrm{N_2}}, \tag{2.1}$$

where $\tilde{u}_{\mathrm{MIX}}$ is the estimated bubble volume of the mixture at the required temperature and pressure, $x_{\mathrm{N_2}}$ is the concentration of nitrogen at the bubble point as quoted in the literature, $v_{\mathrm{CO_2}}$ is the molar volume of pure carbon dioxide at this temperature and pressure, $v_{\mathrm{N_2}}$ is the molar volume of pure nitrogen at this temperature and pressure, and ξ_{BP} is a novel, empirically determined constant included in order to calibrate this estimation for different mixtures. This dimensionless quantity, which

we call the "Bubble Constant", is dependent only on the mixture itself, and its values for different mixtures are given in Table 2.2.

2.4.2 Mixture Dew Point Volume Estimation

For the dew volume estimation we first tried an analogous definition to that given in Equation 2.1 for the bubble point volume. It was immediately clear such a definition did not work however, giving an unphysical behaviour. Specifically, we found that it predicted a mixture dew point volume higher than that of the pure carbon dioxide dew volume at the same temperature, which is impossible. We felt this discrepancy was due to the difference in liquid and vapour compressibilities, and it necessitated a slight deepening of our definition for dew volume estimations.

As a result, we introduced the concept of the temperature–dependent "Dew Ratio", $\Upsilon(T)$ in order to bring the dew volume estimates back into the region of relevance. The dew ratio $\Upsilon(T)$ was defined as being the ratio of the difference in volume between the pure CO_2 dew volume and the pure N_2 volume at the same temperature, and the the difference in volume between the pure CO_2 bubble volume and the pure N_2 volume at the same temperature. It is a dimensionless scaling factor which is dependent on the mixture components as well as the temperature. It must necessarily take a value between 0 and 1, and at each temperature was calculated by:

$$\Upsilon_{\text{MIX}} := \frac{v_{\text{N}_2} - w_{\text{CO}_2}}{v_{\text{N}_2} - u_{\text{CO}_2}}. \tag{2.2}$$

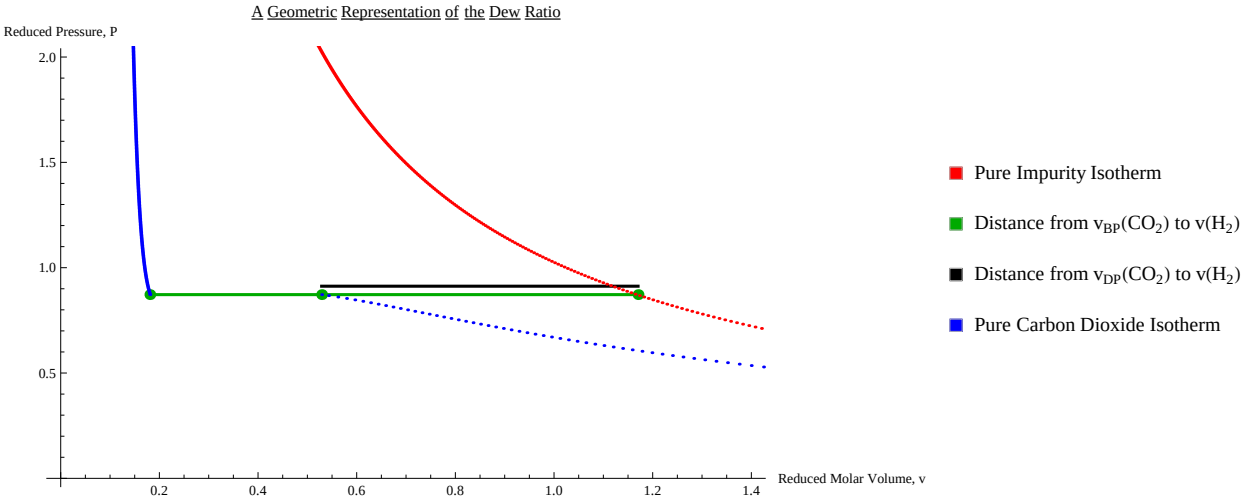

Figure 2.1: A graphical representation of the geometric quantities used in calculating the Dew Ratio, Υ

We could then give the definition for the estimated dew volume as

$$\tilde{w}_{\mathrm{MIX}} := y_{\mathrm{N_2}}^{\xi_{\mathrm{DP}}} v_{\mathrm{CO_2}} + v_{\mathrm{N_2}}(\Upsilon_{\mathrm{MIX}}(1 - y_{\mathrm{N_2}}^{\xi_{\mathrm{DP}}}) + (y_{\mathrm{N_2}} - x_{\mathrm{N_2}})^{\chi_{\mathrm{DP}}}), \tag{2.3}$$

where $\tilde{w}_{\mathrm{MIX}}$ is the estimated bubble volume of the mixture at the required temperature and pressure, $y_{\mathrm{N_2}}$ is the concentration of nitrogen in the vapour phase as quoted in the literature, $x_{\mathrm{N_2}}$ is the coexisting mole fraction in the liquid phase, with ξ_{DP}, which we call the "Dew Constant", and χ_{DP}, which we call the "Critical Constant" playing a similar role to the quantity ξ_{BP} introduced earlier. We note that the presence of the second term in the large bracket on the right–hand–side of Equation (2.3) ensures correct asymptotic behaviour as the pressure increases and the top of the phase boundary is reached, by ensuring that at this point,

$$\tilde{u}_{\mathrm{MIX}} = \tilde{w}_{\mathrm{MIX}} \tag{2.4}$$

As mentioned, the Bubble Constant ξ_{BP}, the Dew Constant ξ_{DP}, and the Critical Constant χ_{DP} are dependent only on the mixture itself, and were empirically determined by trial and error until Equations (2.1) and (2.1) gave visually good estimations. We state the values for these quantities for the binary mixtures CO_2–N_2, CO_2–H_2, and CO_2–O_2 which we found to allow good approximations to the VLE volumes we were seeking:

Mixture	ξ_{BP}	ξ_{DP}	χ_{DP}
CO_2–N_2	1.25	0.68	1.01
CO_2–H_2	1.51	0.48	1.19
CO_2–O_2	1.55	0.47	0.73

Table 2.2: A summary of the values for ξ_{BP}, ξ_{DP}, and $\bar{\xi}_{\mathrm{DP}}$ which we used

During the fitting stages of this project, where the literature data did contain the volumes, we would use these rather than our volume estimation method, instead reserving this for the scenario where the volumes were missing. We highlight the major benefit of this method as being that it allows a substitute value for the missing coexisting volumes, which often were not quoted, to be calculated using only the pure density data which was readily available through NIST [74] and the coexisting molar fractions, which often were quoted.

2.4.3 Performance of Our Volume Estimation Method

Of course, it was necessary to ensure that the volume estimation method functioned appropriately. We did this by employing the method to estimate volumes for a se-

lection of data sets which did contain the volumes, and testing against those data sets to check the method reconstructed the volume data with reasonable accuracy. We reiterate that the volume estimation method only needed the pure density data and the coexisting mole fractions.

We carried out this test for the CO_2–N_2 system at 273.15K [54] and 288.15K [53], for the CO_2–H_2 system at 258.15K and 273.15K [92], and for the CO_2–O_2 system at 273.15K [54]. The comparisons of these estimations with the quoted data are given in Tables 2.3, 2.4, and 2.5.

T(K)	P(MPa)	v_{BP} % Error	v_{DP} % Error
273.15	3.792	1.269	10.320
273.15	4.137	2.718	12.772
273.15	4.482	4.263	13.365
273.15	4.826	5.493	12.653
273.15	5.171	6.527	10.975
273.15	5.516	9.834	9.111
273.15	5.861	8.386	6.507
273.15	6.205	9.322	5.150
273.15	6.550	9.890	4.283
273.15	6.895	10.931	2.536
273.15	7.240	11.383	1.315
273.15	7.584	12.254	0.849
273.15	7.929	12.652	0.202
273.15	8.274	12.961	1.112
273.15	8.618	13.154	2.403
273.15	8.963	13.147	3.481
273.15	9.308	13.237	3.459
273.15	9.653	13.044	4.476
273.15	9.997	13.262	6.535
273.15	10.342	12.900	7.725
273.15	10.687	12.454	8.790
273.15	11.032	11.393	9.822
273.15	11.376	9.905	11.406
273.15	11.721	8.052	12.666
273.15	11.893	5.299	14.720
273.15	11.997	2.534	17.365
288.15	5.695	1.6	9.0
288.15	6.737	2.7	4.0
288.15	7.589	3.1	1.1
288.15	8.105	2.6	3.5
288.15	8.509	1.6	7.2
288.15	9.069	0.2	14.1
288.15	9.463	3.9	16.3
288.15	9.642	6.5	19.6
288.15	9.756	12.7	24.08

Table 2.3: A summary of the performance of our volume estimation method for the binary system carbon dioxide–nitrogen

T(K)	P(MPa)	v_{BP} % Error	v_{DP} % Error
258.15	6.915	7.401	9.358
258.15	13.789	8.375	2.294
273.15	6.895	8.469	1.376
273.15	13.796	11.112	2.205

Table 2.4: A summary of the performance of our volume estimation method for the binary system carbon dioxide–hydrogen

T(K)	P(MPa)	v_{BP} % Error	v_{DP} % Error
273.15	3.792	0.145	8.803
273.15	4.137	2.035	14.095
273.15	4.482	1.088	16.838
273.15	4.826	1.624	17.906
273.15	5.171	2.081	18.657
273.15	5.516	2.453	18.269
273.15	5.861	2.809	17.297
273.15	6.205	2.985	15.580
273.15	6.550	3.145	13.998
273.15	6.895	3.598	11.245
273.15	7.239	3.757	9.069
273.15	7.584	3.727	7.558
273.15	7.929	3.641	5.570
273.15	8.274	3.481	3.616
273.15	8.618	3.311	1.910
273.15	8.963	3.050	0.095
273.15	9.308	2.739	2.264
273.15	9.653	2.417	4.474
273.15	9.997	2.314	7.390
273.15	10.342	1.562	9.796
273.15	10.687	0.744	11.998
273.15	11.032	0.426	13.320
273.15	11.376	2.846	11.965
273.15	11.549	4.107	10.886
273.15	11.742	16.043	2.124

Table 2.5: A summary of the performance of our volume estimation method for the binary system carbon dioxide–oxygen

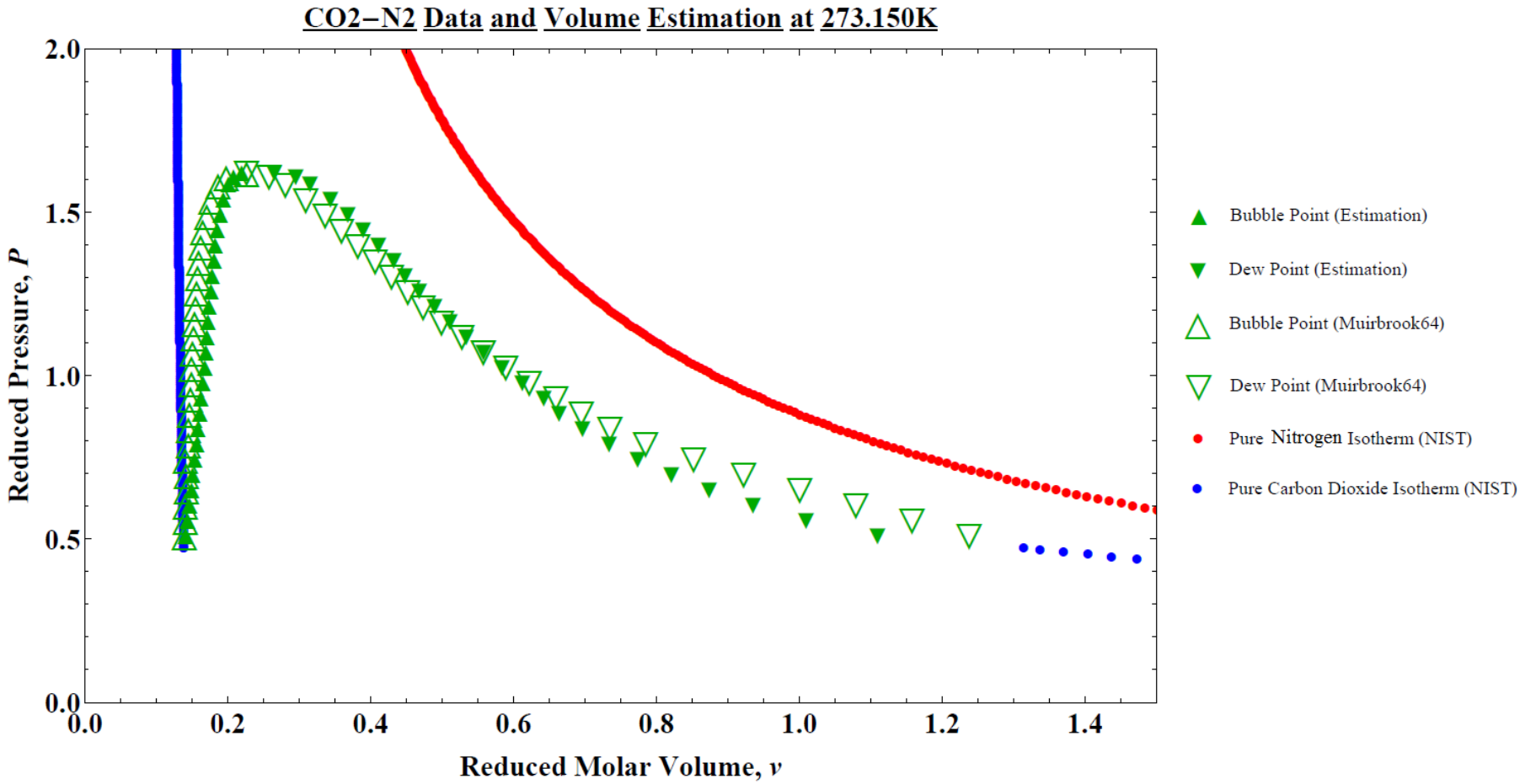

Figure 2.2: Behaviour of the volume estimation method compared to literature data at 273.15K for a carbon dioxide–nitrogen mixture

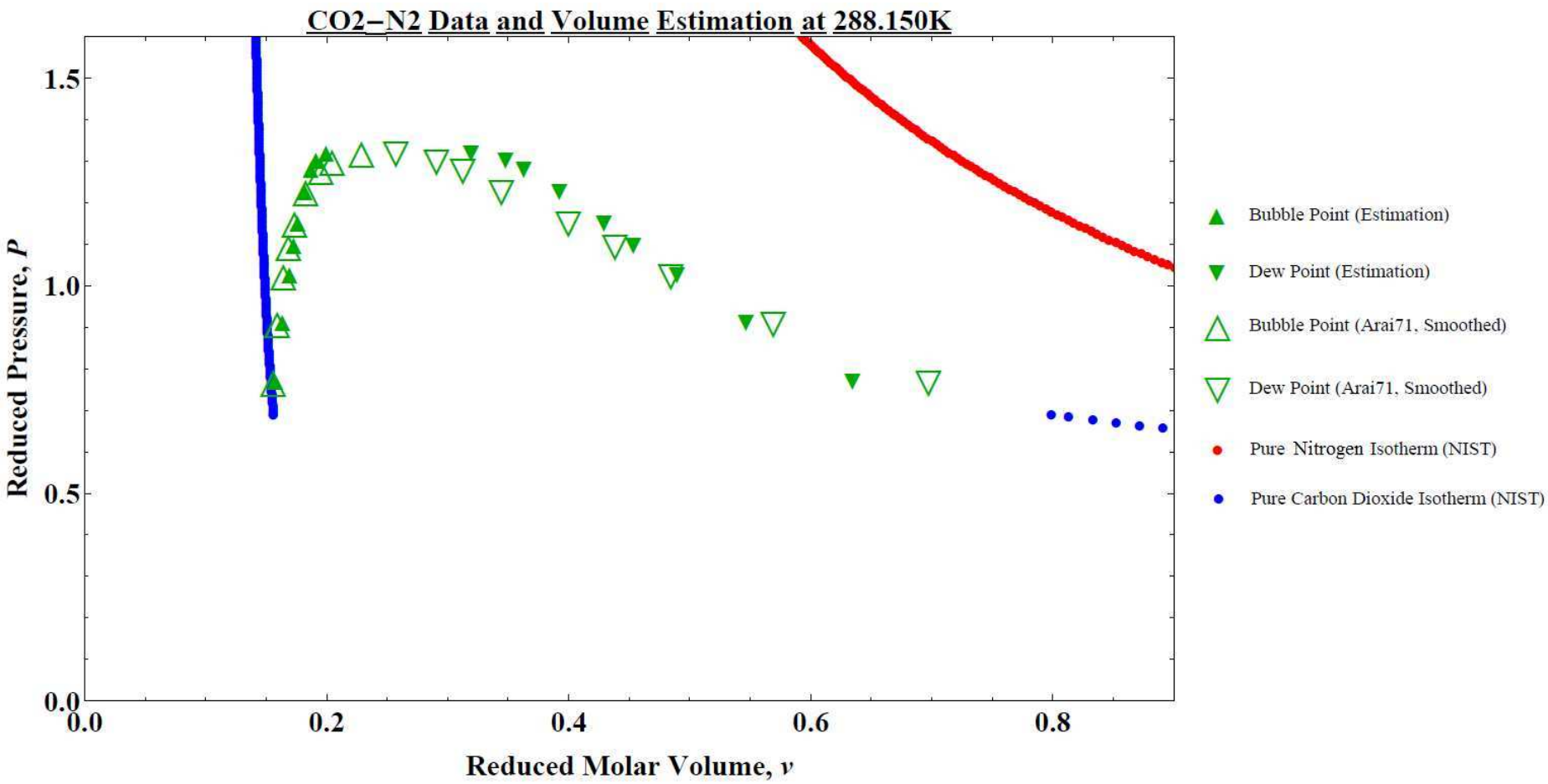

Figure 2.3: Behaviour of the volume estimation method compared to literature data at 288.15K for a carbon dioxide–nitrogen mixture

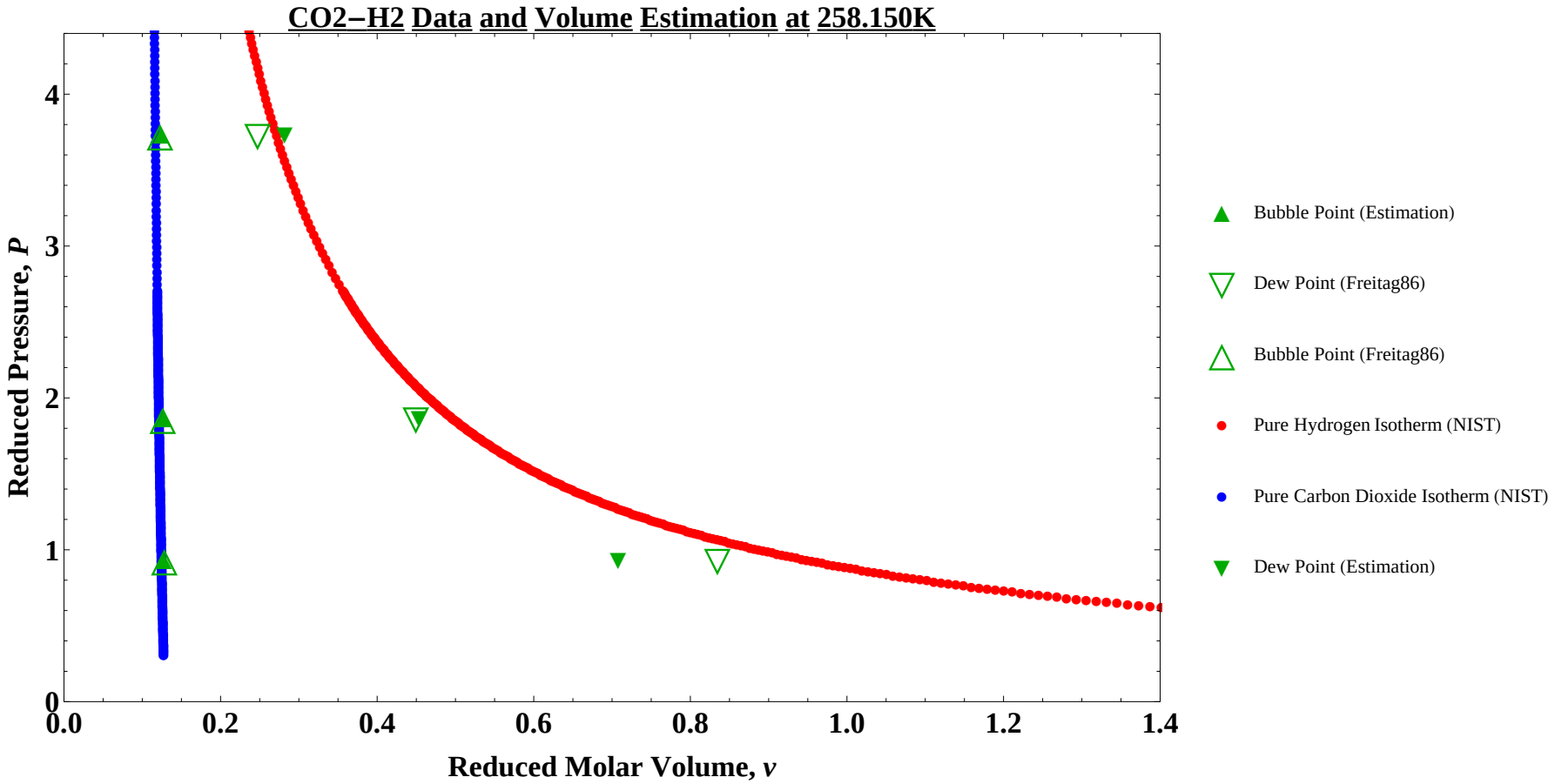

Figure 2.4: Behaviour of the volume estimation method compared to literature data at 258.15K for a carbon dioxide–hydrogen mixture

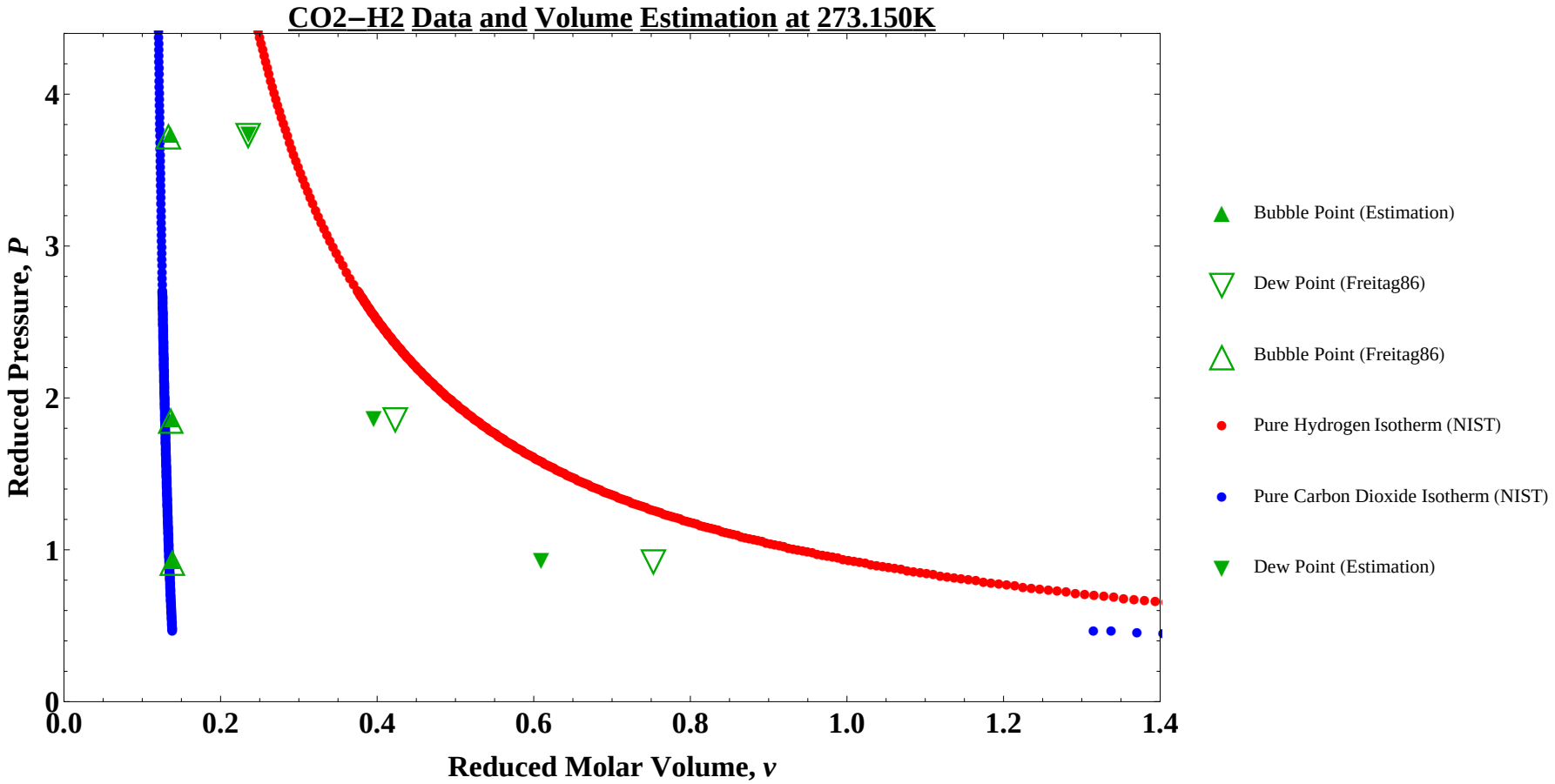

Figure 2.5: Behaviour of the volume estimation method compared to literature data at 273.15K for a carbon dioxide–hydrogen mixture

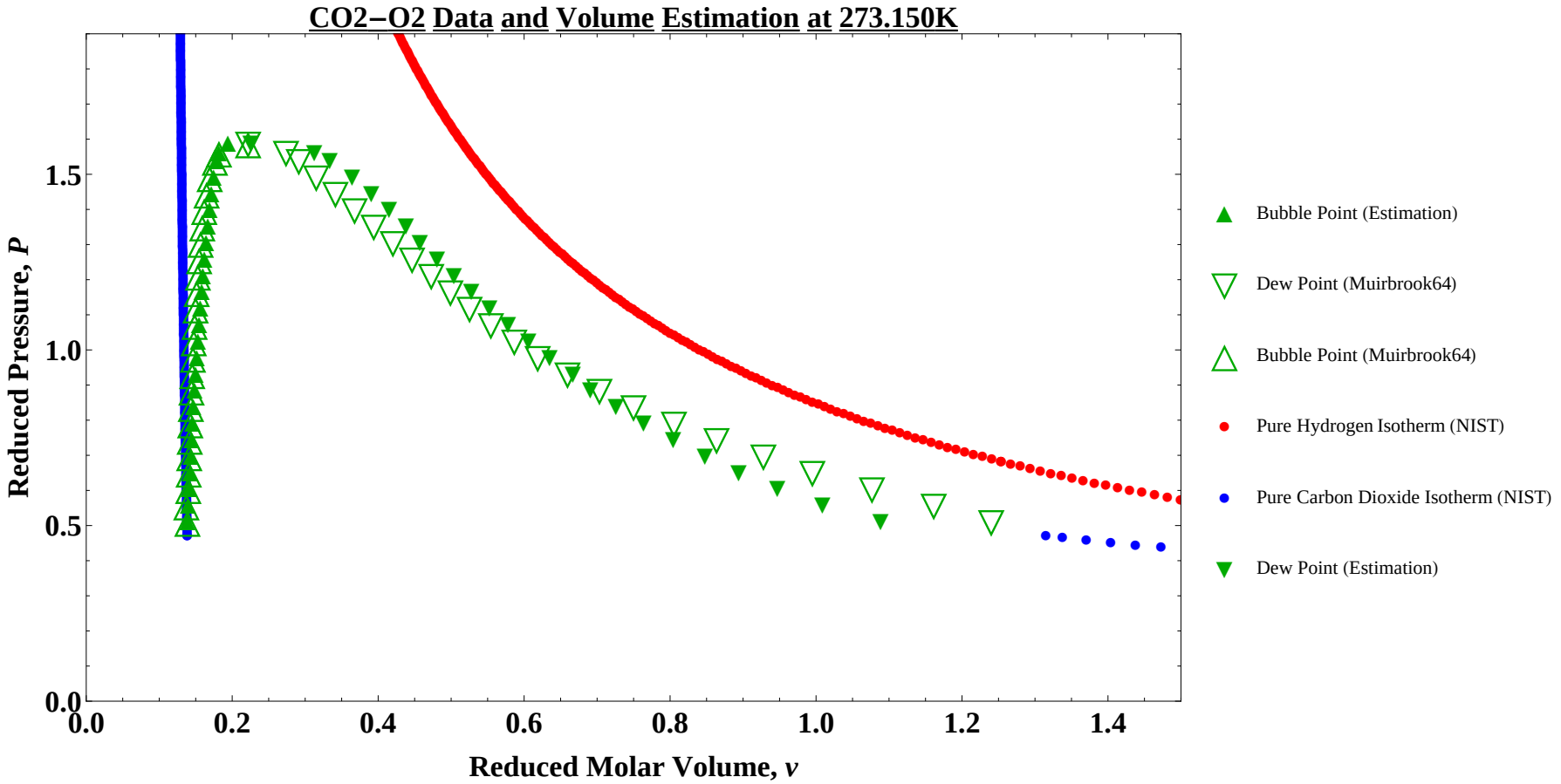

Figure 2.6: Behaviour of the volume estimation method compared to literature data at 273.15K for a carbon dioxide–oxygen mixture

In the binary system CO_2–N_2 our estimation method recovered the volumes with an average percentage error of 7.95% and a maximum percentage error of 24.08%, for CO_2–H_2 with an average percentage error of 6.32% and a maximum percentage error of 11.11%, whilst in the binary system CO_2–O_2 it recovered them with an average percentage error of 3.05% and a maximum percentage error of 18.66%. We felt that these accuracy figures were very similar to the anticipated level of accuracy of the majority of experimental thermodynamic measurements of the type reported in the literature, so on this basis, felt confident that we could employ our volume estimation method to reconstruct the missing data from the literature with a similar accuracy to that with which it would have been presented anyway.

We acknowledge the limitation of this method that it only appeared to give valid estimations within the temperature range from around 260K to 300K: In attempting to estimate the carbon dioxide–nitrogen data at 303.3K, we found the method to perform badly enough that we could not use the resultant estimations. We also note that in the system containing hydrogen, at 258.15K, in Figure 2.4, the estimation of the dew point at the highest pressure was also invalid, and we neglected this estimation for subsequent fittings. Nevertheless, we generally considered that this method would be extremely valuable in substituting for the missing coexisting volumes.

2.5 Estimation of Homogeneous Phase Molar Volumes

Since we were trying to fit to two types of data, and bearing in mind that there were very few temperatures where both VLE and homogeneous density data existed, we felt it would be beneficial for the fitting regimes to extend the volume estimation method described in Section 2.4 to also include estimations for mixture molar volumes in the homogeneous liquid and vapour phases. This was necessary as we wished to constrain the model to give physically relevant homogeneous density predictions, even in situations where this data was not available.

2.5.1 Liquid Phase Volume Estimation

For the liquid phase molar volume estimations we again did this by a weighted average between the pure carbon dioxide molar volume and that of the second component in the binary mixture, where the weighting constant was defined so as

to give consistent behaviour approaching the liquid saturation line:

$$\lambda = \frac{\tilde{u}_{\mathrm{MIX}} - v_{\mathrm{CO_2}}}{v_{\mathrm{N_2}} - v_{\mathrm{CO_2}}}, \tag{2.5}$$

where for any given temperature and pressure, $\tilde{u}_{\mathrm{MIX}}$ is the coexisting bubble volume estimated by the method in Section 2.4, and v_{CO2} and v_{H2} are the pure molar volumes for carbon dioxide and nitrogen (or respectively, whichever the second component in the mixture is) at the given temperature and pressure. We then defined the liquid phase mixture volume to be

$$\tilde{v}_{\mathrm{MIX}} = (1 - \lambda)v_{\mathrm{CO_2}} + \lambda v_{\mathrm{N_2}}. \tag{2.6}$$

We found it useful to establish the homogeneous phase volumes up to the limit of the phase boundary. We reiterate that that quantity λ ensures behaviour is consistent upto the phase boundary, as shown in Figure 2.7

2.5.2 Vapour Phase Volume Estimation

The vapour phase volume estimation was a little more straightforward as the weighting constant was simply taken to be the molar concentration of the impurity:

$$\tilde{v}_{\mathrm{MIX}} = (1 - y_{\mathrm{N_2}})v_{\mathrm{CO_2}} + y_{\mathrm{N_2}}v_{\mathrm{N_2}}, \tag{2.7}$$

where $y_{\mathrm{N_2}}$ is the concentration of impurity in the vapour phase. We note that since at the transition from vapour phase through the multi–phase region and into the liquid phase the molar volume of the pure carbon dioxide jumps suddenly, this definition was only valid upto the vapour pressure at the given temperature, and that these volume estimations for the vapour phase could not therefore be extended all the way to the two–phase boundary.

2.5.3 Behaviour of the Homogeneous Phase Volume Estimation

There was no homogeneous volume data to compare this method to so we are unable to specify its performance in terms of a percentage error. We can however illustrate that it gave a physically relevant behaviour in both the liquid and vapour phases as shown in Figures 2.7 and 2.8.

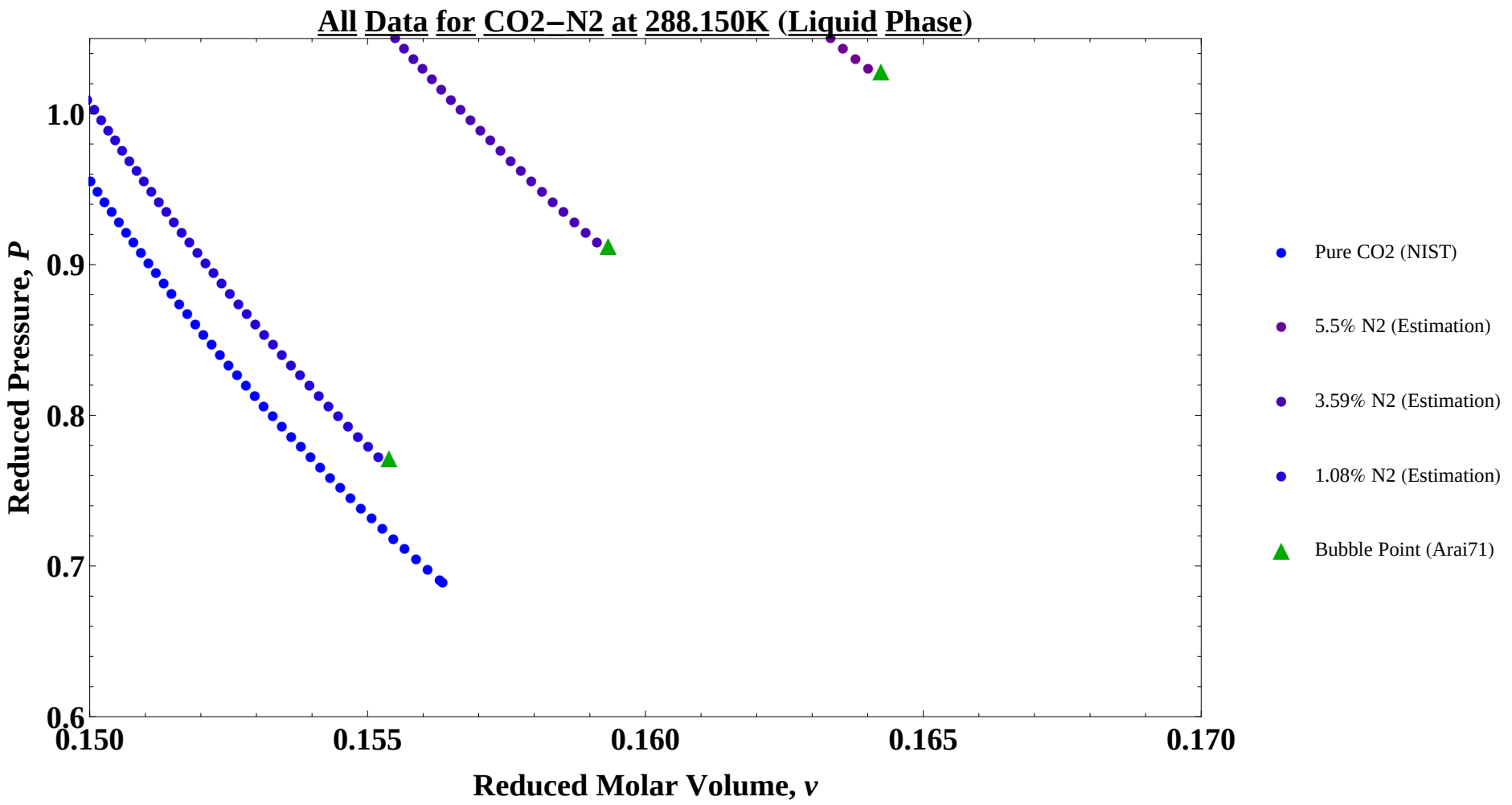

Figure 2.7: Behaviour of the volume estimation method in the liquid phase, upto the bubble point, at 288.15K for a carbon dioxide–nitrogen mixture

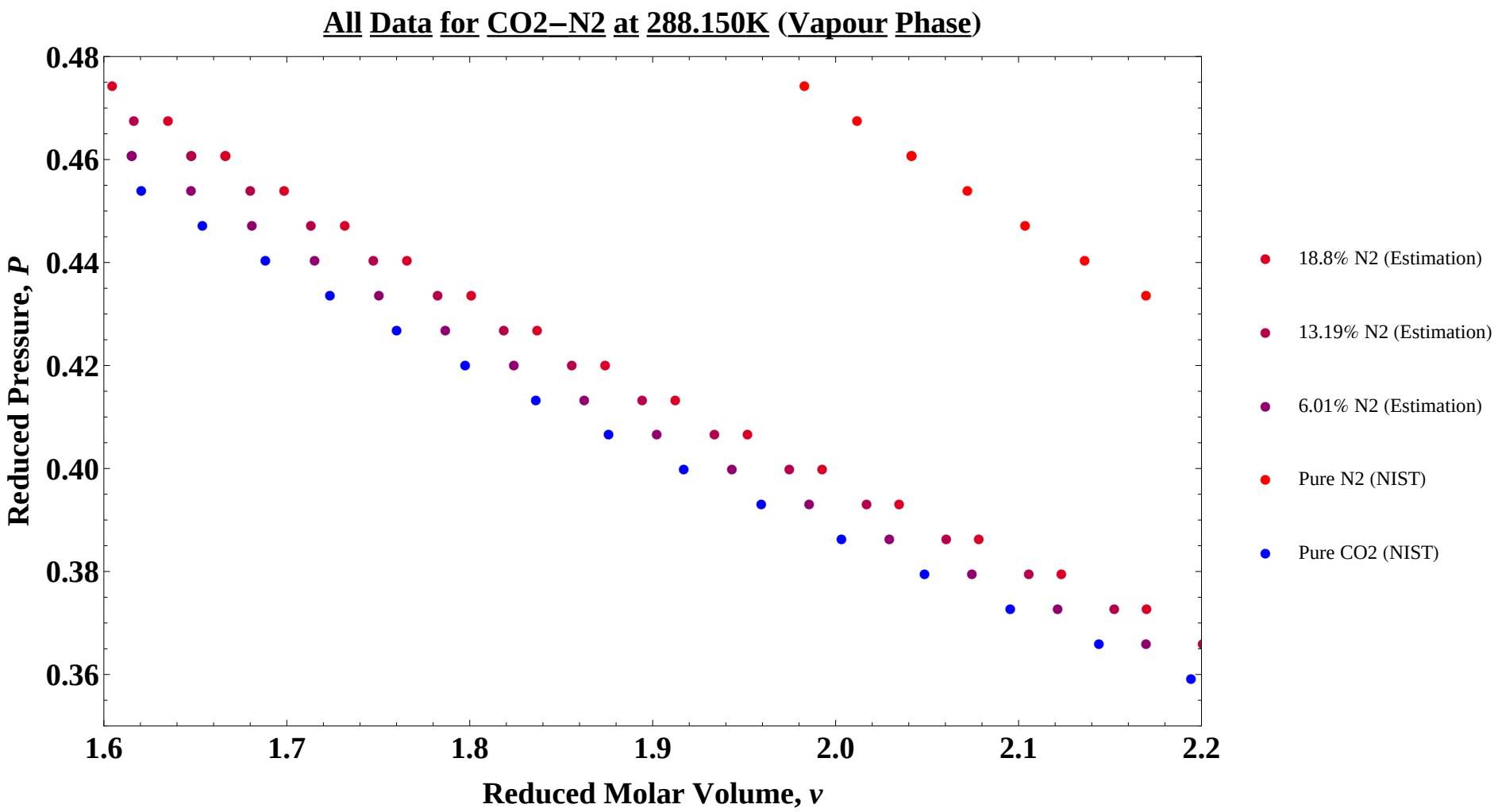

Figure 2.8: Behaviour of the volume estimation method in the vapour phase at 288.15K for a carbon dioxide–nitrogen mixture

2.5.4 Benefits of the Homogeneous Phase Volume Estimation

We felt the benefits of the homogeneous phase mixture volume estimation method were clear as, supplemented with the VLE coexisting volume method outlined in Section 2.4, it allowed us to construct a framework of data against which to fit the proposed equation of state. Without these methods, we would simply have been unable to do this in a meaningful way. The true value of these two methods combined, given that we had identified very few temperatures where homogeneous density and VLE data were both given, was that it meant we could fit the model at any temperature at which merely VLE data was given, and that even then, it needn't have contained the molar volumes.

In terms of attempting to fit the model to as many data points as possible in order to incorporate as much physical relevance to the model as possible, we considered this to be highly beneficial.

2.6 Mathematical Techniques Used for Fitting

At this point we highlight that we viewed our method as one of mathematical modelling, as opposed to physical modelling. Our outlook was that the parameters of the system were quantitative tools that allowed us to fit the proposed model to the data, and any dimensional equivalence with physical quantities is purely coincidental. We list here the main mathematical techniques used for fitting the model to the data which we used in our work.

2.6.1 Simulated Annealing

Simulated annealing [93, 94] is a process of global non–linear optimisation, a technique we used to start our method of fitting to the literature data. It is a stochastic process which searches extensively throughout a parameter space to find an optimum solution, working particularly well in scenarios where a desired global optimum may be hidden amongst a large number of mere local optima.

The term "annealing" stems from the analogy of this process to the cooling of liquids into crystalline structures, in which a slow cooling will permit large crystals of a low energy state to be formed, whereas fast cooling will limit the size of the crystals to be formed, whereby a higher energy state will have been achieved. The key is that by cooling slowly, the individual atoms can mobilise into positions al-

lowing the larger crystal to be formed, but under a quick cooling, energy is lost too quickly and the atoms cannot align to form such large structures in time.

The important feature of simulated annealing is that, just as slowly cooling atoms can retain enough kinetic energy despite the diminishing thermal energy in order to move into an optimal position, it can search through a parameter space in such a way that it may occasionally move against a gradient. This prevents a scenario whereby it doesn't automatically find the nearest local optima, but can have a chance to find the desired global optimum, or at least a very good local optimum. Traditional downhill methods of optimisation do not allow for this as they their algorithmic greediness will not allow the search to progress away from the nearest optimum, and in doing so, will very rarely yield the global optimum.

This means that simulated annealing is perfect for our requirement of finding a desired optimum in a large and potentially complicated parameter space containing a multitude of local optima, as it will not get stuck in the wrong location. Specifically, it works best in scenarios where there may be very many (perhaps arbitrarily many) local optima, in which case traditional downhill search algorithms cannot (usually) hope to find the global optimum. It searches by looking over wide areas to begin with before determining where the best local optima are likely to be located, and zooming in on these areas, repeating this process until a "good" local optimum which may approximate the global optimum is found. In this way, simulated annealing cannot be assumed to always give the very best possible solution, but it will usually return an optimum that gives very good approximations to it. Given that we are going to be searching high–dimensional parameter spaces whilst using our method, an exact optimum is not always necessary for our application; just a good approximation of it. To this end, simulated annealing is a method which is easily accessible in Wolfram Mathematica under the "NMinimize" command. It is a sufficiently powerful tool for us to not need to worry about the results it will return to us, as we deemed it suitable to use in order to produce an initial set of parameters to fit to data where no previous solutions had been determined. We were able to tailor our use of simulated annealing by altering the various search parameters offered by Mathematica: "SearchPoints" allowed us to control with how many simultaneous attempts the algorithm would search the landscape for an optima, "PerturbationScale" would control the size of the jumps the routine took in searching the landscape, and "MaxIterations" controlled how long the routine would look for before declaring itself to have found or not found an optimum.

2.6.2 Local Minimisation

Local minimisation is fundamentally different to simulated annealing in so far as it cannot under any circumstances usually hope to find a global optimum. It finds a local optimum in a perfunctory way by employing a standard downhill simplex method [94] to find a location in the parameter space at which a local optimum occurs, even though it may not be close in value to the true global optimum. This is the main difference to simulated annealing.

In addition, where simulated annealing does not need to have a starting location for its search specified, local minimisation does, and goes "downhill" from there. For application in our method this was actually beneficial as we could use the optimal solution from the previous temperature point as the starting point for the search for parameter values at the new temperature, and in doing so, hope to ensure smoothness of the temperature–dependent variation of each parameter. Another key difference between simulated annealing and local minimisation was the deterministic nature of local minimisation, used in Mathematica under the command "FindMinimum". This means that given a particular starting point local minimisation will always find its way to the same optimum, as it employs a gradient–based method to search for any local minimum. The major drawback of this is that sometimes we found the "FindMinimum" command converging to optima that were irrelevant to us, in which case we had to manipulate other search parameters to persuade it to find one which was acceptable. One benefit of local minimisation over simulated annealing was that it tended to converge quicker, due to the deterministic nature, resulting in reduced uncertainty, in its direction of search. Local minimisation was also controlled in Mathematica by a set of search parameters: "AccuracyGoal" would control how close to the actual optimum we wanted the routine to get, "PrecisionGoal" would control the number of significant figures quoted in the output, "WorkingPrecision" would control the extent to which inter–stage rounding errors could build up to affect the final answer, and "MaxIterations" was as with simulated annealing. We used local minimisation in our work to find parameter values after the initial set had been found using simulated annealing.

2.7 Creating the Fugacity Constraints

2.7.1 The Fugacity of A Chemical Component when in Mixture

Equation (1.19) gives us the fugacity of a single particular chemical component whilst in mixture. Setting $V = Nv$, where V is the total volume, v is the molar volume, and N is the number of moles of the substance, we get

$$\log_i(\bar{\phi}(v)) = \frac{1}{RT}\int_{\hat{v}=\infty}^{\hat{v}=v}\left(\frac{RT}{\hat{v}} - \left(\frac{\partial P}{\partial N_i}(\hat{v})\right)_{T,\hat{v},N_{j\neq i}}\right)\mathrm{d}\hat{v} - \log\left(\frac{RT}{Pv}\right), \tag{2.8}$$

where the bar in "$\bar{\phi}$" denotes that this is the mixture fugacity as opposed to pure case fugacity, and the subscript i denotes the chemical species being referred to in this equation. After the following non–dimensionalisation to allow all variables to take similar numerical values:

$$P = P_c P^\star, \tag{2.9}$$

$$T = T_c T^\star, \tag{2.10}$$

$$v = \left(\frac{RT_c}{P_c}\right)v^\star, \tag{2.11}$$

this becomes:

$$\log_i(\bar{\phi}) = \frac{1}{T}\int_{\hat{v}=\infty}^{\hat{v}=v}\left(\frac{T}{\hat{v}} - \left(\frac{\partial P}{\partial N_i}(\hat{v})\right)_{T,\hat{v},N_{j\neq i}}\right)\mathrm{d}\hat{v} - \log\left(\frac{Pv}{T}\right), \tag{2.12}$$

with all quantities in this expression being the non–dimensional equivalents. Equation (2.12) will have to be used repeatedly in our work in ensuring correct mixture VLE predictions. In order to achieve a state of thermodynamic equilibrium between different chemical components and different phases within those components, we require that the volumes given by each of these are matched at the point of equilibrium.

2.7.2 Pure Substance Fugacity

Equation (1.18) gives us the fugacity of a pure substance. Again setting $V = Nv$, we get

$$\log(\phi(v)) = \frac{1}{RT}\int_{\hat{v}=\infty}^{\hat{v}=v}\left(\frac{RT}{\hat{v}} - P(\hat{v})\right)\mathrm{d}\hat{v} - \log\left(\frac{Pv}{RT}\right) + \left(\frac{Pv}{RT}\right) - 1 \tag{2.13}$$

and after the same nondimensionalisation as in Equations (2.9) — (2.11) this becomes:

$$\log(\phi) = \frac{1}{T}\int_{\hat{v}=\infty}^{\hat{v}=v}\left(\frac{T}{\hat{v}} - \frac{\partial P}{\partial N}(\hat{v})\right)\mathrm{d}\hat{v} - \log\left(\frac{Pv}{T}\right) + \left(\frac{Pv}{T}\right) - 1, \tag{2.14}$$

again with all quantities in this expression being the non–dimensional equivalents. Equation (2.14) will also have to be used repeatedly in this work in ensuring correct pure VLE predictions.

Chapter 3

Formulation of the Model

3.1 Physical Constraints and Expected Qualitative Behaviour of an Equation of State

As established in the opening chapter, we aimed to propose a new equation of state which was simultaneously both sufficiently accurate and easy to implement. We aimed for the simplicity element to be achieved by our proposal of a model with an appropriate degree of functional complexity. In particular, we set out to only permit an EoS containing rational functions. To ensure relevance and accuracy of behaviour, there were two sets of physical constraints that the model had to satisfy. Firstly, we required that an accurate description of the volume–pressure relation must always be given. Next, for the pure case, at the critical temperature T_c the critical pressure P_c must be predicted at the critical molar volume v_c. This gave us the constraint:

$$P(v_c, T_c) = P_c, \tag{3.1}$$

where T_c, P_c, and v_c were as quoted in Table 1.4 for CO_2. At this temperature, there must also be a saddle point in $P(v)$ at the critical molar volume, yielding two more constraints:

$$\frac{\partial^2 P}{\partial v^2}(v_c, T_c) = \frac{\partial P}{\partial v}(v_c, T_c) = 0. \tag{3.2}$$

Recalling the aim for the equation to be able to model the phase behaviour accurately, it was necessary that, at sub–critical temperatures, we could accurately

predict the bubble point $(v_{\mathrm{BP}}, P_{\mathrm{vap}})$ and the dew point $(v_{\mathrm{DP}}, P_{\mathrm{BP}})$, where v_{DP} is the molar volume at which the bubble point occurs, v_{DP} is the molar volume at which the dew point occurs, and P_{vap} is the vapour pressure corresponding to both. In order to do this, we observed that at the bubble and dew volumes the fugacity for each chemical component (see Section 2.7 on VLE and fugacity) should be matched and therefore that Equation (1.18) evaluated at these two volumes should take equal values. In addition, the model must ensure that the predicted pressure at each of the the bubble and dew volumes was equal to the vapour pressure. Thus, for temperatures below T_c, we had two sets of constraints to impose; those ensuring correct pressures at the points of coexistence were described:

$$P(v_{\mathrm{BP}}) = P_{\mathrm{vap}}, \tag{3.3}$$
$$P(v_{\mathrm{DP}}) = P_{\mathrm{vap}}, \tag{3.4}$$

and those ensuring correct phase behaviour are described:

$$\log \phi(v_{\mathrm{BP}}) = \log \phi(v_{\mathrm{DP}}). \tag{3.5}$$

In Equations (3.3) to (3.5), v_{DP}, v_{BP}, and P_{vap} were values given by NIST. We use Equation (1.18) to enforce the constraint in Equation (3.5).

At super–critical temperatures there were no phase behaviour constraints as there could be no VLE there, and we were free to focus entirely on fitting to the density experimental data. These physical constraints were incorporated into fitting of the proposed model at the critical temperature by imposing Equations (3.1) and (3.2) and below the critical temperature by imposing Equations (3.3) to (3.5).

For the case of binary mixtures we again had two types of constraint to impose in order to ensure correct physical behaviour. Once more we had to impose the condition that correct pressures were predicted at the mixture bubble and dew points:

$$P(v_{\mathrm{BP,MIX}}) = P_{\mathrm{vap,MIX}}, \tag{3.6}$$
$$P(v_{\mathrm{DP,MIX}}) = P_{\mathrm{vap,MIX}}, \tag{3.7}$$

as well as to ensure that the fugacity at each of these coexisting volumes for each different chemical species within the mixture was the same

$$\log \bar{\phi}_i(v_{\mathrm{BP}}) = \log \bar{\phi}_i(v_{\mathrm{DP}}), \tag{3.8}$$

where $P(v)$ is the formulation we propose, $v_{\mathrm{BP,MIX}}$ is the molar volume at the bubble point, $v_{\mathrm{DP,MIX}}$ is the molar volume at the dew point, $P_{\mathrm{vap,MIX}}$ is the vapour pressure of the mixture at these volumes, and $\bar{\phi}_i$ denotes the mixture fugacity for component i as opposed to ϕ_i which denotes the fugacity of pure component i. Thus, there are would be as many constraints of the type shown in Equation (3.8) as there were components in the mixture.

3.2 Finding Vapour–Liquid Equilibrium

In the pure case, we are able to compute VLE by solving for the three unknown variables v_{BP}, v_{DP} and P_{DP} from the three Equations (3.3) to (3.5) for each temperature step. This required parameter values at the given temperature to be known so that $P(v)$ would be fully determined. We thus highlight the distinction between the initial process of finding parameter values which allowed the model to fit the data, and the subsequent process of implementing these parameter values and solving the system of three unknowns in three equations to generate a picture of the VLE behaviour of the system.

For binary mixtures this situation is the same, but there are four variables v_{BP}, v_{DP}, the composition of the liquid phase $x_{\mathrm{CO_2}}$ and the composition of the vapour phase $y_{\mathrm{CO_2}}$ from the four equations, noting that in a binary case Equation (3.8) yields two constraints; one each for both components. Again, we highlight that before this stage can be carried out, fitting to the data to find parameter values that would allow $P(v)$ to be defined would have had to have been done beforehand. In solving this system of equations we can thus find the binary mixture VLE for any specified temperature and the pressure.

This would allow us to calculate the VLE. Whether fitting the model to the data in the pure case or in a binary mixture however, it was also as necessary to ensure that correct pressure behaviour was described by the model. In the case of modelling the pure CO_2 we took the pressure data from the NIST database and included this data in the fitting regime to ensure the model could give accurate pressure descriptions. Whilst modelling mixtures, we again took both of the pure case pressure data sets from NIST, and any available pressure data for intermediate mixtures found within the literature, a comprehensive review of which was included in the Appendices.

3.3 Proposed Equation of State

We began the quest for a new functional form of equation that would satisfy the aims set out in Chapter 1 by considering the advantages and disadvantages of the most commonly used Equations [36]. We then used the general form of the many existing cubic equations of state as a template. As most of these equations were all modifications to the van der Waals equation, itself an adaptation of the ideal gas law, this was the starting point for our search. We decided early on that a pressure explicit equation of the form $P(v,T)$, would allow us both to calibrate against the data and to incorporate the fugacity constraints discussed previously most easily.

The evolution in functional forms from the ideal gas law towards the PREoS and beyond to the SWEoS, as noted in the literature review was used as a motivation for the type and complexity of the function we should be looking for in terms of both the degree and the number of parameters within. The equation we chose, having tried many variations on this theme, and the equation of state we propose as part of this thesis is:

$$P(v,T;a,b,c,d,e,f,g) = \frac{RT}{v+a} - \frac{b^2}{v^2+c^2} - \frac{d^3}{v^3+e^3} + \left(\frac{f}{v-g}\right)^6 \tag{3.9}$$

Immediately we are able to verify that this equation satisfied the requirement of being functionally quite easy to manage, there are relatively few terms (only four) and relatively few parameters (only seven), which most modern computers and software should have little problem in manipulating and using to perform calculations. From here it was a matter of also satisfying the primary requirement of giving accurate pressure and phase behaviour predictions compared with the complied data. To do this we proceeded by determining the combination of the seven parameter values which best allowed Equation (3.9) to describe the data. This was done by the process of finding an initial set of parameter values using simulated annealing then subsequent values at different temperatures using local minimisation, as mentioned in the methodology in Chapter 2.

In Equation (3.9), P was the pressure in MPa, v was the molar volume in $\mathrm{m^3.mol^{-1}}$, T was absolute temperature in K, and a through g were parameters of the system which allowed us to fit to the data at every temperature. Our motivations for suggesting this form of equation were as follows:

- All terms ensure it exhibited behaviour resembling the ideal gas law at low pressures, with $T \to 0$ as $v \to \infty$.

- A high–powered term to allow the model to retain enough flexibility to model the liquid–like incompressibility at high pressures, including the very sharp upturn of pressure immediately above the critical point. With this in mind, the final term of (3.9) was specifically chosen with a higher power than is usually seen in equations of state of similar complexity in order to allow fitting to the steep up–turn in pressure that exists above the critical point; a feature which cubic equations of state such as PREoS frequently miss out on (see Figures 4.26 to 4.28 for an illustration).

- A suitable number of parameters to allow the model to accurately fit the elongated plateau in $P(v)$ in the region of v_c at the critical temperature.

3.4 Nondimensionalisation

Equation (3.9) was nondimensionalised according to a similar regime as used to nondimensionalise the fugacity constraints (1.18) and (1.19), by the following set of substitutions:

$$P = P_c P^\star; \tag{3.10}$$
$$T = T_c T^\star; \tag{3.11}$$
$$v = \left(\frac{RT_c}{P_c}\right) v^\star; \tag{3.12}$$
$$a = \left(\frac{RT_c}{P_c}\right) a^\star; \tag{3.13}$$
$$b = \left(\frac{(RT_c)^2}{P_c}\right) b^\star; \tag{3.14}$$
$$c = \left(\frac{RT_c}{P_c}\right)^2 c^\star; \tag{3.15}$$
$$d = \left(\frac{(RT_c)^3}{P_c^2}\right) d^\star; \tag{3.16}$$
$$e = \left(\frac{RT_c}{P_c}\right)^3 e^\star; \tag{3.17}$$
$$f = \left(\frac{RT_c}{P_c^{5/6}}\right) f^\star; \tag{3.18}$$
$$g = \left(\frac{RT_c}{P_c}\right) g^\star, \tag{3.19}$$

where $\star$ denotes a dimensionless quantity. We nondimensionalised each quantity within our model against a suitable typical quantity, according to the regime noted

in Equations (3.10) to (3.19). For example, temperature T was scaled against the carbon dioxide critical temperature T_c so as to allow us to work with values which were all roughly of order 1. Crucially, we saw that this would give the numerical optimisation algorithms (simulated annealing and local minimisation) a better chance of finding good optima during the fitting process as they could focus on a particular region of the parameter space. After nondimensionalisation we had:

$$P(v^\star, T^\star; a^\star, b^\star, c^\star, d^\star, e^\star, f^\star, g^\star) = \frac{T^\star}{v^\star + a^\star} - \frac{b^{\star 2}}{v^{\star 2} + c^{\star 2}} - \frac{d^{\star 3}}{v^{\star 3} + e^{\star 3}} + \left(\frac{f^\star}{v^\star - g^\star}\right)^6, \tag{3.20}$$

and from this point forwards we dealt exclusively with nondimensionalised units (unless otherwise stated), and dropped the $\star$'s for notational convenience. This yielded the dimensionless version of our equation of state:

$$P(v, T; a, b, c, d, e, f, g) = \frac{T}{v + a} - \frac{b^2}{v^2 + c^2} - \frac{d^3}{v^3 + e^3} + \left(\frac{f}{v - g}\right)^6. \tag{3.21}$$

For example, applying the proposed model (3.21) to the pure fugacity constraint defined in Equation (2.14) gave:

$$\begin{aligned} \log \phi(v) \;=\; & -\frac{f^6}{5T(g-v)^5} + \log\left(\frac{v}{a+v}\right) + \frac{d}{3Te^{2/3}} \log\left(\frac{\sqrt[3]{e} + v}{\sqrt{e^{2/3} - \sqrt[3]{e}v + v^2}}\right) \\ & + \frac{b}{T\sqrt{c}} \arctan\left(\frac{v}{\sqrt{c}}\right) + \frac{d}{T\sqrt{3e^2}} \arctan\left(\frac{2v - \sqrt[3]{e}}{\sqrt{3}\sqrt[3]{e}}\right) \\ & - \frac{\pi}{2T}\left(\frac{b}{\sqrt{c}} + \frac{d}{\sqrt{3}e^{2/3}}\right) - \log\left(\frac{P(v)v}{T}\right) + \left(\frac{P(v)v}{T}\right) - 1 \end{aligned} \tag{3.22}$$

This expression plays a key role in enforcing the coexistence constraints and finding suitable parameter values to optimise the model against the data.

Chapter 4

Calibration of the Pure Carbon Dioxide Equation

4.1 Getting the Search Started: Fitting the Critical Point

Work carried out in this chapter was presented in a published paper [40] in May 2013. For the calibration of the pure CO_2 equation we needed only data from NIST. Whereas this data was itself generated using the an equation of state, it was done so using a far more complicated version (SWEoS) [74], which has scope to be highly accurate at the cost of functional simplicity, as has already been noted. We determined that the data was thus akin to high–accuracy experimental measurements, and could be treated as such. It is worth noting that the NIST data is well known for being used as a benchmark for high accuracy, so for our purposes, we were satisfied that using it to calibrate our equation should cause no problems.

To begin with we ran the simulated annealing package discussed in the opening chapter to seek the parameter values a through g at the critical temperature T_c. This process searched the the seven–dimensional space for a good combination of these parameters which would allow the proposed dimensionless Equation (3.21) to match most closely the NIST data at this temperature. We recognised the possibility that either there was no exact match given the functional form we had proposed, in which case no combination of parameter values would suggest to us we had a perfect agreement, or that it might be the case that even if there was one, the search

algorithm might not find it.

4.1.1 Error Function

To allow us to carry out this search, we defined an error function $E(a, b, c, d, e, f, g)$, depending on the system parameters, for Equation (3.21). This would work by assigning a comparatively high score for a bad fit of the data, a lower score for a better fit of the data, and a score of zero for a perfect match. The error function was to be dependent on the parameters in such a way that by minimising the value of this error function using simulated annealing, we would find the parameter values that had brought about such an optimum. At the critical temperature, the simulated annealing search algorithm progressed through the seven–dimensional space trying out different combinations of parameters, giving us output values for parameters a to g. Again, it was important to understand that these values might not have been found at a global optimum, but merely at a good local optimum, which for our purposes was sufficient.

The error function we used was arbitrarily defined, but as long as it exhibited the property that a closer agreement to the data resulted in a lower score, it was suitable for our needs. The error function $E(a, b, c, d, e, f, g)$ which we chose to use at each temperature T was:

$$E(a, b, c, d, e, f, g) = W\left(\sum_{i=1}^{n}\left(\frac{P(v_{\mathrm{NIST}}^{(i)}, T) - P_{\mathrm{NIST}}^{(i)}}{P_{\mathrm{NIST}}^{(i)}}\right)^2\right) + (1 - W)\Gamma, \qquad (4.1)$$

where Γ represents the type of behaviour being modelled (density and VLE in the coexistence region, just density in the homogeneous region, or the limiting behaviour between). The first term on the right–hand–side of Equation (4.1) was responsible for enforcing the density constraints whilst the second term was responsible for enforcing any coexistence constraints. We can visually verify that Equation (4.1) satisfies the requirements for the error function as outlined above. The The data we took from NIST went from 0.05MPa to 20MPa, approximately three times the critical pressure for pure carbon dioxide, at intervals of 0.05MPa. We chose this range to ensure the model was fit to the CCS pipeline relevant range of pressures, but in doing so, noted that much of the literature suggested a pressure of 20MPa would be far too high for this purpose. Nevertheless, by fitting at higher pressures, we would incorporate this enhanced range of operation of the model in case it might be needed for modelling during the repressurisation stages of CCS pipelines. In this model, T_c was the critical temperature for CO_2, taken to be the value given in Table

1.4, and the quantity $W \in [0,1]$ was a weighting function, which we chose manually, whose role was two–fold: Firstly, it would ensure that a suitable balance between predictions of the model for VLE and pressure was found. Secondly, it would allow us to perturb the parameter values in order that we might try to impose smooth temperature dependence for each.

In Equation (4.1), the first term ensured the pressure constraints were fit, whilst the second term ensured the coexistence constraints were fit. To be consistent with our work leading up to this point, each of the quantities in Equation (4.1) were in reduced (nondimensionalised) units, again because it allowed the search algorithm to focus more closely in a particular region of the seven–dimensional parameter space rather than having to search a wider region.

Γ was a quantity which depended on the temperature at which we were fitting and had the role of capturing the coexistence behaviour. We note that whereas coexistence could only ever occur below the critical temperature, the pressure data had to be accurately modelled at every temperature point. Below the critical temperature there were the VLE coexistence constraints to be enforced, whilst at the critical temperature there were the critical point constraints, and above the critical temperature there were no extra constraints. Thus, following on from Equations (3.1) and (3.2) for fitting at the critical temperature, we set:

$$\Gamma = \left(P(v,T)\Big|_{v=v_c,T=T_c} - P_c \right)^2 + \left(\frac{\mathrm{d}P}{\mathrm{d}v}(v,T)\Big|_{v=v_c,T=T_c} \right)^2 + \left(\frac{\mathrm{d}^2P}{\mathrm{d}v^2}(v,T)\Big|_{v=v_c,T=T_c} \right)^2, \tag{4.2}$$

and this fully defined our error function $E(a,b,c,d,e,f,g)$ which we could then ask simulated annealing to work with, because our equation of state was dependent on temperature, molar volume, and each of the parameters $P(v,T;a,b,c,d,e,f,g)$. We note at this point that all the quantities in the error function E were squared quantities, thus imposing the restriction that E could never take a negative value, and only take a zero value if the NIST data were fully satisfied was ensured. This fulfilled our requirement for it to act as an error function.

The two types of constraint in the error function were quantities that also had to be taken into consideration in order for the solution to be physically relevant. It would not have been good enough simply to fit the NIST pressure–volume data with no regard for the phase behaviour of the system.

In reality, we found that several runs of the fitting procedure with different values for W were needed to generate a feel for what would give a good balance, and find an acceptable compromise between fitting the two types of constraint for density and VLE fitting. We highlight that a value of W close to 0 meant the search algorithm would look more closely for parameter combinations that would fit the coexistence constraints, whilst a value of W close to 1 meant that it would instead prioritise pressure fitting the pressure data.

For the first guess using simulated annealing we eventually came to the realisation that it was important to set W quite high within the range 0 to 1 to take account of the fact that the pressure data must be accurately modelled in the first place in order for all the subsequent fittings to also be accurate: We felt a good pressure behaviour was slightly more fundamental to an accurate equation of state than phase behaviour at this stage of the development as correct phase behaviour can be inferred from pressure, but not the other way round. For example, setting $W = 0$ would remove the term for pressure considerations from Equation (4.1) and make the search algorithm look only for parameters that would yield a good VLE description. Conversely, setting $W = 1$ would remove the term for VLE considerations from Equation (4.1) and make the search algorithm look only for parameters that would yield a good pressure description. Bearing in mind the overall aims we set out for the model, specifically that it must give accurate descriptions for both density and VLE behaviours, we had to find the optimum value of W that would ensure a proportionate fit to both types of data. After some trial and error to determine this optimum value, we settled on a value of $W = 0.75$ for the very first fitting at the critical temperature, as this would allow the fitting regime to find parameters which would give a good performance in predicting the pressure whilst maintaining some consideration for the requirement to include a good phase behaviour prediction.

4.2 Generalising to Sub–Critical Temperatures

After the first set of parameters had been established for T_c, we moved our attention to a very slightly lower temperature (304K). Given that our aim was to build an idea of how the proposed EoS behaved at a range of temperatures up to and including T_c, we again sought to minimise the value of E over the set of seven parameters a to g at this new temperature, much as before. The significant difference in this fitting was that we would no longer be using simulated annealing, but the default local minimisation algorithm programmed into Mathematica as described in Chapter 2, where we would take as our starting point the set of parameter values determined

at the previous temperature point, in this case T_c. Our reason for this was that the local minimisation technique starts its search of the seven–dimensional space from a specified location, whereas simulated annealing does not. In this way we would be able to influence the search for the optimum set of parameters to look in a region of the space close to the region where the previous set of optimum parameters were found. This was beneficial because ultimately we would need to specify a temperature dependence for each of the model parameters, and if we could ensure that as the temperature varied so too would the value of the parameter in a smooth way, we might hope that the continuous nature of the physical behaviour might be borne out by smoothly varying parameters.

At sub–critical temperatures we again used the error function (4.1), this time with the constraints as given in Equations (3.3) to (3.5):

$$\Gamma = \Big(\log\phi(v_{\mathrm{DP}}) - \log\phi(v_{\mathrm{BP}}) \Big)^2 + \left(P(v,T)\Big|_{v=v_{\mathrm{DP}}} - P_{\mathrm{vap}} \right)^2 + \left(P(v,T)\Big|_{v=v_{\mathrm{BP}}} - P_{\mathrm{vap}} \right)^2 . \tag{4.3}$$

Again, this allowed us to fully define the error function which the Mathematica local minimisation routine mentioned in Chapter 2 would be able to use in order to find the set of parameters at the new temperature which optimised our model.

In this way we repeated the process of fitting to the NIST data at a comprehensive range of temperatures below the critical temperature. We used the default local optimisation procedure for these steps and again after some experimentation to find a value for the weighting function, we found a value of $W = 0.01$ to usually work well, although while fitting at some temperatures we occasionally perturbed this slightly to affect either a smooth variation of the model parameters with temperature or a better balance between the pressure accuracy and predictions of VLE behaviour. Ultimately, our criterion for selecting a value for W was that the average percentage errors in predictions of the two types of behaviour should be similar. We note that at subsequent temperature fittings W took on a much lower value than the first time as a solution exhibiting a good pressure behaviour had been "locked in" by the initial stage where W was higher. Thus, we were free to look a little more closely at ensuring phase behaviour was accurately modelled.

4.3 Generalising to Super–Critical Temperatures

We note that fitting to temperatures above T_c was also possible in this set–up by setting

$$\Gamma = 0, \tag{4.4}$$

as there is no coexistence constraint to be enforced here, and using the error function as before. We note that the range of ambient temperatures found in the majority of locations where CCS is proposed (for example, Northern Europe), is expected to operate significantly below the supercritical temperatures (approximately 31°C and over), yet we extend our model to this elevated temperature range as it may prove to be a useful addition to the model, for example in describing behaviour in the latter stages of the pipeline transport process before the injection stage of CCS, which can sometimes occur at temperatures around 35°C, or at the exit of the compression stage where temperatures can reach 40—50°C.

4.4 Variation of Model Parameters with Respect to Temperature

We repeated this process at the many different temperature points in our intended region of fitting. We chose this to be from 260K and 335K, as we identified this to be a slightly wider temperature range than CCS pipelines could be expected to encounter, so by fitting to this range, bearing in mind the pressure range we had selected, we would ensure the model could be of use in any CCS pipeline scenario. We fit the parameter values obtained by the search routines to a function in T, thus allowing us to formulate a picture of how each parameter $a(T), b(T), \ldots, g(T)$ varied continuously with temperature. This fully determined the equation of state, giving an expression for P in terms of just v and T. Having done this, we report in Table 4.1 the parameter values we found to optimise the system at each temperature. We wanted to ensure we had proposed a relevant temperature variation for each parameter, which would closely match the values in this table. In order to be able to employ some mathematical insight into this, we also present the values quoted in Table 4.1 graphically for each parameter. For example, values for parameter a_{CO_2} obtained through the sequential process of using simulated annealing and local minimisation at different temperatures as described above, where the subscript CO_2 denotes specifically that this value of parameter a corresponds to the pure carbon dioxide case, are shown for temperatures below T_c in Figure 4.1 and above T_c in a similar plot in Figure 4.2.

T(K)	a_{CO_2}	b_{CO_2}	c_{CO_2}	d_{CO_2}	e_{CO_2}	f_{CO_2}	g_{CO_2}
260	0.369524	0.367818	0.125183	-0.000374	0.780747	0.098833	0.045463
265	0.363018	0.356758	0.127792	-0.000374	0.780747	0.099351	0.045960
270	0.356738	0.345941	0.130935	-0.000374	0.780747	0.100522	0.046091
273.15	0.353753	0.339103	0.133745	-0.000374	0.780747	0.101314	0.046273
275	0.352635	0.334360	0.135155	-0.000374	0.780747	0.100010	0.047680
278.15	0.349700	0.327409	0.138206	-0.000374	0.780747	0.100852	0.047762
280	0.347979	0.323392	0.140225	-0.000374	0.780747	0.101620	0.047543
285	0.343788	0.312494	0.146504	-0.000374	0.780747	0.104030	0.046656
288.15	0.342452	0.304852	0.151022	-0.000374	0.780747	0.103906	0.047526
290	0.341598	0.300542	0.154080	-0.000374	0.780747	0.104501	0.047415
290.15	0.341531	0.300195	0.154336	-0.000374	0.780747	0.104560	0.047408
291	0.334409	0.304063	0.162855	-0.000374	0.780747	0.100603	0.050768
292	0.333988	0.301780	0.164693	-0.000374	0.780747	0.100958	0.050712
293	0.333391	0.299669	0.166641	-0.000374	0.780747	0.101837	0.050200
293.15	0.333442	0.299248	0.166944	-0.000374	0.780747	0.101643	0.050411
294	0.333217	0.297275	0.168698	-0.000374	0.780747	0.101877	0.050429
294.5	0.333293	0.295975	0.169781	-0.000374	0.780747	0.101581	0.050826
295	0.332991	0.294970	0.170886	-0.000374	0.780747	0.102211	0.050397
295.5	0.327151	0.298688	0.176698	-0.000374	0.780747	0.100414	0.051963
296	0.327087	0.297534	0.177863	-0.000374	0.780747	0.100485	0.052041
296.5	0.327160	0.296298	0.179083	-0.000374	0.780747	0.100277	0.052370
297	0.327371	0.294982	0.180368	-0.000374	0.780747	0.099785	0.052956
297.5	0.327344	0.293857	0.181672	-0.000374	0.780747	0.099934	0.052965
298	0.327498	0.292628	0.183056	-0.000374	0.780747	0.099714	0.053308
298.15	0.327501	0.292295	0.183478	-0.000374	0.780747	0.099757	0.053310
298.5	0.327488	0.291539	0.184468	-0.000374	0.780747	0.099972	0.053217
299	0.327705	0.290322	0.185984	-0.000374	0.780747	0.099769	0.053546
299.5	0.327841	0.289195	0.187556	-0.000374	0.780747	0.099864	0.053600
300	0.316831	0.297393	0.196327	-0.000374	0.780747	0.096801	0.056346
300.5	0.317132	0.296246	0.198061	-0.000374	0.780747	0.096403	0.056870
301	0.317278	0.295254	0.199853	-0.000374	0.780747	0.096562	0.056878
301.5	0.317632	0.294200	0.201836	-0.000374	0.780747	0.096365	0.057214
302	0.317896	0.293291	0.203947	-0.000374	0.780747	0.096660	0.057086
302.5	0.318518	0.292290	0.206393	-0.000374	0.780747	0.096350	0.057516
303	0.315041	0.294811	0.211153	-0.000374	0.780747	0.095212	0.058670
303.15	0.315262	0.294589	0.212058	-0.000374	0.780747	0.095178	0.058740
303.5	0.315713	0.294227	0.214359	-0.000374	0.780747	0.095333	0.058680
304	0.229488	0.361051	0.236202	-0.000374	0.780747	0.091201	0.062049
304.1282	0.271294	0.332617	0.238762	-0.000374	0.780747	0.078770	0.074028
304.5	0.220559	0.357053	0.217490	-5.384474E-13	0.780747	0.104931	0.050584
305	0.220559	0.357053	0.217490	-5.384474E-13	0.780747	0.104931	0.050584
305.5	0.220559	0.357053	0.217490	-5.384474E-13	0.780747	0.104931	0.050584
306	0.220559	0.357053	0.217490	-5.384474E-13	0.780747	0.104931	0.050584
306.5	0.218855	0.354471	0.219015	-2.692236E-13	0.780747	0.106345	0.049896
307	0.218226	0.353668	0.219518	-2.692236E-13	0.780747	0.106846	0.049642
307.5	0.218226	0.353668	0.219518	-2.692236E-13	0.780747	0.106846	0.049642
308	0.218226	0.353668	0.219518	-2.692236E-13	0.780747	0.106846	0.049642
308.5	0.215691	0.351925	0.221185	-2.692236E-13	0.780747	0.108419	0.048817
309	0.214702	0.351501	0.221777	-2.687911E-13	0.780747	0.108962	0.048525
309.5	0.213678	0.351120	0.222378	-2.292181E-13	0.780747	0.109514	0.048224
310	0.212633	0.350769	0.222983	-2.292181E-13	0.780747	0.110075	0.047917
310.5	0.212633	0.350769	0.222983	-2.292181E-13	0.780747	0.110075	0.047917
311	0.210520	0.350117	0.224197	-2.292181E-13	0.780747	0.111223	0.047278
311.5	0.209466	0.349802	0.224803	-1.954713E-13	0.780747	0.111809	0.046948
312	0.209466	0.349802	0.224803	-1.954713E-13	0.780747	0.111809	0.046948
312.5	0.207387	0.349168	0.226006	-1.954712E-13	0.780747	0.113005	0.046267
313	0.206369	0.348843	0.226603	-1.954712E-13	0.780747	0.113615	0.045916
313.5	0.206369	0.348843	0.226603	-1.954712E-13	0.780747	0.113615	0.045916
314	0.203427	0.347799	0.228363	-1.954711E-13	0.780747	0.115495	0.044820
314.5	0.202490	0.347421	0.228938	-1.954709E-13	0.780747	0.116138	0.044439
315	0.201577	0.347026	0.229507	-1.954708E-13	0.780747	0.116791	0.044050
316	0.199829	0.346174	0.230626	-3.909416E-14	0.780747	0.118125	0.043248
317	0.198190	0.345232	0.231715	-1.954708E-14	0.780747	0.119498	0.042411
318	0.196666	0.344191	0.232774	-1.954708E-14	0.780747	0.120914	0.041536
319	0.195259	0.343044	0.233802	-1.954708E-14	0.780747	0.122373	0.040622
320	0.193968	0.341788	0.234800	-1.954708E-14	0.780747	0.123877	0.039669
325	0.189045	0.333994	0.239438	-1.954708E-14	0.780747	0.132034	0.034325
330	0.185791	0.324454	0.243890	-1.954708E-14	0.780747	0.141024	0.028211
335	0.183236	0.314125	0.248578	-1.954708E-14	0.780747	0.150615	0.021512

Table 4.1: Parameter values for pure carbon dioxide at each temperature

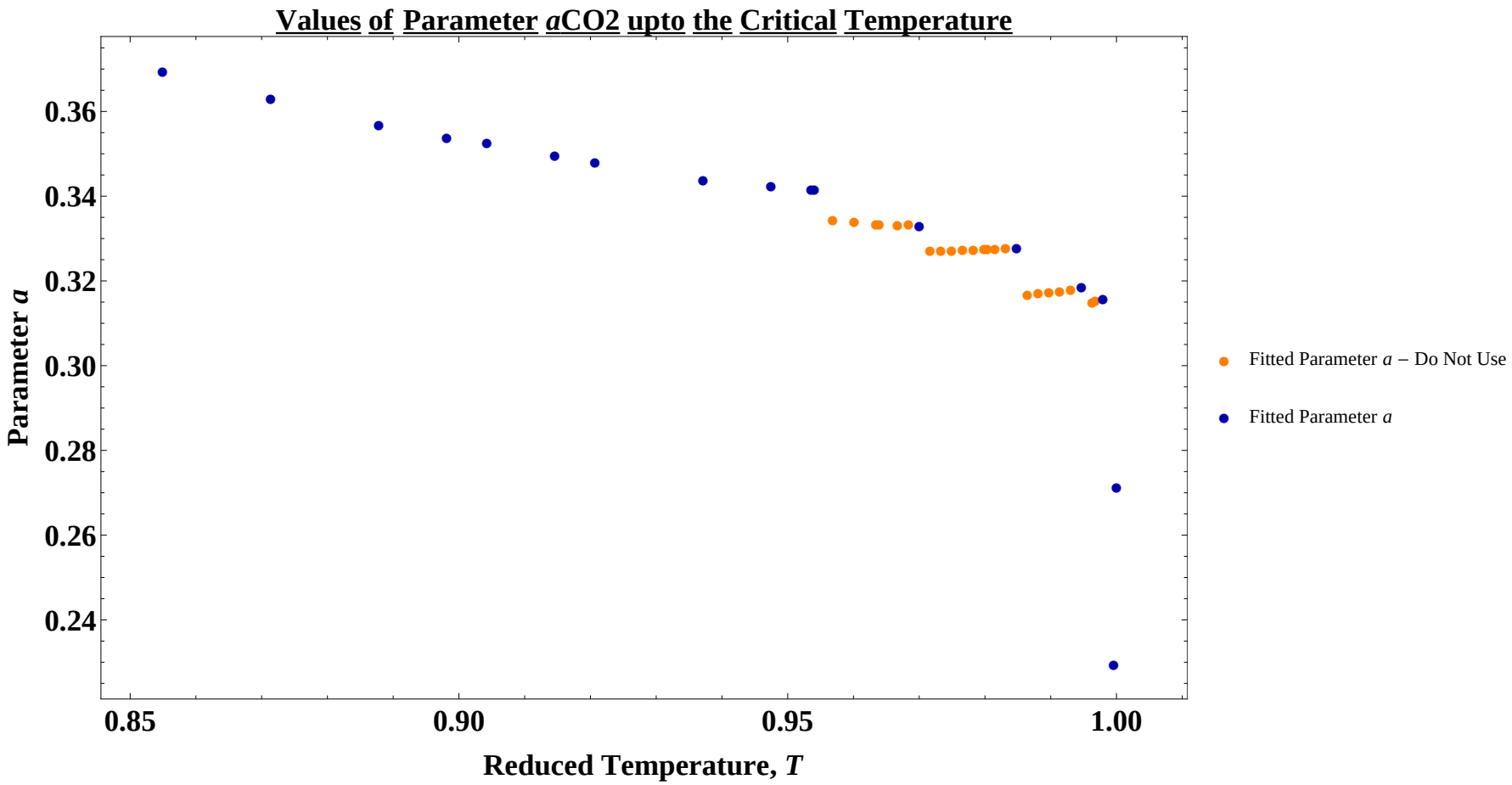

Figure 4.1: Values of parameter a_{CO_2} at sub–critical temperatures

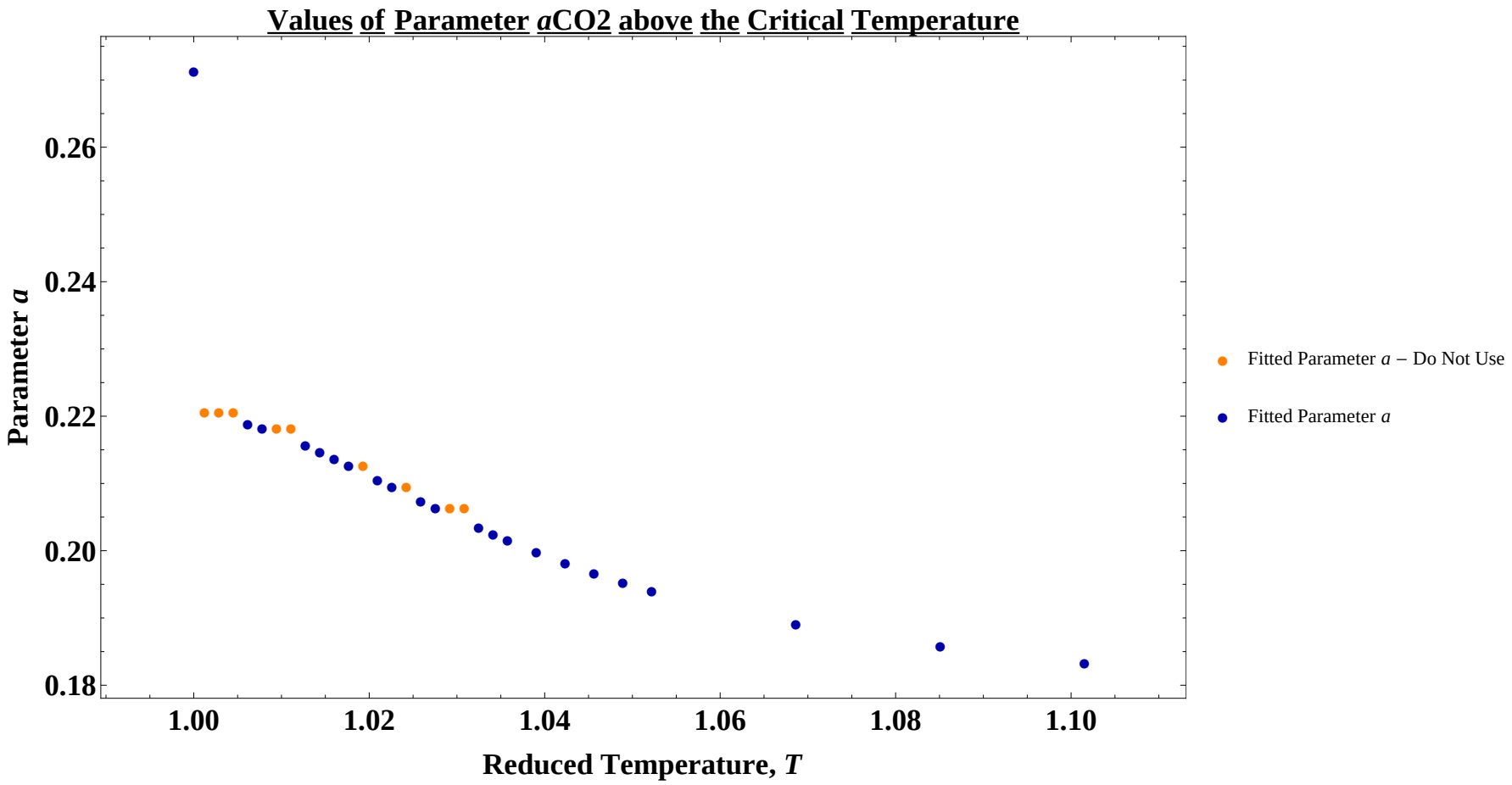

Figure 4.2: Values of parameter a_{CO_2} at super–critical temperatures for pure carbon dioxide

The orange markers in Figures 4.1 and 4.2 were those values of parameter a_{CO_2} which were seen not to obey the overall trend of the other parameter values throughout the temperature range (hence the legend identifies that these were not to be used). In the original fitting steps we could have compensated for this by altering the value of W where necessary, as detailed previously. This would have allowed all the points to align in a smooth way, but we skipped the step of actually doing this, instead discarding those points for which this would need to be done, and moving straight to the second–stage fitting of each parameter with T, as it would potentially have been a time consuming process to find the exact value of W which gave this good alignment, and we would have arrived at the same conclusion anyway. The end result that we would have a smooth curve for the temperature dependence of each parameter would have been the same if we neglected those values at this stage and fit without them.

We wished to have each parameter vary smoothly with T up to, including, and beyond the critical temperature, but we observed from Figures 4.1 and 4.2 what appears to be behaviour resembling a non–analytic variation of a_{CO_2} with T, as T_c was approached from either side. Taking inspiration from the Frobenius Method for series solutions close to singular points, where the gradient can become very steep, we suggested the following general form for each parameter in the pure CO_2 case for our model:

$$a_{\text{var}}(T; a_1, a_2, a_3, a_4) = |T-1|^{a_1}\big(a_2|T-1|^2 + a_3|T-1| + a_4\big) + a_{\text{FIT}}(T_c), \qquad (4.5)$$

where $a_{\text{FIT}}(T_c)$ was the exact value given in Table 4.1 determined in the fitting stages. This would ensure an excellent prediction of the critical point. We again established an error function similar in construction to the that in Equation (4.1):

$$\Gamma_a = \sum_{\text{all } T} (a_{\text{FIT}}(T) - a_{\text{var}}(T))^2, \qquad (4.6)$$

where $a_{\text{FIT}}(T)$ is the value for parameter a given in Table 4.1 and $a_{\text{var}}(T; a_1, a_2, a_3, a_4)$ is the form of temperature dependence we assigned to parameter a in (4.5). We then minimised this using simulated annealing to find numerical values for a_1 to a_4, thus giving us the complete temperature variation of a with T. This process was carried out twice; once below the critical temperature and once above, each time anchoring the variation at the critical temperature to the value given in Table 4.1, in doing so ensuring an excellent prediction of the critical point and a continuous (albeit non-differentiable at T_c) form for the parameter.

Our final derived expression for the parameter a, both below and above T_c, obtained using this method, was,

$$a_{\mathrm{CO}_2}(T) = \begin{cases} |T-1|^{0.626207}(33.9261|T-1|^2 - 8.10461|T-1| \\ + 0.805812) + 0.27129411630837575312 & T \leq 1 \\ |T-1|^{5.514209492375366\text{E-}9}(3.556|T-1|^2 - 0.765078|T-1| \\ - 0.0467569) + 0.27129411630837575312 & T \geq 1 \end{cases} \tag{4.7}$$

a plot of which in the region of interest is as shown in Figure 4.3. We carried out exactly the same process to determine the other six parameters $b_{\mathrm{CO}_2}(T)$ — $g_{\mathrm{CO}_2}(T)$. Below the critical temperature, b took values as demonstrated in Figure 4.1 and above the critical temperature as shown in Figure 4.5.

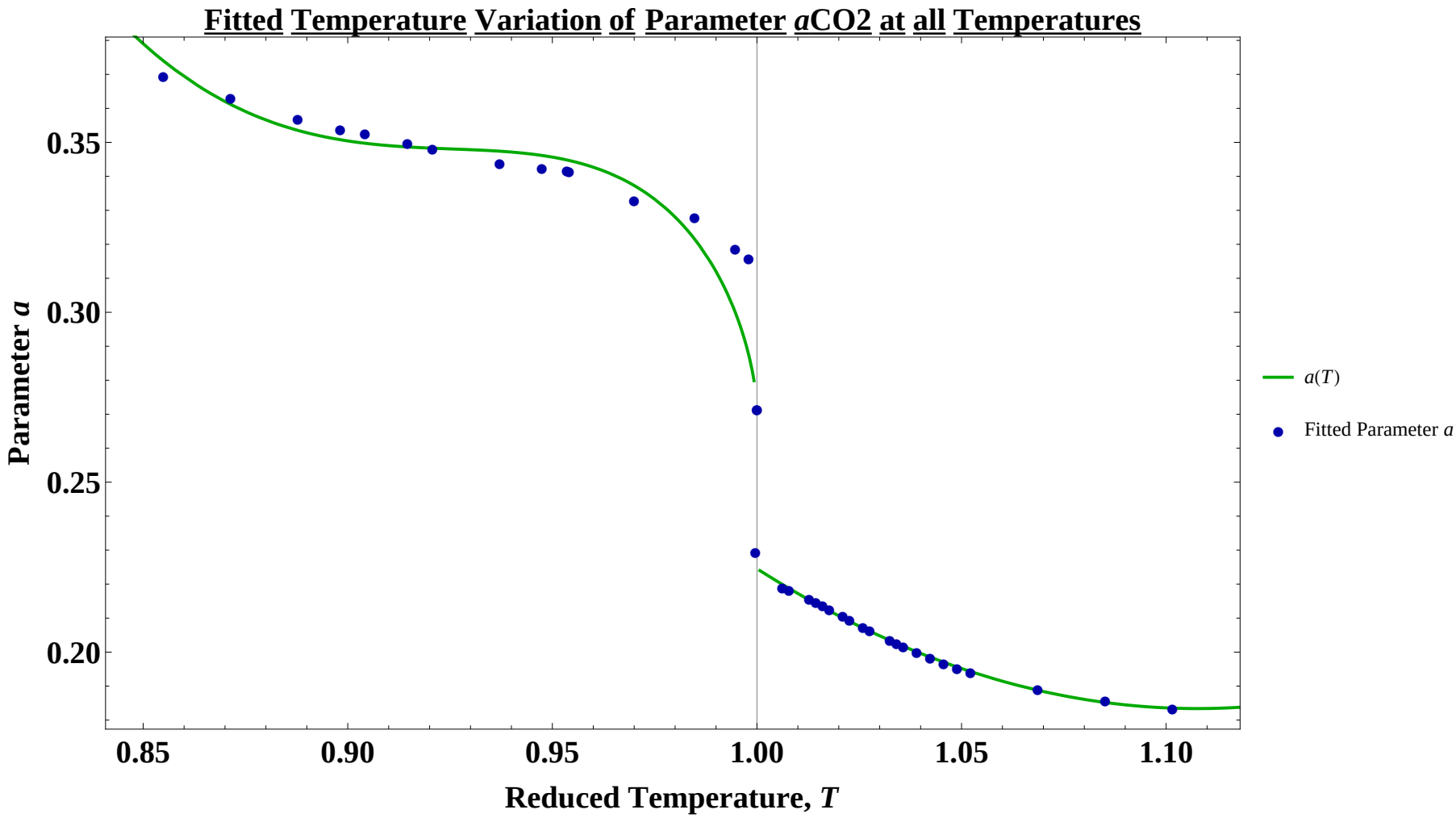

Figure 4.3: Variation of parameter a_{CO_2} at all temperatures

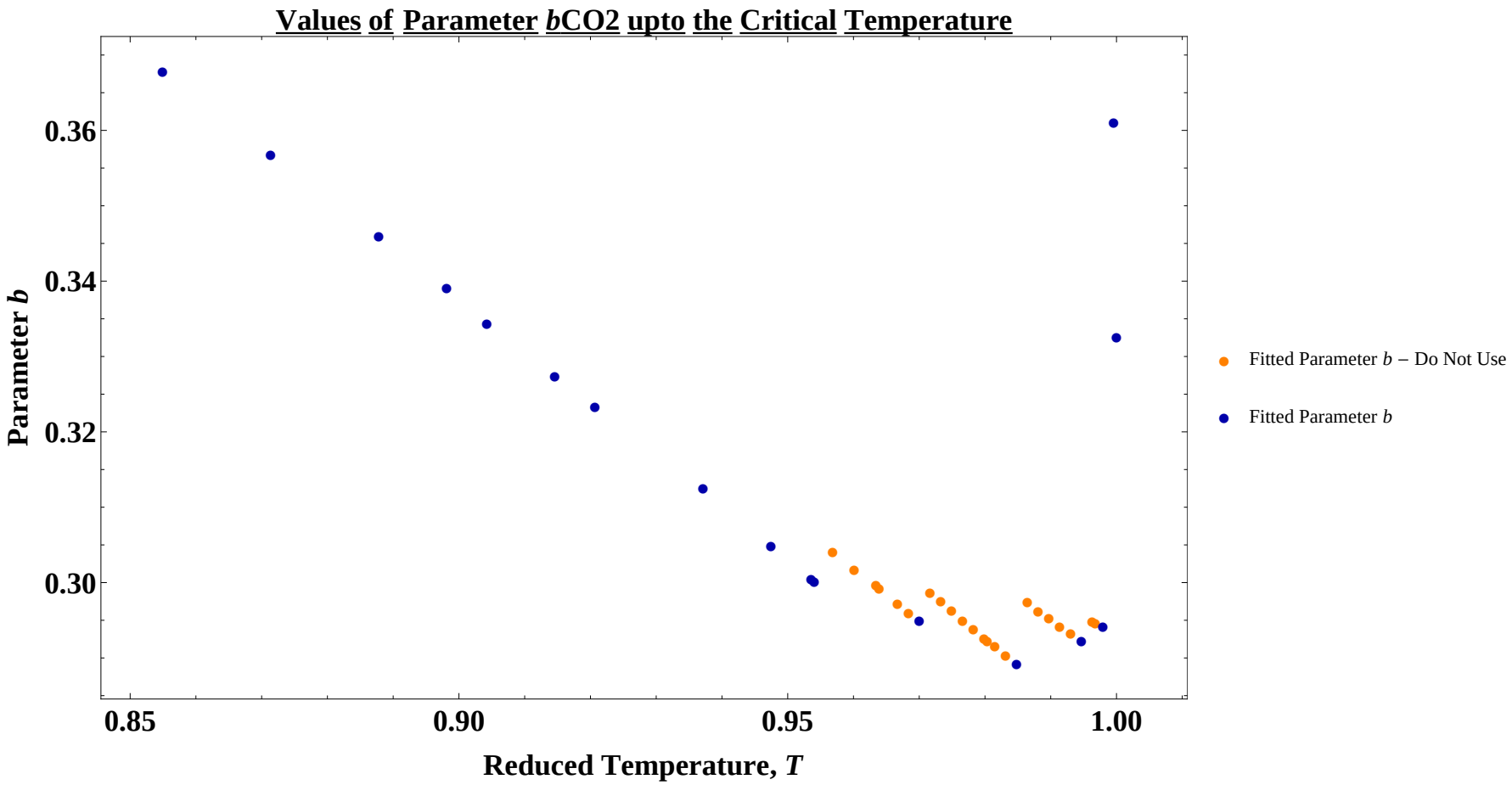

Figure 4.4: Values of parameter b_{CO_2} at sub–critical temperatures for pure carbon dioxide

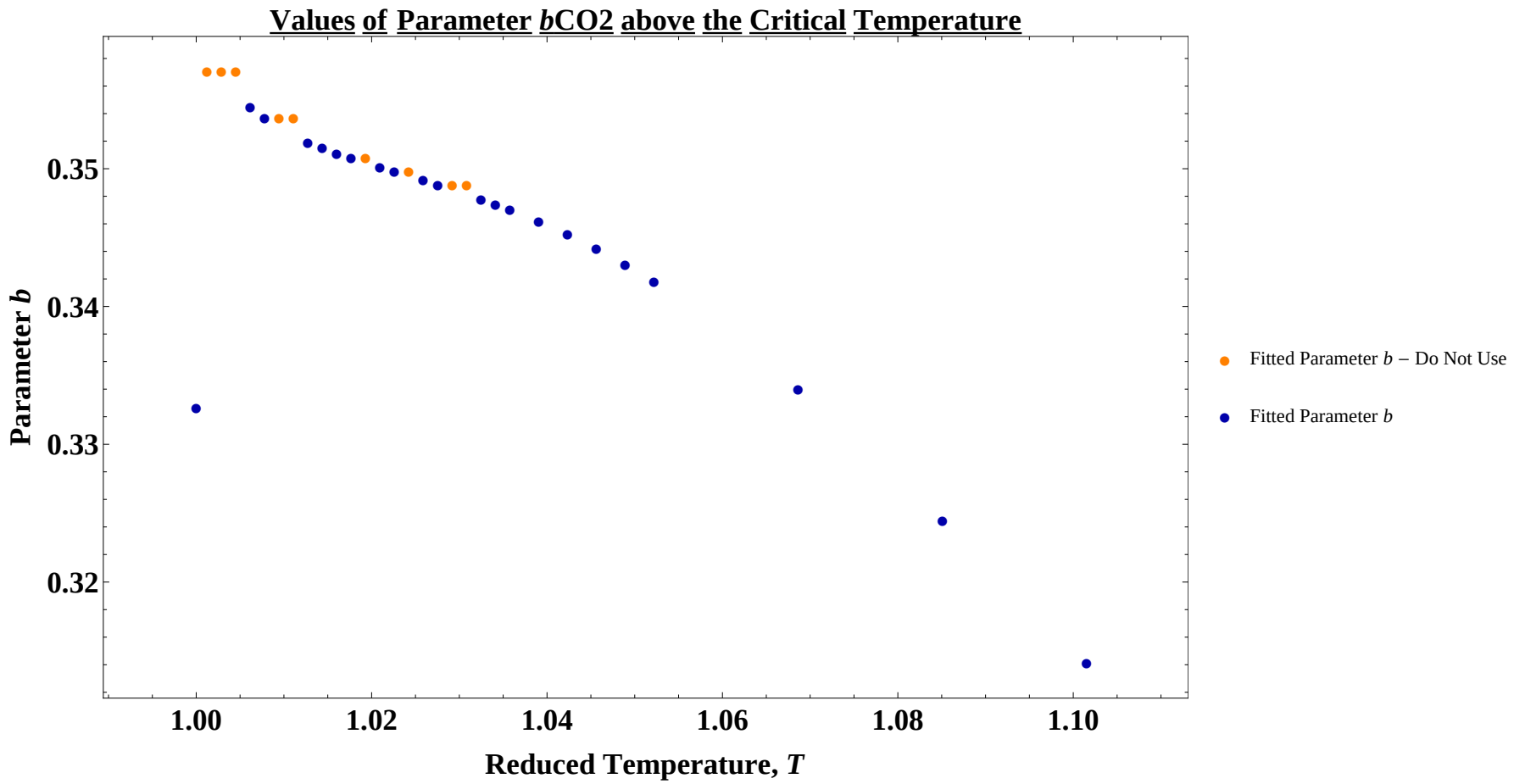

Figure 4.5: Values of parameter b_{CO_2} at super–critical temperatures for pure carbon dioxide

We again specified a functional form for b_{CO_2} in the same way as for a_{CO_2}:

$$b_{\mathrm{var}}(T; b_1, b_2, b_3, b_4) = |T-1|^{b_1}\left(b_2|T-1|^2 + b_3|T-1| + b_4\right) + b_{\mathrm{FIT}}(T_c), \tag{4.8}$$

and upon minimising an analogous error function to that shown in Equation (4.6), obtained the following temperature definition for b_{CO_2}:

$$b_{\mathrm{CO}_2}(T) = \begin{cases} |T-1|^{0.405254}(-13.5708|T-1|^2 + 4.48534|T-1| - 0.295229) & \\ \quad + 0.33261690686926754767 & T \leq 1 \\ |T-1|^{5.5792801817977416\mathrm{E}\text{-}9}(-3.07866|T-1|^2 - 0.0767956|T-1| & \\ \quad + 0.0210443) + 0.33261690686926754767 & T \geq 1 \end{cases} \tag{4.9}$$

a plot of which is shown in Figure 4.6.

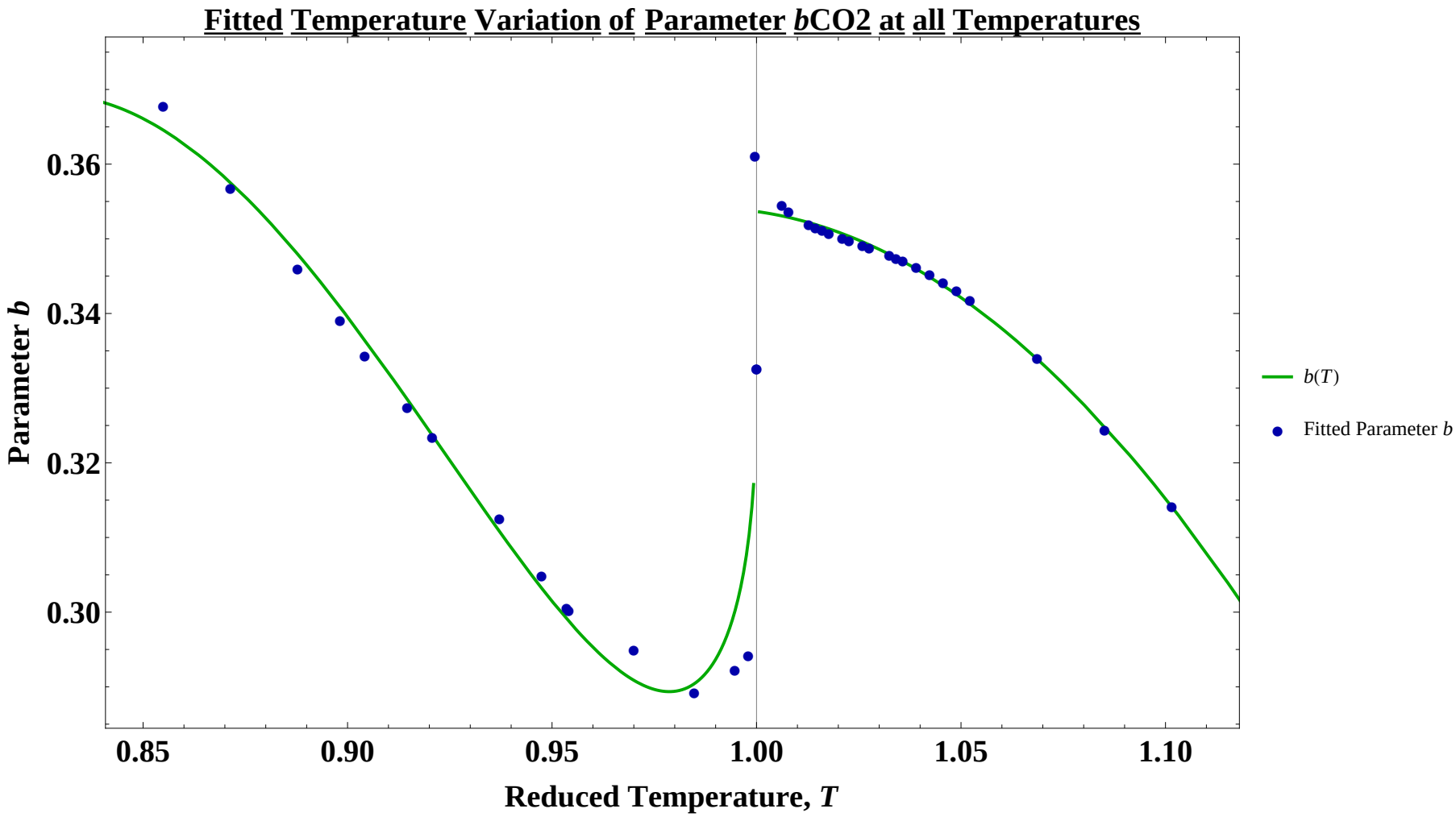

Figure 4.6: Variation of parameter b_{CO_2} at all temperatures in the CCS pipeline relevant range

For the remaining pure carbon dioxide parameters $c_{CO_2}(T)$ through to $g_{CO_2}(T)$, we carried out the same process, noting the slightly more complicated behaviour for parameter d in Figure 4.9, where we increased the order of the temperature dependence by one, and the minuscule variation of e with respect to T, where we opted for a different approach for this parameter, instead defining it to be take on a constant value; that being taken at the critical temperature.

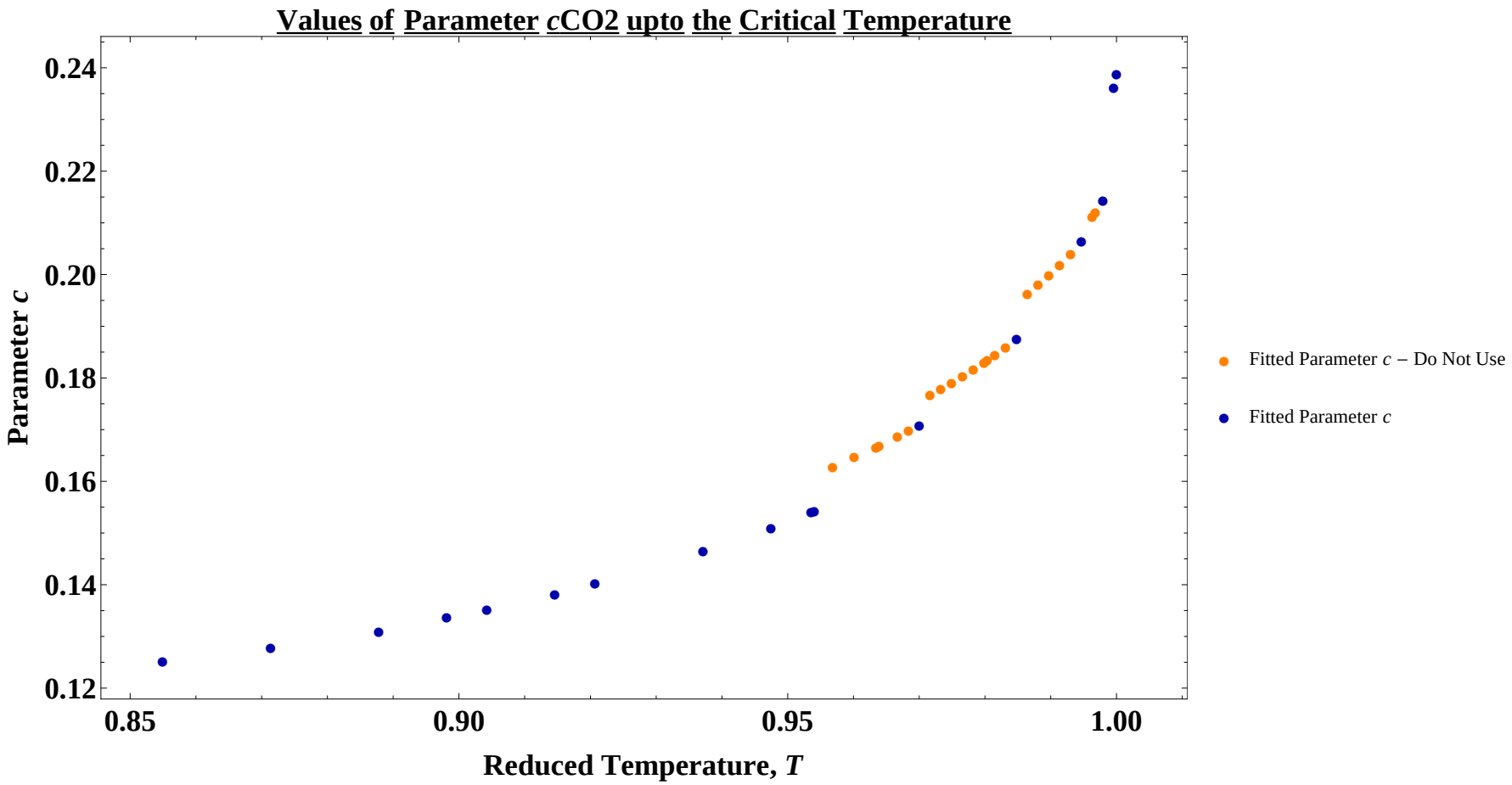

Figure 4.7: Values of parameter c_{CO_2} at sub–critical temperatures for pure carbon dioxide

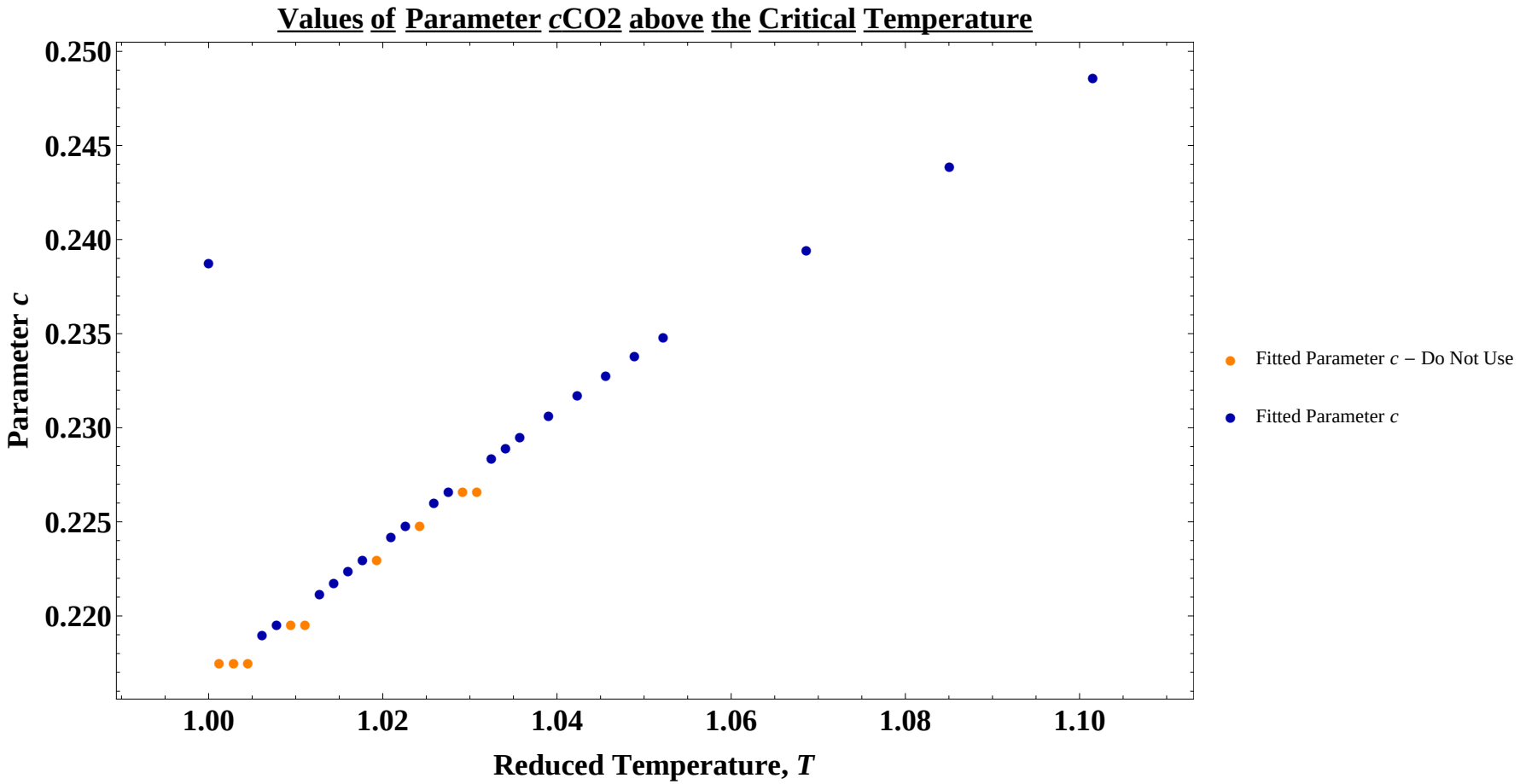

Figure 4.8: Values of parameter c_{CO_2} at super–critical temperatures for pure carbon dioxide

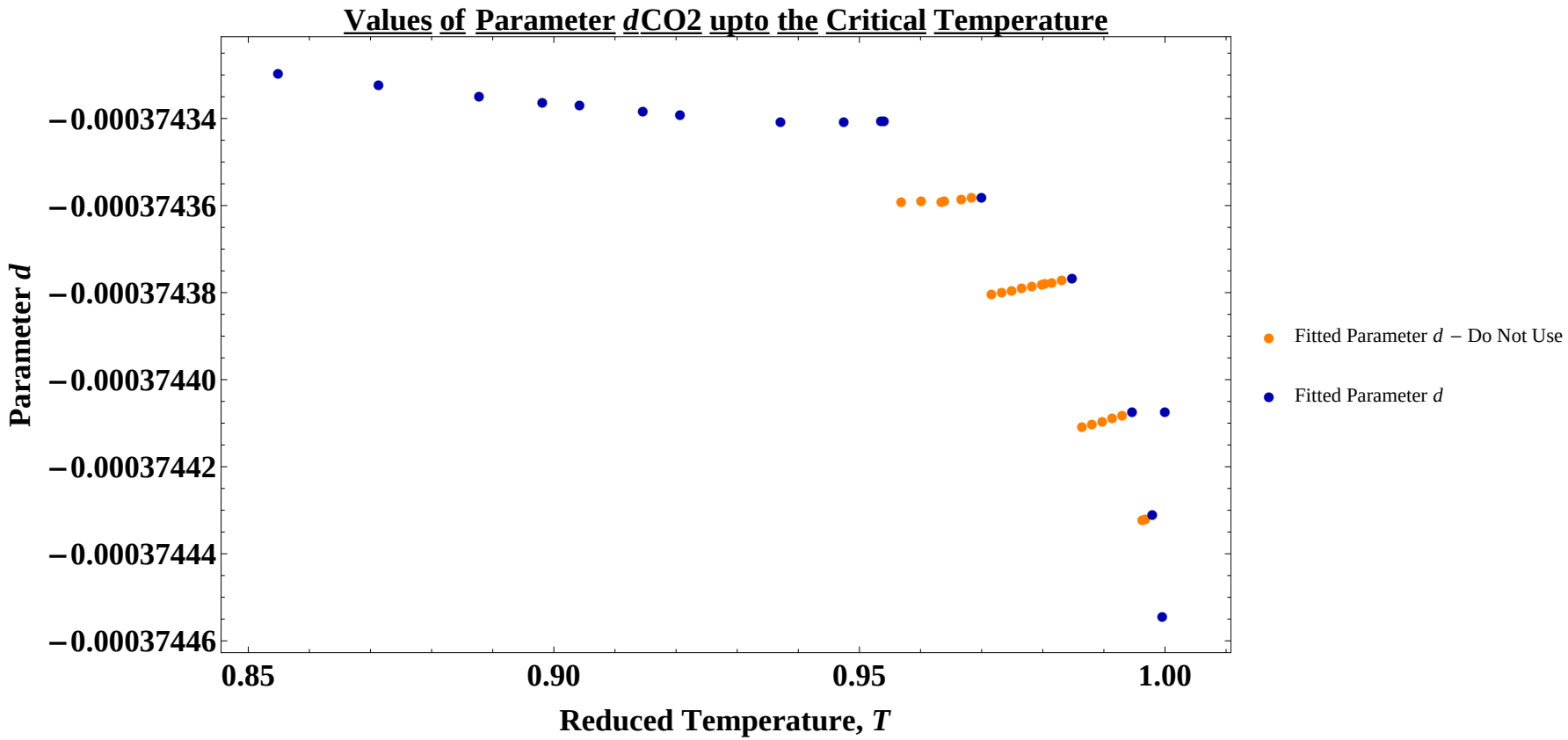

Figure 4.9: Values of parameter d_{CO_2} at sub–critical temperatures for pure carbon dioxide

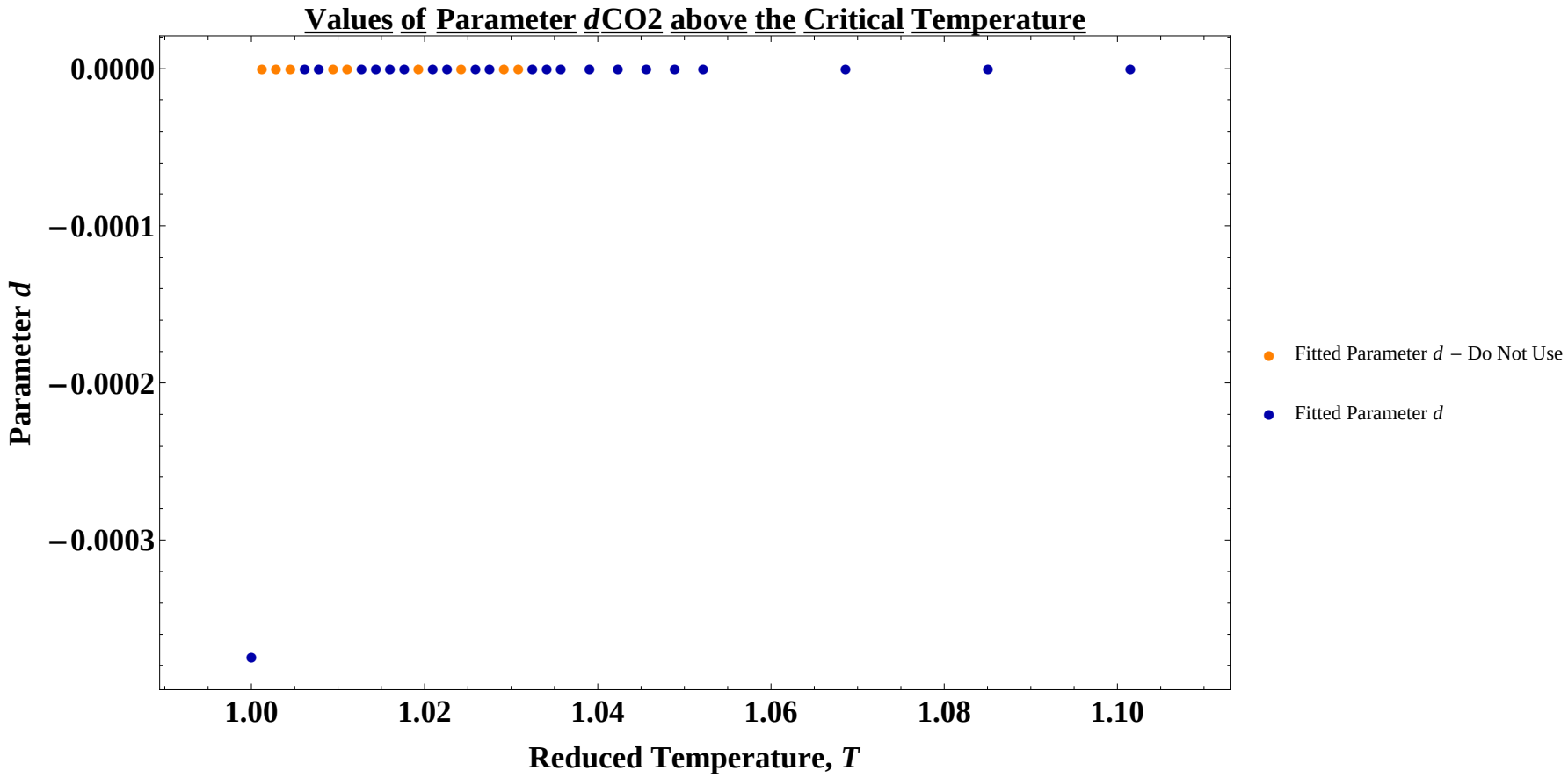

Figure 4.10: Values of parameter d_{CO_2} at super–critical temperatures for pure carbon dioxide

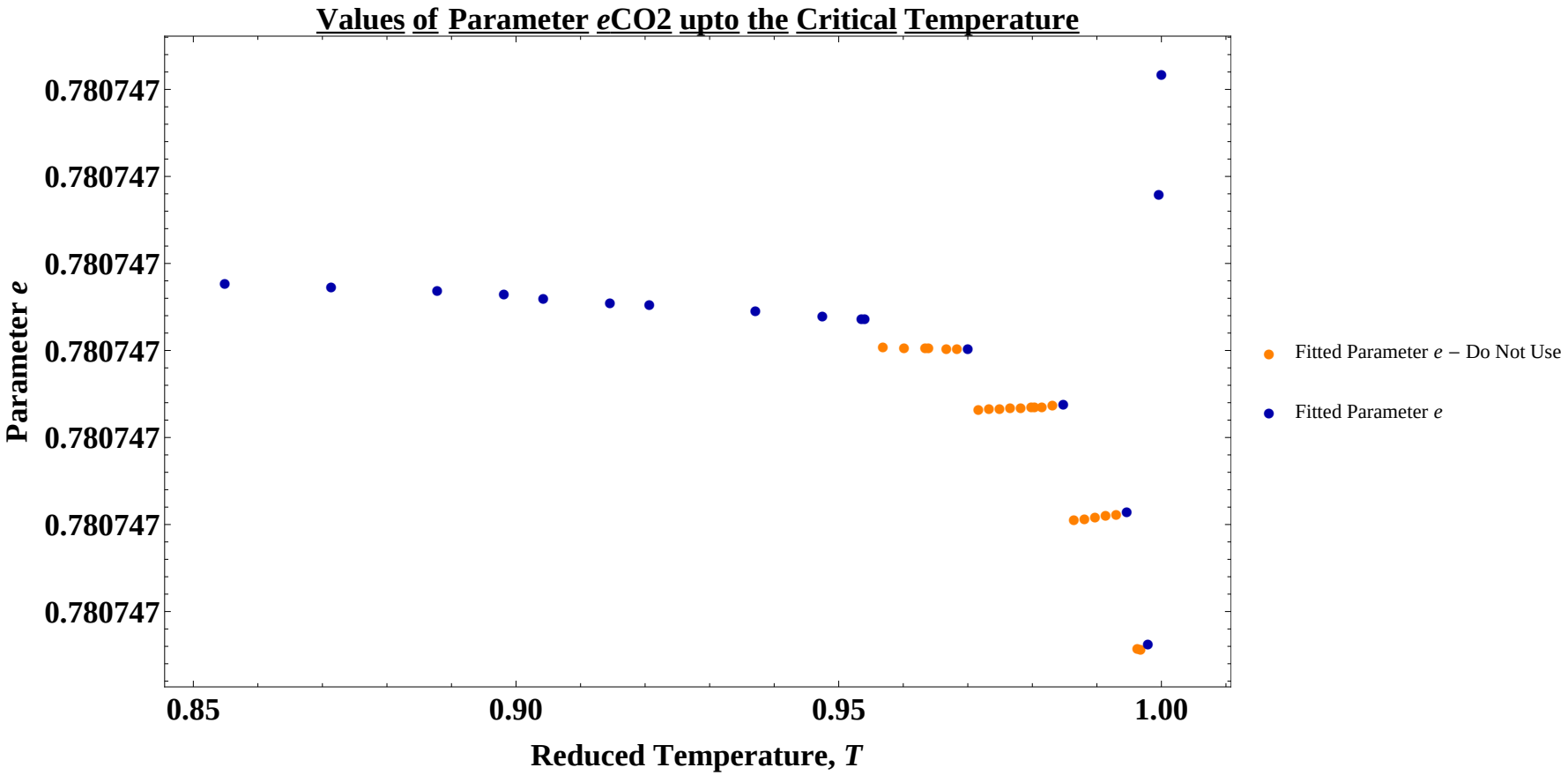

Figure 4.11: Variation of parameter e_{CO_2} at sub–critical temperatures for pure carbon dioxide

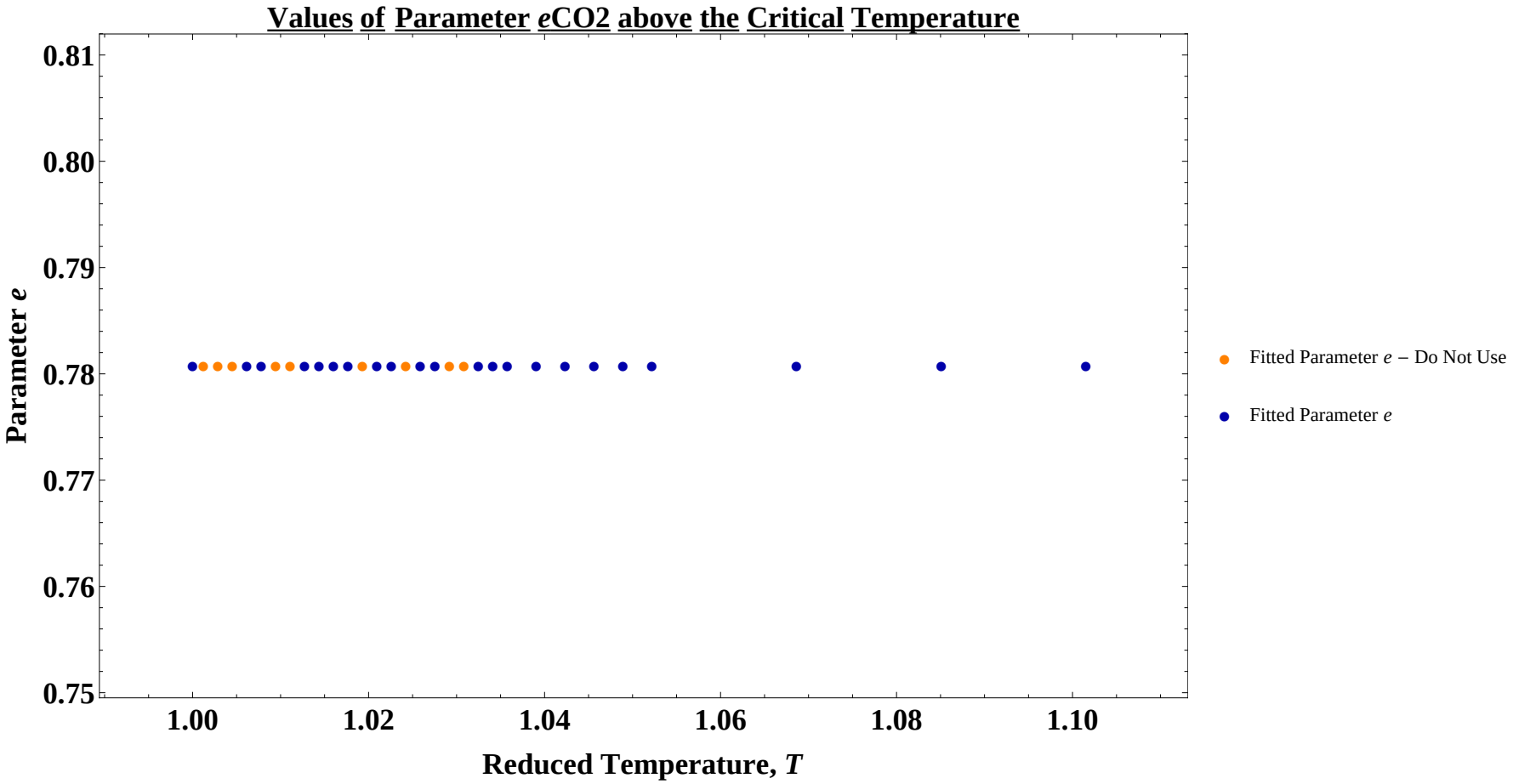

Figure 4.12: Values of parameter e_{CO_2} at super–critical temperatures for pure carbon dioxide

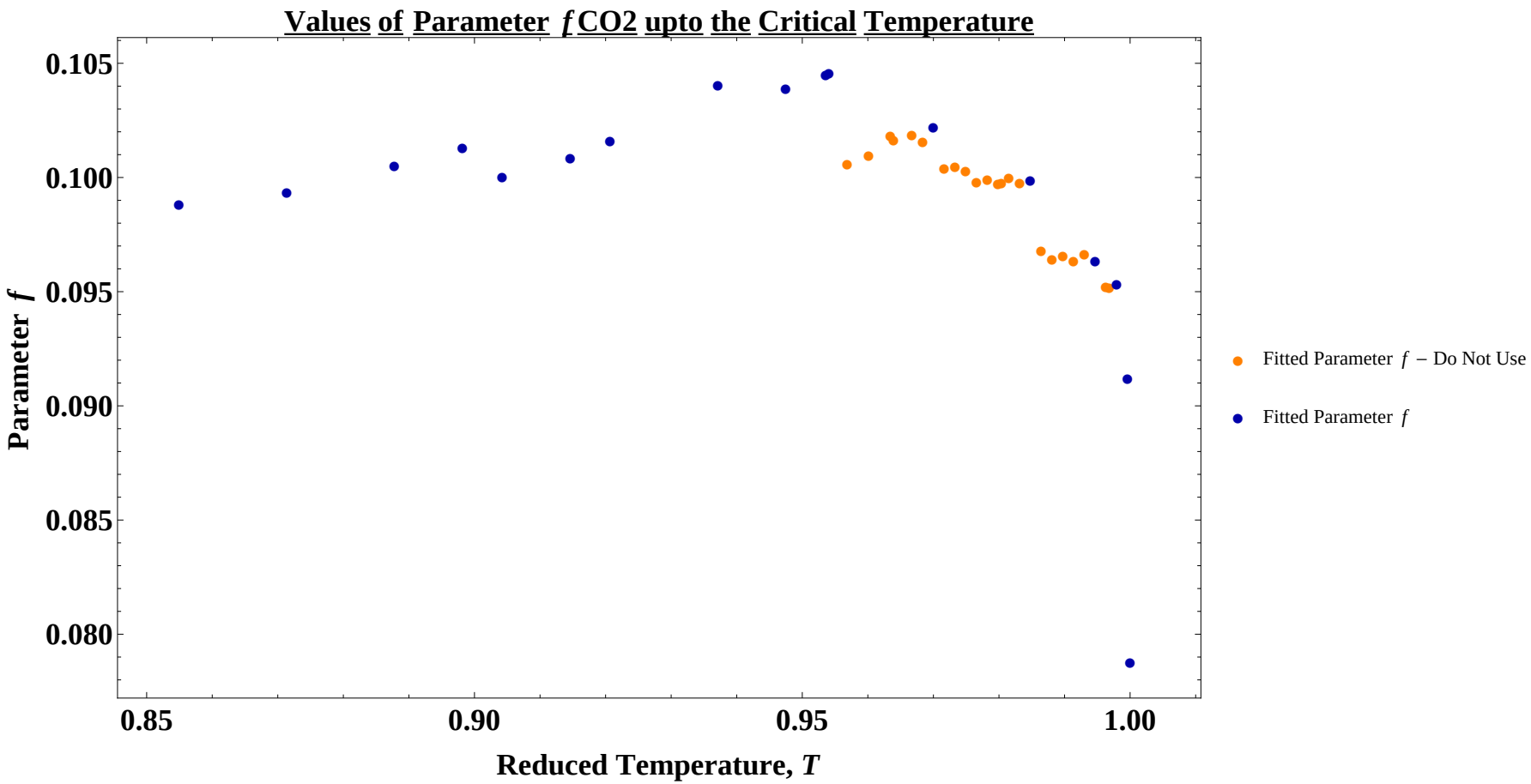

Figure 4.13: Values of parameter f_{CO_2} at sub–critical temperatures for pure carbon dioxide

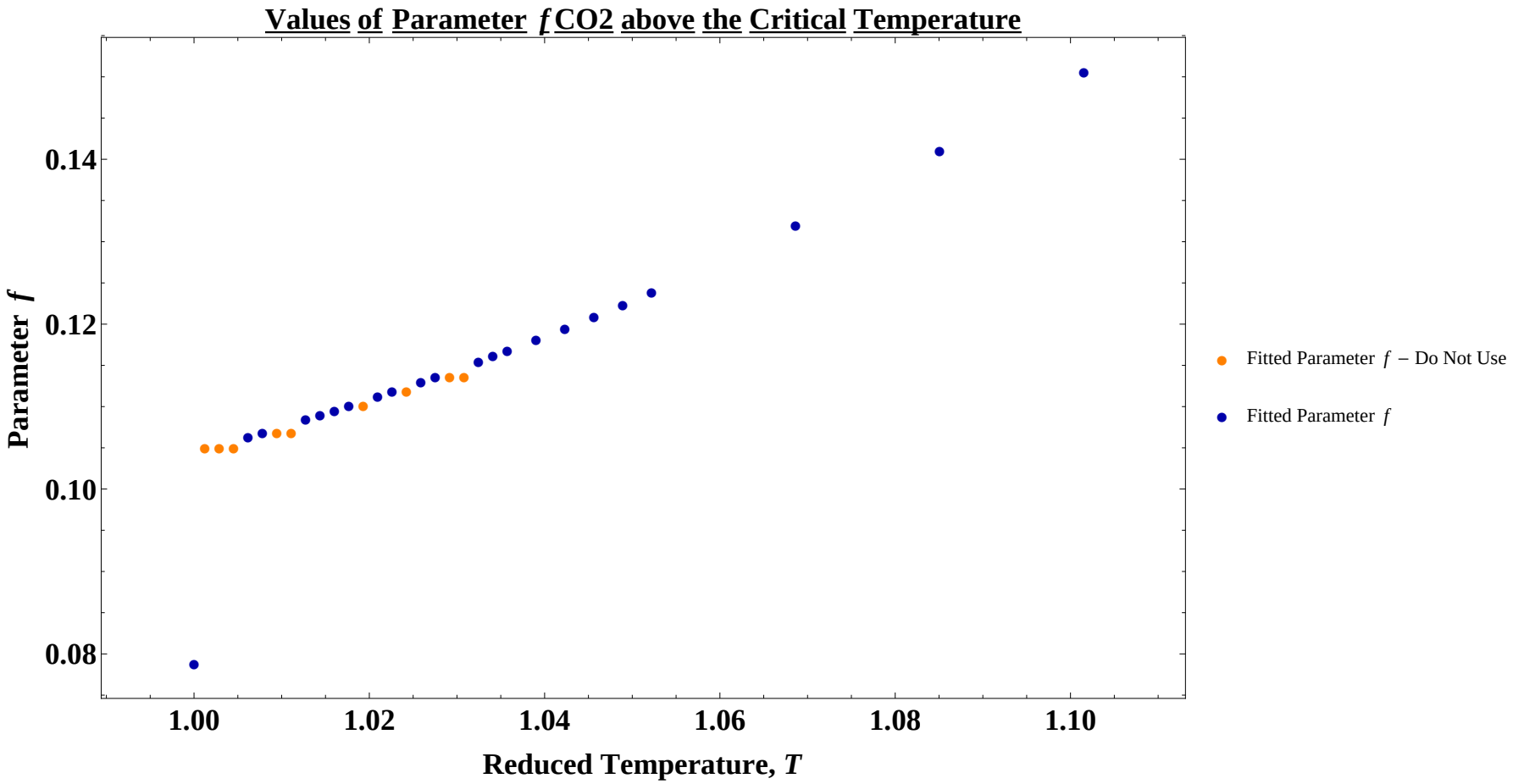

Figure 4.14: Values of parameter f_{CO_2} at super–critical temperatures for pure carbon dioxide

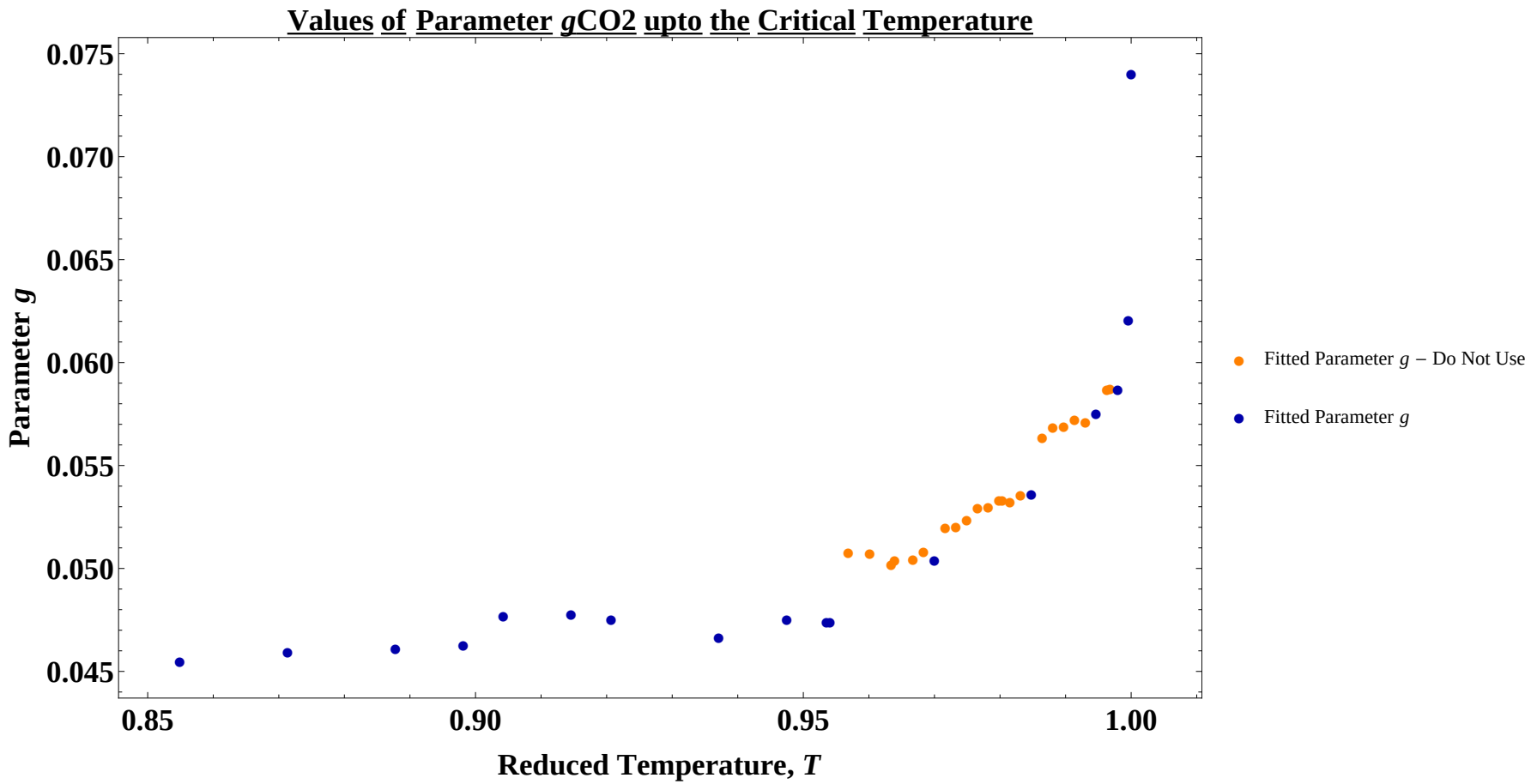

Figure 4.15: Values of parameter g_{CO_2} at sub–critical temperatures for pure carbon dioxide

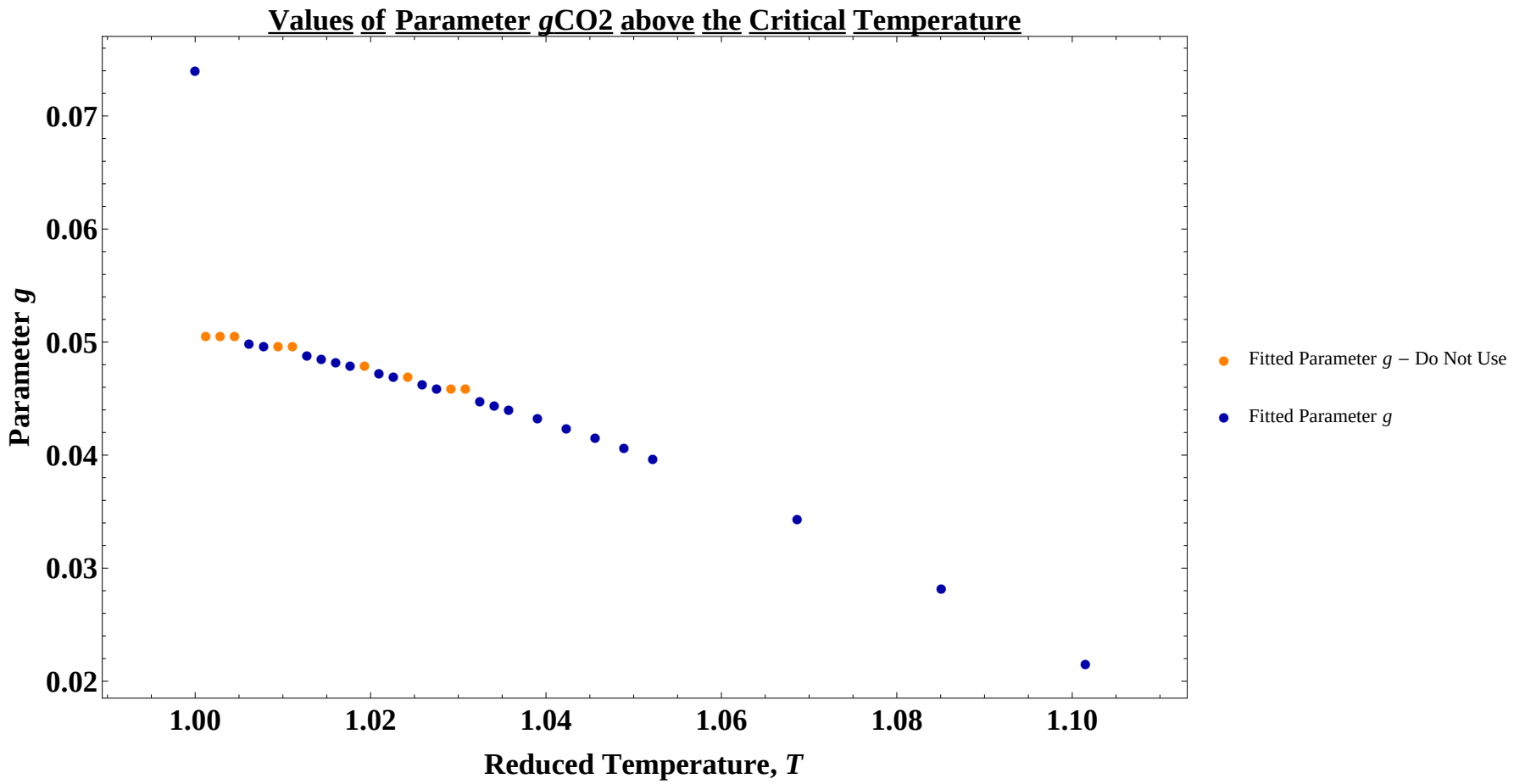

Figure 4.16: Values of parameter g_{CO_2} at super–critical temperatures for pure carbon dioxide

$$c(T) = \begin{cases} |T-1|^{0.515789}(-3.77054|T-1|^2 + 1.72673|T-1| \\ -0.478733) + 0.23876225996324883019 & T \leq 1 \\ |T-1|^{0.00608516}(-0.823306|T-1|^2 + 0.405298|T-1| \\ -0.0229758) + 0.23876225996324883019 & T \geq 1 \end{cases} \tag{4.10}$$

$$d(T) = \begin{cases} |T-1|^{1.27068}(0.000634507|T-1|^3 - 8.327888244017052\text{E-}6|T-1|^2 \\ -0.0000382867|T-1| + 4.661593764290955\text{E-}6) + \\ -0.0003744073550274074144 3 & T \leq 1 \\ 0.000374402|T-1|^{4.7618206193929816\text{E-}7} + \\ -0.0003744073550274074144 3 & T \geq 1 \end{cases} \tag{4.11}$$

$$e(T) = 0.78074651436175671059, \tag{4.12}$$

$$f(T) = \begin{cases} |T-1|^{0.192269}(0.210429|T-1|^2 - 0.199813|T-1| \\ +0.0528131) + 0.078770114175749938219 & T \leq 1 \\ |T-1|^{6.022611289345914\text{E-}9}(1.7061|T-1|^2 + 0.281852|T-1| \\ +0.0257812) + 0.078770114175749938219 & T \geq 1 \end{cases} \tag{4.13}$$

$$g(T) = \begin{cases} |T-1|^{0.198411}(-0.185594|T-1|^2 + 0.0931741|T-1| \\ -0.0510056) + 0.074028115340316985540 & T \leq 1 \\ |T-1|^{2.1304304817762944\text{E-}9}(-1.51507|T-1|^2 - 0.135147|T-1| \\ -0.0232326) + 0.074028115340316985540 & T \geq 1 \end{cases} \tag{4.14}$$

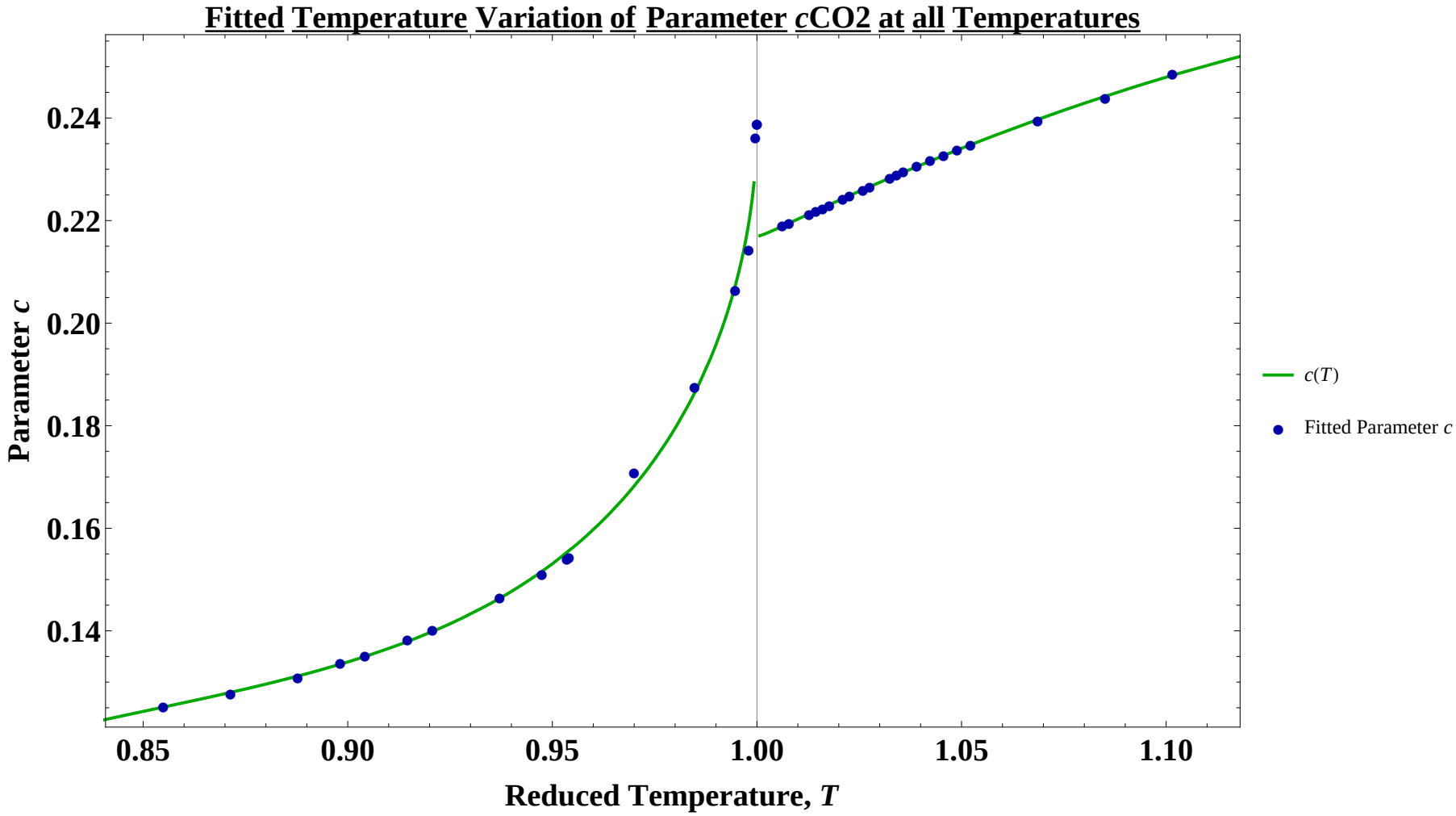

Figure 4.17: Variation of parameter c_{CO_2} at all temperatures in the CCS pipeline relevant range

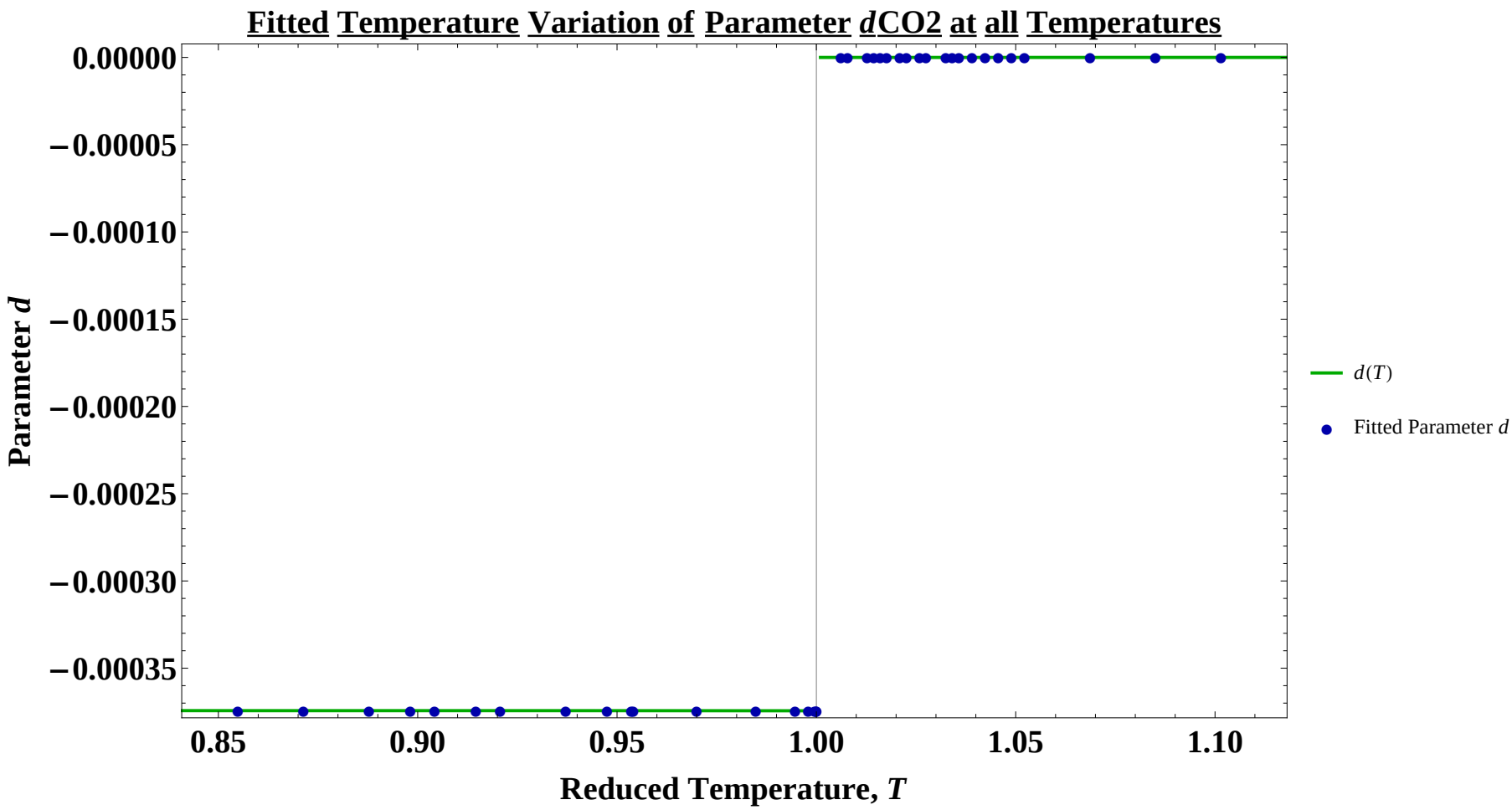

Figure 4.18: Values of parameter d_{CO_2} at sub–critical temperatures for pure carbon dioxide

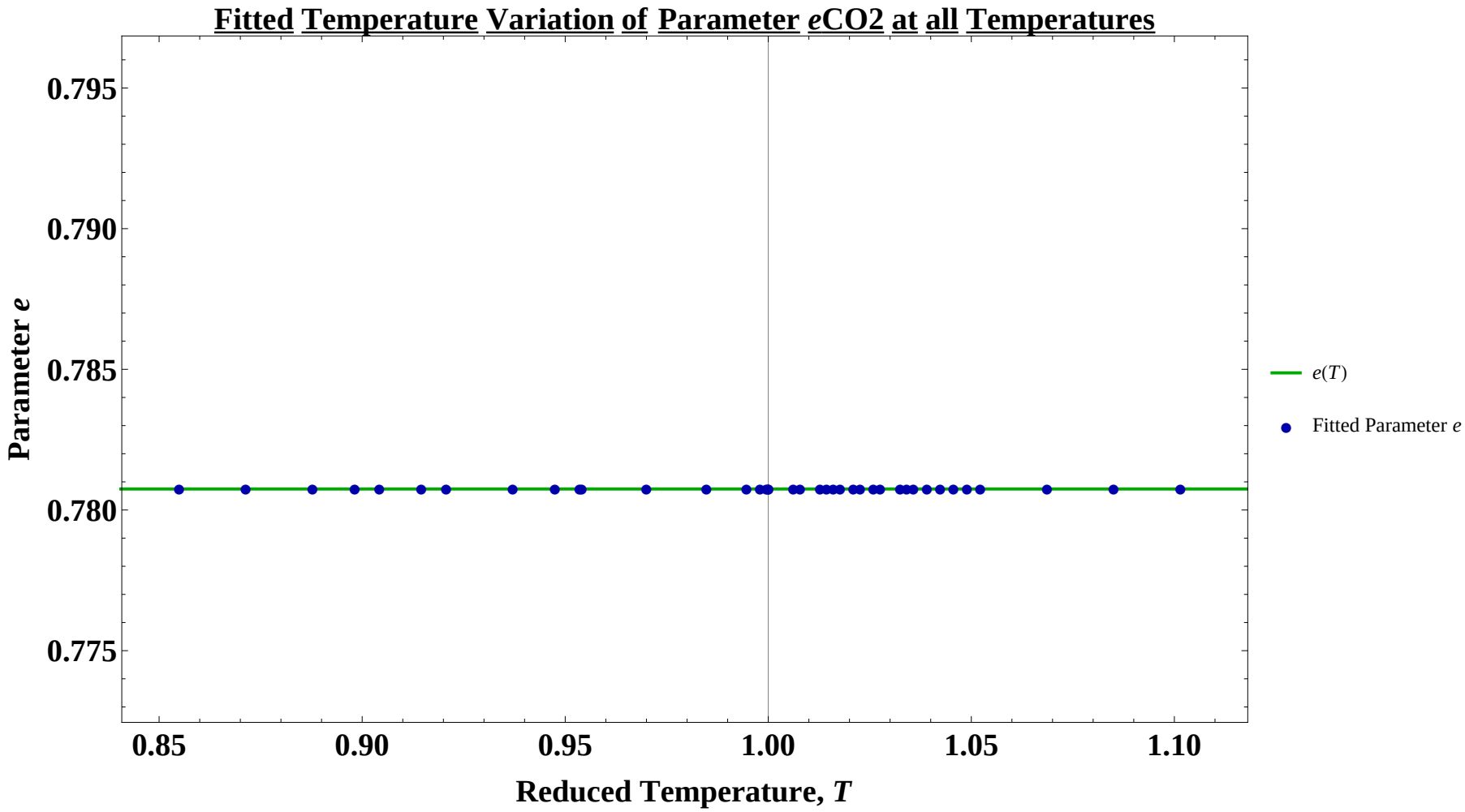

Figure 4.19: Variation of parameter e_{CO_2} at all temperatures in the CCS pipeline relevant range

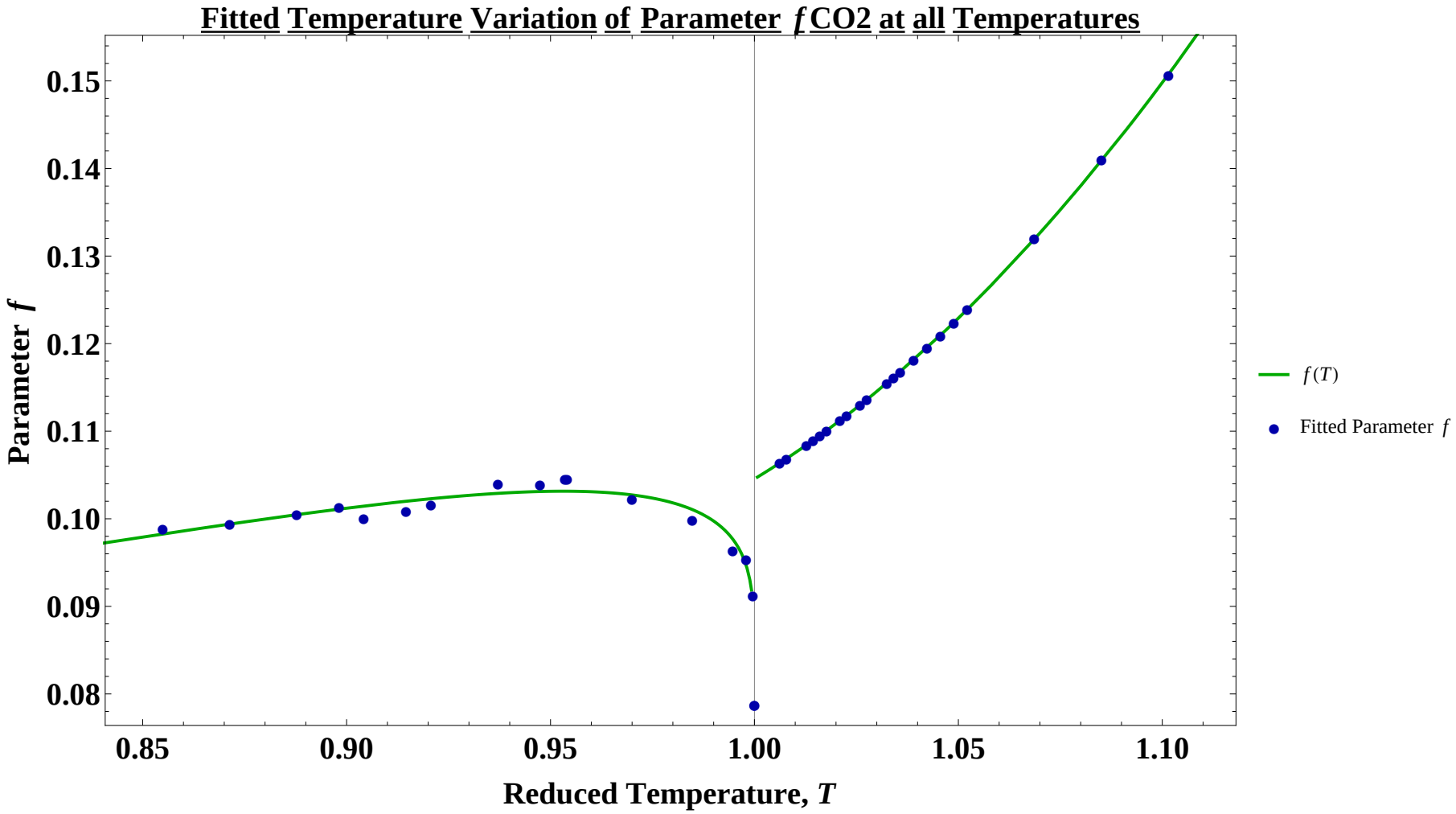

Figure 4.20: Variation of parameter f_{CO_2} at all temperatures in the CCS pipeline relevant range

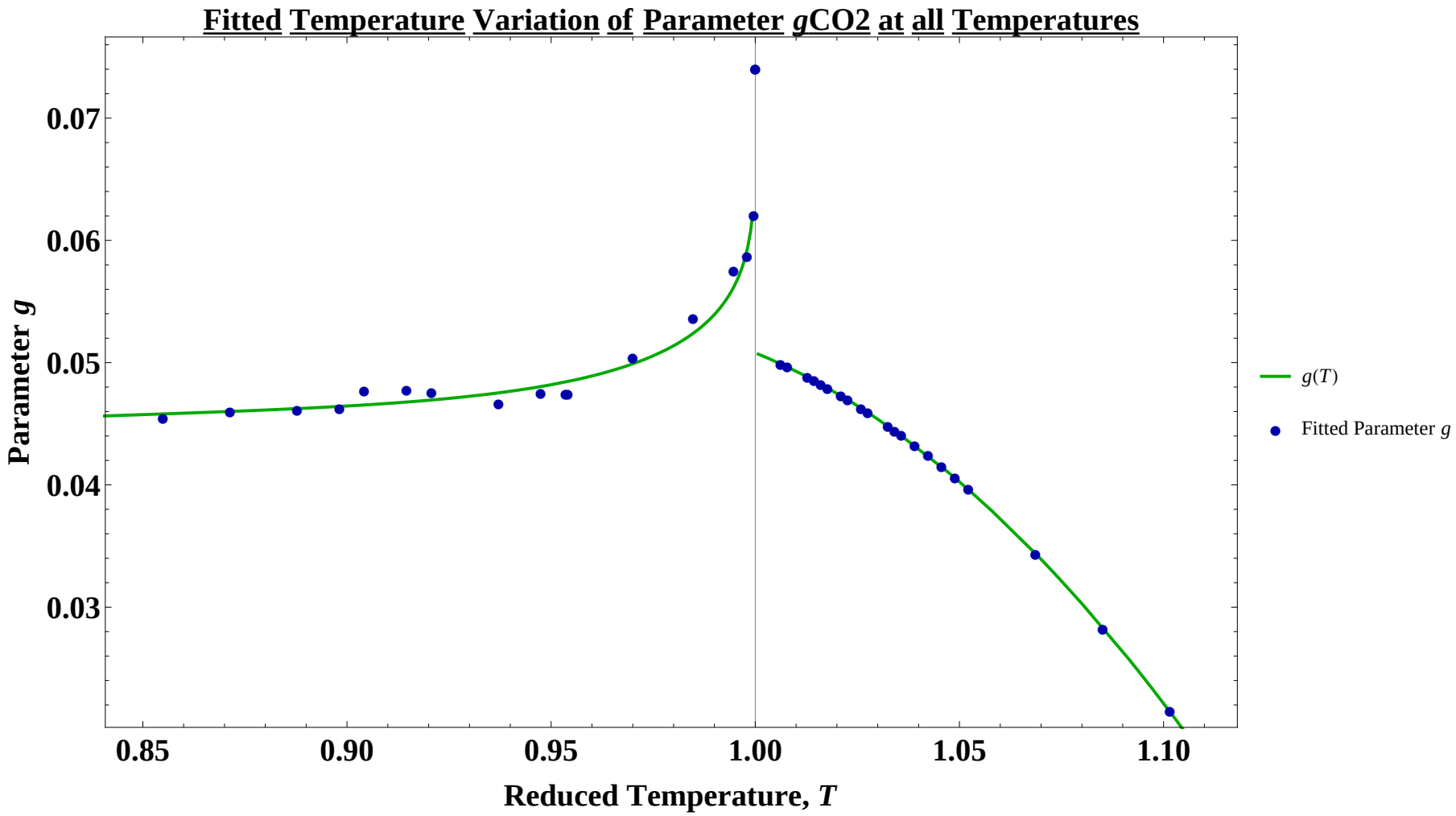

Figure 4.21: Variation of parameter g_{CO_2} at all temperatures in the CCS pipeline relevant range

Thus each parameter was fully defined and this completed the model in the case of pure carbon dioxide. We note that the parameter variations given here differ slightly from those proposed in our published work [40]. The model proposed here extends to the elevated temperatures, and has a better performance than that suggested previously.

4.5 Performance of the Proposed Model in the Case of Pure Carbon Dioxide

Having established the continuous temperature dependences for each model parameter, we subsequently found our model to very accurately reconstruct the data provided by NIST. Over the following pages we have plotted the behaviour at a range of different temperatures (including T_c) throughout the range of relevance for CCS pipelines in order to demonstrate the usefulness of the proposed equation within this range.

Figures 4.22 to 4.31 show a direct comparison between pressure predictions of our equation of state (dark green line) and the Peng–Robinson equation of state (dark red line) against the NIST data (dark blue markers), as well as the phase behaviour in the form of the bubble and dew points, shown for each model by triangles in its respective colour, and for the NIST data by the large hollow triangles. We can easily verify that the proposed model (3.21) incorporating parameters a to g as defined in Equations (4.7), (4.9), (4.10), (4.11), (4.12), (4.13) and (4.14) gives a very accurate description.

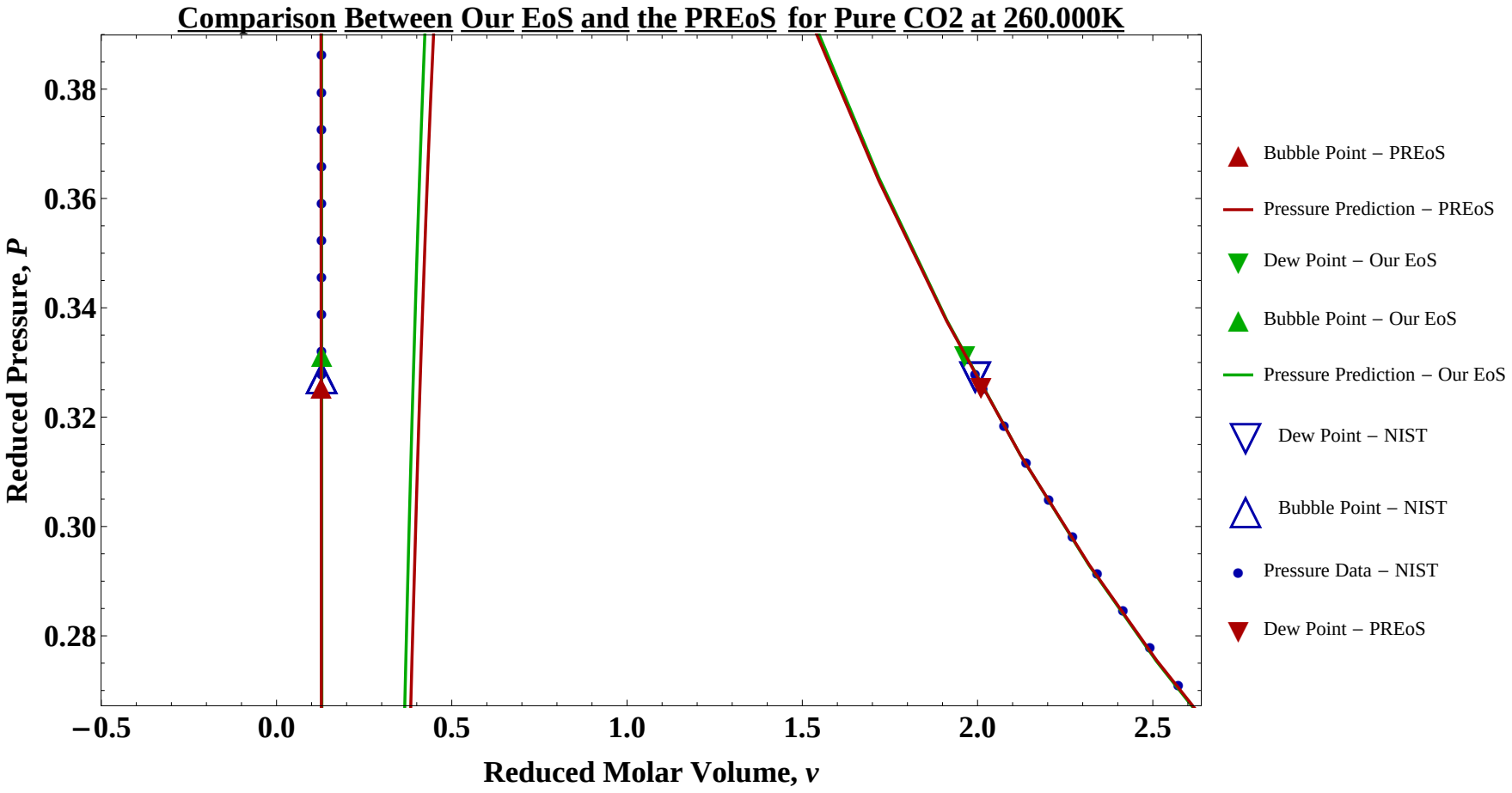

Figure 4.22: A comparison between the proposed EoS and the PREoS against the NIST data at 260K

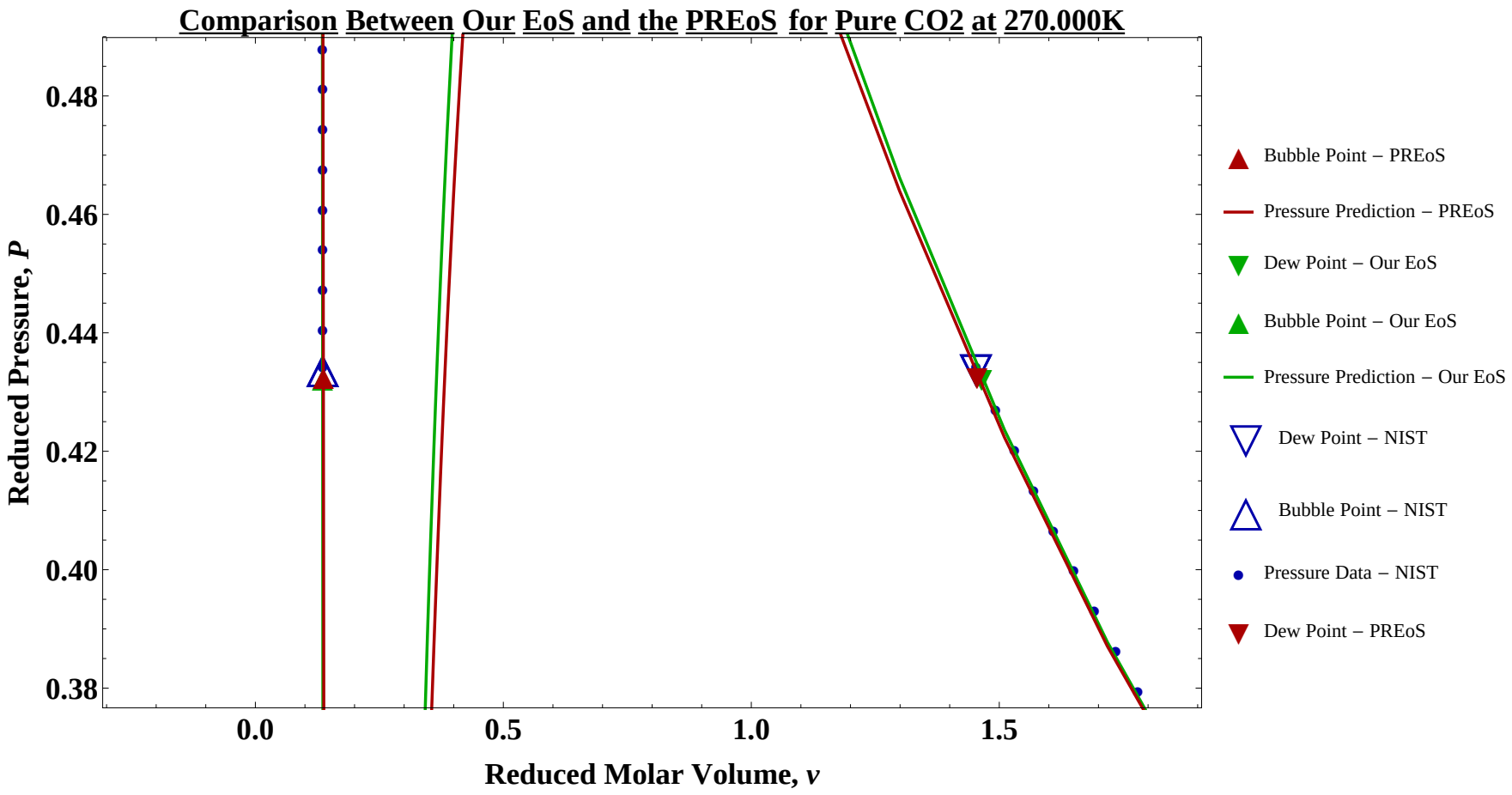

Figure 4.23: A comparison between the proposed EoS and the PREoS against the NIST data at 270K

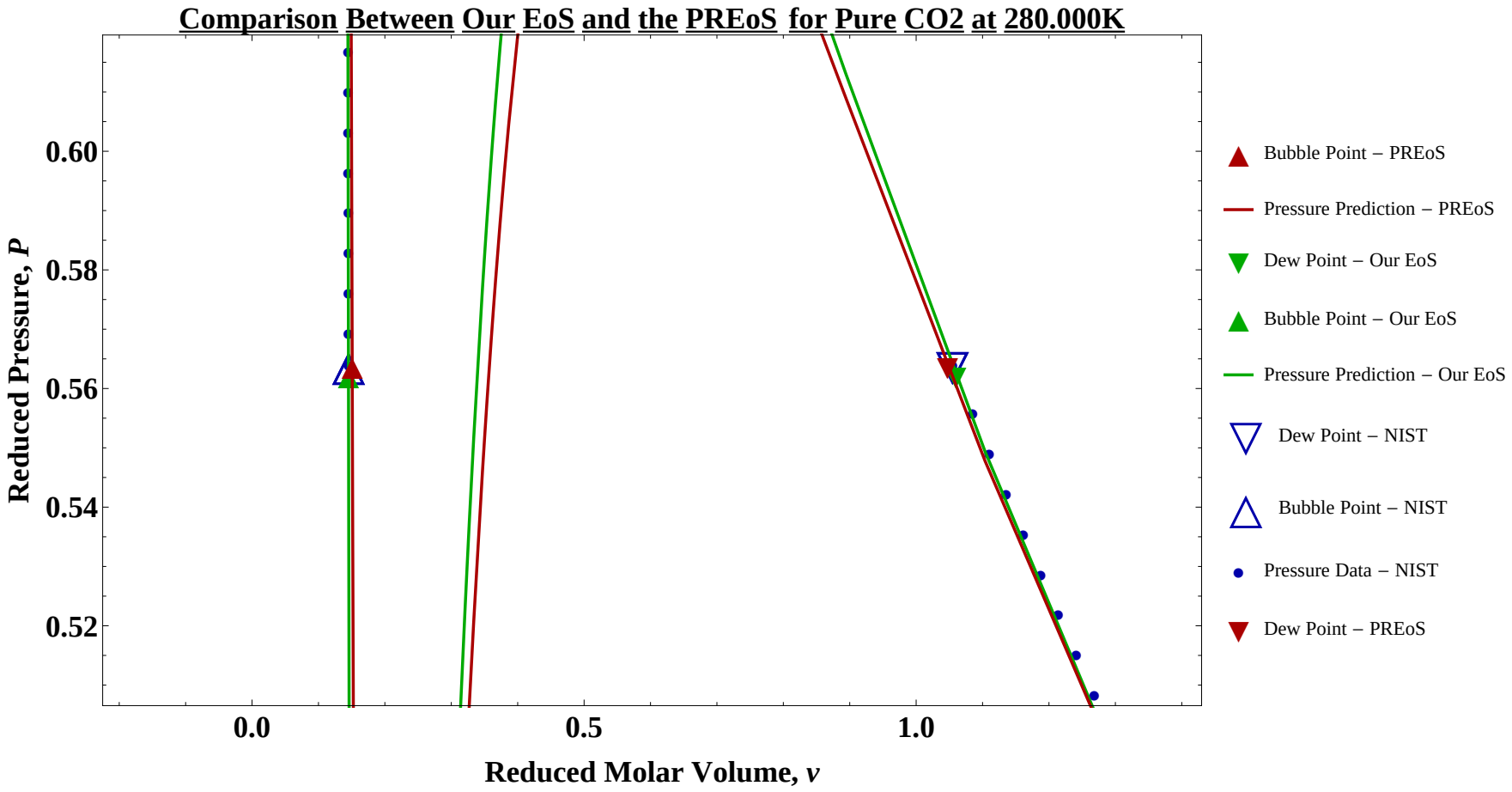

Figure 4.24: A comparison between the proposed EoS and the PREoS against the NIST data at 280K

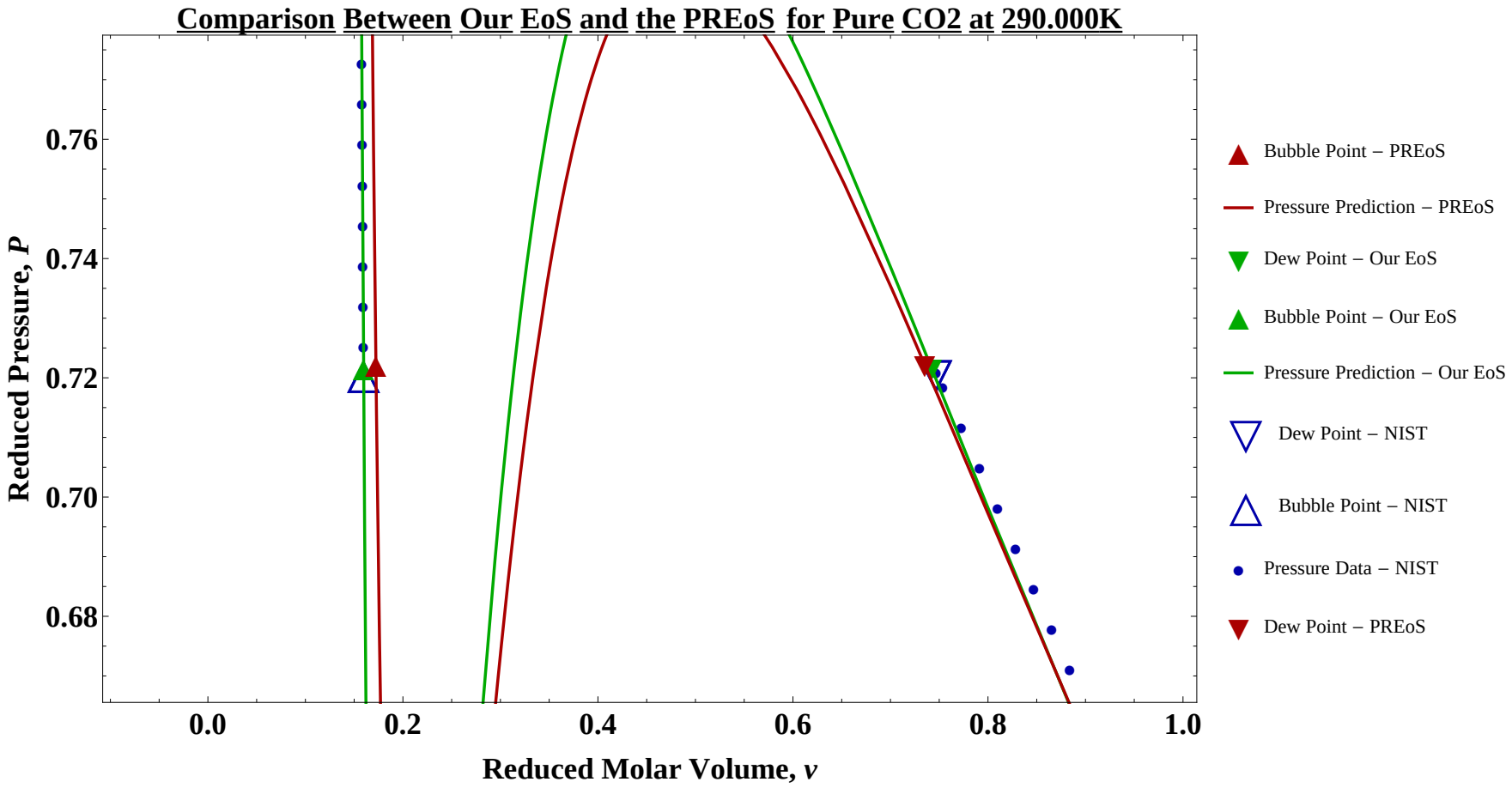

Figure 4.25: A comparison between the proposed EoS and the PREoS against the NIST data at 290K

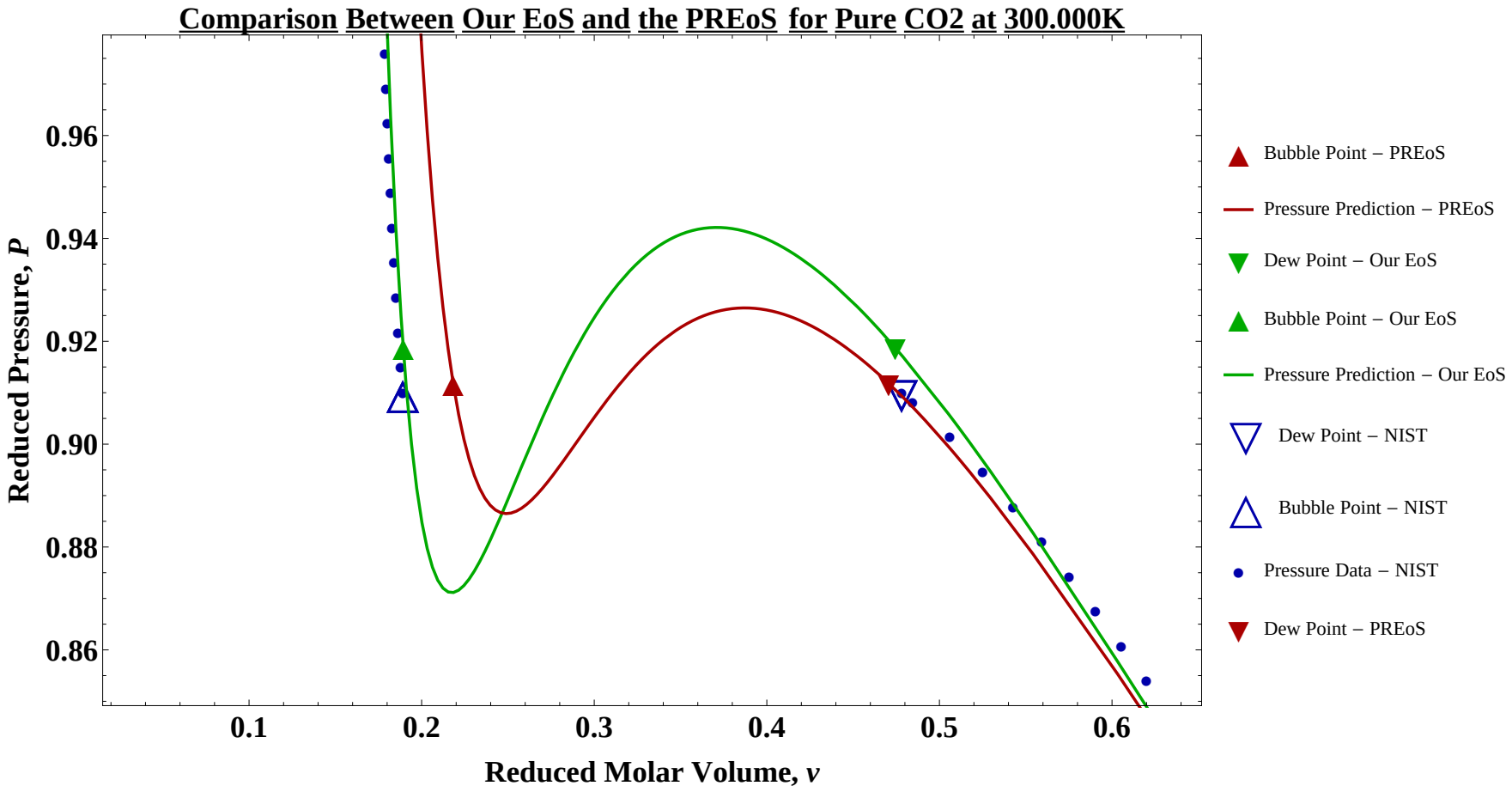

Figure 4.26: A comparison between the proposed EoS and the PREoS against the NIST data at 300K

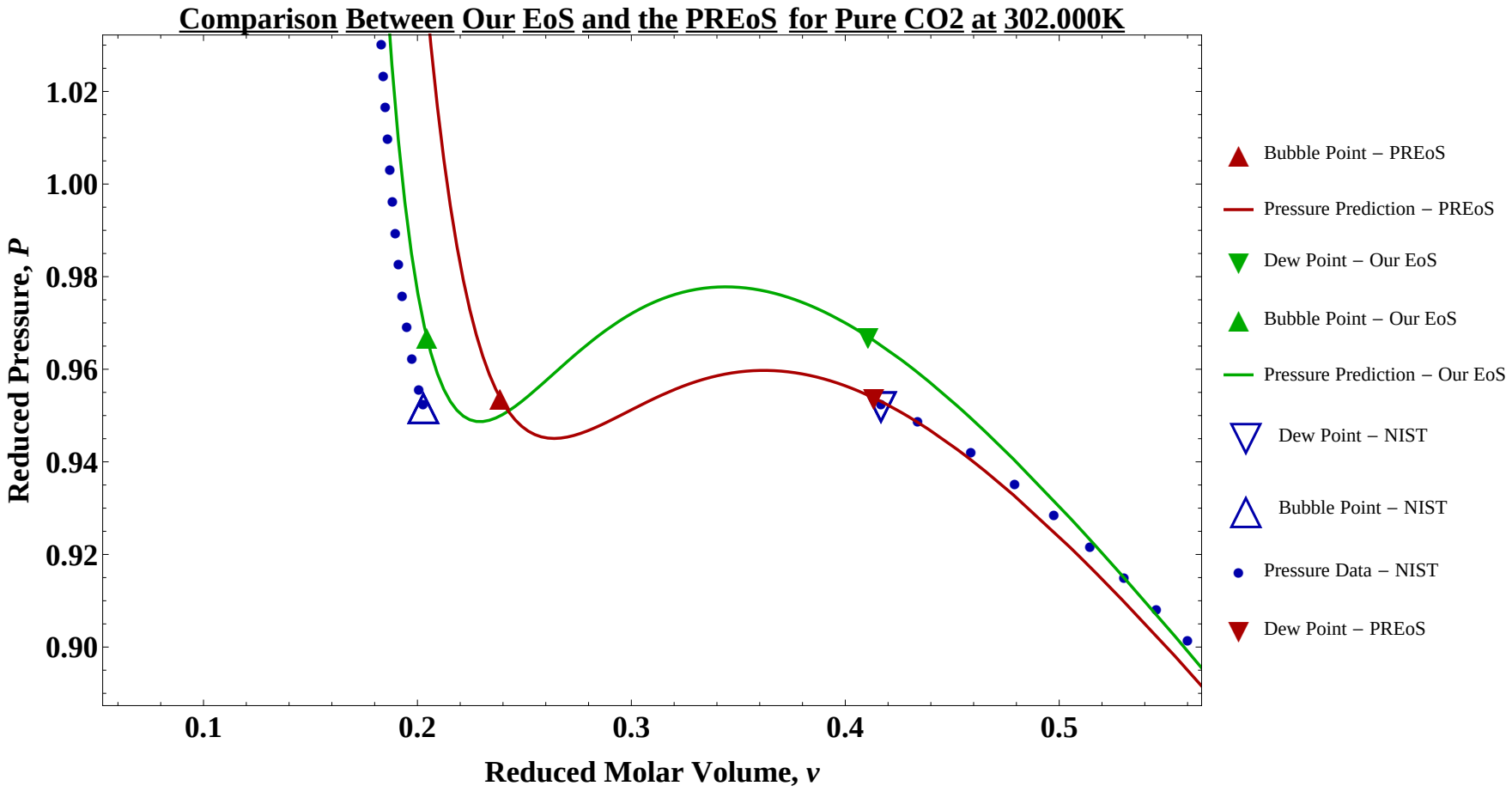

Figure 4.27: A comparison between the proposed EoS and the PREoS against the NIST data at 302K

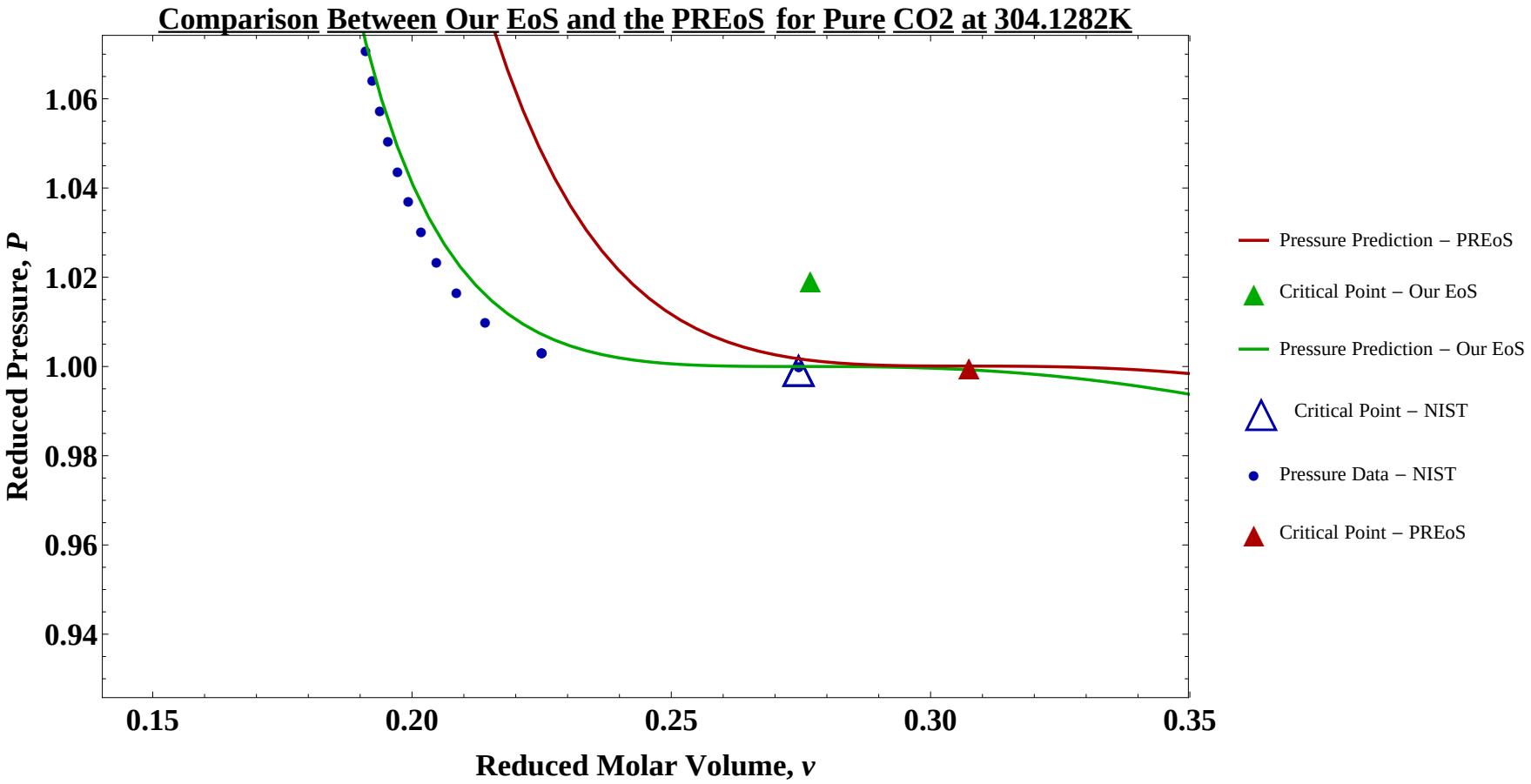

Figure 4.28: A comparison between the proposed EoS and the PREoS against the NIST data at the critical temperature

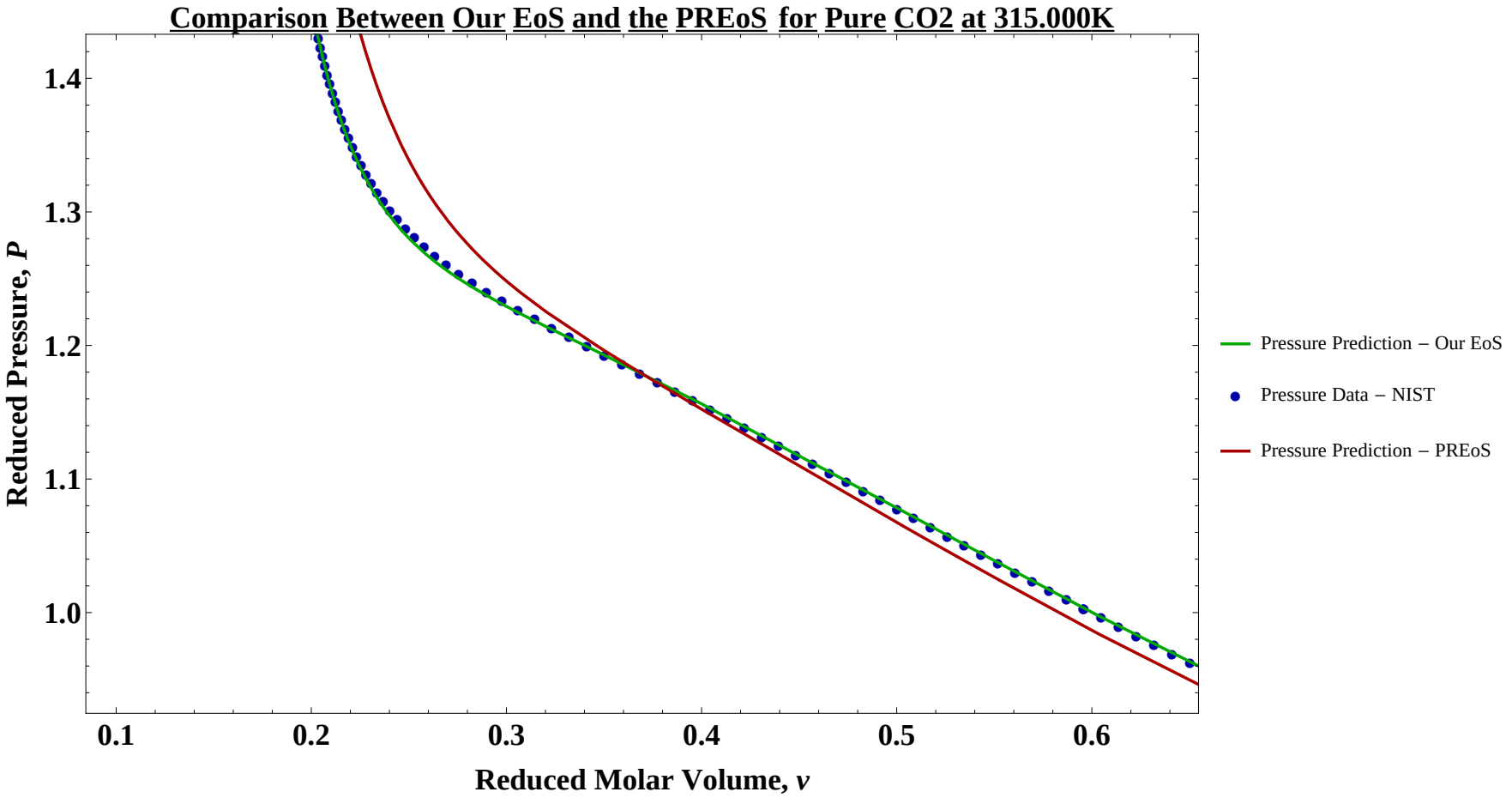

Figure 4.29: A comparison between the proposed EoS and the PREoS against the NIST data at 315K

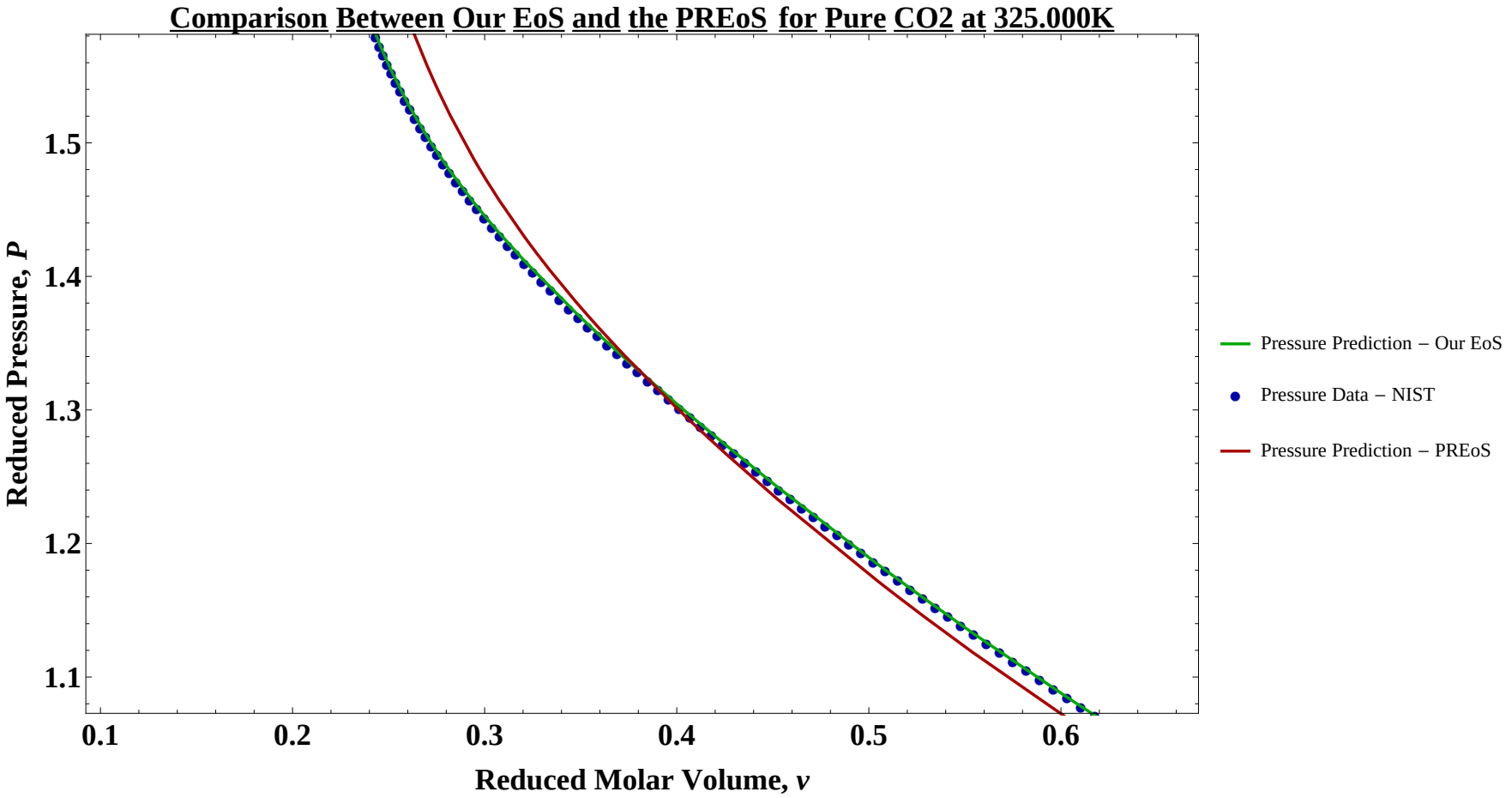

Figure 4.30: A comparison between the proposed EoS and the PREoS against the NIST data at 325K

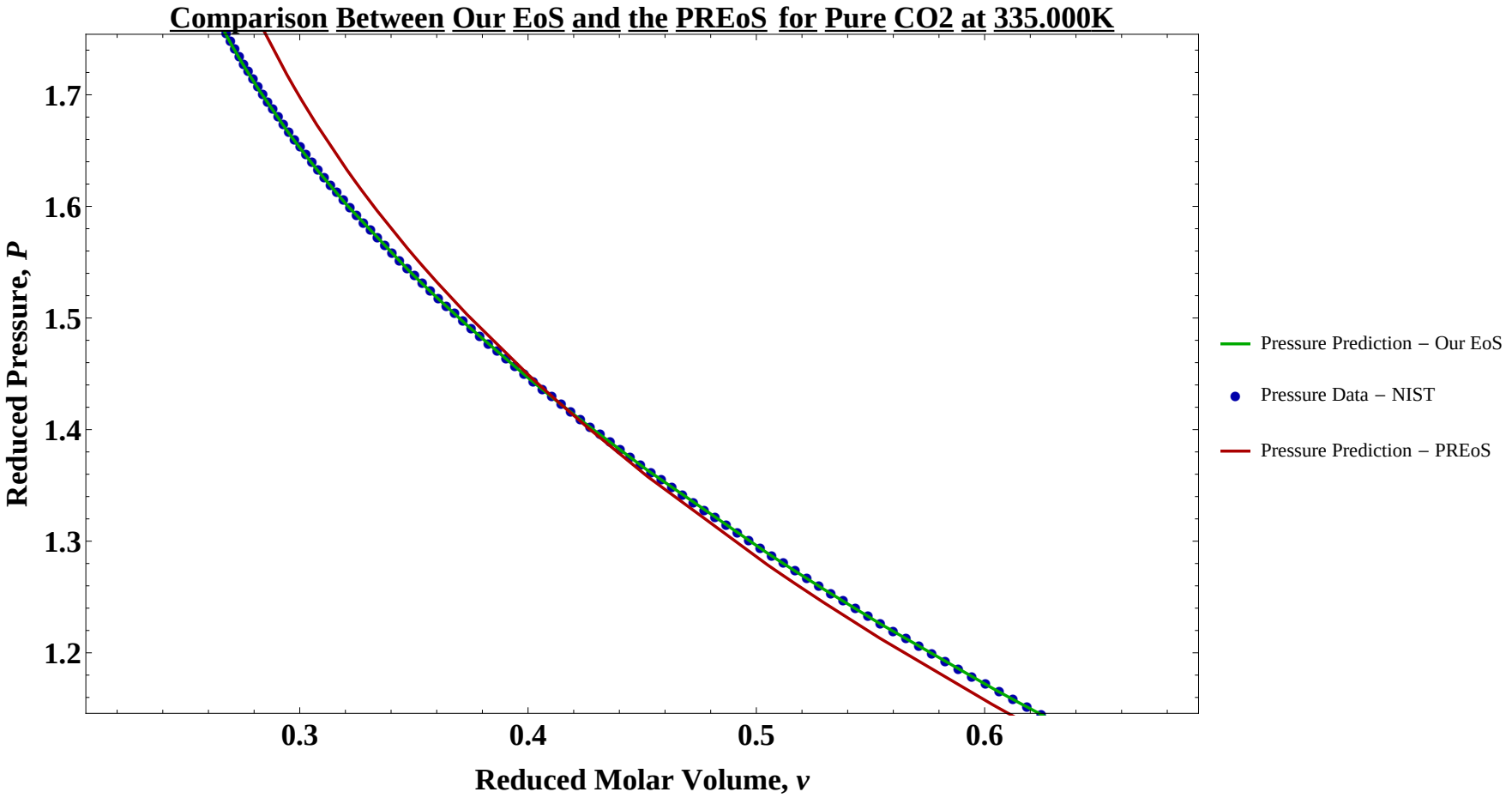

Figure 4.31: A comparison between the proposed EoS and the PREoS against the NIST data at 335K

In particular, we note the following:

- In the high pressure region there is a much better agreement with the NIST data for our model than PREoS.
- We also note the closeness of agreement with the NIST bubble and dew points and the predicted bubble and dew points of the proposed EoS, thus suggesting that our model is as accurate as had aimed for.
- Looking closely at the multi–phase region we can see that in the liquid phase, the PREoS fails to model the pressure behaviour accurately enough for CCS. In this region, we can see from Table 4.2 that it can be as much as 41% out in the relevant range of temperatures, whereas the proposed EoS never exhibits more than a 5.5% error compared to the NIST data, and rarely more than a 2% error.

Broadly speaking we found the proposed model to very accurately reconstruct the pressure and phase behaviour prescribed by the NIST database. The phase behaviour was generally found to be well within our target range of a 2% error, as shown in Table 4.2. Specifically, we found the pressure predictions to almost exclusively be within this target range, apart from in the immediate vicinity of the critical point. We conjecture that having enforced the model to vary smoothly, this may account for the slight loss of comparable accuracy in this region. Despite this however, we note that our model still appears to offer significant advantages in accuracy over the PREoS.

The values for percentage errors are given in the Table 4.2, with a comparison against the PREoS demonstrating the potential of our model. For the proposed equation, percentage errors were calculated using Equation (4.1), and for the PREoS an analogous equation was used. In Table 4.3 we also note the critical property predictions of the proposed model, and Figure 4.32 compares the prediction of the pure case phase boundary made by our model to that of the PREoS.

Temperature (K)	Maximum Percentage Error in P		Average Percentage Error in P		Percentage Error in P_{vap}		Percentage Error in v_{BP}		Percentage Error in v_{DP}	
	(3.21)	PREoS	(3.21)	PREoS	(3.21)	PREoS	(3.21)	PREoS	(3.21)	PREoS
260	14.979	45.332	1.730	38.109	1.068	0.664	0.113	0.991	1.520	0.847
265	2.672	38.337	1.746	25.379	0.004	0.520	0.052	0.013	0.099	0.528
270	4.093	31.811	2.467	17.202	0.439	0.365	0.038	1.053	0.793	0.161
273.15	4.259	31.564	2.291	14.320	0.500	0.265	0.233	1.624	0.886	0.093
275	3.848	35.412	2.052	13.029	0.484	0.207	0.060	2.264	0.845	0.248
278.15	2.734	39.602	1.560	11.472	0.400	0.109	0.090	3.088	0.651	0.524
280	2.002	40.852	1.264	10.765	0.329	0.053	0.087	3.627	0.481	0.691
285	1.363	40.529	0.670	9.463	0.106	0.084	0.105	5.236	0.091	1.147
288.15	1.551	38.005	0.564	8.944	0.035	0.157	0.019	6.555	0.449	1.425
290	1.654	35.814	0.582	8.627	0.117	0.191	0.048	7.375	0.625	1.574
290.15	1.662	35.615	0.584	8.639	0.123	0.194	0.041	7.436	0.638	1.586
291	1.705	34.431	0.599	8.533	0.161	0.207	0.150	7.929	0.702	1.649
292	1.752	32.913	0.618	8.364	0.208	0.221	0.148	8.413	0.764	1.717
293	1.793	31.267	0.639	8.207	0.257	0.232	0.059	8.846	0.808	1.776
293.15	1.798	31.009	0.643	8.218	0.264	0.234	0.090	8.953	0.813	1.784
294	1.827	29.531	0.663	8.132	0.311	0.240	0.076	9.404	0.834	1.825
294.5	1.842	28.715	0.675	8.024	0.340	0.243	0.128	9.735	0.839	1.844
295	1.854	27.945	0.688	7.989	0.372	0.245	0.041	9.950	0.838	1.859
295.5	1.864	27.218	0.701	7.888	0.407	0.246	0.007	10.207	0.834	1.870
296	1.871	26.527	0.714	7.854	0.444	0.247	0.015	10.510	0.824	1.875
296.5	1.875	25.874	0.728	7.819	0.485	0.246	0.023	10.862	0.811	1.874
297	1.877	25.254	0.740	7.726	0.531	0.244	0.111	11.267	0.796	1.867
297.5	1.875	24.663	0.752	7.692	0.582	0.240	0.091	11.585	0.778	1.851
298	1.870	24.102	0.762	7.604	0.639	0.236	0.137	11.969	0.760	1.825
298.15	1.868	23.939	0.765	7.610	0.658	0.234	0.133	12.070	0.756	1.815
298.5	1.861	23.568	0.772	7.570	0.704	0.230	0.099	12.286	0.746	1.788
299	1.848	23.057	0.780	7.488	0.777	0.223	0.152	12.688	0.739	1.737
299.5	1.830	22.568	0.788	7.453	0.860	0.214	0.157	13.049	0.744	1.668
300	1.815	22.103	0.795	7.376	0.955	0.203	0.140	13.390	0.770	1.578
300.5	2.020	21.656	0.806	7.339	1.065	0.191	0.291	13.865	0.830	1.460
301	2.263	21.229	0.823	7.267	1.191	0.176	0.356	14.241	0.943	1.305
301.5	2.553	20.818	0.857	7.228	1.336	0.159	0.566	14.694	1.141	1.100
302	2.898	20.424	0.924	7.162	1.506	0.139	0.757	15.038	1.481	0.819
302.5	3.307	20.044	1.081	7.099	1.702	0.116	1.313	15.507	2.078	0.421
303	3.792	19.680	1.319	7.057	1.925	0.090	2.321	15.936	3.214	0.182
303.15	3.952	19.573	1.403	7.034	1.996	0.081	2.822	16.063	3.765	0.429
303.5	4.343	19.329	1.630	7.000	2.157	0.058	4.815	16.329	5.952	1.217
304	4.628	18.990	1.963	6.945	2.137	0.020	11.017	16.015	16.092	3.849
304.1282	5.483	18.905	2.141	6.922	—	—	—	—	—	—
304.5	1.450	18.664	0.453	6.902	—	—	—	—	—	—
305	1.405	18.349	0.365	6.863	—	—	—	—	—	—
305.5	1.405	18.349	0.365	6.863	—	—	—	—	—	—
306	1.342	18.044	0.303	6.823	—	—	—	—	—	—
306.5	1.279	17.750	0.256	6.784	—	—	—	—	—	—
307	1.217	17.465	0.225	6.743	—	—	—	—	—	—
307.5	1.157	17.189	0.204	6.701	—	—	—	—	—	—
308	1.098	16.922	0.187	6.658	—	—	—	—	—	—
308.5	1.041	16.663	0.175	6.614	—	—	—	—	—	—
309	0.984	16.411	0.165	6.569	—	—	—	—	—	—
309.5	0.929	16.167	0.156	6.523	—	—	—	—	—	—
310	0.874	15.931	0.150	6.476	—	—	—	—	—	—
310.5	0.820	15.701	0.144	6.429	—	—	—	—	—	—
311	0.770	15.478	0.138	6.380	—	—	—	—	—	—
311.5	0.721	15.261	0.133	6.331	—	—	—	—	—	—
312	0.672	15.049	0.127	6.281	—	—	—	—	—	—
312.5	0.624	14.844	0.122	6.230	—	—	—	—	—	—
313	0.530	14.449	0.110	6.126	—	—	—	—	—	—
313.5	0.485	14.260	0.104	6.073	—	—	—	—	—	—
314	0.440	14.075	0.098	6.019	—	—	—	—	—	—
314.5	0.399	13.896	0.091	5.965	—	—	—	—	—	—
315	0.358	13.720	0.084	5.911	—	—	—	—	—	—
316	0.279	13.383	0.070	5.800	—	—	—	—	—	—
317	0.205	13.062	0.057	5.687	—	—	—	—	—	—
318	0.138	12.756	0.046	5.574	—	—	—	—	—	—
319	0.119	12.465	0.039	5.459	—	—	—	—	—	—
320	0.138	12.187	0.038	5.343	—	—	—	—	—	—
325	0.209	10.968	0.099	4.762	—	—	—	—	—	—
330	0.150	9.971	0.080	4.192	—	—	—	—	—	—
335	0.143	9.132	0.061	3.655	—	—	—	—	—	—

Table 4.2: Maximum and average percentage errors in P, and errors for P_{vap}, v_{BP} and v_{DP} for both the proposed EoS and the PREoS

Model	Critical Temperature		Critical Pressure		Critical Volume	
	Predicted (K)	Error (%)	Predicted (MPa)	Error (%)	Predicted ($m^3.mol^{-1}$)	Error (%)
PREoS	304.121	0.002	7.3768	0.007	1.0537×10^{-4}	11.957
Proposed Model	304.422	0.097	7.5210	1.948	9.4875×10^{-5}	0.803
Actual Value	304.1282	—	7.3773	—	9.41185×10^{-5}	—

Table 4.3: Comparison of critical point predictions

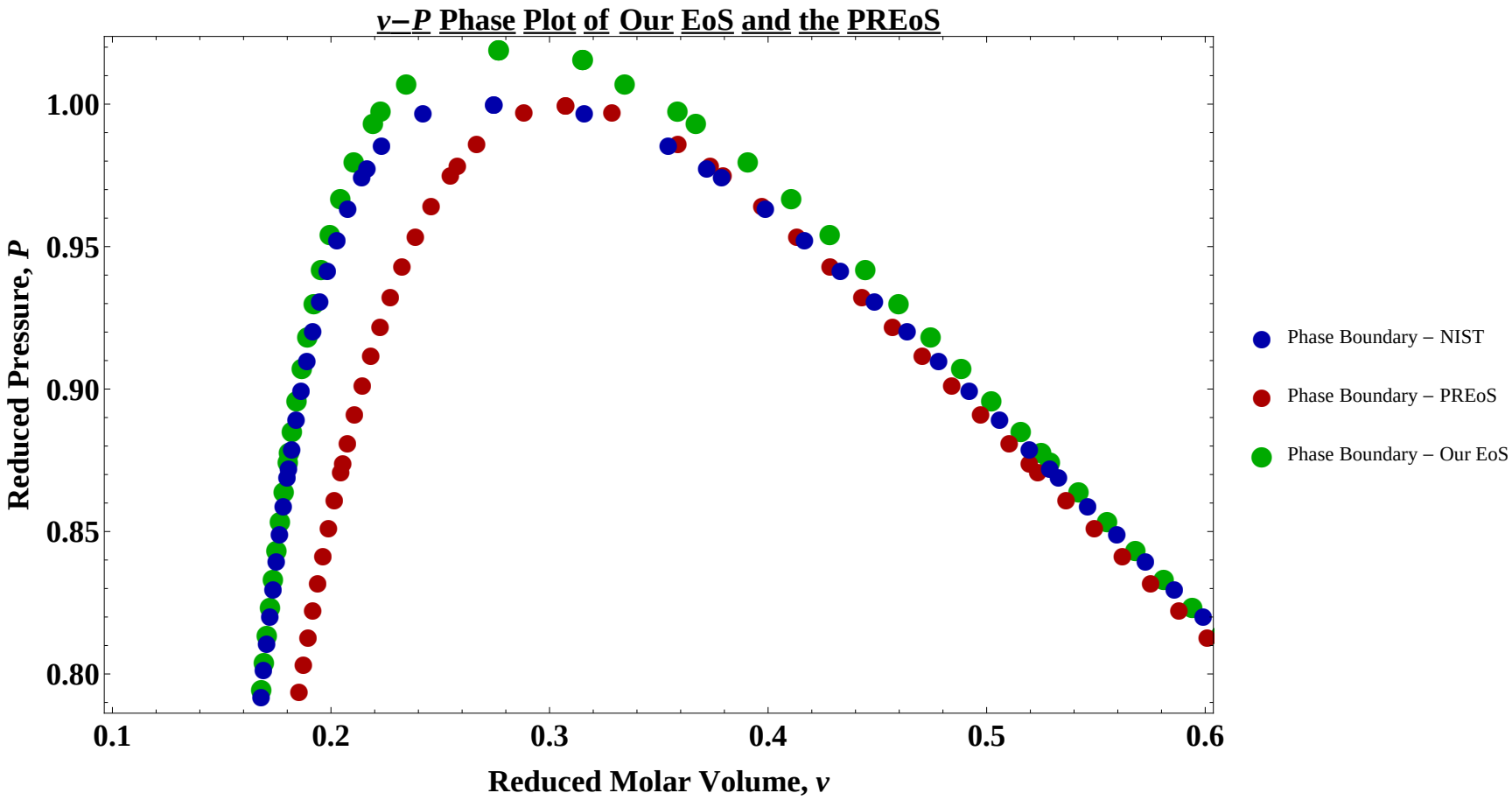

Figure 4.32: A comparison between predictions of the two–phase region boundary of our EoS compare to the PREoS

4.6 Discussion

As we can see from Figures 4.22 to 4.31 and 4.32, and Tables 4.2 and 4.3, the proposed equation of state certainly appears to have great potential in modelling the physical behaviour of pure carbon dioxide when compared directly with the PREoS, without any significant overburden of complexity. Our analyses revealed that there was hardly ever a time in the window 260–335K and 0.05-20MPa when the Peng–Robinson EoS predicted the pressure behaviour more accurately than the proposed EoS, except for when it happens to pass through zero error on the way from over–estimating to under–estimating (or vice–versa). The data in columns two to five of Table 4.2 substantiate this claim by showing that at any given temperature both the maximum and average errors of the proposed EoS compare extremely favourably to those of the Peng–Robinson EoS. This is definitely an excellent starting point from which to extend the EoS to a wider range of temperatures if deemed necessary and into predictions for physical behaviour of the CCS pipeline relevant mixtures.

Predictions of the bubble $(v_{\mathrm{BP}}, P_{\mathrm{vap}})$ and dew $(v_{\mathrm{DP}}, P_{\mathrm{vap}})$ points also seem to have been reasonably accurate although the proposed EoS is not quite so dominant over the Peng–Robinson EoS in this regard. In the region just below the critical point the Peng–Robinson EoS appears to do a better job of predicting the dew volume v_{DP} and the vapour pressure P_{vap}. We attribute this to our insistence that the model should give a smooth description of the behaviour at all temperatures, at the expense of some amount of the model's flexibility, yielding an apparently unfavourable performance in this small region very close to the critical point. We also note the slight overestimation of the critical point, although with the intended application of this model to be the operation of CCS pipelines, this could ensure users err on the side of caution and stay away from the multi–phase region.

Nevertheless, we feel the model we proposed for the case of pure carbon dioxide is a significant step forward in modelling carbon dioxide behaviour in the CCS pipeline relevant region. We highlight that within the window of 260–335K and upto 200bar, our equation actually delivers its best performance in the region that really matters to CCS pipeline design and operation: the dense liquid and supercritical phases upto and including the liquid saturation line. The percentage errors we associate with our model were found, generally speaking, to be within our target range. At this stage of the research, we were happy to apply the pure CO_2 equation developed in this chapter to the case of binary mixtures.

Chapter 5

Calibration of the Binary Mixture Model

5.1 Generalising Fugacity Constraints to the Case of Mixtures

We begin this chapter by specifying a novel method which allows the fugacity of a substance when in mixture to be directly calculated from the fugacity when in the pure case. In Chapter 4, we established the pure fugacity constraint, which holds when a substance is on its own. The method we will show here allows us to enforce the fugacity requirements much more conveniently whilst fitting the binary mixture data, and furthermore, this works for any given form of equation of state and any mixing rules.

For this process we return briefly to working with dimensional units. Assuming we have an equation of state which explicitly gives the pressure P as a function of the molar volume v and some model parameters $\mathbf{a}(N_i) = (a_1(N_i), a_2(N_i), \ldots, a_m(N_i))$, where N_i is the number of moles of substance i, and m is the number of components in the mixture, we may consider P to be in the form $P = f(v, \mathbf{a}(N_i))$. Recalling Equation (2.3.1) from [72], given in a slightly different form in this thesis in Equation (1.19):

$$\log(\phi(V)) = \frac{1}{RT}\int_{\hat{V}=\infty}^{\hat{V}=V}\left(\frac{1}{\hat{V}} - \left(\frac{\partial P}{\partial N}\right)_{T,\hat{V},N_{j\neq i}}\right)\mathrm{d}\hat{V} - \log(Z), \tag{5.1}$$

we apply the chain rule to the derivative in the integrand:

$$\begin{aligned}
\frac{\partial P}{\partial N_i} &= \frac{\partial P}{\partial v}\frac{\partial v}{\partial N_i} + \sum_j^m \frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i} && (5.2)\\
&= -\frac{V}{N^2}\frac{\partial P}{\partial v} + \sum_j^m \frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i} && (5.3)\\
&= -\frac{V}{N^2}\frac{\partial P}{\partial (V/N)} + \sum_j^m \frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i} && (5.4)\\
&= -\frac{V}{N}\frac{\partial P}{\partial V} + \sum_j^m \frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i}, && (5.5)
\end{aligned}$$

where $a_j(N_i)$ denotes the jth parameter in $\mathbf{a}(N_i)$. Substituting this expression for $\frac{\partial P}{\partial N_i}$ back into (1.19) gives

$$\begin{aligned}
\log(\bar{\phi}_i(V)) &= \frac{1}{RT}\int_\infty^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N}\frac{\partial P}{\partial \hat{V}} - \sum_j^m \frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i}\right)\mathrm{d}\hat{V}\\
&\quad - \log(Z) && (5.6)\\
&= \left[\frac{1}{RT}\int_\infty^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N}\frac{\partial P}{\partial \hat{V}}\right)\mathrm{d}\hat{V} - \log(Z)\right]\\
&\quad - \left[\frac{1}{RT}\sum_j^m \int_\infty^V \left(\frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i}\right)\mathrm{d}\hat{V}\right]. && (5.7)
\end{aligned}$$

Considering the first square–bracketed term of Equation (5.7):

$$\begin{aligned}
\frac{1}{RT}\int_\infty^V \left(\frac{RT}{\hat{V}} + \frac{\hat{V}}{N}\frac{\partial P}{\partial \hat{V}}\right)\mathrm{d}\hat{V} - \log(Z) &= \frac{1}{RT}\int_\infty^V \left(\frac{RT}{\hat{V}}\right)\mathrm{d}\hat{V}\\
&\quad + \frac{1}{RT}\int_\infty^V \left(\frac{\hat{V}}{N}\frac{\partial P}{\partial \hat{V}}\right)\mathrm{d}\hat{V}, \quad (5.8)
\end{aligned}$$

and we perform integration by parts on the second integral on the right hand side of Equation (5.8) to get:

$$\begin{aligned}
\frac{1}{RT}\int_\infty^V \left(\frac{\hat{V}}{N}\frac{\partial P}{\partial \hat{V}}\right)\mathrm{d}\hat{V} &= \frac{1}{RT}\left[\frac{P\hat{V}}{N}\right]_\infty^V - \frac{1}{RT}\int_\infty^V \left(\frac{P(\hat{V})}{N}\right)\mathrm{d}\hat{V} && (5.9)\\
&= Z - 1 - \frac{1}{RT}\int_\infty^V \left(\frac{P(\hat{V})}{N}\right)\mathrm{d}\hat{V}, && (5.10)
\end{aligned}$$

and upon substituting this back into Equation (5.8) we get

$$\frac{1}{RT}\int_{\infty}^{V}\left(\frac{RT}{\hat{V}}+\frac{\hat{V}}{N}\frac{\partial P}{\partial \hat{V}}\right)\mathrm{d}\hat{V}-\log(Z) = \frac{1}{RT}\int_{\infty}^{V}\left(\frac{RT}{\hat{V}}-\frac{P}{N}\right)\mathrm{d}\hat{V} - \log(Z)+Z-1, \tag{5.11}$$

the right hand side of which we recognise from Equation (2.3.9) in [72] as being the same expression for the fugacity coefficient in pure form, but with mixture parameters accounted for.

It would be beneficial if we could relate the two expressions for the pure and mixture case fugacity, as this would allow us to work out one from the other. We now considering the second square–bracketed term of (5.7), and begin by making the following definition:

$$F := \log(\phi_i(V))+\log(Z)-Z+1 \tag{5.12}$$

$$= \frac{1}{RT}\int_{\infty}^{V}\left(\frac{RT}{\hat{V}}-\frac{P}{N}\right)\mathrm{d}\hat{V}, \tag{5.13}$$

where the second equality follows from Equation (2.8). We differentiate this expression for F with respect to a_j to get a term that can be used to simplify the second square–bracketed term in Equation (5.7):

$$N\frac{\partial F}{\partial a_j} = N\frac{\partial}{\partial a_j}\left(\frac{1}{RT}\int_{\infty}^{V}\left(\frac{RT}{\hat{V}}-\frac{P}{N}\right)\mathrm{d}\hat{V}\right) \tag{5.14}$$

$$= \frac{1}{RT}\int_{\infty}^{V}\left(-N\frac{\partial}{\partial a_j}\left(\frac{P}{N}\right)\mathrm{d}\hat{V}\right) \tag{5.15}$$

$$= \frac{1}{RT}\int_{\infty}^{V}\left(-\frac{\partial P}{\partial a_j}\right)\mathrm{d}\hat{V}, \tag{5.16}$$

and substituting this into the second square bracket from Equation (5.7) gives

$$-\frac{1}{RT}\int_{\infty}^{V}\left(-\frac{\partial P}{\partial a_j}\frac{\partial a_j}{\partial N_i}\right)\mathrm{d}\hat{V} = N\frac{\partial F}{\partial a_j}\frac{\partial a_j}{\partial N_i}. \tag{5.17}$$

Combining Equation (5.11) and (5.17) into Equation (5.7) gives

$$\log(\bar{\phi}_i(V)) = \log(\phi_i(V))+N\sum_{j}^{m}\frac{\partial F}{\partial a_j}\frac{\partial a_j}{\partial N_i}. \tag{5.18}$$

Supposing then that we have model parameters $\mathbf{a}$ (this vector notation meaning

(a, b, c, d, e, f, g)) dependent on the relative molar concentrations of each chemical component in the mixture, such that for each parameter

$$a = a(\mathbf{x}), \tag{5.19}$$

where $\mathbf{x} = (x_1, x_2, \ldots x_n)$ is the vector of concentrations of chemical species within a mixture of n components. Now, since

$$\sum_{i}^{n} x_i = 1, \tag{5.20}$$

then by allowing the number of moles of each component to vary independently of the number of moles of other substances such that it is possible to increase the number of moles of one component without having to decrease another, we have:

$$x_i = \frac{N_i}{N_i + N_{\text{rest}}}, \tag{5.21}$$

$$x_j = \frac{N_j}{N_i + N_{\text{rest}}}, \tag{5.22}$$

where N_{rest} is this sense is the total number of moles of other substances. We can again apply the chain rule, this time to the second term of Equation (5.18), to obtain

$$\frac{\partial a_j}{\partial N_i} = \frac{\partial a_j}{\partial x_i}\frac{\partial x_i}{\partial N_i} + \sum_{k \neq i} \frac{\partial a_j}{\partial x_k}\frac{\partial x_k}{\partial N_i}. \tag{5.23}$$

Noting that

$$\frac{\partial x_i}{\partial N_i} = \frac{\partial}{\partial N_i}\left(\frac{N_i}{N_i + N_{\text{rest}}}\right) \tag{5.24}$$

$$= \frac{1}{N_i + N_{\text{rest}}} - \frac{N_i}{(N_i + N_{\text{rest}})^2} \tag{5.25}$$

$$= \frac{1}{N} - \frac{N_i}{N^2}, \tag{5.26}$$

$$\tag{5.27}$$

in which case

$$N\frac{\partial x_i}{\partial N_i} = 1 - x_i, \tag{5.28}$$

and also that for $k \neq i$

$$\begin{aligned} \frac{\partial x_k}{\partial N_i} &= \frac{\partial}{\partial N_i}\left(\frac{N_k}{N_i + N_{\text{rest}}}\right) && (5.29)\\ &= -\frac{N_k}{(N_i + N_{\text{rest}})^2} && (5.30)\\ &= -\frac{N_k}{N^2}, && (5.31)\\ & && (5.32) \end{aligned}$$

whereby

$$N\frac{\partial x_k}{\partial N_i} = -x_k \tag{5.33}$$

for $k \neq i$. We can compile the effect of the mixing rules into Equation (5.18) to obtain a practical relation between the pure and mixture fugacity for chemical component i:

$$\log(\bar{\phi}_i(v)) = \log(\phi_i(v)) + \sum_j^m \frac{\partial F}{\partial a_j}\left(\frac{\partial a_j}{\partial x_i} - \sum_k^n x_k \frac{\partial a_j}{\partial x_k}\right). \tag{5.34}$$

We highlight Equation (5.34) as allowing us to conveniently evaluate the mixture fugacity constraint for component i, denoted $\log(\bar{\phi}_i(v))$, directly from the its pure fugacity constraint, denoted $\log(\phi_i(v))$, and the mixing rules $a_1(x_1, \ldots, x_n)$, …, $a_m(x_1, \ldots, x_n)$.

5.2 Mixing Rules

As a chemical impurity is introduced to the mixture, we wish for our model to be able to predict the changes in pressure and phase behaviour that will be brought about as a result. In order to do this, we allow the model parameters to not merely vary with changing temperature, but also with the composition of the mixture. In this way, the effect of impurities can be included in the modelling of the CCS pipeline transport conditions.

Thus, for each parameter of the model we needed to propose a mixing rule. Returning now to dimensionless units, and taking inspiration from the mixing rules offered in the PREoS [34], we opted to impose the quadratic binary mixing rule for each of the model parameters in Equation (3.21) for increased flexibility. In the case of the

binary mixture for carbon dioxide and nitrogen for example, these are:

$$
\begin{aligned}
a(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 a_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} a_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 a_{\mathrm{N_2}}(T) \quad (5.35)\\
b(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 b_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} b_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 b_{\mathrm{N_2}}(T) \quad (5.36)\\
c(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 c_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} c_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 c_{\mathrm{N_2}}(T) \quad (5.37)\\
d(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 d_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} d_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 d_{\mathrm{N_2}}(T) \quad (5.38)\\
e(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 e_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} e_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 e_{\mathrm{N_2}}(T) \quad (5.39)\\
f(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 f_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} f_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 f_{\mathrm{N_2}}(T) \quad (5.40)\\
g(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) &= x_{\mathrm{CO_2}}^2 g_{\mathrm{CO_2}}(T) + x_{\mathrm{CO_2}} x_{\mathrm{N_2}} g_{\mathrm{CO_2,N_2}}(T) + x_{\mathrm{N_2}}^2 g_{\mathrm{N_2}}(T), \quad (5.41)
\end{aligned}
$$

where $a_{\mathrm{CO_2}}(T)$, $b_{\mathrm{CO_2}}(T)$, ... are as defined in Chapter 4 for the pure carbon dioxide equation, $a_{\mathrm{N_2}}(T)$, $b_{\mathrm{N_2}}(T)$, ... are the analogous quantities for nitrogen which we need to specify, and $a_{\mathrm{CO_2,N_2}}(T)$,$b_{\mathrm{CO_2,N_2}}(T)$, ... are the binary interaction parameters, which also need to be determined.

We note at this stage that since in a binary system

$$x_{\mathrm{N_2}} = 1 - x_{\mathrm{CO_2}}, \quad (5.42)$$

the number of dependent variables for the mixing rules can be reduced to two. The above equations can be defined analogously for the other binary mixtures we are considering.

5.3 Carbon Dioxide–Nitrogen Binary Mixture

5.3.1 Data Availability

We begin this section by noting the literature data that was available for us to fit to for the CO_2–N_2 mixture. As specified in Chapter 2, we would require isothermal VLE data including coexisting vapour and liquid points to be given at the same temperature as homogeneous phase density data. A tabulated summary of the relevant available data is given in Table 5.1, ordered by temperature.

We can see from Table 5.1 that the literature data contained just four temperature points where complete VLE data existed: at 273.15K [53, 54], 288.15K [53], 301.3K [91] and 303.3K [91], however, of these, we had to neglect the data at 303.3K on the grounds that it did not appear to give a true description of behaviour. We can also see from Table 5.1 that there were very few temperatures at which both VLE,

whether with volumes or not, and homogeneous density data existed. Without the estimation techniques described in Chapter 2, this would have left us with just two temperature points to fit the parameters for this particular binary system; 273.15K and 288.15K. With these methods, we were able to build the model around more temperature points.

Temperature (K)	Homogeneous Density Data Sources	VLE Data Sources
260	[82], [75], [88]	
265	[86], [83]	
270	[75], [88]	[95]†, [96]†, [97]†, [98]†
273.15	[53], [82], [99]	[53], [100]†, [54], [101]†, [102]†, [84]†, [103]†
273.2		[104]†
275	[86], [83], [75], [88], [105]	
280	[75], [88]	
285	[86], [77], [83], [75], [88]	
288.15	[53]	[53], [100]†
288.3		[106]†
288.706	[82]	
290	[75], [88]	
293.2	[107]	
293.3		[106]†
295	[75], [88]	
298.15	[108]	[100]†
298.2		[104]†
300	[82], [85], [86], [77], [83], [75], [88], [78], [105]	
301.3		[91]
303.22	[109]	
303.3		[91]
† means the VLE data in this source did not contain volumes		

Table 5.1: A summary of available data by spurce for carbon dioxide–nitrogen mixtures

5.3.2 Fitting the Carbon Dioxide–Nitrogen Binary Model Parameters

We proceeded first by determining the pure nitrogen parameters a_{N_2} to g_{N_2} at the available temperature points by the same sequence of optimisation techniques as used in the pure carbon dioxide case. Specifically, we minimised an error function which was exactly analogous to that in Equation (4.1), which in the case of a binary mixture, was

$$\begin{aligned} E(a,b,c,d,e,f,g,h) &= W\sum_{i=1}^{n}\left(\frac{P(v_{\mathrm{DATA}}^{(i)},T,x_{\mathrm{DATA}}^{(i)})-P_{\mathrm{DATA}}^{(i)}}{P_{\mathrm{DATA}}^{(i)}}\right)^2 \\ &\quad +(1-W)\sum_{j=1}^{m}\Bigg((\log\bar{\phi}_{\mathrm{CO}_2}(v_{\mathrm{DP}}^{(j)})-\log\bar{\phi}_{\mathrm{CO}_2}(v_{\mathrm{BP}}^{(j)}))^2 \\ &\quad +(\log\bar{\phi}_{\mathrm{N}_2}(v_{\mathrm{DP}}^{(j)})-\log\bar{\phi}_{\mathrm{N}_2}(v_{\mathrm{BP}}^{(j)}))^2 \\ &\quad +(P(v_{\mathrm{DP}}^{(j)},T,x^{(j)})-P_{\mathrm{vap}}^{(j)})^2 \\ &\quad +(P(v_{\mathrm{BP}}^{(j)},T,x^{(j)})-P_{\mathrm{vap}}^{(j)})^2\Bigg), \end{aligned} \tag{5.43}$$

where the first term after the equals sign is for fitting the homogeneous phase den-

sity and all subsequent terms are for fitting VLE at the phase boundary. In this equation n is the number of homogeneous density points at this temperature and m is the number of VLE coexistence points. Just as in the pure case, we minimised this initially by using simulated annealing at the first temperature point, then worked down the temperature values, at each subsequent one using local root finding.

In order to find the pure nitrogen parameter values, we temporarily introduced a linear mixing rule for each of the seven parameters, of the form

$$a_{\mathrm{N_2}}(T, x_{\mathrm{CO_2}}, x_{\mathrm{N_2}}) = x_{\mathrm{CO_2}} a_{\mathrm{CO_2}}(T) + x_{\mathrm{N_2}} a_{\mathrm{N_2}}(T), \tag{5.44}$$

and similarly for parameters $b_{\mathrm{N_2}}$ through $g_{\mathrm{N_2}}$. We did this because we found simulated annealing to struggle with more than seven parameters at any one time. In particular, we felt asking it to optimise an error function which was dependent on fourteen parameters would have been too demanding, and would have diminished the accuracy of the results it gave. We highlight that we were able to temporarily introduce this linear mixing rule as both it and the quadratic mixing rule as specified in Equation (5.35) give the same values when evaluated at either extreme of compositions.

Setting $W = 0.99$ to focus on fitting the homogeneous density data to begin with, we were able to generate values for each of the seven pure nitrogen parameters at each of the temperature points in this way. Having done this, we then reintroduced the quadratic mixing rules as given in Equation (5.35), in which both the pure carbon dioxide parameters $a_{\mathrm{CO_2}}$ and the pure nitrogen parameters $a_{\mathrm{N_2}}$ were now known. Following exactly the same procedure as having temporarily introduced a linear mixing rule, and setting $W = 0.05$ to allow the binary interaction parameters to focus on fitting the VLE behaviour, we repeated the process for the seven Binary Interaction Parameters (BIP) at each of the temperature points.

For the pure nitrogen parameters and the binary interaction parameters, the values we found by following this method are summarised in Table 5.2:

5.3.3 Preliminary Indications of Performance

After having found the fourteen parameters at each temperature point, we evaluated the performance of the proposed model to check the fitting that had been achieved through the optimisation of the error function (5.43) rendered a suitable representation of the data that had been used to calibrate it in each case.

T(K)	a_{N_2}	b_{N_2}	c_{N_2}	d_{N_2}	e_{N_2}	f_{N_2}	g_{N_2}
301.3	-0.067690	-0.069072	0.051949	0.394802	0.213906	0.707765	-0.395181
298.15	-0.112859	-0.778754	-1.142430	0.363730	-0.088425	0.544037	-0.269156
293.3	0.043030	-0.306196	-0.125938	-0.225702	-0.112868	0.996458	-0.659658
288.15	0.021057	-0.183572	0.028688	-0.175184	-0.126123	0.584742	-0.321931
273.15	0.053949	-0.146277	0.520106	-0.192693	-0.117818	0.631785	-0.410574
270	0.009311	-0.241595	0.451289	-0.151992	-0.126193	0.454463	-0.243880

T(K)	a_{CO_2,N_2}	b_{CO_2,N_2}	c_{CO_2,N_2}	d_{CO_2,N_2}	e_{CO_2,N_2}	f_{CO_2,N_2}	g_{CO_2,N_2}
301.3	2.311730	-1.546690	-1.291800	-3.533050	-0.560407	1.616910	-0.987250
298.15	0.422929	-0.048641	0.067566	-1.071050	-0.655508	0.409527	-0.071220
293.3	1.392655	-0.491103	0.706931	-1.985994	1.171984	-0.036535	0.177126
288.15	0.128213	0.410874	0.907126	0.527336	-2.189245	0.330155	-0.040261
273.15	0.112001	0.639749	0.926503	0.296718	-1.149070	0.450452	-0.150223
270	2.872352	2.739344	3.937239	-1.362795	-1.182876	-0.290171	-0.124155

Table 5.2: Fitted parameter values for the carbon dioxide–nitrogen binary system

We did this by checking the percentage errors of the values suggested by our model for both the homogeneous density and VLE. A summary is in Table 5.3.

Temperature (K)	Homogeneous Density		v_{BP} †		v_{DP} †		x_{N_2} †		y_{N_2} †	
	Maximum	Average	Maximum	Average	Maximum	Average	Maximum	Average	Maximum	Average
301.3	34.23	4.45	15.34	11.84	31.35	23.92	1.40	1.05	3.09	1.78
298.15	19.77	6.70	17.14	17.14	94.13	94.13	3.84	3.84	14.17	14.17
293.3	18.80	6.21	7.52	3.31	33.00	11.96	2.50	1.13	8.19	2.41
288.15	9.56	2.97	21.75	10.61	32.36	14.12	5.92	4.02	21.17	8.15
273.15	9.20	1.79	13.26	5.78	40.64	19.64	12.74	5.37	36.98	21.70
270	135.14	43.56	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
† where convergence to a meaningful solution had been possible										

Table 5.3: Preliminary testing of predictions made by our model for the carbon dioxide–nitrogen binary system

We note at this stage that there was a particularly good fit of all the data types at 293.3K, 288.15K, and 273.15K. At these temperatures, where a relevant fitting had been achieved, a good behaviour was allowed by our proposed model and fitting technique. With the exception of the temperature points at which a poor fit had been achieved (301.3K, 298.15K, 270K), the average percentage errors for all quantities fell close to or under our target of 5%. We highlight in particular a very good fit to the homogeneous density data at the other three temperature points (293.3K, 288.15K, 273.15K). Unsurprisingly, when a poor fit had been found, the errors were quite large, and at 270K where a very poor fit had been found, convergence of the numerical search algorithms in finding the VLE had not been possible at all. With performance at 293.3K, 288.15K, and 273.15K having been demonstrated as being very reasonable, we fit the temperature dependence of the fourteen mixture parameters to the values taken at these points, discarding the parameter values at the other temperature points.

5.3.4 Variation of Model Parameters with Temperature

For each parameter we thus had only three temperature values at which reliable behaviour had been demonstrated. Analysing the values of the parameters at these three temperatures, we decided to fit a quadratic dependence, such as

$$a_{\mathrm{N}_2}(T) = \alpha_1 T^2 + \alpha_2 T + \alpha_3, \tag{5.45}$$

where α_1, α_2, and α_3 would allow us to fit the values given in Table 5.2, and analogously for the other thirteen parameters.

In order to find the numerical values for α_1, α_2, and α_3, we did this for each of the parameters by minimising a similar error function to that in Equation (5.45), and in doing so, the temperature dependences of the carbon dioxide–nitrogen parameters were found.

These were:

$$\begin{aligned}
a_{\mathrm{N}_2}(T) &= 25.8842 - 55.39T + 29.6505T^2 && (5.46)\\
b_{\mathrm{N}_2}(T) &= -82.7613 + 179.897T - 97.8833T^2 && (5.47)\\
c_{\mathrm{N}_2}(T) &= 20.1581 - 33.1472T + 12.5615T^2 && (5.48)\\
d_{\mathrm{N}_2}(T) &= -43.3875 + 93.347T - 50.3857T^2 && (5.49)\\
e_{\mathrm{N}_2}(T) &= 12.249 - 26.6624T + 14.3552T^2 && (5.50)\\
f_{\mathrm{N}_2}(T) &= 326.012 - 704.801T + 381.364T^2 && (5.51)\\
g_{\mathrm{N}_2}(T) &= -281.263 + 607.427T - 328.147T^2 && (5.52)\\
a_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= 954.634 - 2070.54T + 1122.05T^2 && (5.53)\\
b_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= -619.712 + 1349.86T - 733.905T^2 && (5.54)\\
c_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= -145.516 + 317.986T - 172.507T^2 && (5.55)\\
d_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= -1970.24 + 4269.39T - 2310.74T^2 && (5.56)\\
e_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= 2838.05 - 6137.84T + 3314.23T^2 && (5.57)\\
f_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= -244.155 + 532.828T - 290.023T^2 && (5.58)\\
g_{\mathrm{CO}_2,\mathrm{N}_2}(T) &= 134.094 - 293.271T + 160.111T^2 && (5.59)
\end{aligned}$$

We can see from the following two (randomly chosen) examples how these temperature dependences resembled the parameter values at the chosen three temperature points.

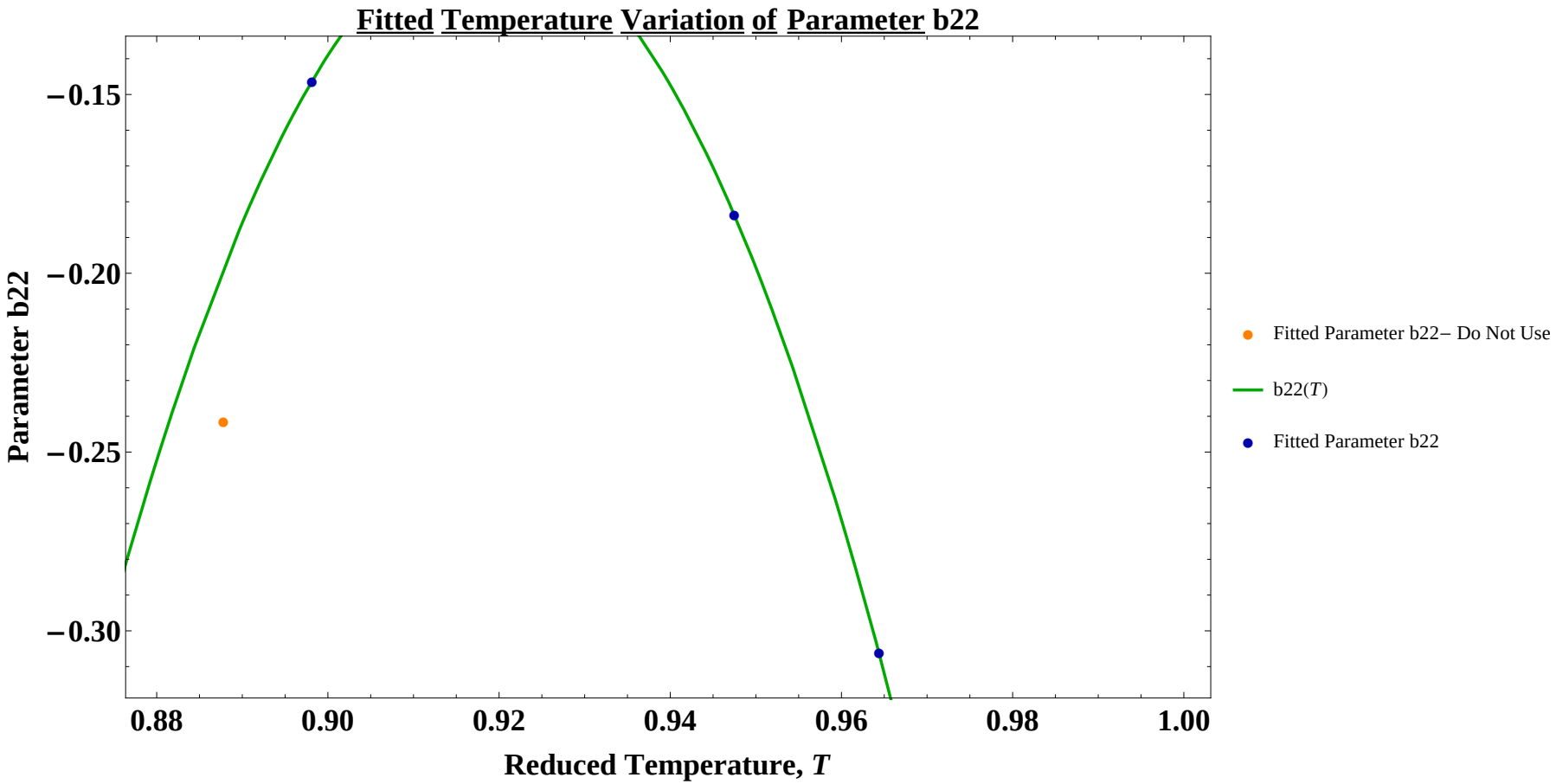

Figure 5.1: Temperature dependence for the pure nitrogen parameter b_{N_2} (denoted in the graph by b_{22})

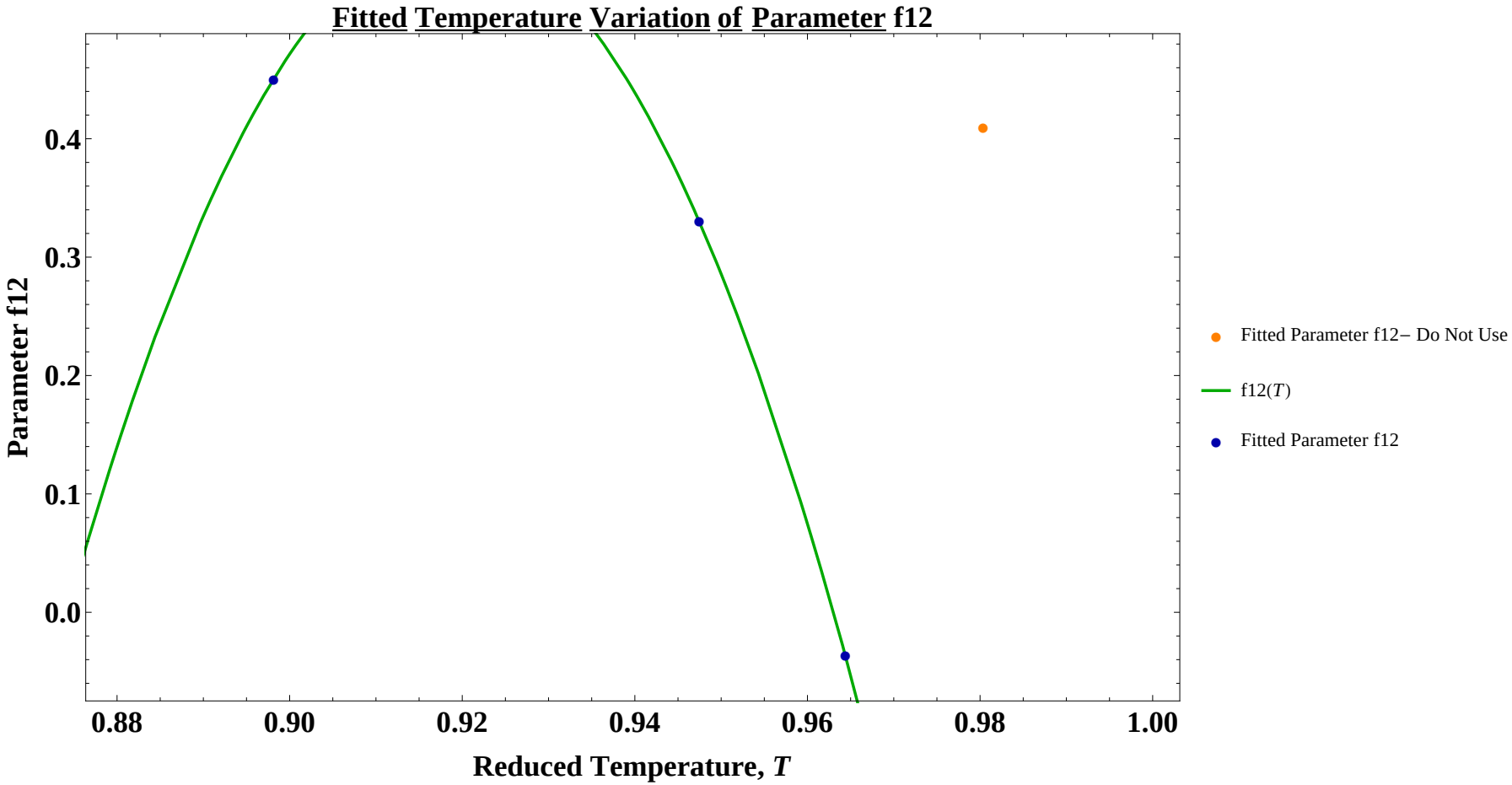

Figure 5.2: Temperature dependence for the binary interaction parameter d_{CO_2,N_2} (denoted in the graph by f_{12})

5.3.5 Performance of the Full Model for Binary Mixtures of Carbon Dioxide and Nitrogen

With the model thus fully defined for the binary system involving carbon dioxide and nitrogen, we were able to assess its performance. We did this in the first instance by comparing the completed model to the same data which had been used to generate the fitted parameters. We then checked the performance of the model at temperatures where no data existed, so as to assess the behaviour as users of the model might experience it. We note that since for the nitrogen model we fit the model parameters between 273.15K and 293.3K, we would not have expected any meaningful descriptions to be given outside this range of temperatures.

We began by comparing the behaviour of the completed model to the homogeneous volume–pressure data at 273.15K.

Nitrogen Composition (%)	Maximum Error (%)	Average Error (%)
2.6 (liquid phase)	9.20	2.75
5.0 (liquid phase)	4.34	1.75
6.7 (liquid phase)	0.87	0.31
5.8 (vapour phase)	1.76	0.39
8.8 (vapour phase)	2.49	0.59
50.8(supercritical phase)	4.83	2.30
100	3.73	1.77
ALL	9.20	1.79

Table 5.4: Pressure performance of model at 273.15

We also compared the behaviour of our model to the VLE data at the same temperature.

Quantity	Maximum Error (%)	Average Error (%)
v_{BP} †	0.99	0.53
v_{DP} †	5.72	3.21
$x_{\mathrm{N_2}}$ †	0.96	0.48
$y_{\mathrm{N_2}}$ †	6.94	3.64
ALL	6.94	1.96
† where convergence to a meaningful solution had been possible		

Table 5.5: VLE performance of model at 273.15K

We noted the excellent performance of the model at this temperature, as compared with the literature data and volume estimations that were used to calibrate the model before smoothing of the parameters with temperature. In particular, nearly all the predictions met our target accuracy. We also highlight that the best performance of our model occurred at the liquid saturation curve (bubble curve), which we understand to be the more relevant consideration for CCS pipelines. Overall, this represented an excellent performance of our model at this temperature. Additionally, we were able to verify in Figure 5.3 that the behaviour of our model was consistent with the density data.

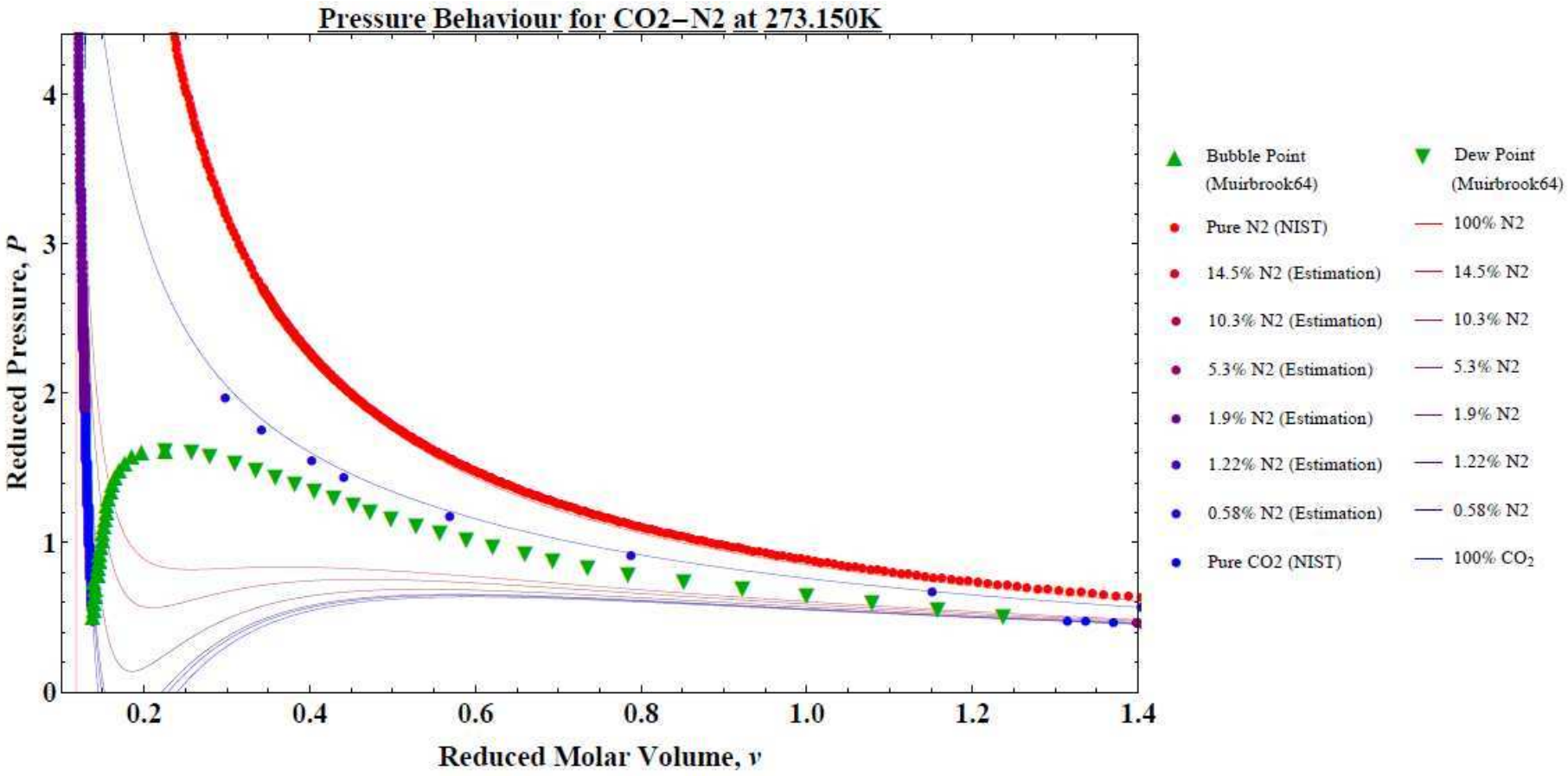

Figure 5.3: Pressure performance of model at 273.15K for carbon dioxide–nitrogen. The thin lines are the density predictions of our model with the more red lines indicating a higher concentration of nitrogen

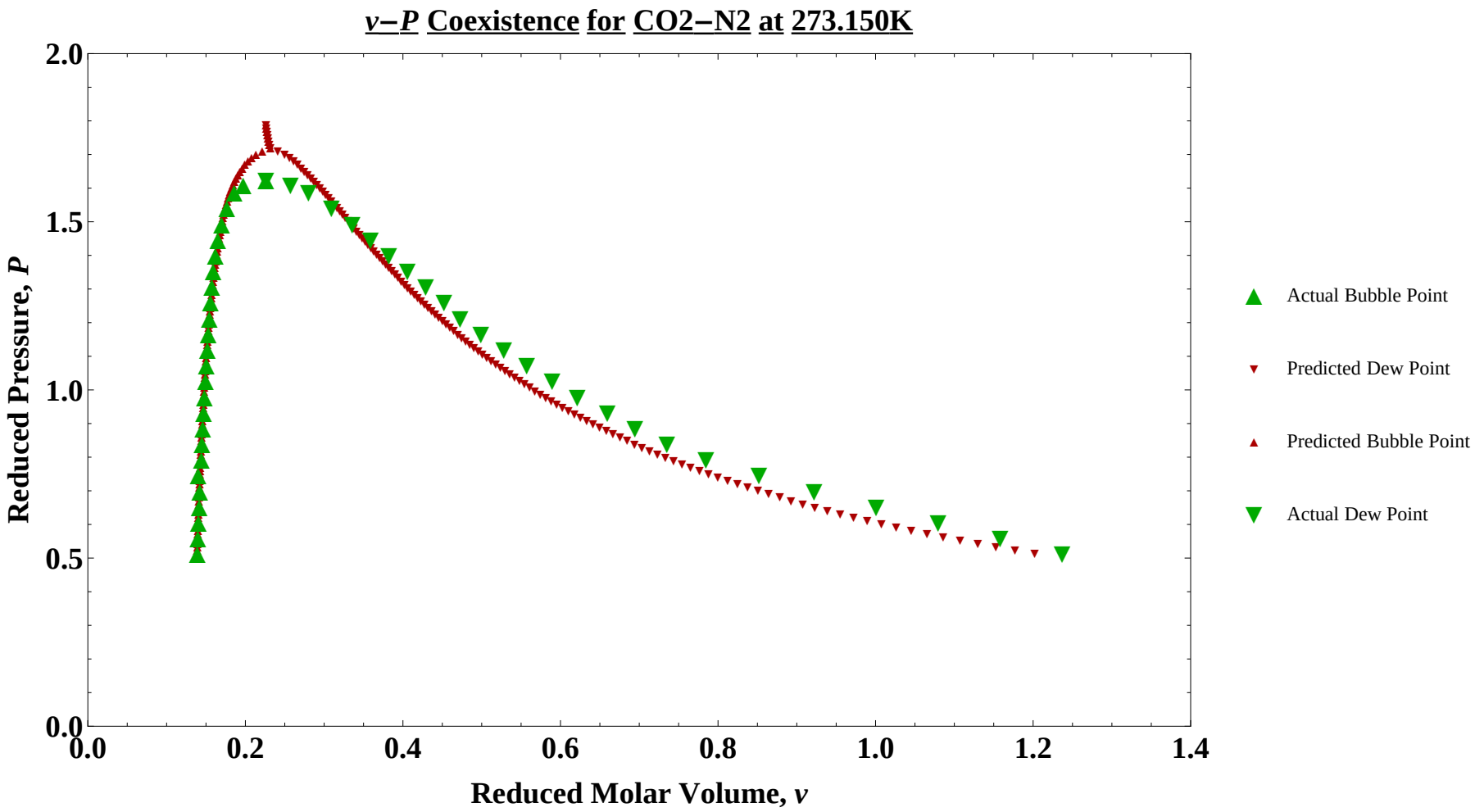

Figure 5.4: VLE coexisting volume performance of model at 273.15K for carbon dioxide–nitrogen. Note that in the interests of not over crowding this plot we do not include equivalent plots for the GERG on the basis that it is not user–friendly enough to be compared here, and we do not include the PREos on the basis that its errors in the mixture case are high

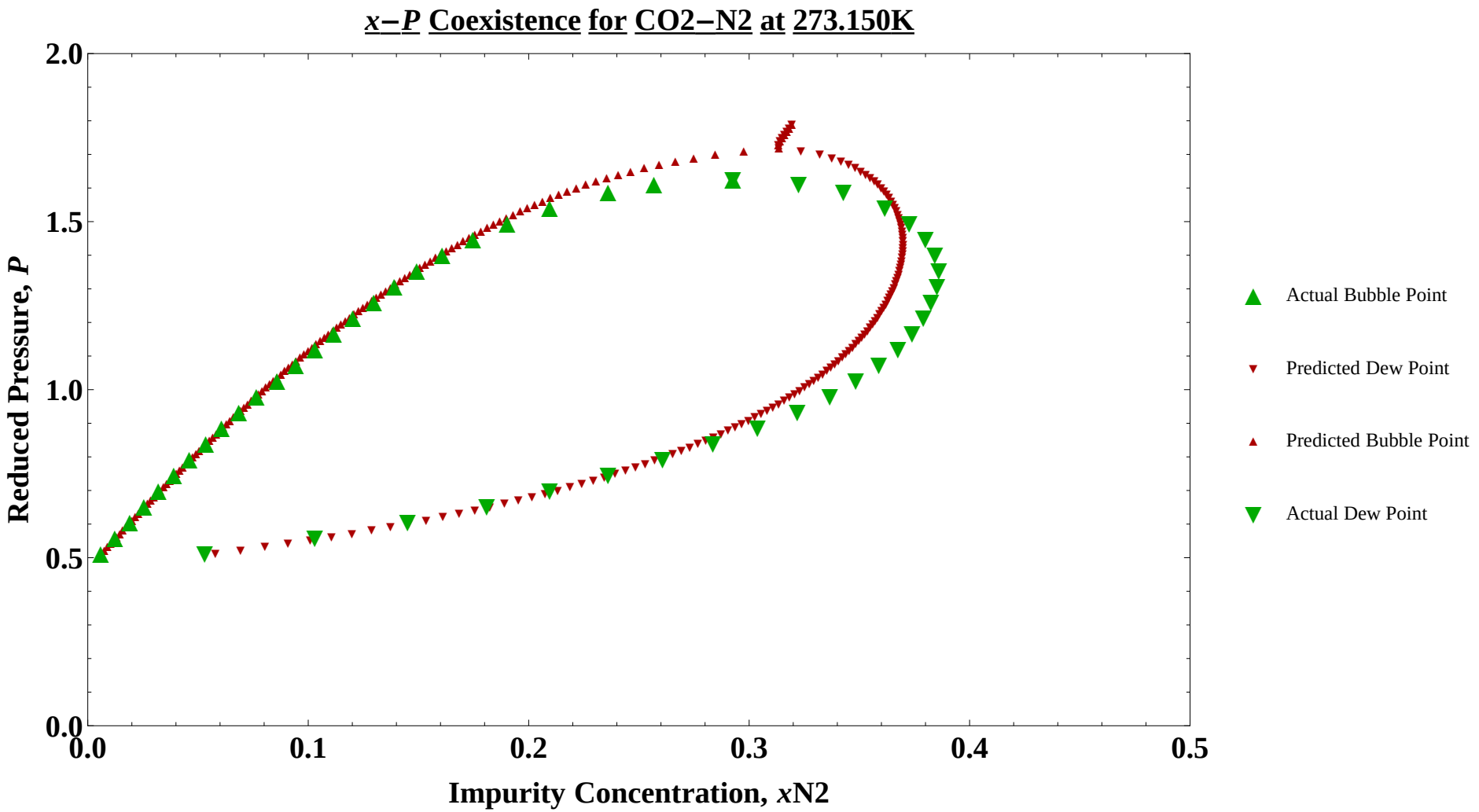

Figure 5.5: VLE coexisting mole fraction performance of model at 273.15K for carbon dioxide–nitrogen. The small "tail" at the top of the envelope is where the numerical search algorithms did not find a solution in the homogeneous region, as expected

We then compared the behaviour of our model to the homogeneous volume–pressure and composition–pressure data at 288.15K.

Nitrogen Composition (%)	Maximum Error (%)	Average Error (%)
3.59 (liquid phase)	4.63	2.07
5.5 (liquid phase)	9.55	2.58
6.01 (liquid phase)	8.53	5.84
13.1 (vapour phase)	2.67	0.58
18.8 (vapour phase)	5.64	1.05
29.8 (supercritical phase)	8.14	1.99
100	3.96	2.03
ALL	9.55	2.97

Table 5.6: Pressure performance of model at 288.15K

We also compared the behaviour of our model to the VLE data at 288.15K:

Quantity	Maximum Error (%)	Average Error (%)
v_{BP} †	1.64	1.22
v_{DP} †	22.21	11.44
x_{N_2} †	2.24	1.14
y_{N_2} †	8.04	4.12
ALL	22.21	4.48
† where convergence to a meaningful solution had been possible		

Table 5.7: VLE performance of model at 288.15K

The performance of the model at higher temperature was similarly excellent to that at 273.15K. We highlight the excellent agreement with the vapour phase pressure data and again that there was a particularly good performance of our model at the liquid saturation line. In visually checking the behaviour of the model in Figures 5.6 to 5.8, we see that at this point of the temperature range, the carbon dioxide–nitrogen model behaves very well. In Figures 5.9 to 5.11 we also include plots demonstrating the behaviour of our model at 293.3K, showing that it also exhibits very strong predictions there as well. Furthermore, we include in Figures 5.12 and 5.13 the VLE behaviour of the model at 298.15K, even though this was outside the range of fitting. These highlight the robustness of the model in predicting physical properties throughout a considerable temperature range. Figure 5.14 compares the VLE behaviour of the model at a range of temperatures.

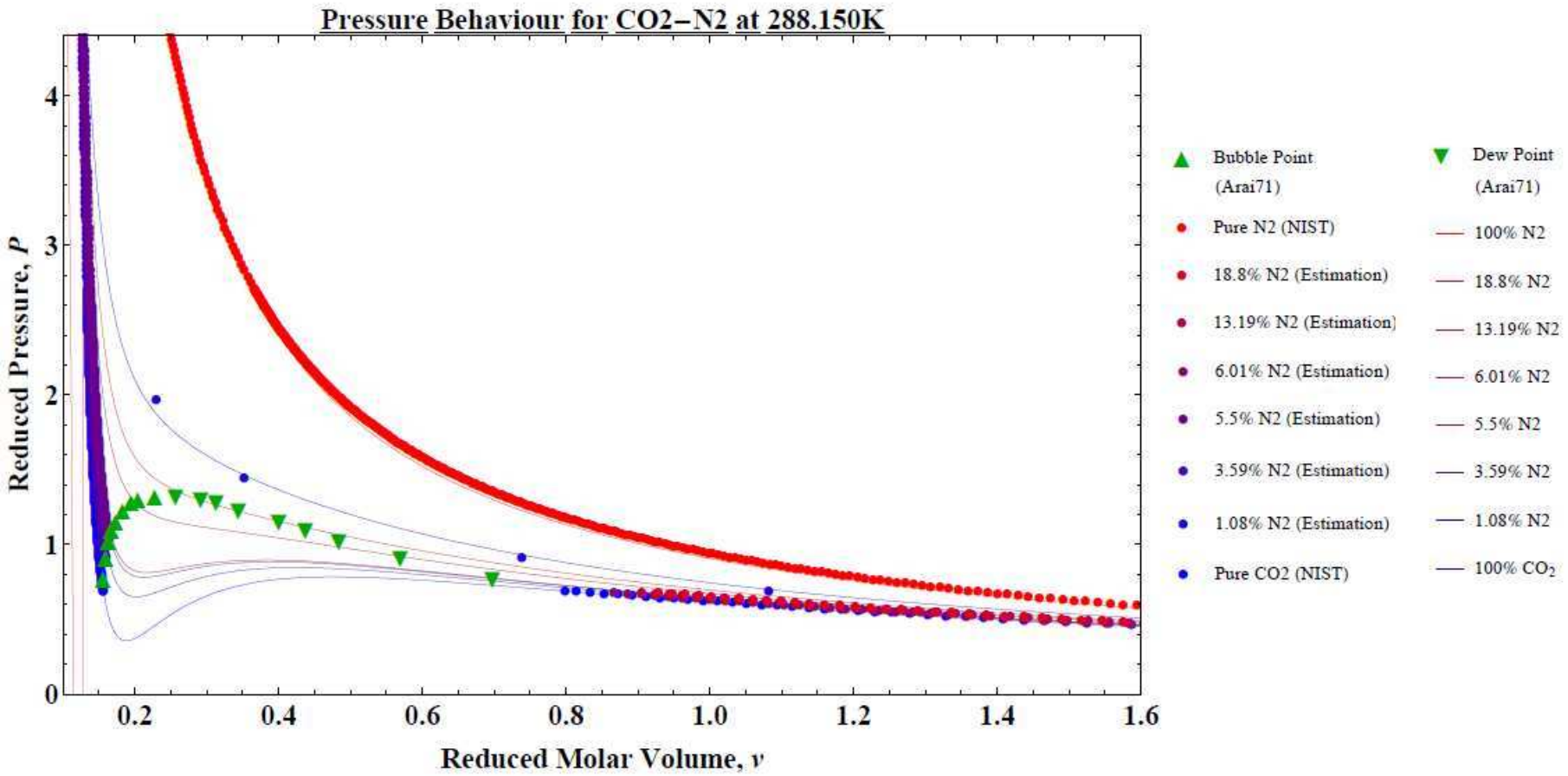

Figure 5.6: Pressure performance of model at 288.15K for carbon dioxide–nitrogen

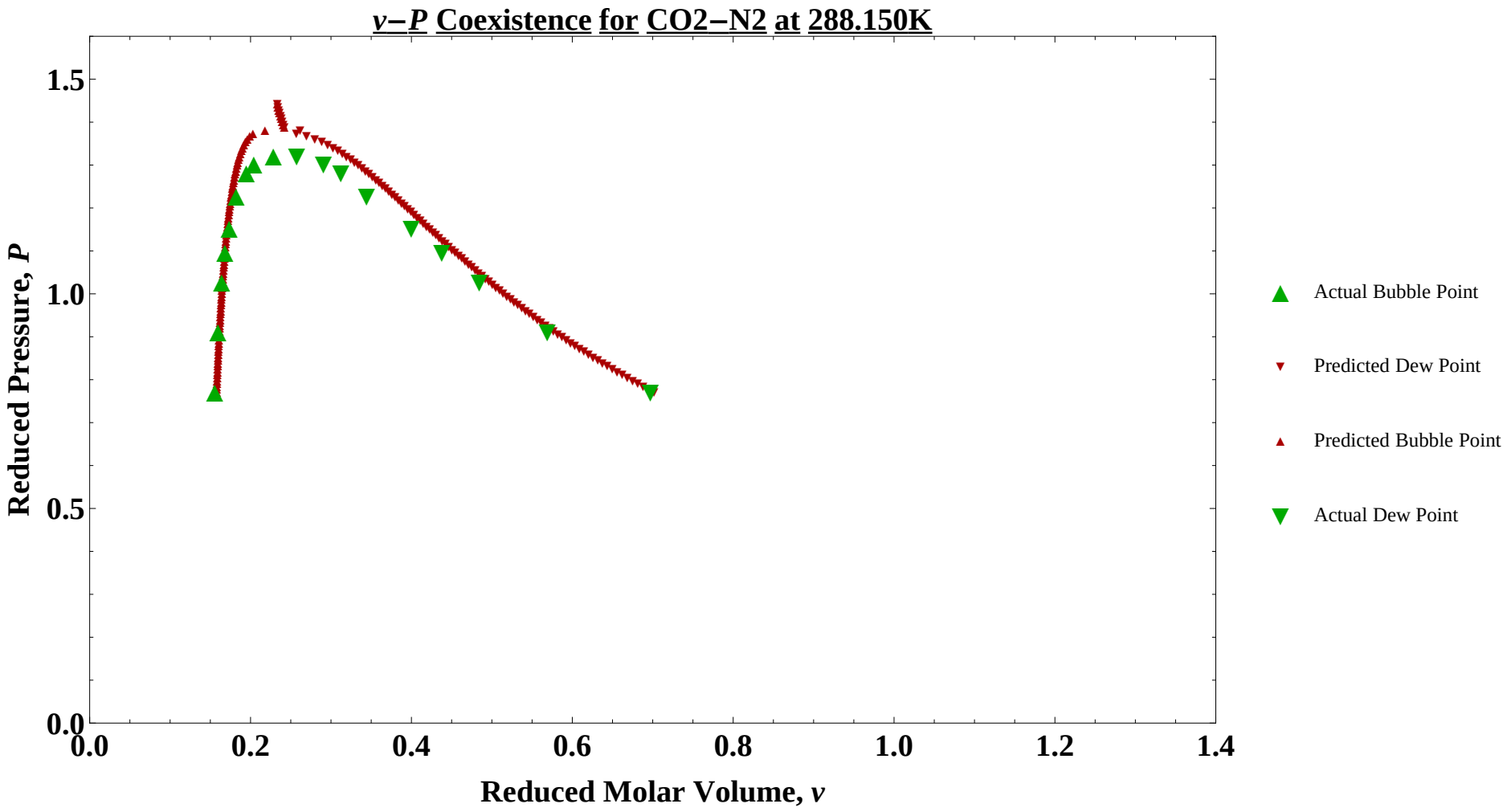

Figure 5.7: VLE coexisting volume performance of model at 288.15K for carbon dioxide–nitrogen

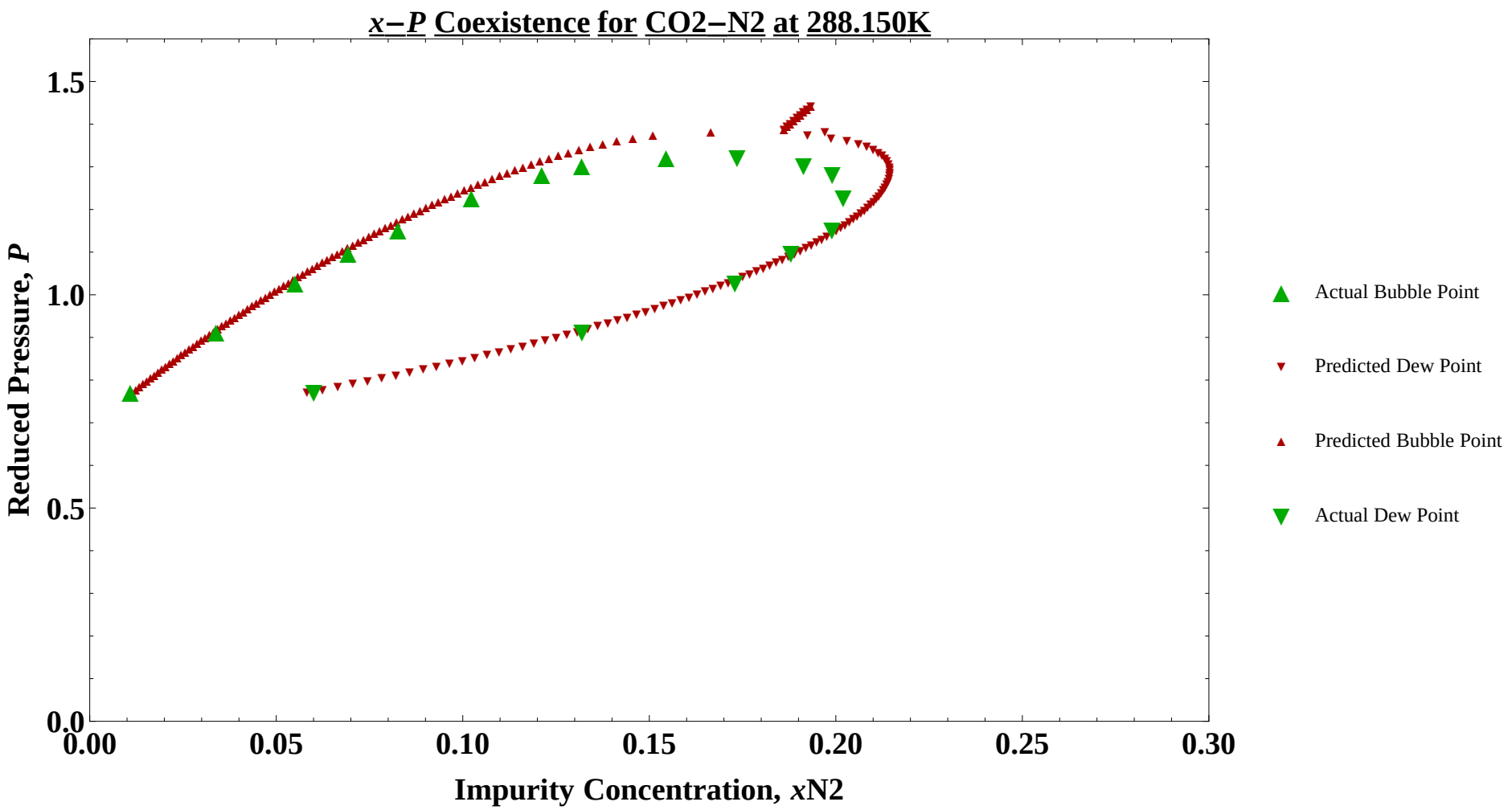

Figure 5.8: VLE coexisting mole fraction performance of model at 288.15K for carbon dioxide–nitrogen

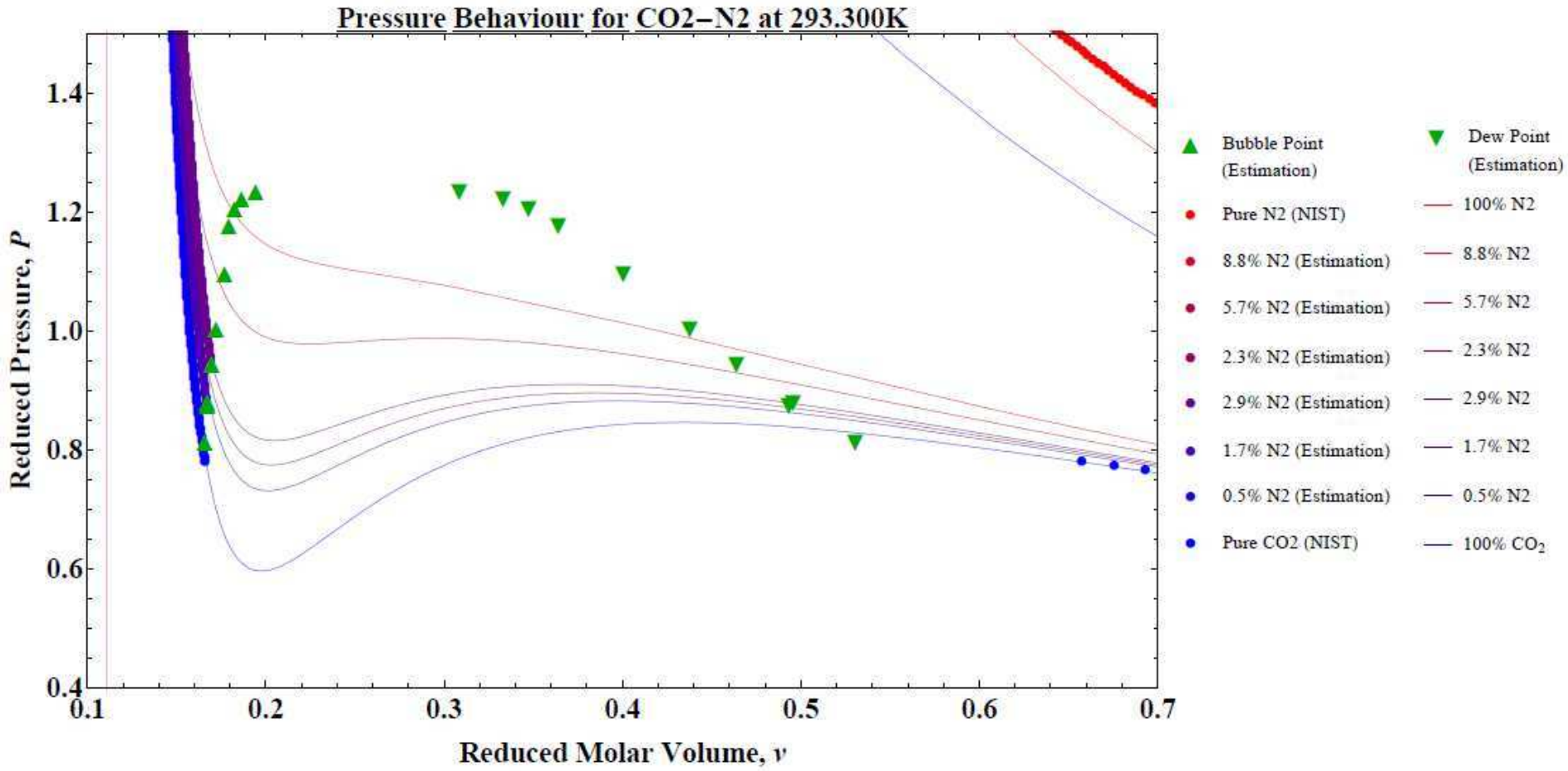

Figure 5.9: Pressure performance of model at 293.3K for carbon dioxide–nitrogen

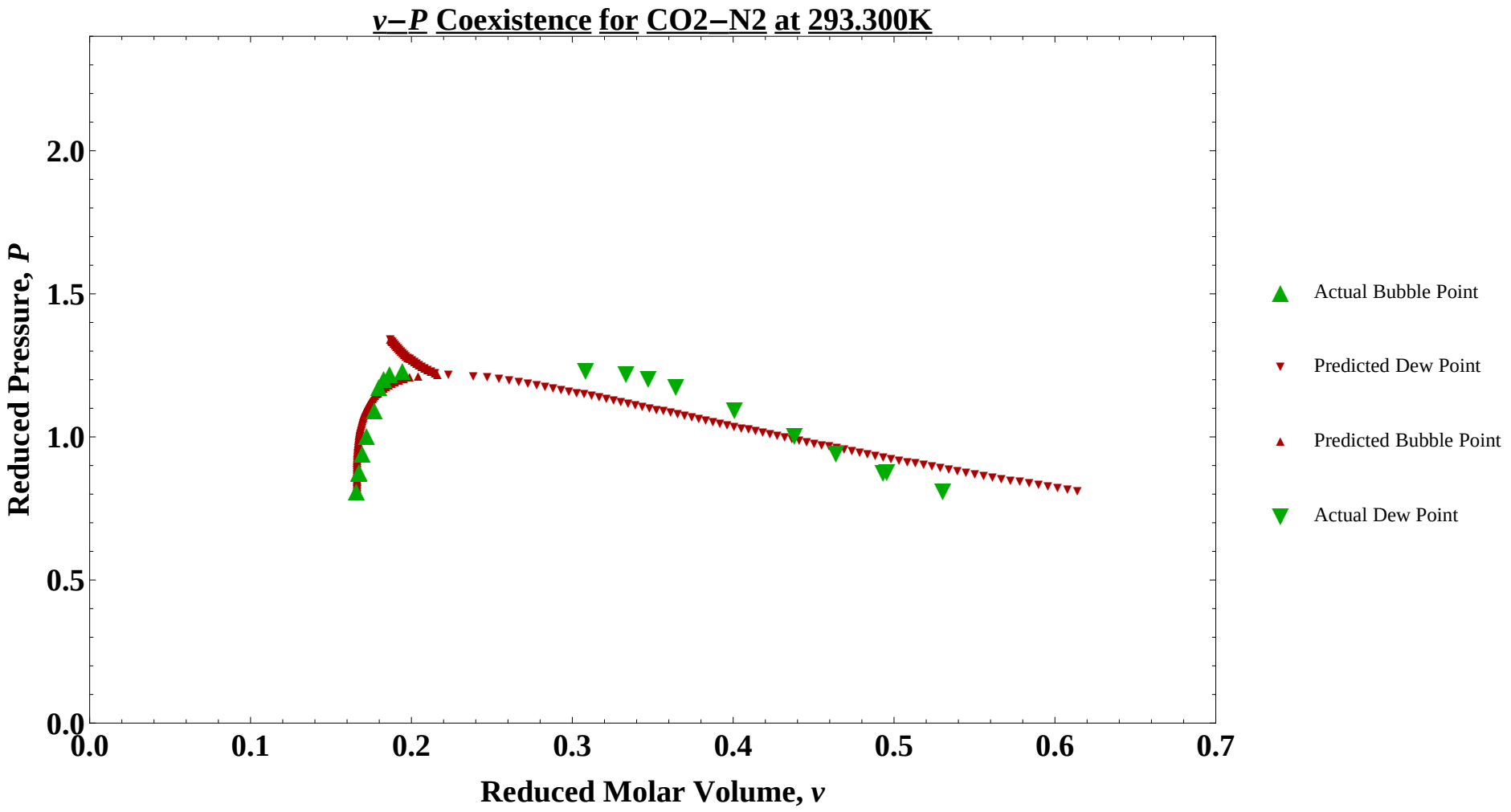

Figure 5.10: VLE coexisting volume performance of model at 293.3K for carbon dioxide–nitrogen

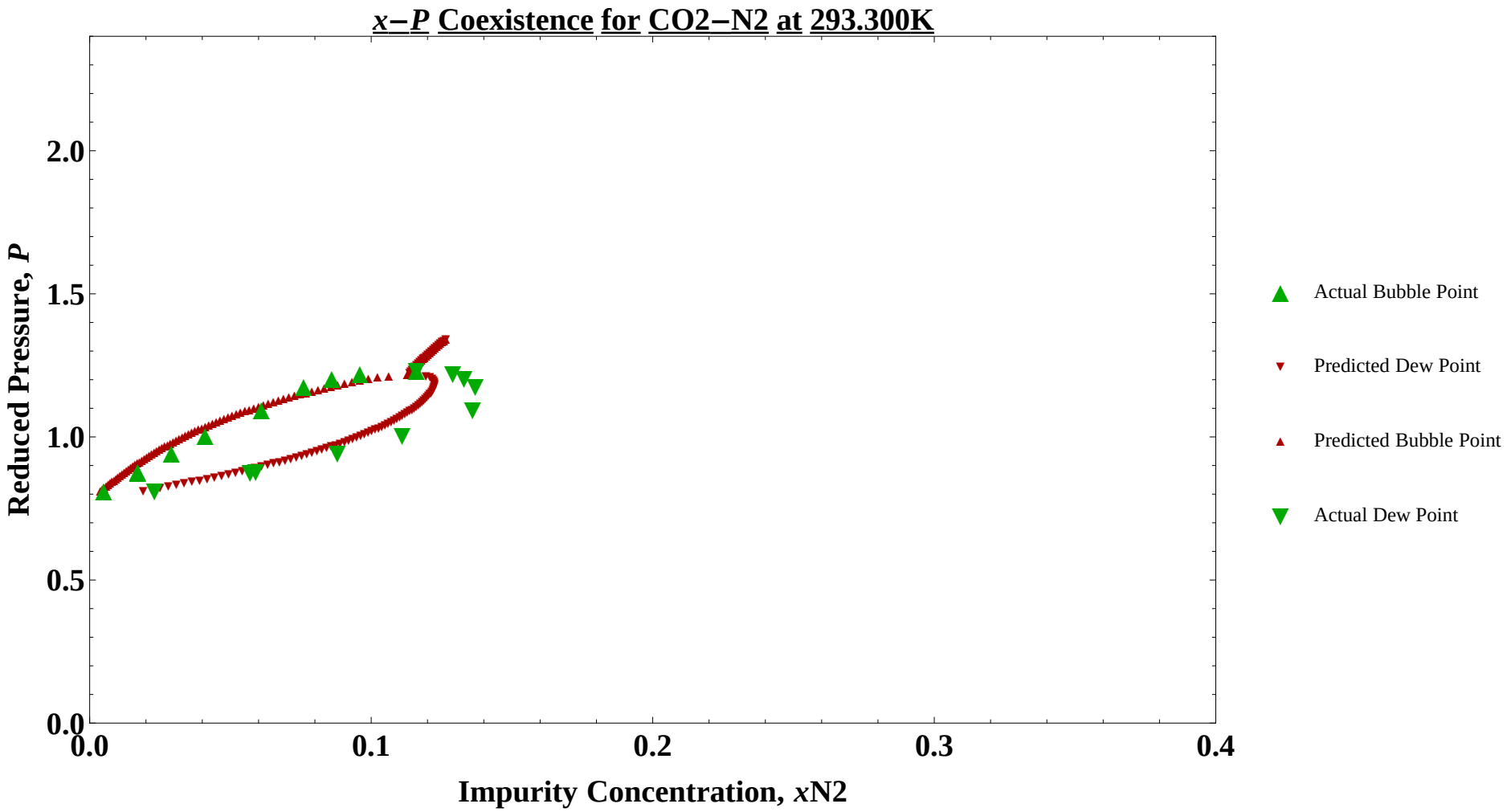

Figure 5.11: VLE coexisting mole fraction performance of model at 293.3K for carbon dioxide–nitrogen

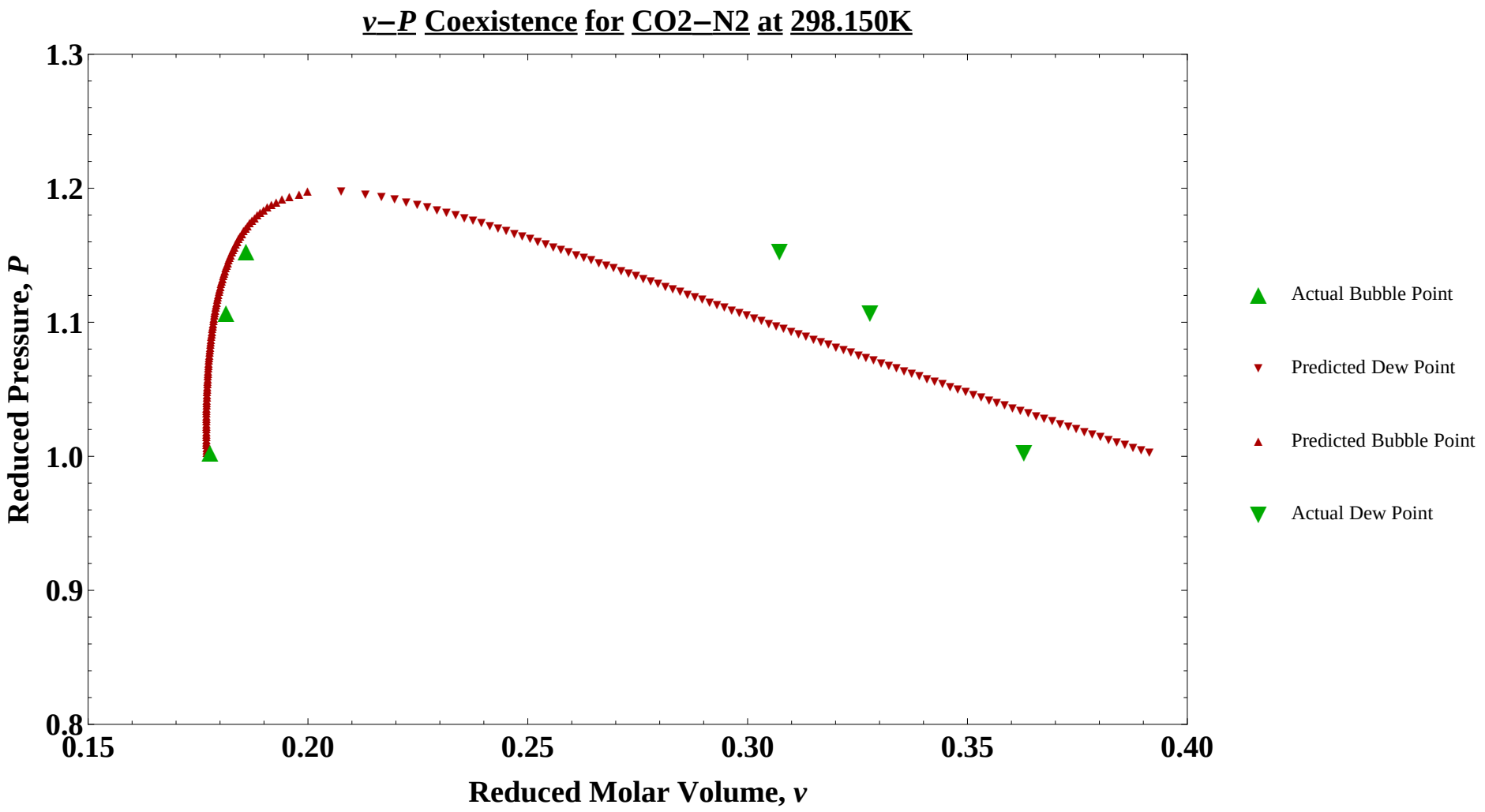

Figure 5.12: VLE coexisting volume performance of model at 298.15K for carbon dioxide–nitrogen

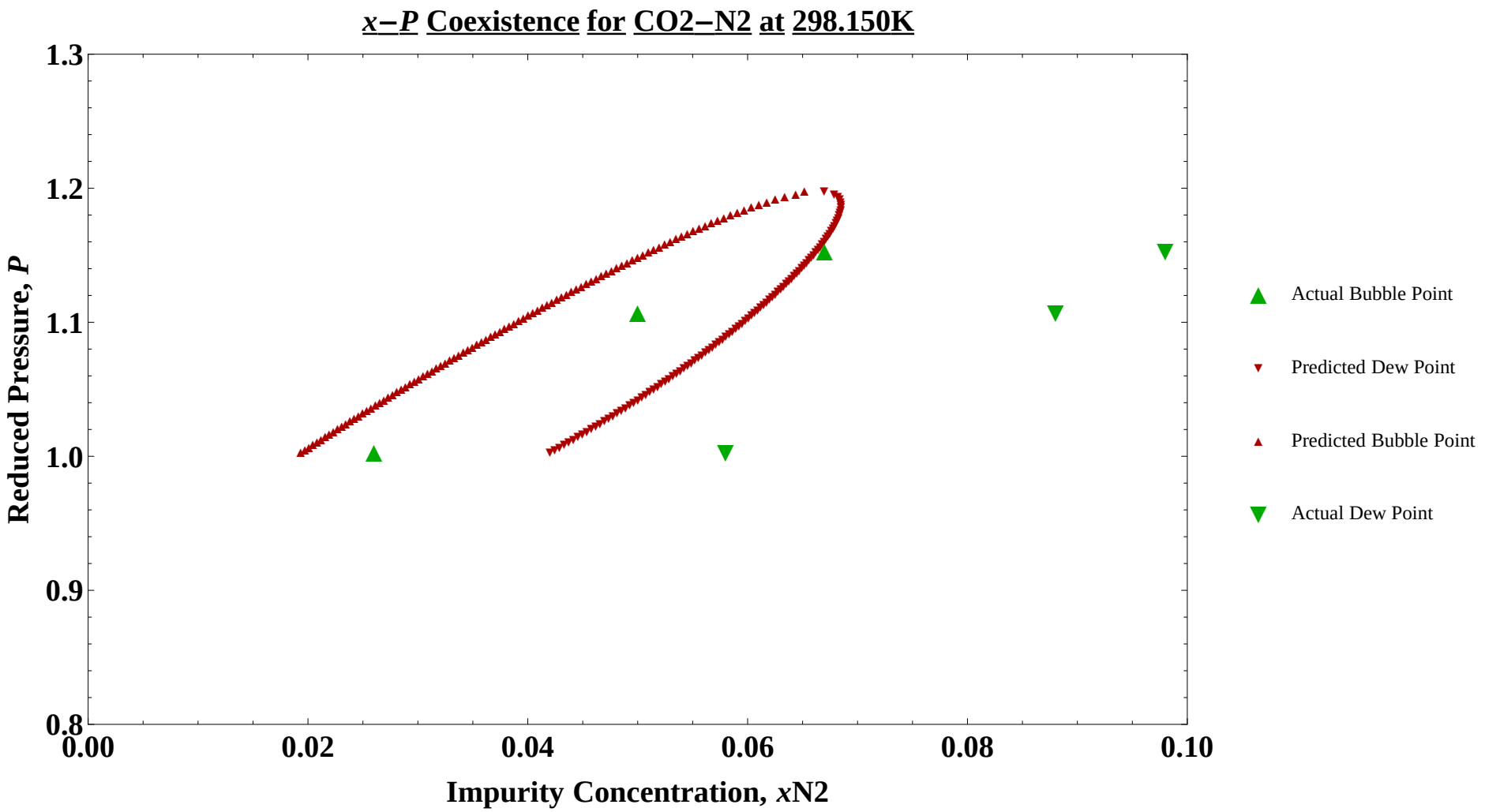

Figure 5.13: VLE coexisting mole fraction performance of model at 298.15K for carbon dioxide–nitrogen. Note that since the phase envelope is very small at this temperature, the prediction made here actually represents a very small absolute error

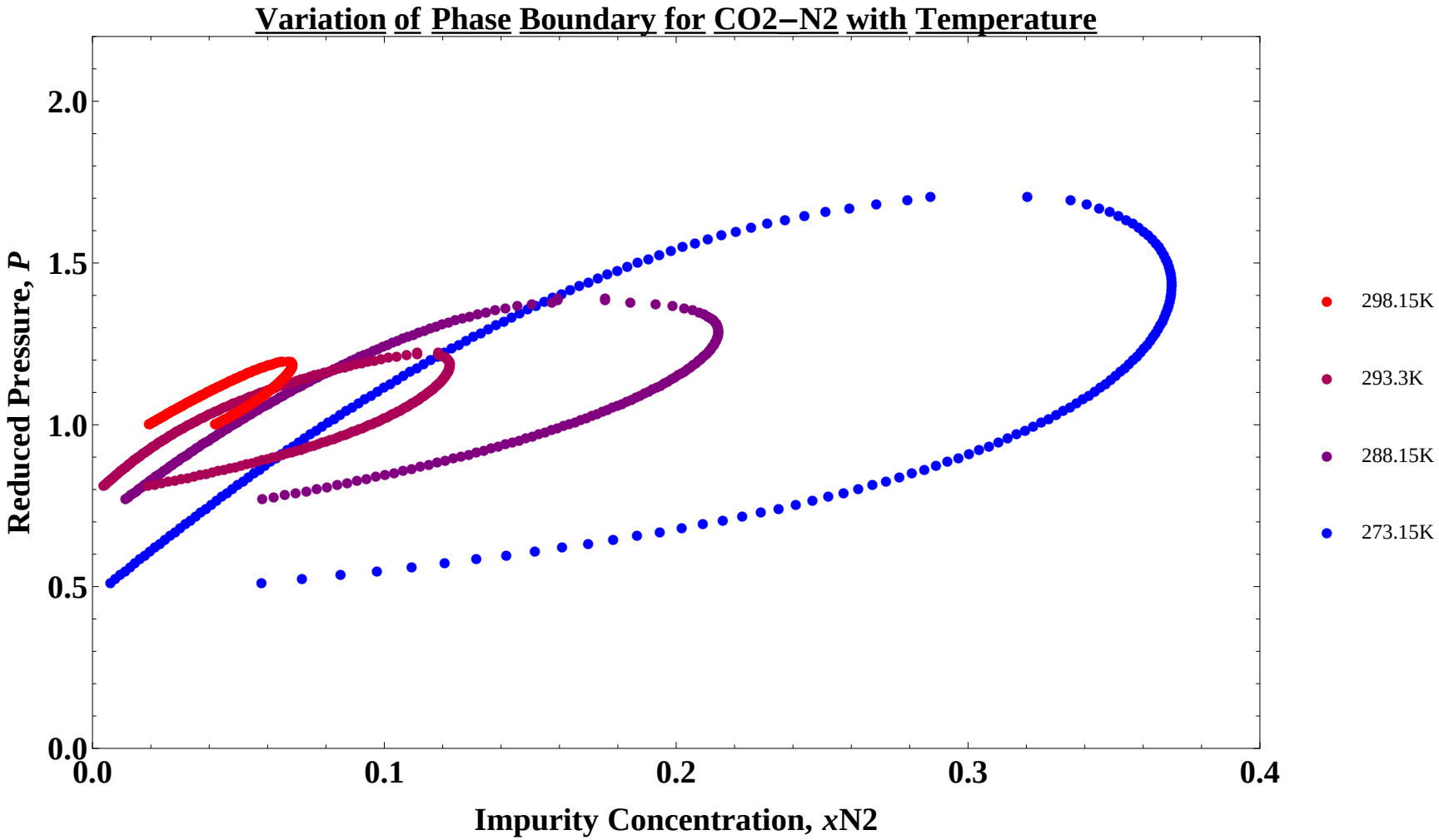

Figure 5.14: Effect of temperature on phase behaviour in the carbon dioxide–nitrogen binary system

There were numerous positives to draw from our fitting to the carbon dioxide–nitrogen data; not least the excellent pressure behaviour of the model at all nitrogen concentrations and temperatures, specifically those in the range of relevance to CCS as specified in Table 1.2. Phase behaviour predictions were also found to be well within the targets. Furthermore, use of our model to calculate the effect of temperature on the carbon dioxide–nitrogen phase boundary was possible, as shown in Figure 5.14.

Overall, for this mixture, we felt that the great promise shown by the model in the pure carbon dioxide case had been borne out. Even though the availability of the required data to affect a comprehensive fitting for a large range of temperatures was low, that data which was available together with the estimation methods had allowed us to calibrate the model in such a way as to demonstrate its true abilities.

We specifically highlight this as being a great success for the model as it proves beyond doubt that when appropriate data exists, it has the ability to give a very true description of it. We felt that if data at more temperatures became available, this would allow for an improved fit at a wider range of temperatures.

5.4 Carbon Dioxide–Hydrogen Binary Mixture

5.4.1 Data Availability

We again open this section by noting the availability of literature data for us to use in fitting the CO_2–H_2 model. There was not a single temperature at which both homogeneous pressure–density and VLE data, whether containing volumes or not, existed. This proved particularly problematic as it meant that even with our method of volume estimation, we did not have the full required amount of data in order to perform the fitting. This motivated our method of homogeneous phase density estimations.

A tabulated summary of the relevant available data is given in Table 5.8, again ordered by temperature. The availability of data in the hydrogen case was even more limited than in that of nitrogen. We can see from Table 5.8 that there were just two temperature points where complete VLE data existed: at 273.15K [92] and 258.15K [92], which is below the relevant range of temperatures for CCS pipelines. In addition, there were no temperatures at which VLE data and homogeneous density data existed. Whereas for the nitrogen case where there were some, albeit not many, temperatures at which both data types existed, for the hydrogen case, this

created a scenario in which without the estimation techniques described in Chapter 2, we would have been unable to perform a single fitting. With these methods however, we were able to build the model around seven temperature points accounting for the validity of some of the data presented, whilst ensuring we covered the correct temperature range; 298.15K, 290K, 280K, 273.15K, 270K, 260K, and the data at 258.15K, which even though we acknowledge is below our range of interest, since it was the full array of VLE data, by including it in our considerations, we hoped it may anchor the model and give some extra accuracy at lower temperatures.

Temperature (K)	Homogeneous Density Data Sources	VLE Data Sources
258.15		[92]
260		[110] †
270		[110] †
273.15		[92] [84] †
278.15		[90] †
280		[110] †
288.15	[111]	
290		[110] †
290.15		[90] †
293.15	[111]	
298.15		[90] †
303.15	[111]	
† means the VLE data in this source did not contain volumes		

Table 5.8: A summary of available data by source for carbon dioxide–hydrogen binary mixtures

5.4.2 Fitting the Carbon Dioxide–Hydrogen Binary Model Parameters

For fitting the carbon dioxide–hydrogen parameters, we proceeded in exactly the same way as for fitting the nitrogen parameters discussed in Section 5.3. We first determined the pure hydrogen parameters a_{H_2} through g_{H_2} at the seven temperature points specified by temporarily introducing a linear mixing rule similar to that given in Equation (5.44), and minimising the error function which found the values of the parameters best describing the two types of data. Again, this was done by simulated annealing at 298.15K and local minimisation at all subsequent temperatures. To find the binary interaction parameters we reintroduced the quadratic mixing rules and carried out the same process.

For finding the pure hydrogen parameters we again set $W = 0.99$ in the error function to persuade the fitting regime to concentrate on finding a good fit for the homogeneous density data to begin with. We again set $W = 0.05$ for finding the binary interaction parameters to force these to influence the search algorithm to focus on fitting the VLE behaviour more carefully.

For the pure hydrogen parameters and the binary interaction parameters of this system, the values we found by following this method are as summarised in Table 5.9.

T(K)	a_{H_2}	b_{H_2}	c_{H_2}	d_{H_2}	e_{H_2}	f_{H_2}	g_{H_2}
298.15	-0.036120	-0.268687	-0.140686	0.000064	-0.342518	0.841807	-0.570231
290	-0.001527	-0.115780	-0.010731	-0.041427	-0.341615	0.532446	-0.283406
280	-0.010139	-0.203360	-0.000606	-0.039236	-0.350992	0.449553	-0.202573
273.15	-0.016366	-0.285983	0.044472	-0.071323	-0.358931	0.668197	-0.354539
270	-0.036633	-0.261411	0.066326	-0.061539	-0.359609	0.666215	-0.395087
260	-0.025148	-0.241830	0.061862	-0.064112	-0.356514	0.607538	-0.338173
258.15	0.033329	-0.150848	-0.052928	0.087893	-0.835536	0.458757	-0.205049
T(K)	a_{CO_2,H_2}	b_{CO_2,H_2}	c_{CO_2,H_2}	d_{CO_2,H_2}	e_{CO_2,H_2}	f_{CO_2,H_2}	g_{CO_2,H_2}
298.15	1.020390	-0.599860	-0.714769	-0.200111	0.071537	0.994452	-0.543545
290	23.672552	-1.137099	-0.851500	-0.818970	-1.247985	4.546853	-3.464147
280	0.925204	0.031172	-0.125157	-0.220122	0.070576	1.052079	-0.534298
273.15	0.764031	-0.247773	-0.943430	-0.776950	0.062453	1.681050	-1.033491
270	0.768990	-0.409059	-1.083002	-0.754101	-1.147136	1.675058	-1.037449
260	0.620573	-0.518750	-1.029732	-0.651093	-0.989265	1.378729	-1.474389
258.15	0.810443	-0.490394	-0.905972	-0.632675	-0.172276	1.674597	-1.185195

Table 5.9: Fitted parameter values for the carbon dioxide–hydrogen binary system

5.4.3 Preliminary Indications of Performance

After having found the fourteen parameters at each temperature point, we evaluated the performance of the proposed model to check the fitting that had been achieved through the optimisation of the error function had rendered a suitable representation of the data that was used to calibrate it in each case.

We did this by checking the percentage errors of the values suggested by our model for both the homogeneous density and VLE. A summary is in Table 5.10:

Temperature	Homogeneous Density		v_{BP} †		v_{DP} †		x_{H_2} †		y_{H_2} †	
(K)	Maximum	Average	Maximum	Average	Maximum	Average	Maximum	Average	Maximum	Average
298.15	21.10	3.81	140.95	31.89	81.39	49.02	123.82	22.97	15.80	10.18
290	71.55	28.25	83.96	71.27	74.10	28.26	19.86	9.70	49.84	18.02
280	28.99	8.80	37.88	12.03	21.92	13.10	26.96	16.01	32.11	21.47
273.15	54.80	18.73	17.53	15.36	203.57	70.58	8.23	5.20	266.19	101.21
270	30.98	11.92	2.33	1.91	28.13	12.33	7.97	3.75	30.36	15.76
260	258.63	82.51	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
258.15	104.02	44.80	145.06	69.70	552.57	210.74	71.50	28.51	407.74	233.62
† where convergence to a meaningful solution had been possible										

Table 5.10: Preliminary testing of predictions made by our model for the carbon dioxide–hydrogen binary system, with results suggesting that with smoothly varying parameters the model could be good

It is evident from these figures that where there was a lack of suitable literature data to fit the model parameters to, the model has been unable to recreate that data. Nevertheless, we decided to fit the temperature dependence of the parameters to all the temperature points apart from 260K where a particularly bad fitting had been done, and 290K as the parameter values were significantly different to those surround it.

5.4.4 Variation of Model Parameters with Temperature

We again specified a quadratic temperature dependence, as for the binary mixture involving nitrogen. Following the same procedure as before to determine these dependences, we obtained:

$$a_{H_2}(T) = 2.18375 - 4.48398T + 2.27583T^2 \quad (5.60)$$
$$b_{H_2}(T) = 8.11481 - 17.5501T + 9.19340T^2 \quad (5.61)$$
$$c_{H_2}(T) = -24.007 + 53.8038T - 30.1181T^2 \quad (5.62)$$
$$d_{H_2}(T) = 16.8885 - 36.6077T + 19.7692T^2 \quad (5.63)$$
$$e_{H_2}(T) = -46.8681 + 99.0315T - 52.6178T^2 \quad (5.64)$$
$$f_{H_2}(T) = 13.5063 - 30.4078T + 17.7652T^2 \quad (5.65)$$
$$g_{H_2}(T) = -15.1254 + 34.353T - 19.7936T^2 \quad (5.66)$$
$$a_{CO_2,H_2}(T) = 25.1402 - 54.8628T + 30.8661T^2 \quad (5.67)$$
$$b_{CO_2,H_2}(T) = -58.0063 + 127.15T - 69.9675T^2 \quad (5.68)$$
$$c_{CO_2,H_2}(T) = 20.2645 - 47.7947T + 26.924T^2 \quad (5.69)$$
$$d_{CO_2,H_2}(T) = 59.4809 - 134.987T + 75.5951T^2 \quad (5.70)$$
$$e_{CO_2,H_2}(T) = -31.1574 + 66.5051T - 35.3448T^2 \quad (5.71)$$
$$f_{CO_2,H_2}(T) = -47.6094 + 112.811T - 64.5009T^2 \quad (5.72)$$
$$g_{CO_2,H_2}(T) = 12.9232 - 35.2366T + 21.9309T^2 \quad (5.73)$$

We can see from the following two examples how these temperature dependences resembled the parameter values at the chosen five temperature points.

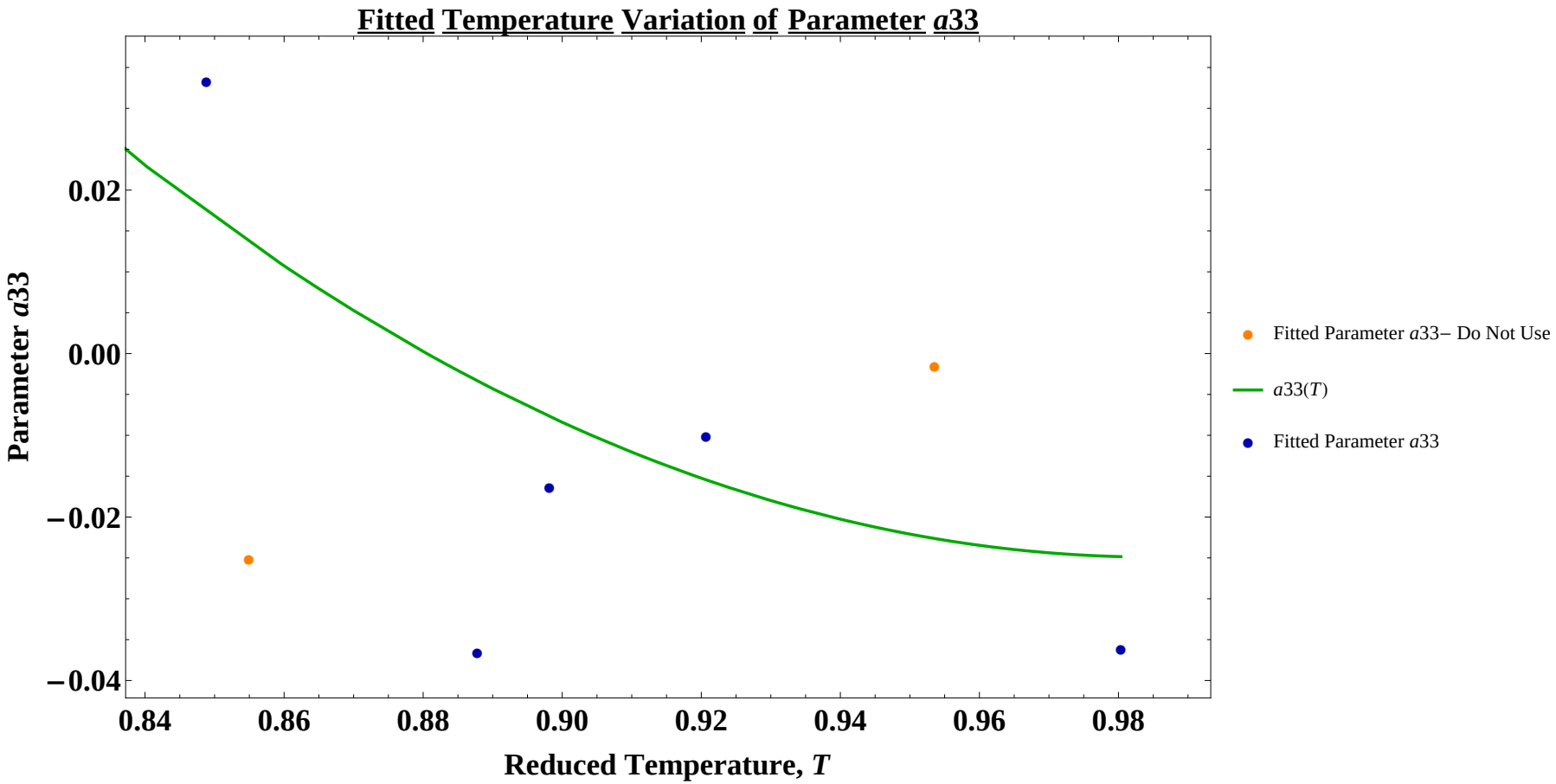

Figure 5.15: Temperature dependence for the pure nitrogen parameter a_{H_2} (denoted in the graph by a_{33})

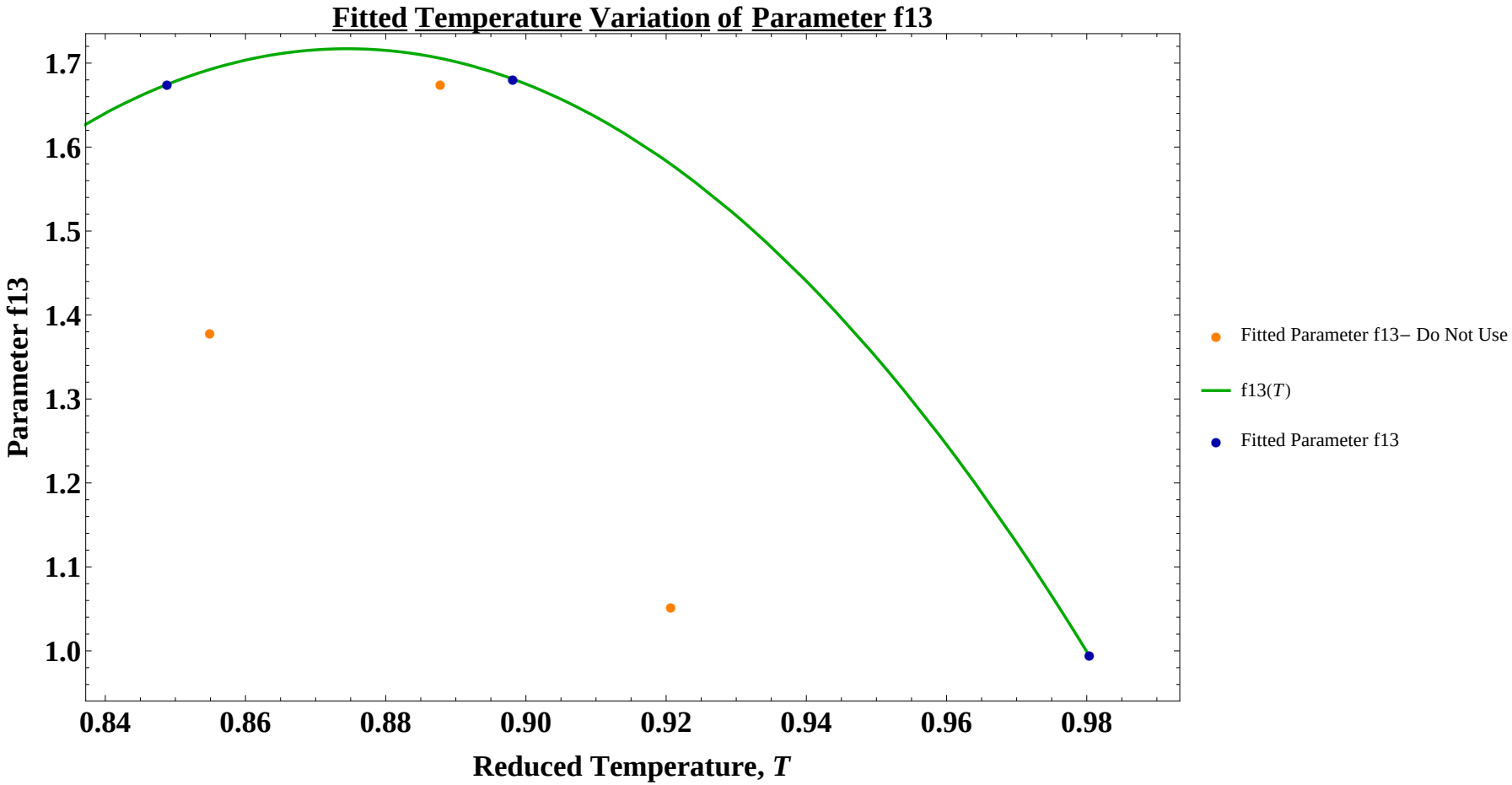

Figure 5.16: Temperature dependence for the binary interaction parameter f_{CO_2,H_2} (denoted in the graph by f_{13})

5.4.5 Performance of the Full Model for Binary Mixtures of Carbon Dioxide and Hydrogen

With the model thus fully defined for the binary system involving carbon dioxide and hydrogen, we were able to assess the performance of the final model for this particular mixture. We did this by once again comparing the model at temperature points which had been used to generate the fitted parameters, and then by checking the performance at temperatures where no data existed in order to check performance there. We note that since we fit the model parameters between 258.15K and 298.15K, we would not expect meaningful descriptions to be given significantly outside this range of particular relevance to CCS pipeline operation.

We began by comparing the behaviour of our model to the homogeneous volume–pressure data at 298.15K.

Hydrogen Composition (%)	Maximum Error (%)	Average Error (%)
0.96 (liquid phase)	21.15	5.90
2.84 (liquid phase)	13.66	3.55
3.82 (liquid phase)	15.33	5.50
4.25 (vapour phase)	4.05	1.10
7.43 (vapour phase)	5.97	1.26
10.06 (vapour phase)	6.91	1.39
100	11.70	5.55
ALL	21.15	4.51

Table 5.11: Pressure performance of model at 298.15K

We also compared the behaviour of our model to the VLE data at 298.15K.

Quantity	Maximum Error (%)	Average Error (%)
v_{BP} †	10.01	8.31
v_{DP} †	61.70	52.35
$x_{\mathrm{N_2}}$ †	1.28	0.98
$y_{\mathrm{N_2}}$ †	3.39	2.02
ALL	61.70	15.92
† where convergence to a meaningful solution had been possible		

Table 5.12: VLE performance of model at 298.15K

We note that with the exception of the dew curve volumes, most predictions either met our target accuracy, or were significantly better. It is worth pointing out that at this temperature we employed volume estimation for the VLE volumes, meaning that although some high percentage errors were given, these are only compared to the estimations, and not the real data. We again highlight that the best performance of our model occurred at the liquid saturation line (bubble curve), which is advantageous for application to CCS pipelines. Overall, we felt this behaviour represented an acceptable performance of our model at this temperature. We can additionally visually verify in Figures 5.17 to 5.19 that the behaviour of our model is broadly consistent with that little data which was available.

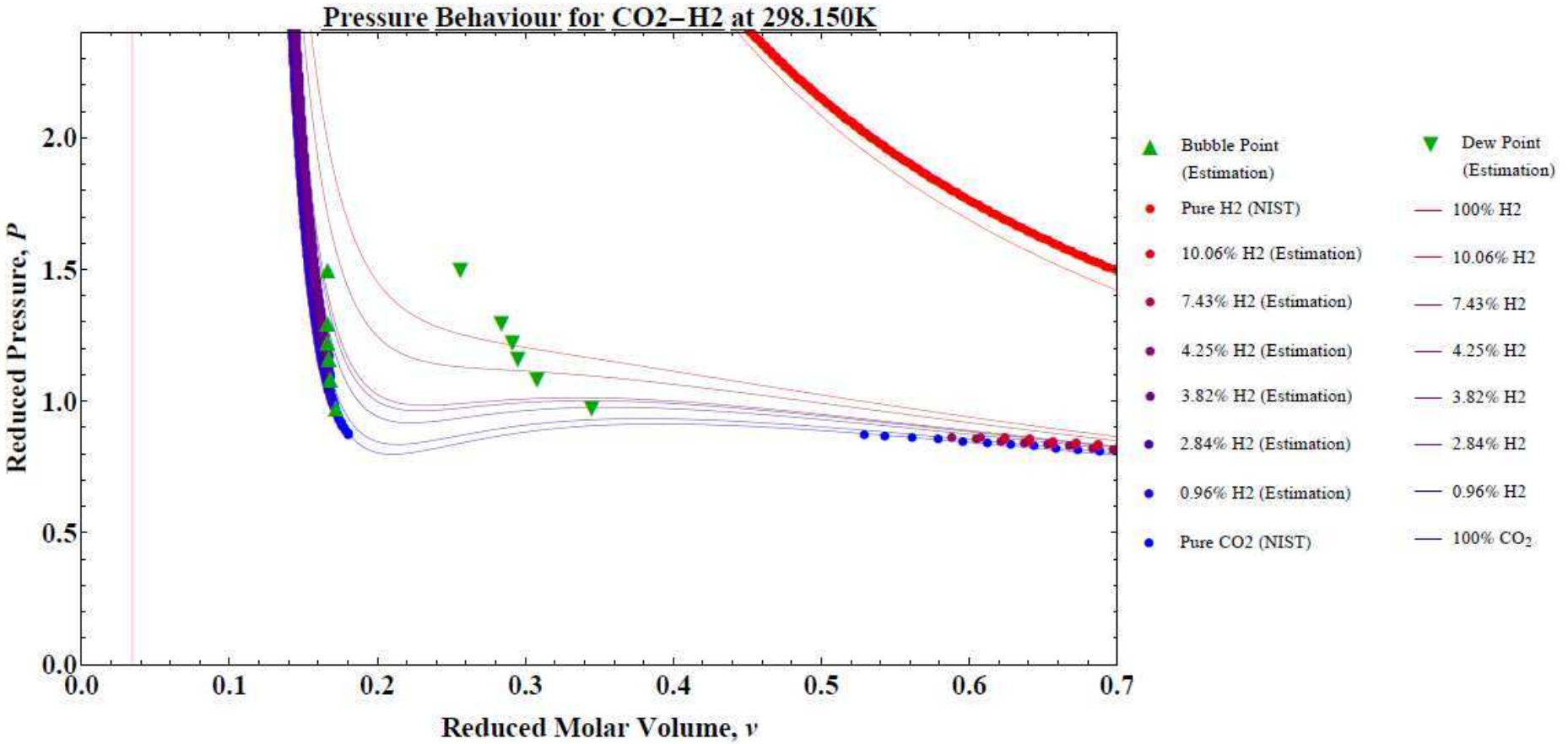

Figure 5.17: Pressure performance of model at 298.15K for carbon dioxide–hydrogen

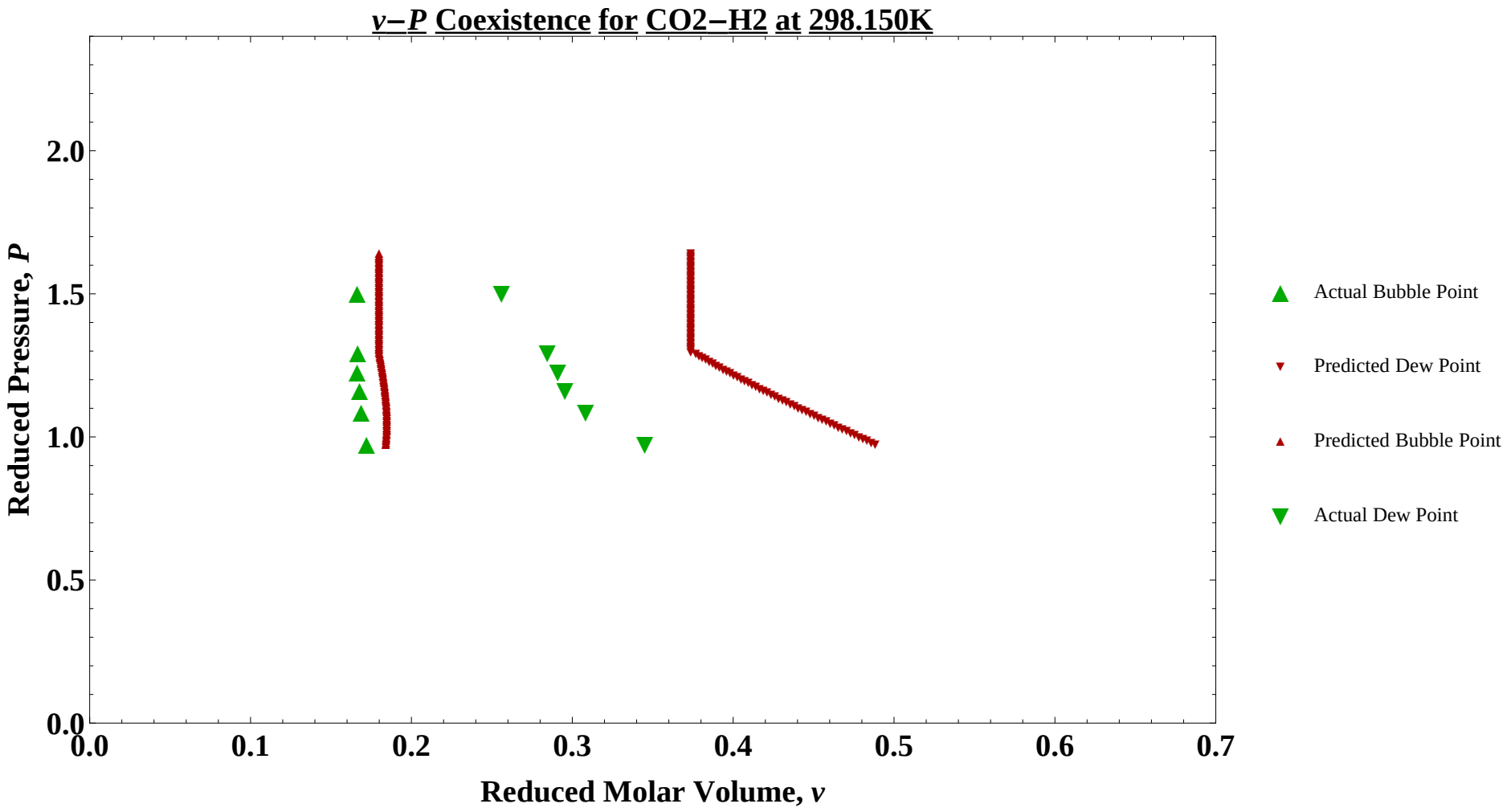

Figure 5.18: VLE coexisting volume performance of model at 298.15K for carbon dioxide–hydrogen

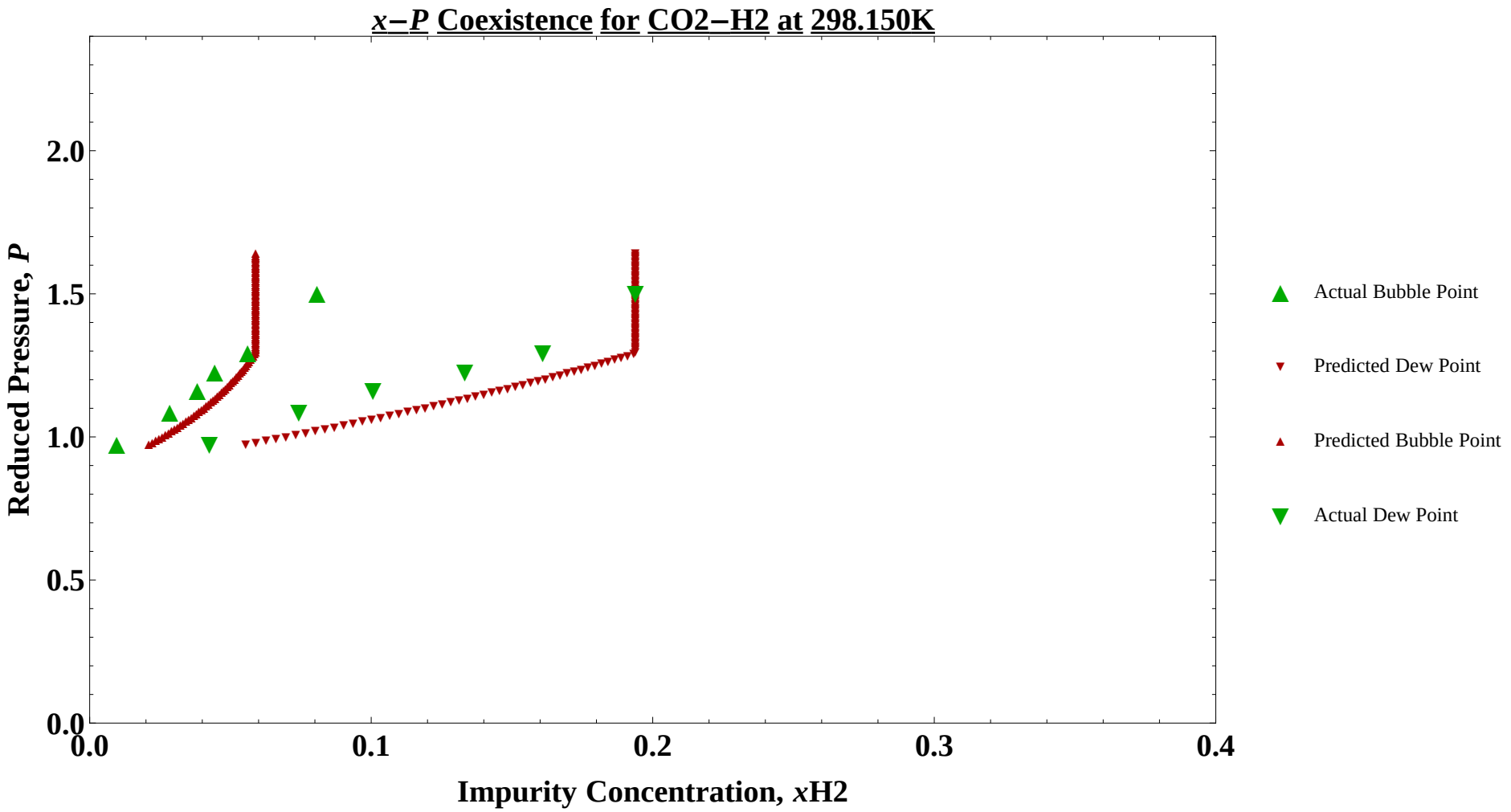

Figure 5.19: VLE coexisting mole fraction performance of model at 298.15K for carbon dioxide–hydrogen

We then compared the behaviour of our model to the homogeneous volume–pressure data at 273.15K.

Hydrogen Composition (%)	Maximum Error (%)	Average Error (%)
2.66 (liquid phase)	23.06	16.04
7.99 (liquid phase)	52.54	33.77
19.3 (liquid phase)	35.80	18.78
36.15 (vapour phase)	2.09	0.56
55 (vapour phase)	1.74	1.23
61 (vapour phase)	2.25	1.59
100	18.58	9.47
ALL	52.54	15.56

Table 5.13: Pressure performance of the model at 273.15K

We also compared the behaviour of our model to the VLE data at 273.15K:

Quantity	Maximum Error (%)	Average Error (%)
v_{BP} †	21.17	10.85
v_{DP} †	47.08	26.22
$x_{\mathrm{N_2}}$ †	4.83	2.90
$y_{\mathrm{N_2}}$ †	10.74	7.95
ALL	47.08	5.99
† where convergence to a meaningful solution had been possible		

Table 5.14: VLE performance of model at 273.15K

The performance of the model at both these temperatures was a little below the standard we had been aiming for. However, in some places, particularly close to the dew curve in the homogeneous vapour phase, we found the model to give good descriptions of the data. In the liquid phase there was also a generally good pressure description. As was the case for the nitrogen binary mixture, the model gave excellent descriptions of the bubble line, either meeting the target aim or falling just outside.

We again visually checked the behaviour of the model in Figures 5.19 to 5.22 for consistency, and we saw that at low concentrations of hydrogen, as is to be anticipated for CCS pipelines, a very good description is given.

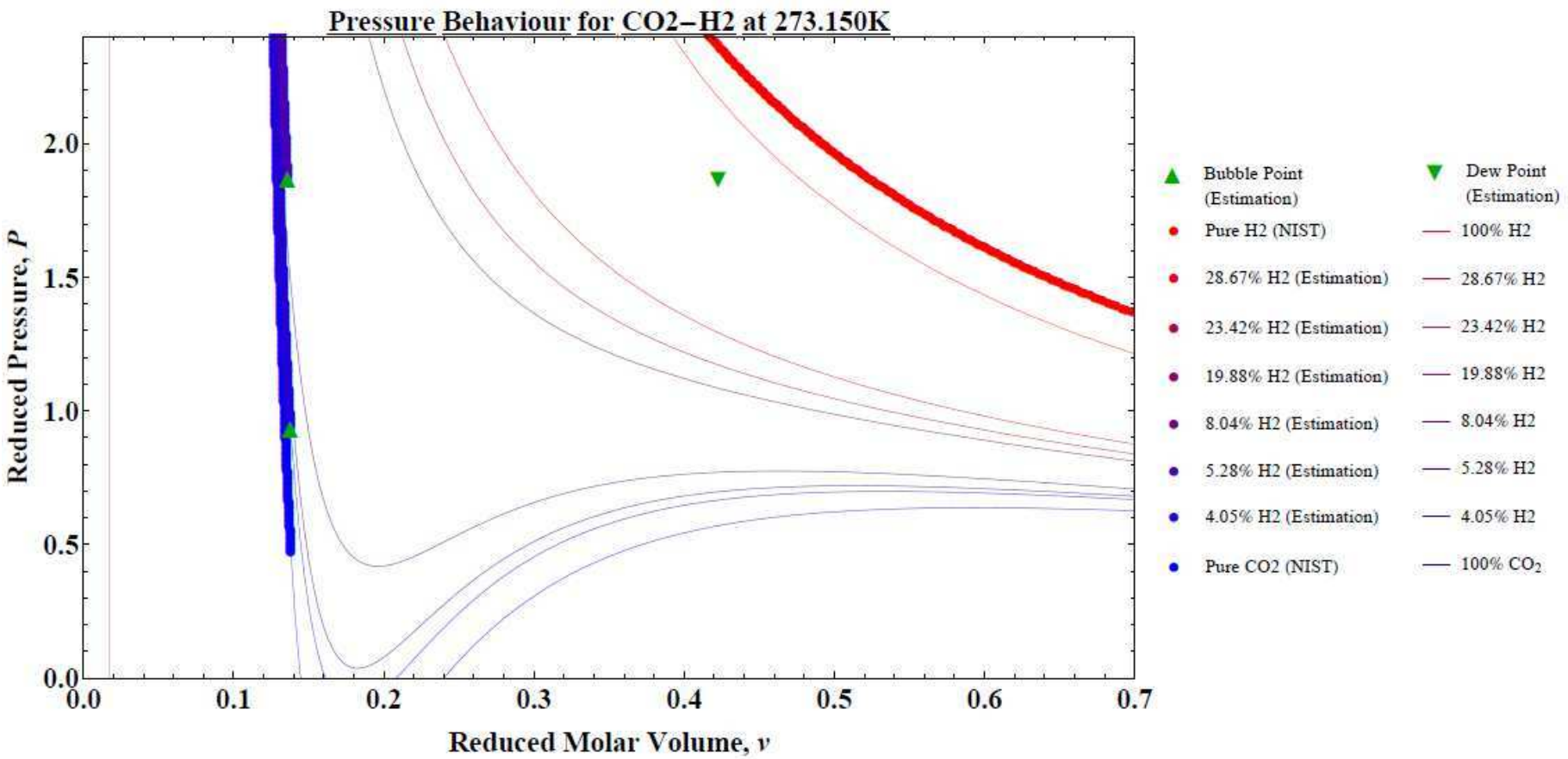

Figure 5.20: Pressure performance of model at 273.15K for carbon dioxide–hydrogen

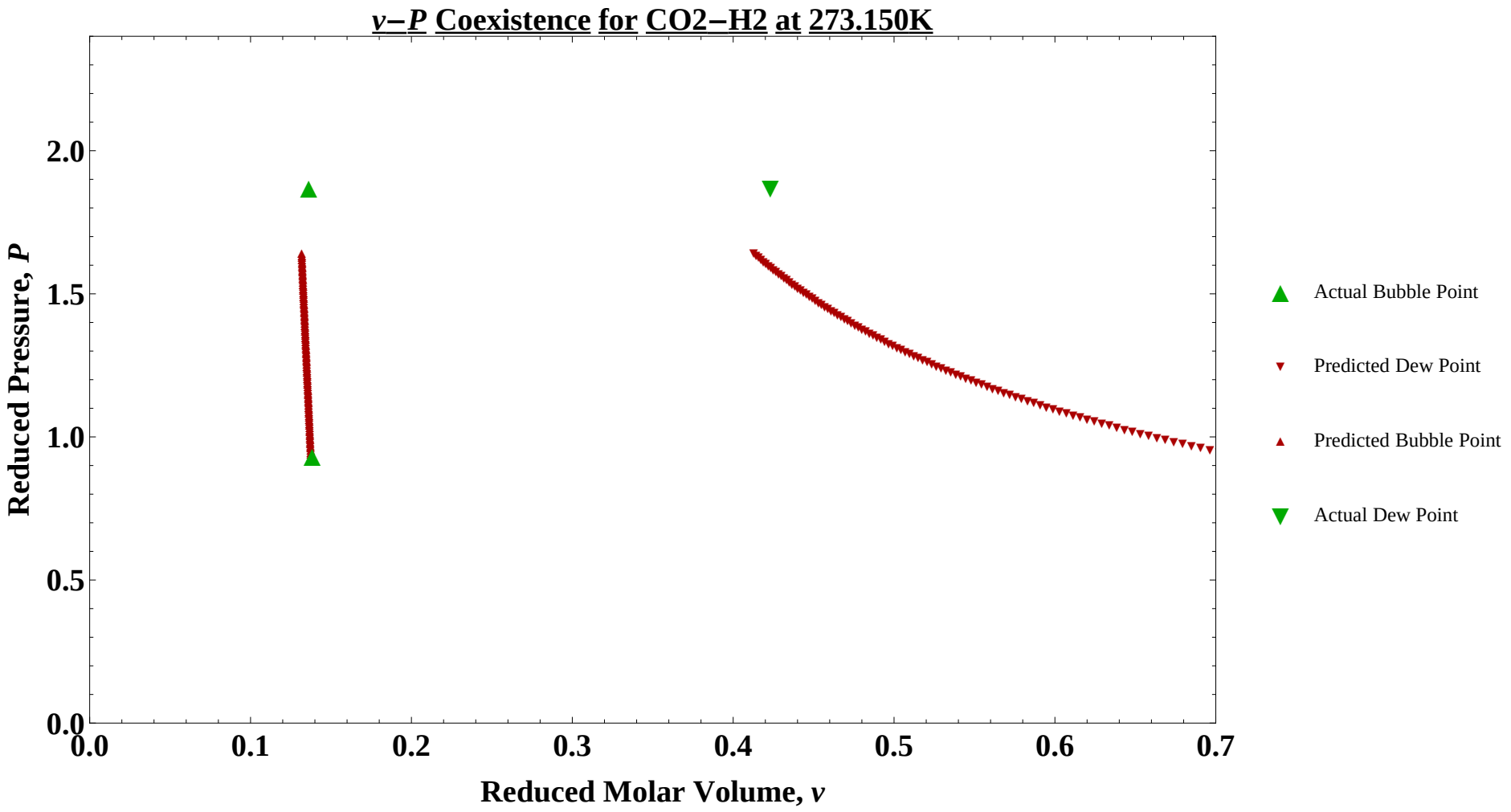

Figure 5.21: VLE coexisting volume performance of model at 273.15K for carbon dioxide–hydrogen

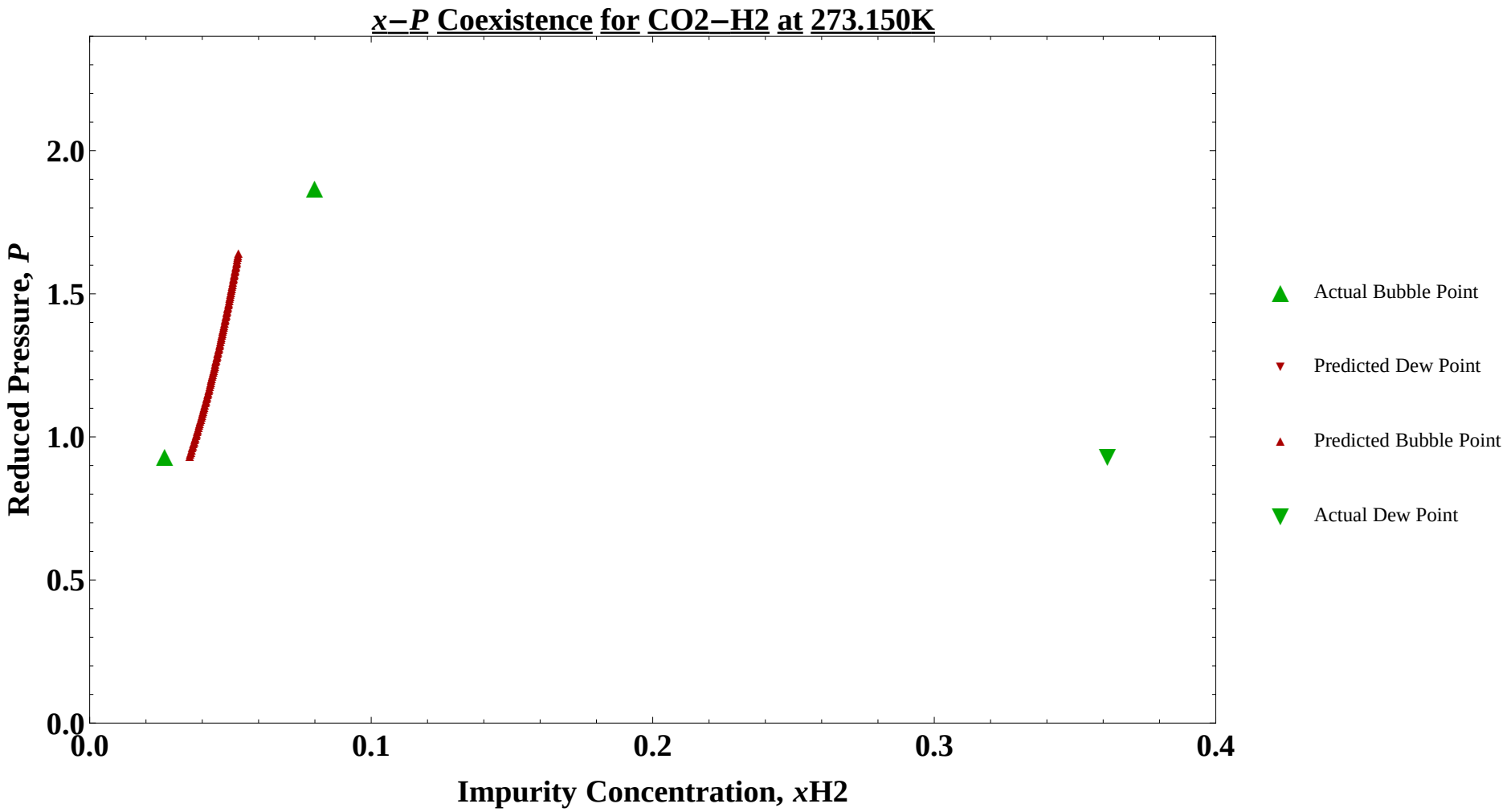

Figure 5.22: VLE coexisting mole fraction performance of model at 273.15K for carbon dioxide–hydrogen

We again suggest that where the model falls down could be a direct result of the lack of data that was available for fitting. Following on from the analyses at 298.15K and 273.15K, we also generated some plots at 285K and 275K; temperatures at which we had no data to fit to, in order to ensure consistent and physical behaviour.

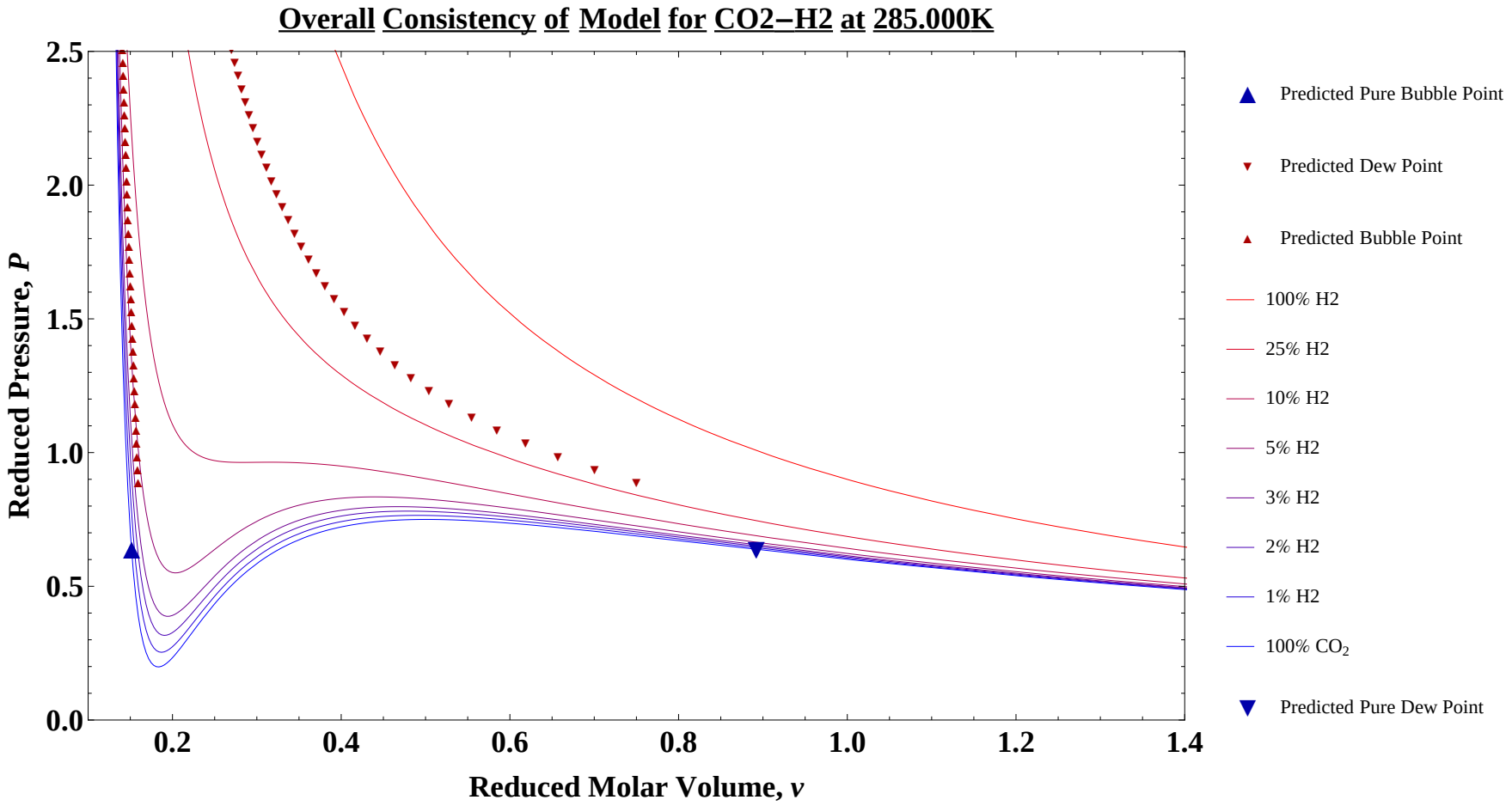

Figure 5.23: Pressure performance of model at 285K for carbon dioxide–hydrogen

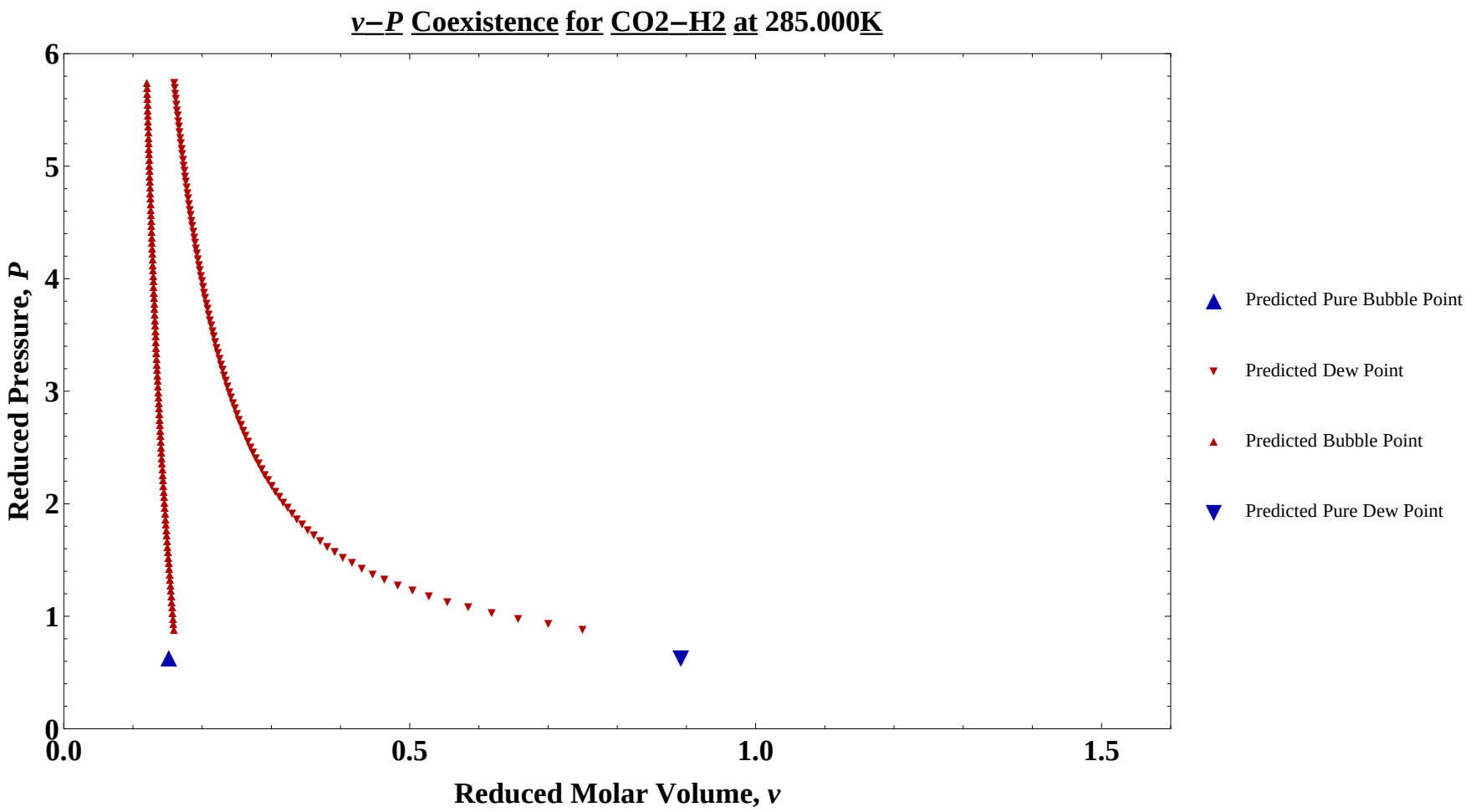

Figure 5.24: VLE coexisting volume performance of model at 285K for carbon dioxide–hydrogen

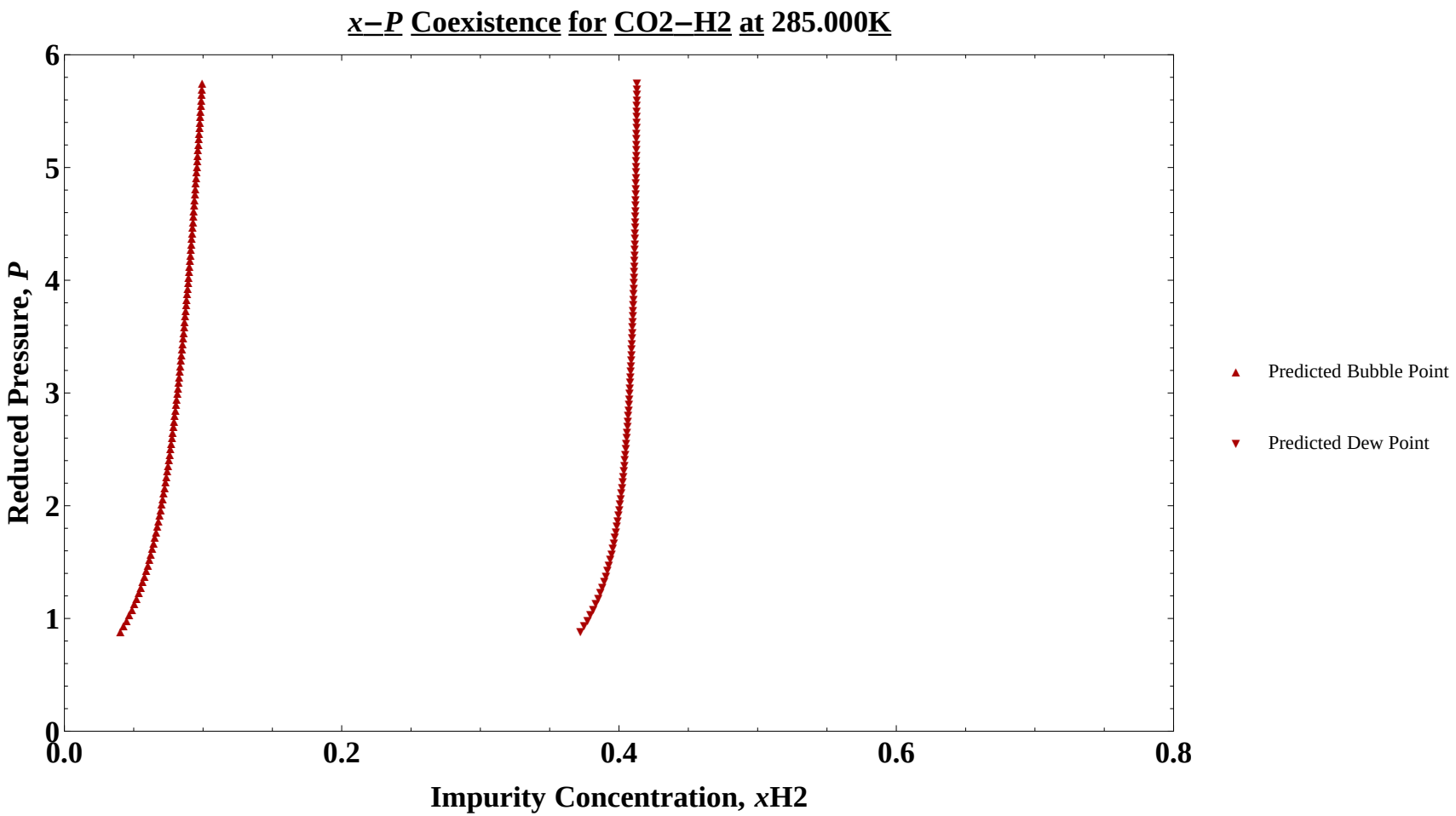

Figure 5.25: VLE coexisting mole fraction performance of model at 285K for carbon dioxide–hydrogen

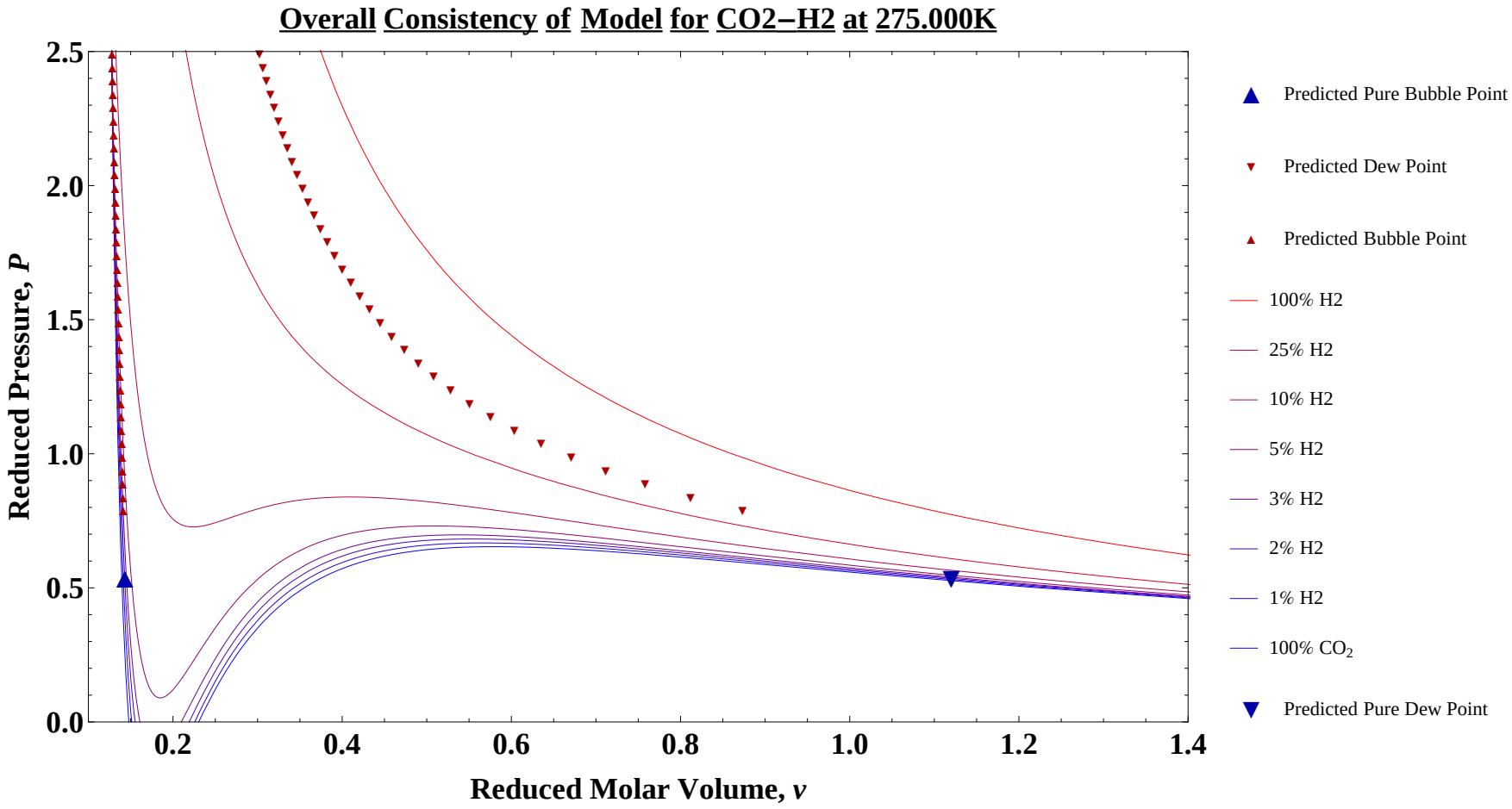

Figure 5.26: Pressure performance of model at 275K for carbon dioxide–hydrogen

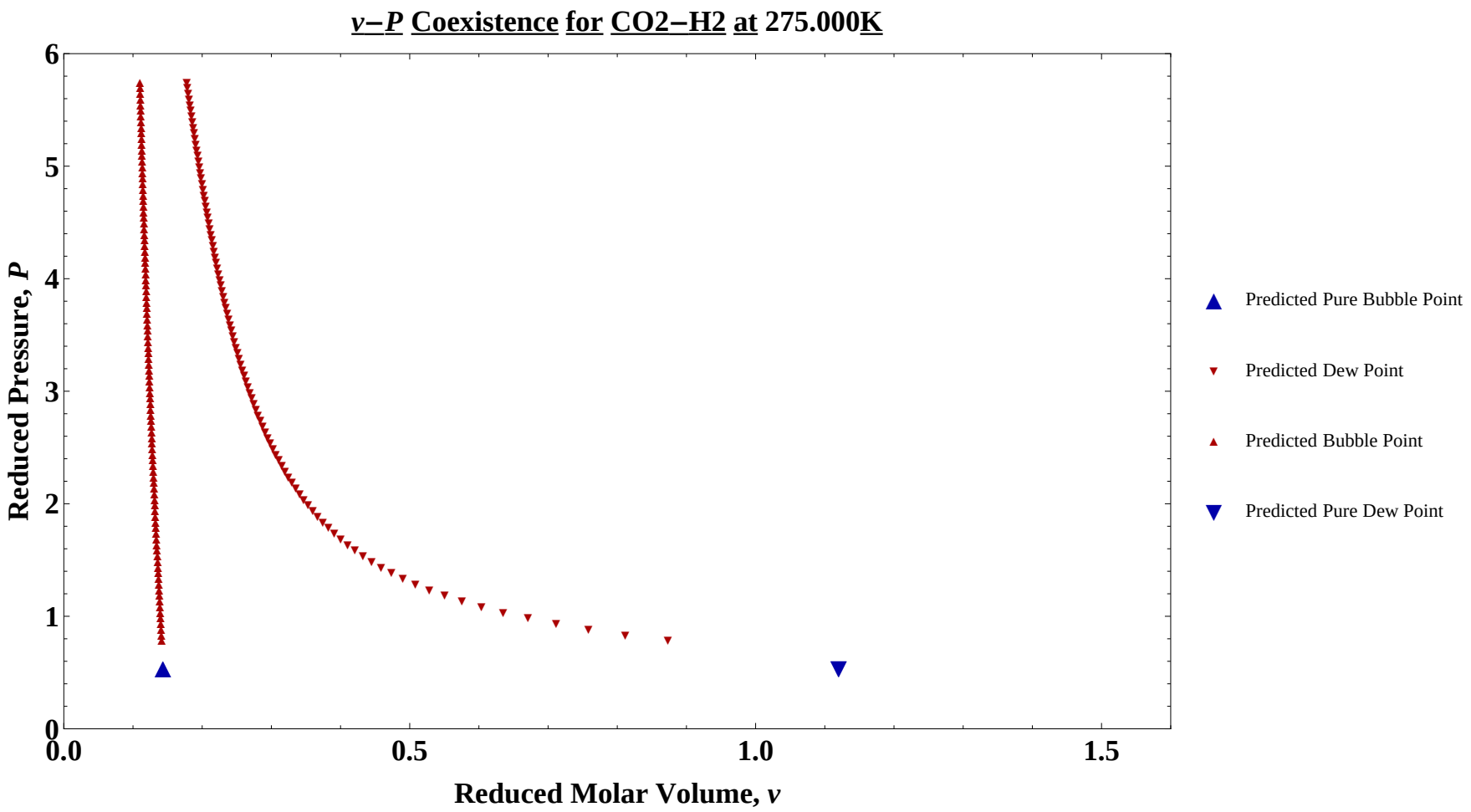

Figure 5.27: VLE coexisting volume performance of model at 275K for carbon dioxide–hydrogen

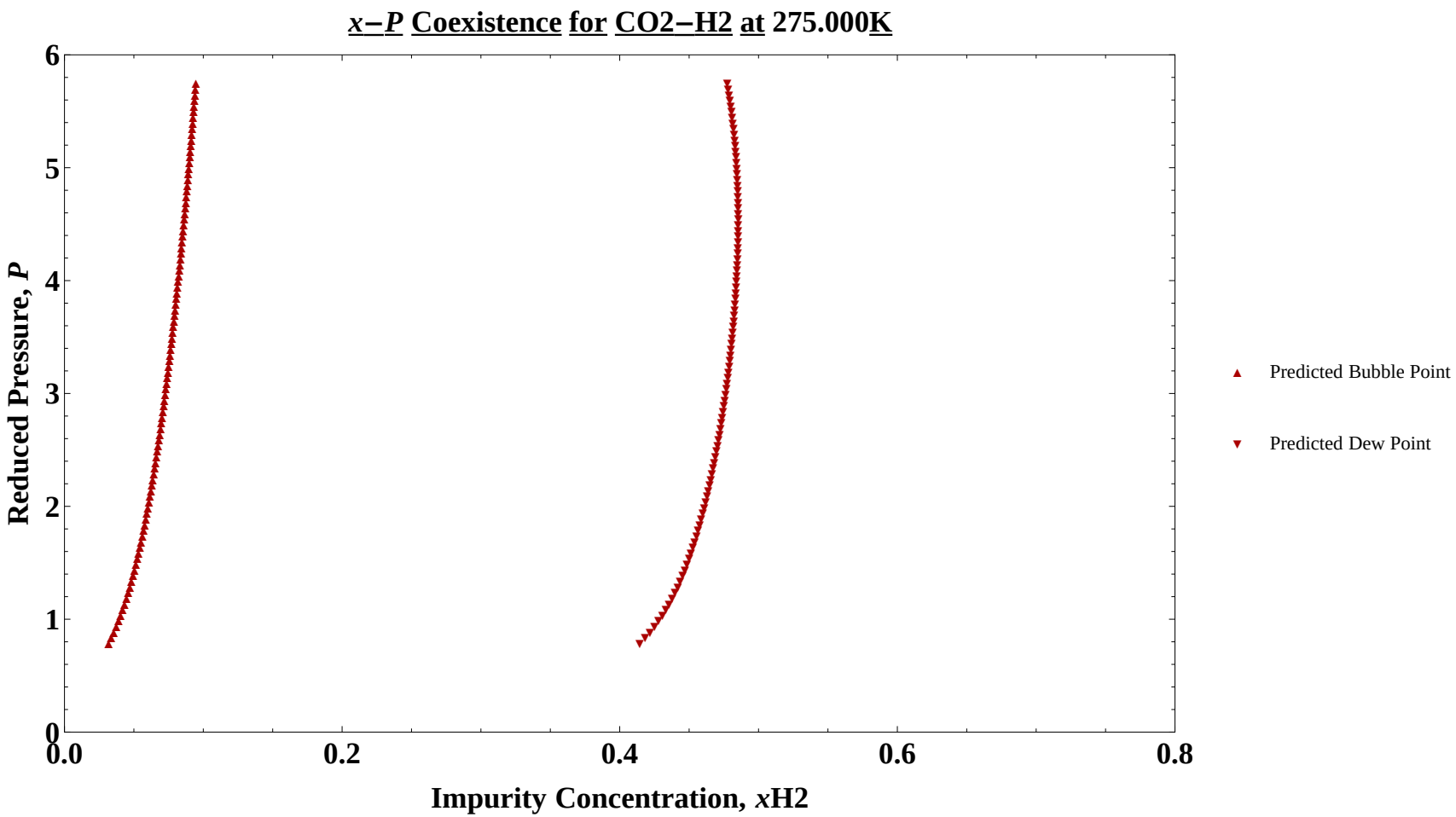

Figure 5.28: VLE coexisting mole fraction performance of model at 275K for carbon dioxide–hydrogen

These revealed a seemingly excellent behaviour, given the lack of literature data, right throughout the relevant range of temperatures. There did not appear to be any unphysical behaviour or contradictions, and the only issue we faced in generating and subsequently analysing these three plots was that at 295K we were unable to solve for the phase boundary, where we saw a lack of convergence at the top of the phase envelope. Nevertheless, in light of the performance of the other plots, we again felt confident that this showed the proposed equation to possess the potential to give good descriptions of the carbon dioxide–hydrogen system. Noting the difference in performance between the nitrogen binary system and the hydrogen binary system, we again attribute this to a lack of available data in the fitting stage which would constrain the VLE behaviour of the model.

5.5 Carbon Dioxide–Oxygen Binary Mixture

5.5.1 Data Availability

The situation with regard to availability of data in the carbon dioxide–oxygen system was found to be even more limited than for hydrogen, which was in turn more limited than for nitrogen. There was a single temperature at which the full array of VLE information was presented, at 273.15K (Muirbrook64 [54]), the highest temperature at which any VLE data was presented of 283.15K, and there was again no temperature at which both VLE and density data was given. A tabulated summary of the relevant available data is given in Table 5.15, again ordered by temperature.

Temperature (K)	Homogeneous Density Data Sources	VLE Data Sources
263.15		[112] †
273.15		[112] †, [54], [103] †
283.15		[112] †
302.22	[109]	
† means the VLE data in this source did not contain volumes		

Table 5.15: A summary of available data by source for carbon dioxide–oxygen binary mixtures

We can see from Table 5.15 that for the carbon dioxide–oxygen binary system there was just a single temperature point where the complete VLE data was given. Data was only presented at four temperature points in the range of interest, and again, we this created a scenario in which without the estimation techniques described in Chapter 2, we would have been unable to perform a single fitting (this again a key justification for our estimation methods). With these methods however, we were able to build the model around three temperature points: 283.15K, 273.15K, and 263.15K.

5.5.2 Fitting the Carbon Dioxide–Oxygen Binary Model Parameters

For fitting the carbon dioxide–oxygen parameters, we proceeded in exactly the same way as for fitting the nitrogen and then the hydrogen parameters, as discussed in Sections 5.3 and Section 5.4 respectively.

For finding the pure oxygen parameters we again set $W = 0.99$ in the error function for the pure oxygen parameters and for finding the binary interaction parameters for this system we set $W = 0.05$.

As a slight difference to how we proceeded before, owing to the smaller number of temperature points for this mixture, and the fact that most complete data set was available at 273.15K, we did the first step with simulated annealing at this temperature, then used local minimisation, taking the parameter values from this middle temperature, at the two other temperatures. The carbon dioxide–oxygen binary system parameters are summarised in Table 5.16.

T(K)	a_{O_2}	b_{O_2}	c_{O_2}	d_{O_2}	e_{O_2}	f_{O_2}	g_{O_2}
263.15	0.094921	-0.208998	-0.126906	-0.132688	-0.029934	0.723007	0.426078
273.15	0.124226	-0.214169	-0.042443	-0.181688	-0.094012	0.776980	-0.494059
283.15	0.029317	-0.205162	-0.043949	-0.136298	-0.106251	0.447834	-0.229049
T(K)	a_{CO_2,O_2}	b_{CO_2,O_2}	c_{CO_2,O_2}	d_{CO_2,O_2}	e_{CO_2,O_2}	f_{CO_2,O_2}	g_{CO_2,O_2}
263.15	0.206934	0.463788	0.062166	0.685644	-1.781140	0.624714	-0.722116
273.15	0.188844	0.430426	0.151882	0.735649	-1.031840	0.882312	-0.445456
283.15	0.080006	0.554140	0.906305	0.639080	-1.830015	0.143994	0.089705

Table 5.16: Fitted parameter values for the carbon dioxide–oxygen binary system

5.5.3 Preliminary Indications of Performance

After having found the fourteen parameters at each temperature point, we evaluated the performance of the proposed model to check the fitting that had been achieved through the optimisation of the error function had rendered a suitable representation of the data that was used to calibrate it in each case.

Just as for the two other binary mixtures, we did this by checking the percentage errors of the values suggested by our model for both the homogeneous density and VLE. A summary is in Table 5.17. We could see from this table that at 273.15K and 283.15K, an all round excellent performance was suggested, even though there was no homogeneous density data within the temperature range we considered. At 263.15K the performance was clearly a lot worse, and we again attribute this to a lack of sufficient data at this temperature.

Temperature (K)	Homogeneous Density		v_{BP} †		v_{DP} †		x_{O_2} †		y_{O_2} †	
	Maximum	Average	Maximum	Average	Maximum	Average	Maximum	Average	Maximum	Average
263.15	302.24	89.10	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
273.15	11.19	2.43	5.82	3.03	34.43	15.76	8.37	4.27	34.69	21.26
283.15	13.28	3.80	7.48	3.88	34.45	17.53	5.63	2.81	20.23	9.60
† where convergence to a meaningful solution had been possible										

Table 5.17: Preliminary testing of predictions made by our model for the carbon dioxide–oxygen binary system

5.5.4 Variation of Model Parameters with Temperature

We again specified a quadratic temperature dependence for each parameter in the carbon dioxide–oxygen system, as for the binary mixtures involving nitrogen and hydrogen. We carried out the same procedure as before to determine these dependences, and obtained the following:

$$a_{O_2}(T) = -45.3188 + 102.191T - 57.4457T^2 \quad (5.74)$$

$$b_{O_2}(T) = 5.0224 - 11.7192T + 6.55663T^2 \quad (5.75)$$

$$c_{O_2}(T) = -33.2466 + 72.6782T - 39.7581T^2 \quad (5.76)$$

$$d_{O_2}(T) = 35.0799 - 78.4664T + 43.6521T^2 \quad (5.77)$$

$$e_{O_2}(T) = 20.2866 - 44.2235T + 23.9734T^2 \quad (5.78)$$

$$f_{O_2}(T) = -138.389 + 314.082T - 177.181T^2 \quad (5.79)$$

$$g_{O_2}(T) = 121.039 - 273.628T + 153.998T^2 \quad (5.80)$$

$$a_{CO_2,O_2}(T) = -31.9314 + 73.4563T - 41.968T^2 \quad (5.81)$$

$$b_{CO_2,O_2}(T) = 57.7945 - 129.114T + 72.6431T^2 \quad (5.82)$$

$$c_{CO_2,O_2}(T) = 236.595 - 539.354T + 307.407T^2 \quad (5.83)$$

$$d_{CO_2,O_2}(T) = -53.3081 + 121.054T - 67.7856T^2 \quad (5.84)$$

$$e_{CO_2,O_2}(T) = -577.655 + 1284.78T - 715.657T^2 \quad (5.85)$$

$$f_{CO_2,O_2}(T) = -364.083 + 820.022T - 460.581T^2 \quad (5.86)$$

$$g_{CO_2,O_2}(T) = 84.9019 - 202.398T + 119.549T^2 \quad (5.87)$$

We can see from Figures 5.29 and 5.30 how these temperature dependences resembled the parameter values at the chosen temperature points.

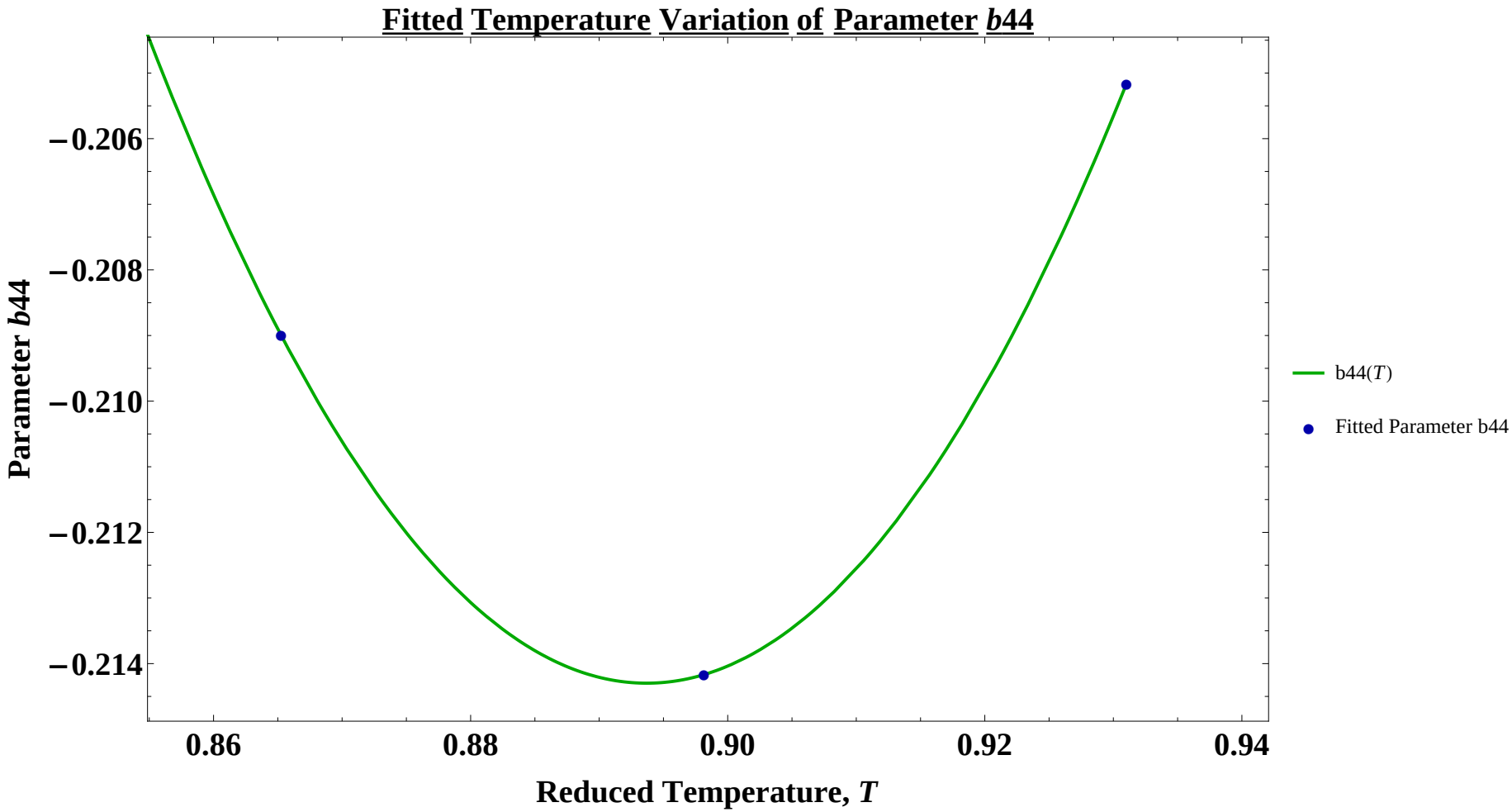

Figure 5.29: Temperature dependence for the pure oxygen parameter b_{O_2} (denoted in the graph by b_{44}

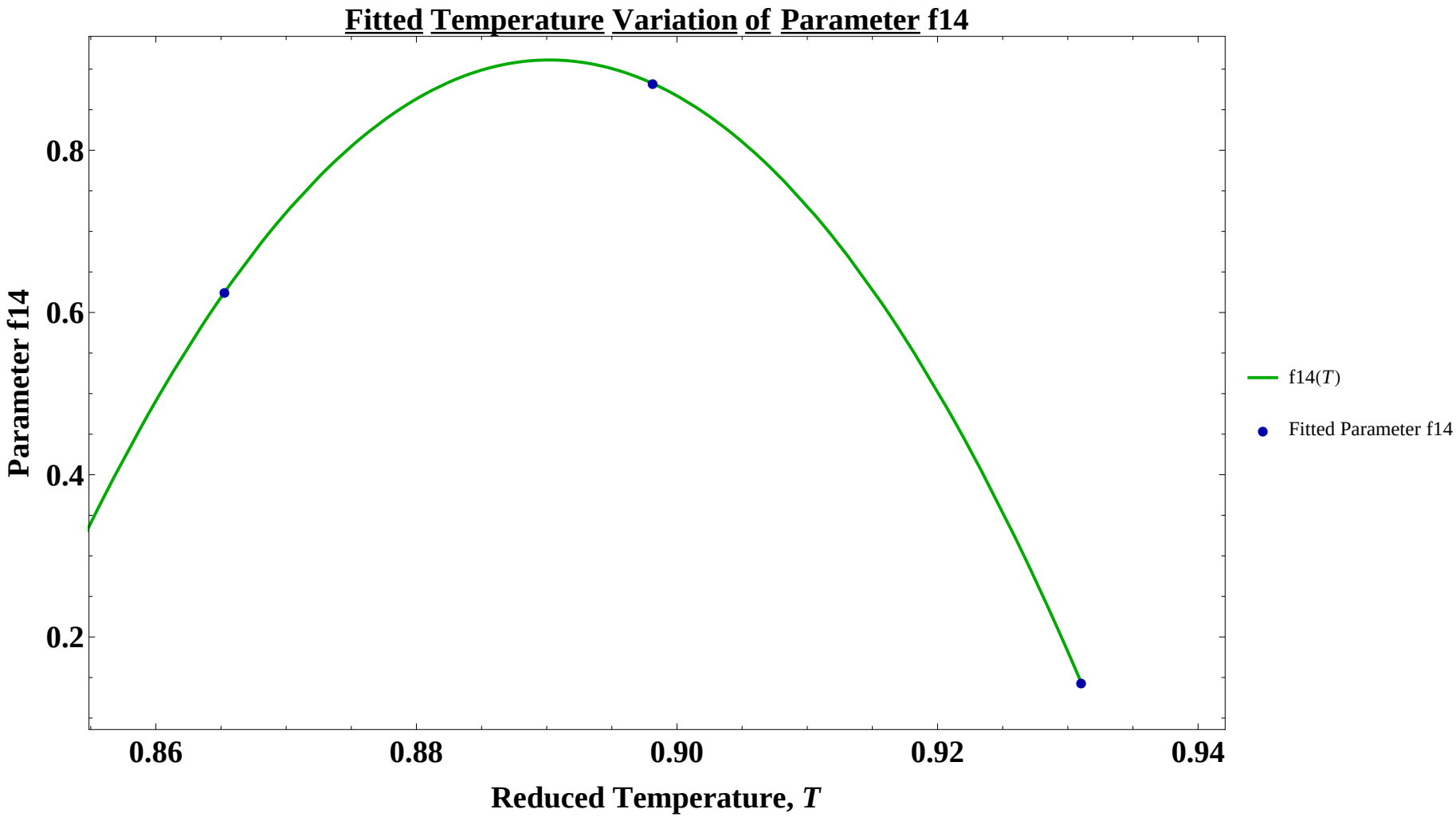

Figure 5.30: Temperature dependence for the binary interaction parameter f_{CO_2,O_2} (denoted in the graph by f_{14}

5.5.5 Performance of the Full Model for Binary Mixtures of Carbon Dioxide and Oxygen

This closed the model for the binary system involving carbon dioxide and oxygen, and with it, all three binary systems we sought to describe. Using this full definition, we were able to assess the performance of the final model for this case. We did this by once again comparing the model at temperature points which had been used to generate the fitted parameters, and then by checking the performance at temperatures where no data existed in order to check performance there. We note that since we fit the model parameters between 263.15K and 283.15K, we would not expect meaningful descriptions to be given significantly outside this range, in particular approaching the carbon dioxide critical temperature.

We began by comparing the behaviour of our model to the homogeneous volume–pressure data at 283.15K:

Oxygen Composition (%)	Maximum Error (%)	Average Error (%)
2.8 (liquid phase)	13.28	3.27
4 (liquid phase)	9.06	3.77
7.1 (liquid phase)	11.19	8.47
11.5 (vapour phase)	3.91	0.74
16.1 (vapour phase)	5.37	1.27
21.8 (vapour phase)	6.99	1.96
100	3.36	1.81
ALL	13.28	3.80

Table 5.18: Pressure performance of the model at 283.15K

We also compared the behaviour of our model to the VLE data at 283.15K:

Quantity	Maximum Error (%)	Average Error (%)
v_{BP} †	6.23	3.42
v_{DP} †	68.75	37.50
$x_{\mathrm{O_2}}$ †	10.72	5.59
$y_{\mathrm{O_2}}$ †	28.25	16.86
ALL	68.75	15.88
† where convergence to a meaningful solution had been possible		

Table 5.19: VLE performance of the model at 283.15K

We note that, as was the case for both nitrogen and hydrogen, most predictions were around our target accuracy range, with the exception of the bubble curve volumes, demonstrating once more that the model possessed sufficient flexibility to be able to also model this binary system with sufficient accuracy for the needs of CCS pipeline operators. Once again we highlight the best performance of our model as occurring at the liquid saturation line. Overall, we felt the behaviour of the model exhibited at this temperature was excellent in light of the fact that there had been no homogeneous density or coexisting volume data here, giving further credibility

to our homogeneous density estimation methods. We can again verify in Figures 5.31 to 5.33 that the behaviour of our model was broadly consistent with the data.

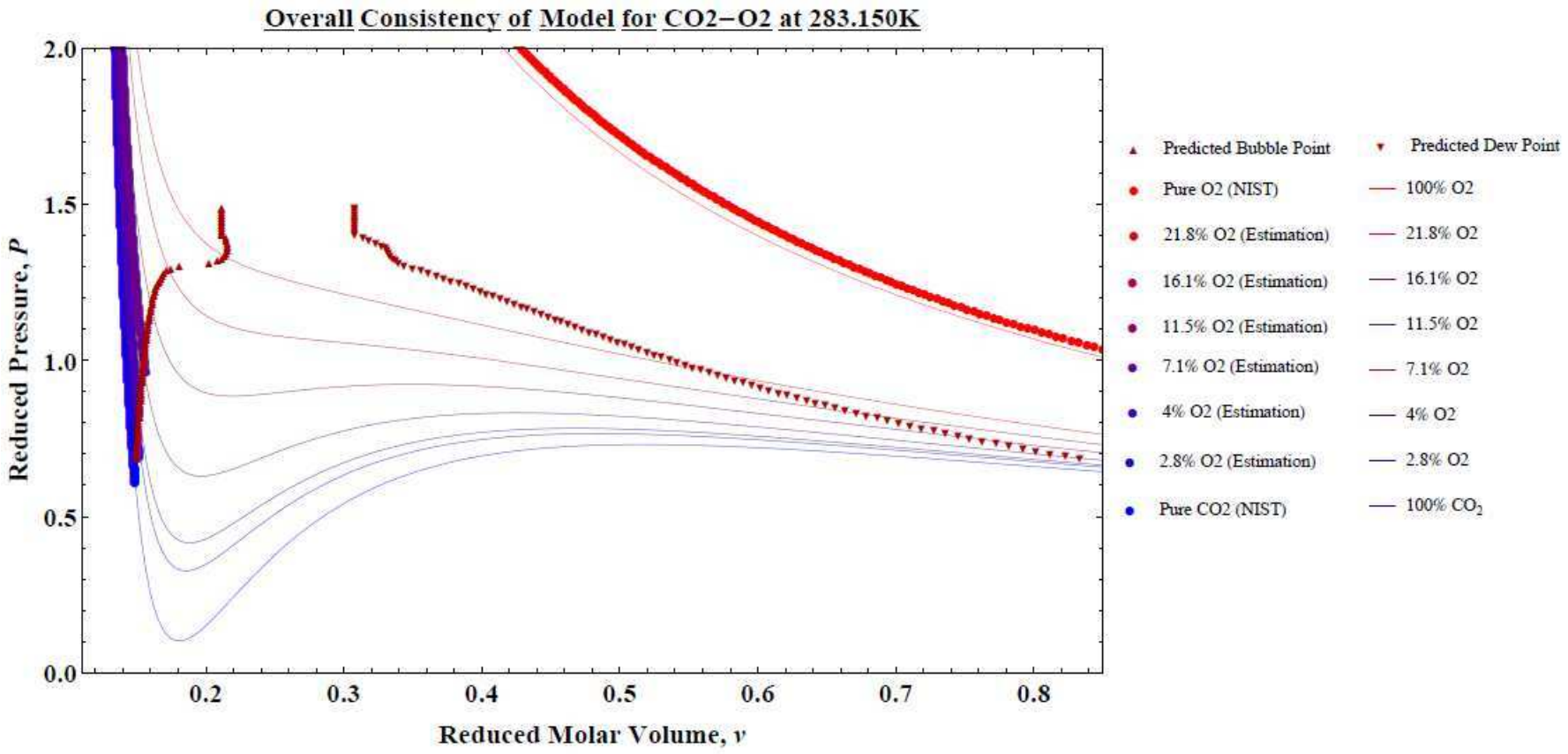

Figure 5.31: Pressure performance of model at 283.15K for carbon dioxide–oxygen

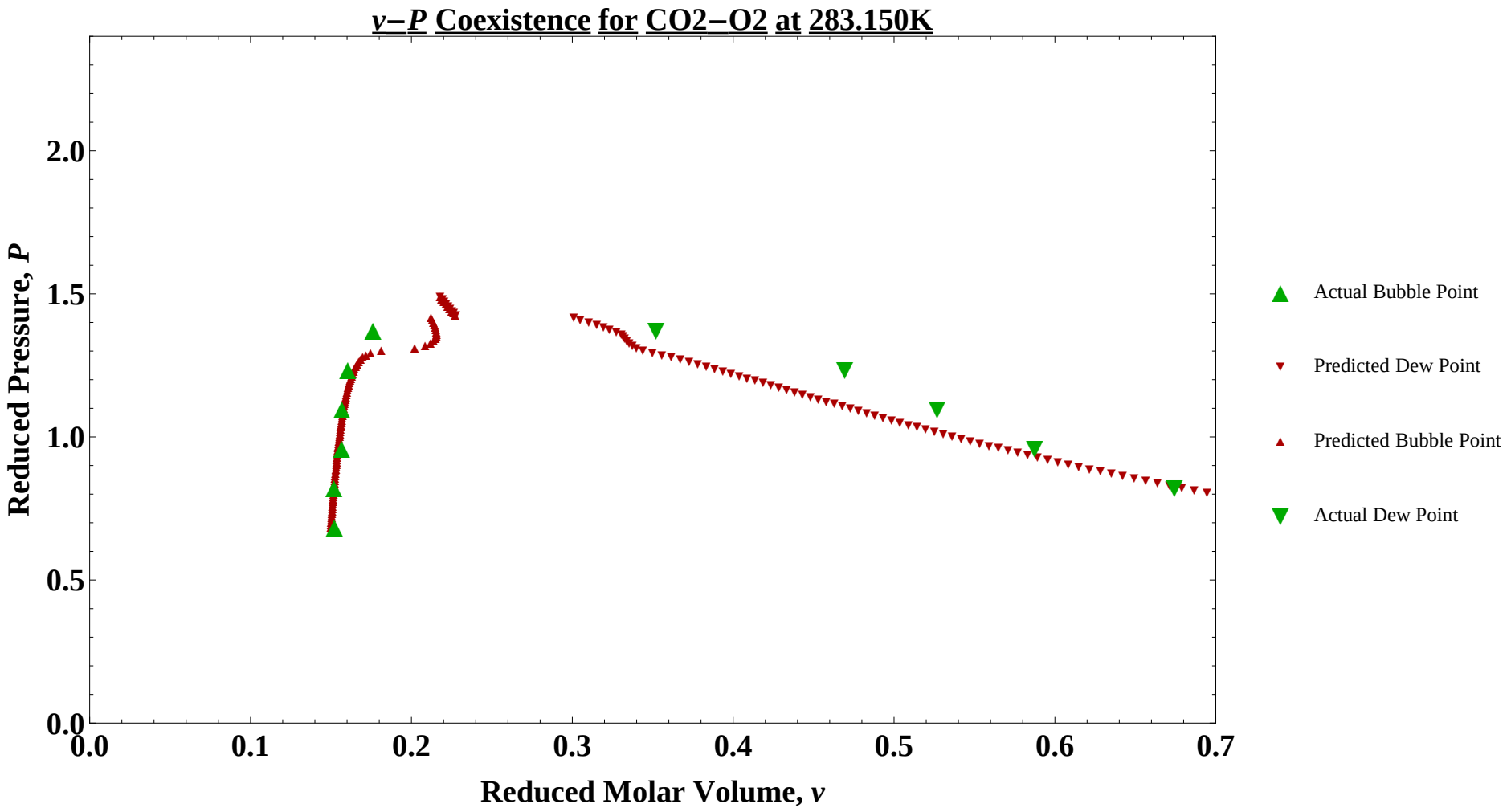

Figure 5.32: VLE coexisting volume performance of model at 283.15K for carbon dioxide–oxygen

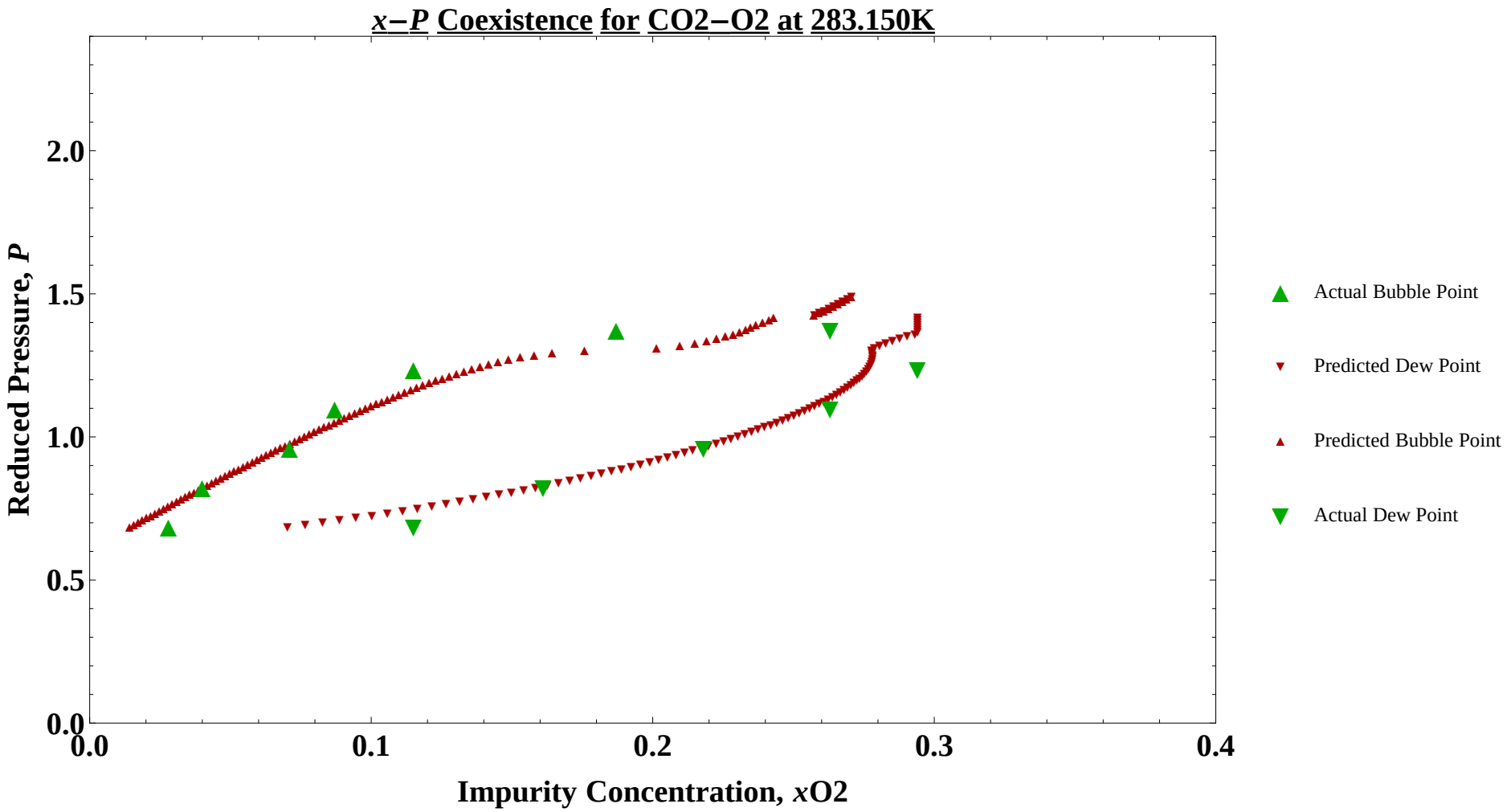

Figure 5.33: VLE coexisting mole fraction performance of model at 283.15K for carbon dioxide–oxygen

We then compared the behaviour of our model to the homogeneous volume–pressure data at 273.15K:

Nitrogen Composition	Maximum Error (%)	Average Error (%)
0.66 (liquid phase)	11.19	2.42
1.41 (liquid phase)	3.57	1.38
2.18 (liquid phase)	4.51	2.60
4.8 (vapour phase)	1.27	0.29
9.9 (vapour phase)	2.55	0.57
14.5 (vapour phase)	3.58	0.98
100	8.71	3.80
ALL	11.19	2.43

Table 5.20: Pressure performance of the model at 273.15K

We also compared the behaviour of our model to the VLE data at 273.15K:

Quantity	Maximum Error (%)	Average Error (%)
v_{BP} †	5.12	1.95
v_{DP} †	85.02	40.35
$x_{\mathrm{N_2}}$ †	9.20	3.88
$y_{\mathrm{N_2}}$ †	29.22	18.12
ALL	85.02	16.08
† where convergence to a meaningful solution had been possible		

Table 5.21: VLE performance of the model at 273.15K

The performance of the model at both these temperatures was again seen to be excellent. Here in particular, we can clearly see the effect of having had high quality literature data such as the VLE measurements which were available at 273.15K in [54]. Such data allowed us to achieve a very good fitting and to produce a model which is extremely faithful to the real behaviour of this binary system, often displaying errors under 1% (see Table 5.20). We checked the behaviour of the model at this temperature for consistency in Figures 5.34 to 5.36, and again saw that at low concentrations of oxygen impurity, as can be expected in CCS pipelines [31], an excellent description is given. Following on from this analysis, we generated one final plot at 275K in order to ensure consistent and physical behaviour at other temperatures.

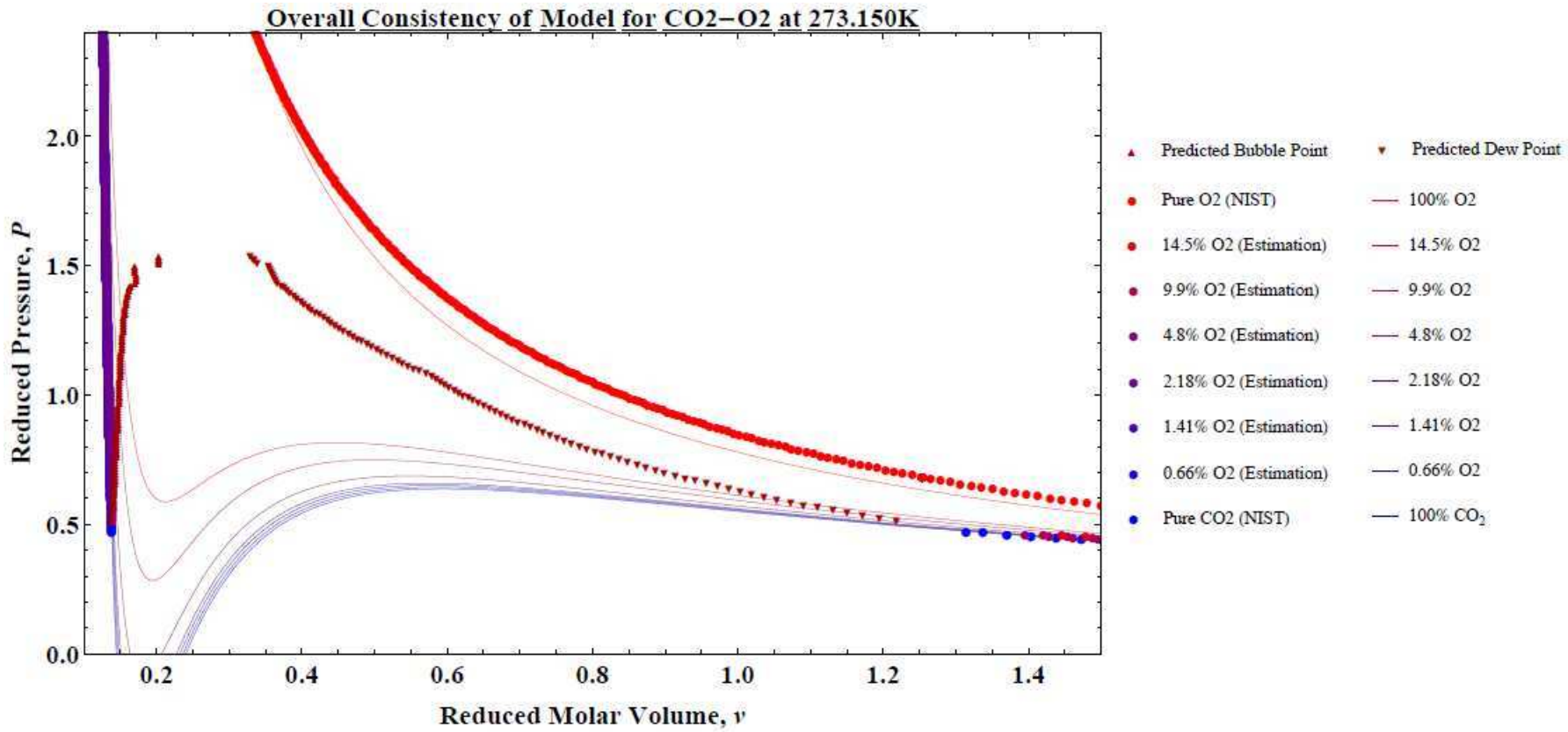

Figure 5.34: Pressure performance of model at 273.15K for carbon dioxide–oxygen

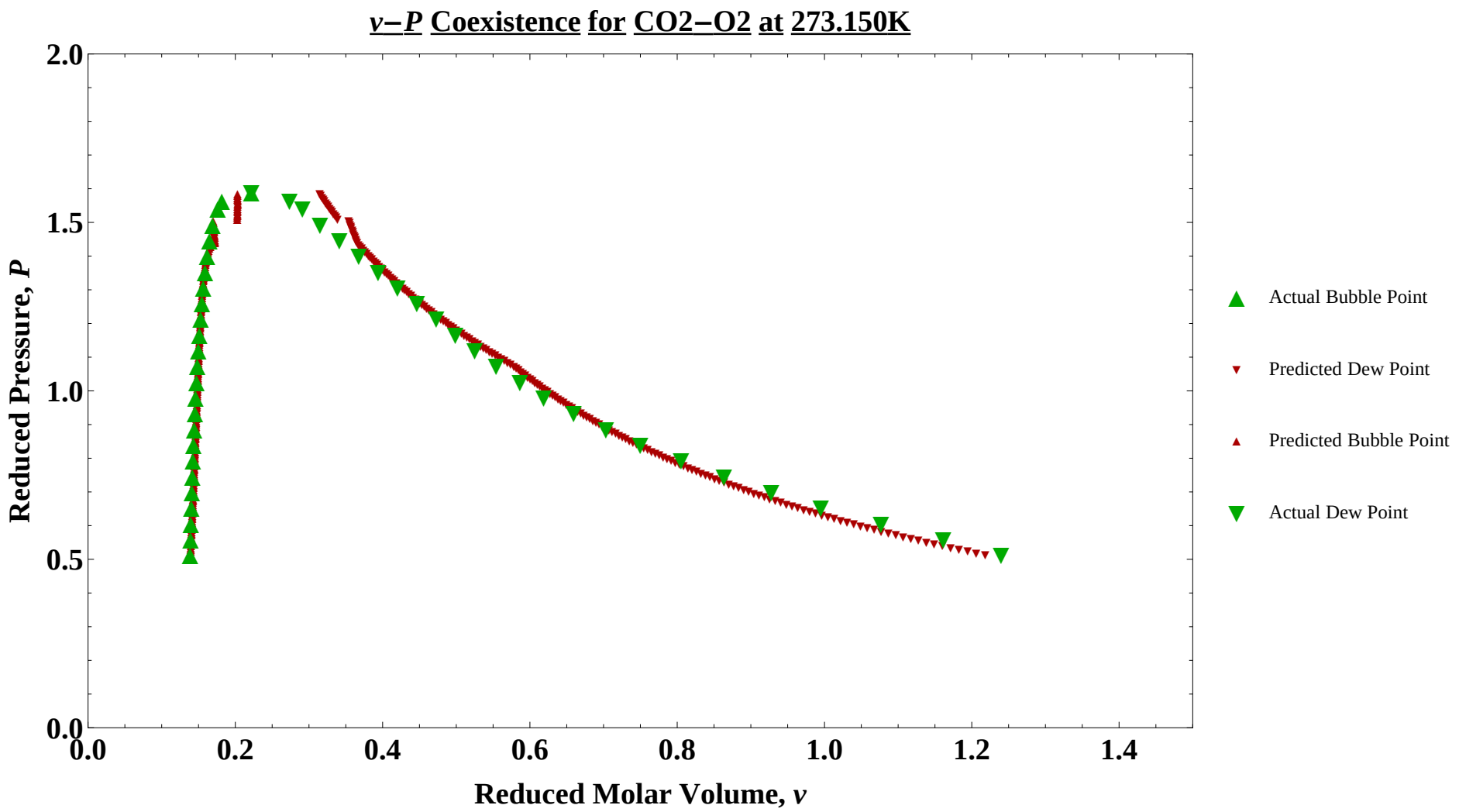

Figure 5.35: VLE coexisting volume performance of model at 273.15K for carbon dioxide–oxygen where a comprehensive data set was available

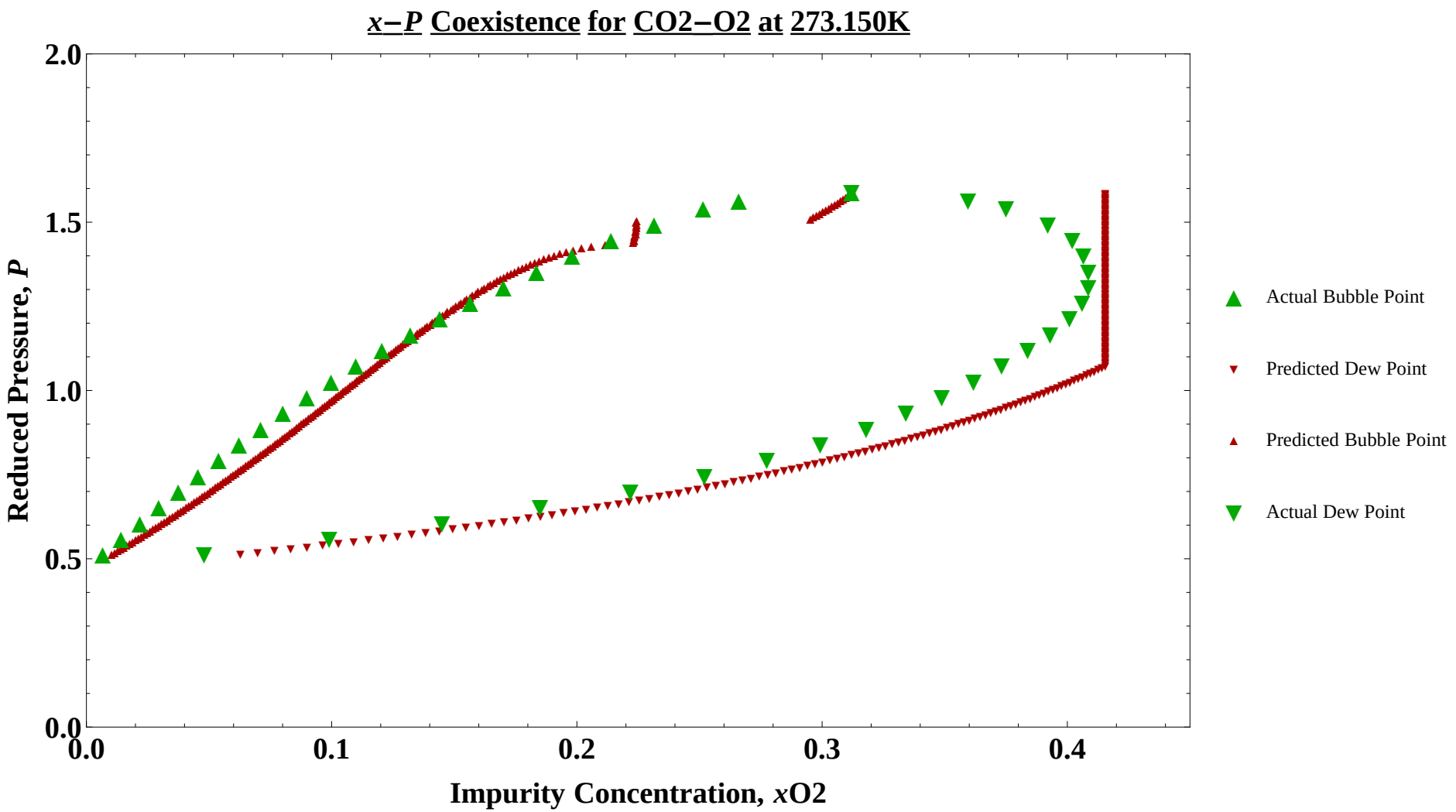

Figure 5.36: VLE coexisting mole fraction performance of model at 273.15K for carbon dioxide–oxygen

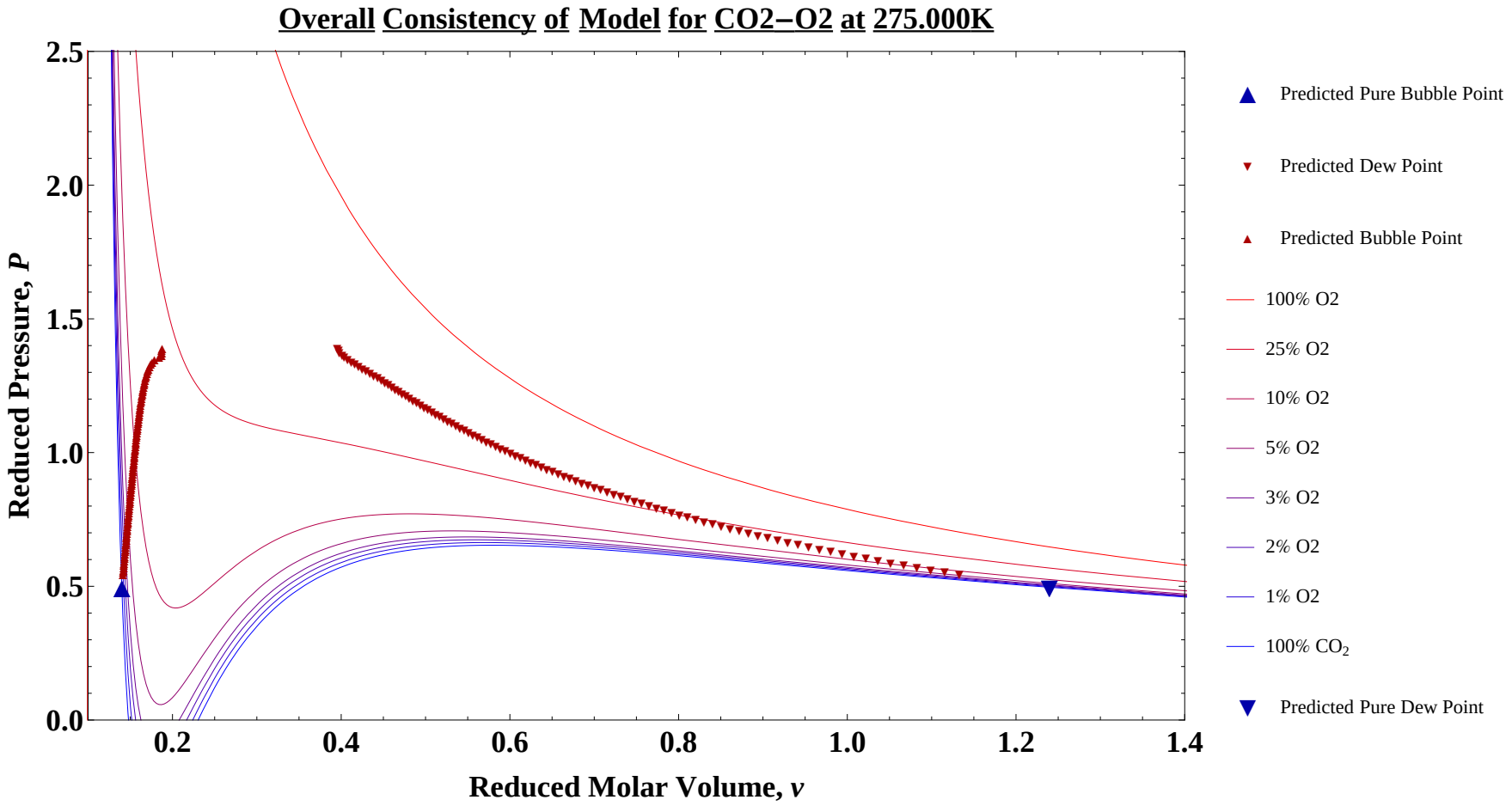

Figure 5.37: Pressure performance of model at 275K for carbon dioxide–oxygen

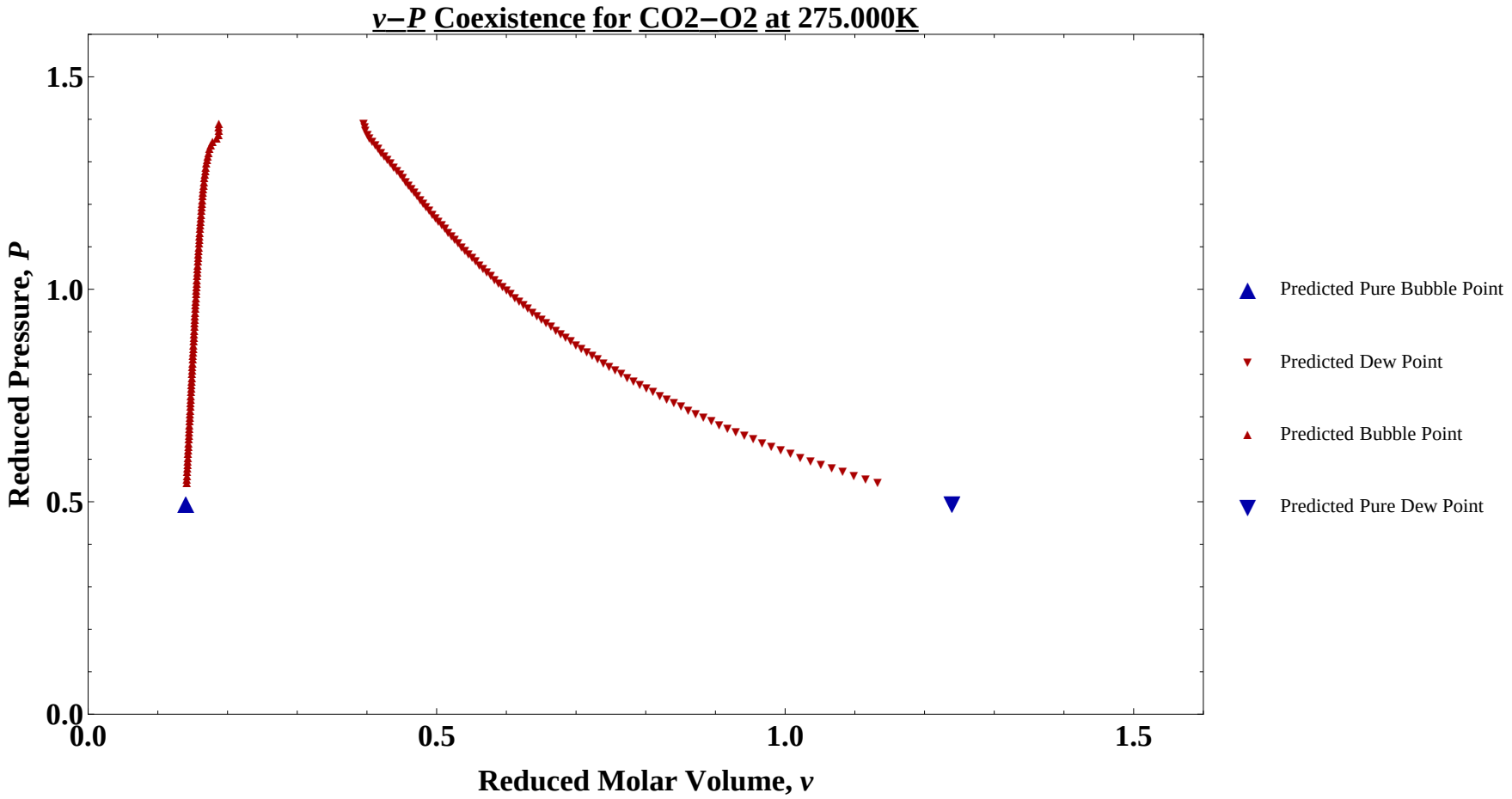

Figure 5.38: VLE coexisting volume performance of model at 275K for carbon dioxide–oxygen

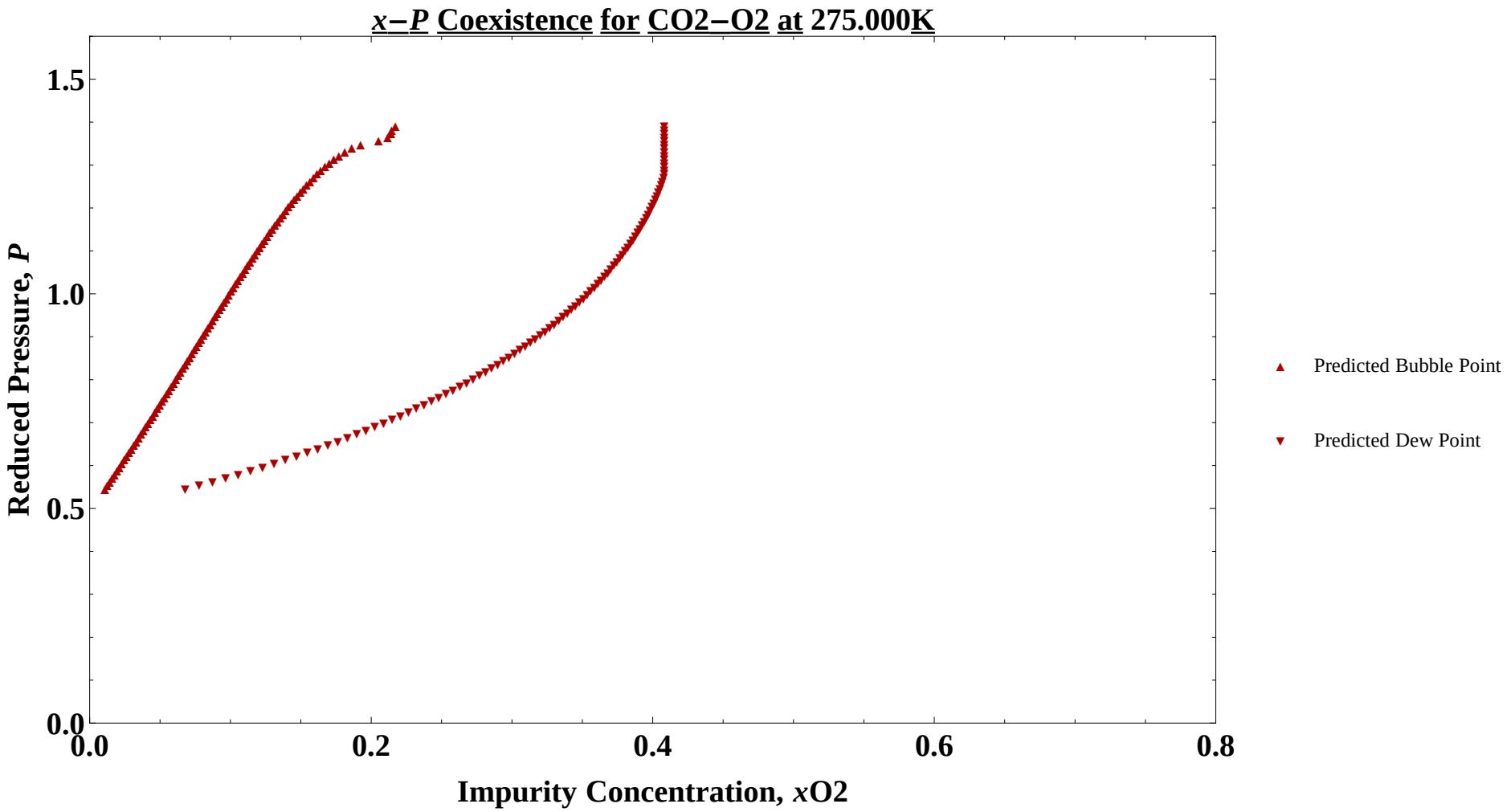

Figure 5.39: VLE coexisting mole fraction performance of model at 275K for carbon dioxide–oxygen

Considering the very limited amount of data we had access to in fitting the carbon dioxide–oxygen model, we felt the performance was again excellent and was further demonstration of the ability of our EoS to predict physical behaviour with a high accuracy. Where the predictions for this mixture were been found to be lacking, specifically in Figures 5.33 and 5.36 where the root finding algorithm for solving to find the VLE fails at some points, we can again attribute this to the lack of middle composition density data which is required to constrain the VLE behaviour close to the critical point. Nevertheless, this capped an excellent performance of our model in reconstructing the binary system of carbon dioxide and oxygen.

Chapter 6

Conclusions and Further Work

6.1 Overview

We set out on this project aiming to develop a new equation of state for use in the design and operation of CCS transport pipelines, which could be relied upon to not be more than 2% out in giving any homogeneous phase density or vapour–liquid equilibrium predictions. Following on from an extensive contextual literature review, we had established that there were many reasons why this was required; principal among them the pressing need for a formulation that would allow users to ensure the pipelines were both safe and cost–effective.

We identified and developed a mathematical method that could be used to calibrate a model which we proposed as part of this work. To allow us to calibrate this proposal into a meaningful equation of state, we began by harvesting a wealth of data for mixtures including homogeneous density and coexistence data from various literature sources and the NIST website.

In the case of pure carbon dioxide we found that the combination of our proposed formulation in Equation (3.9) and the method we had specified in Chapter 2 was able to capture the physical data to a very high degree of accuracy. We had a paper on this part of the work published [40] and in this thesis offered an update that was a slight improvement on this, in terms of accuracy, consistency of behaviour, and of range of validity.

In moving forward to incorporating mixtures to the model we also developed a

formulation relating the fugacity of a substance in a mixture with that of the same substance when in pure form. This allowed us to far more conveniently ensure the correct phase behaviour in fitting the binary data.

There were a number of key outputs from this work:

Firstly, in Equation (3.9) we proposed the formulation for a model which exhibited a high degree of accuracy in describing physical behaviours in the cases where data existed for us to use in fitting the model. We demonstrated the accuracy of our model over the full range of CCS pipeline relevant temperatures and pressures for pure carbon dioxide, as well as in a more limited temperature range in the carbon dioxide–nitrogen binary system, where predictions were seen to be well within the target range. The model also proved extremely useful in reconstructing with great accuracy the behaviour at individual temperature points in the binary systems carbon dioxide–hydrogen and carbon dioxide–oxygen, where a relative lack of data for fitting meant that the same broad accuracy as in the nitrogen case could not be reached, although the predictions still fell broadly within or very close to the target we set. We feel confident that the proposed model could therefore be used throughout the whole range of relevance, if sufficient characterising thermodynamic data were available, specifically middle composition (40-60%) supercritical homogeneous density data, which would constrain the VLE behaviour of the model all the way to the critical point for that mixture at the relevant temperature.

Secondly, we developed a method by which the equation sought in our original aims could be calibrated and developed. Specifically; given a proposed equation in the form $P(v)$ and supplementary mixing rules, we developed a method to obtain all the required fugacity expressions and to fit the model parameters to that data which was available. We utilised this method to fit the proposed model in a range of conditions as allowed by the data we had collected, and we feel confident that once calibrated, our model had the ability to exhibit some very reasonable accuracy. Where suitable data had been available to affect a meaningful fitting, we generally found our models to exhibit errors ranging from 0 to 3% for the two different types of physical predictions.

Thirdly, by way of addressing some of the limitations of the VLE data, we developed a novel method of estimating the molar volumes at the phase boundary where such information had not been reported. We demonstrated the accuracy and suitability of these methods as part of this thesis.

Fourthly, having conducted what we believe to be a thorough review of the thermodynamic data available within the literature, and employed this in the fitting of our model, we are absolutely clear in the reason why we were ultimately unable to finalise the EoS over the whole temperature range. This was because of a lack of sufficient data in the literature which the model could be calibrated to. Specifically, we found that there was an almost total lack of any cases of homogeneous density data being given at the same temperature as VLE data. Furthermore, the majority of the VLE data did not quote the full thermodynamic description, often missing coexisting molar volumes, and so we were not, without some extra insight, able to provide a fitting which simultaneously rendered a useful description of both density and coexistence conditions. Furthermore, we were able, as part of the conclusions of this work, to identify the thermodynamic data which was missing from the literature, and in doing so specify precisely which measurements need to be taken by the CCS community at large in order for our method of calibration to be used. These are highlighted in Section 6.5. If this would be possible, then based on the success of our model and method where data had been available, we felt the aims could be achieved in their entirety.

We have established an effective framework for deriving a new equation of state, calibrating a proposed form to literature data. Our work opens up many new avenues for future research.

6.2 Key Results and Outputs

Chapter 2 highlighted the key physical constraints that needed to be enforced if physically correct behaviour was to be predicted by the model. We specified these for both VLE coexistence conditions, which were imposed at the boundary of the two–phase region, and for the homogeneous density, which were imposed away from the two–phase region in the homogeneous phase. This was in the form of an error function which we could seek to minimise by use of the simulated annealing and local root finding routines programmed in the Mathematica software. We also performed nondimensionalisations of these so that when a nondimensional EoS was presented, these routines could search more easily through the parameter space.

We outlined the features the data had to possess in order to be of any use to us in fitting, and subsequently noted that much of the VLE data presented in the literature was missing a volumetric element at coexistence. In order to compensate for this, we developed a novel method of estimating these values, based on weighted

averages of molar volumes of the carbon dioxide and the second component of the binary mixture being considered. Our methods of volume estimation later proved invaluable in fitting binary mixtures in each of the three cases we worked with.

Chapter 3 saw a proposal of a new, seven–parameter equation of state for use in determining the physical properties of pure CO_2 in the case of pipeline transport for CCS. This would lay the foundation to allow us extend the model into descriptions of the mixture behaviour, as well as to allow us to easily to extend the range of temperatures and pressures if this was deemed necessary. Given our aim of finding an equation which exhibited accuracy superior to the Peng–Robinson Equation of State [34] without necessitating a significant additional functional complexity, we were immediately able to verify that our equation was comparable to the PREoS in terms of complexity, as required. We motivated the form of our equation to allow the reader to confirm that it would render a sufficient flexibility to model the data whilst retaining a faithfulness to the broad physical behaviours that are to be expected.

In Chapter 4 we fitted the seven model parameters to the carbon dioxide data taken from NIST, itself calculated using the Span–Wagner Equation of State [35]. This data came in the form of homogeneous phase volume–pressure isotherms and pure carbon dioxide two–phase boundary volumes and vapour pressures. We deployed the methodologies outlined in Chapter 2 to find values for the seven parameters which would allow the model to most closely match the behaviour given by the NIST data. For fitting the critical temperature isotherm, a strong emphasis was placed on excellent agreement with the pressure (density) data to ensure qualitative behaviour was described accurately, including an excellent estimation of the critical point itself and of the density data either side of the critical volume. The variation of each parameter with temperature was obtained through a sequence of small perturbations in temperature, followed by recalibration of the parameters through local root finding at the new temperature. The disagreement with the pressure and coexistence data was also measured at each subsequent temperature to ensure we had generated a minimum of the error function in which the proposed equation closely resembled the behaviour described by the NIST database. This allowed us to formulate the temperature dependence of each parameter, and in this way the model for describing pure carbon dioxide was finalised. The performance of the model in this case was seen to be well within our aims and we had a paper on this stage of the work published [40] in early 2013.

In Chapter 5 we carried out the fitting to the various mixture data we had col-

lected for the three binary systems we were targeting. We were able to perform the fitting with a high degree of accuracy at a range of temperature points, and as a result draw up a temperature dependence for each model parameter between these temperatures. In doing so, we were able to show that the overall behaviour of the model between and in the vicinity of points at which a fitting had been possible was very good, and we took confidence from this as it showed that our equation was powerful enough to capture the behaviour of these binary mixtures where such data existed.

For the carbon dioxide–nitrogen fitting, we could start to see some of the implications of the current state of the literature data. Indeed, of the five temperature points at which VLE data was available for this mixture, only two of them within the relevant temperature range also had homogeneous mixture density data to allow us to conduct a fitting. This had previously necessitated the development of our methods for coexisting volume estimation and homogeneous density estimation.

In extending the work to the carbon dioxide–hydrogen mixture, we again faced difficulties: There were only two temperature points at which VLE data containing the full array of thermodynamic information was given, one of these being below the range of interest. Furthermore, there were no temperatures at which both homogeneous mixture density and VLE data, whether with volumes or not, existed. Without our volume estimation technique, we would therefore have only been able to fit a single temperature point in a meaningful way. At this temperature, the model was found to give an excellent description of the behaviour, and using the estimation techniques we were able to get acceptable descriptions at some other temperature points.

The carbon dioxide–oxygen binary mixture data was in a similar state. This time there was only a single temperature point at which the full array of VLE information was given, and again, no temperature points at which both VLE and homogeneous density data simultaneously existed. At the few temperature points at which we had been able to perform a fitting, these were again found to be very good.

6.3 Strengths of the Proposed Model

As we can see from Tables 4.2, 4.3, and Figure 4.32, our proposed equation of state appeared to have great potential when compared directly with the PREoS, even though it possessed only slight extra functional complexity. It gave a consistently

superior description of the pressure–density behaviour throughout the CCS–relevant temperature range, which we found to be very close to that of the SWEoS at all but a few points. It also gave, even in the worst cases, a comparably accurate description of the phase behaviour to the PREoS, although usually far superior. For descriptions of the bubble line, which we considered to be the more important consideration for CCS pipeline transport, the predictions were significantly better than the PREoS at all times, again approaching the SWEoS in terms of accuracy in some places.

From our analysis, it seemed the only place the proposed model did not match the high standard exhibited elsewhere was in the immediate vicinity of the critical point. As had been demonstrated in our paper, the model had flexibility to predict the critical point exactly, but this came at the cost of a worse performance around the critical point, so for this thesis we deliberately imposed a high tariff on the model exhibiting a generally more consistent behaviour. The table and figures would seem to suggest that there was nowhere in the window 260–335K, 1–200bar where the PREoS described the pressure behaviour more accurately than the proposed EoS. Moreover, the dominance of the proposed equation suggested that we had established an excellent starting point from which to extend this model to descriptions of physical behaviour of CCS–relevant mixtures.

For creating descriptions of the binary mixtures in those cases where we had been able to perform a fitting to a more comprehensive data set, superior agreements, such as in the case of the oxygen mixture at 273.15K were gained. When possible, we found the average percentage errors to fall within or very close to our target range. This was a sign that we had proposed both a model that had sufficient scope to achieve the aims, and a method by which to develop and calibrate it.

A further strength of the methods we used to develop our model was that they are general enough to allow scope for new data to be incorporated at the fitting stage as and when it becomes available. This generality means that we would expect our method to allow the proposed model to be continually refined and updated as new data is published.

6.4 Limitation of the Proposed Model

We are clear that the proposed model did not generalise to all temperatures within the range of interest for binary mixtures. Nevertheless, we were able to clearly

identify why this was the case, and in Section 6.5 we suggest actions that could be taken to further the work we have done. The development of auxiliary methods such as that for the estimation of volumes at the phase boundary and that relating pure and mixture fugacities would enable this to be done. As such, we are confident that we have put everything in place so that once the correct thermodynamic data becomes available, our methods can be employed exactly as prescribed in this thesis to bring about the equation of state currently needed for understanding CCS pipeline transport.

6.5 Future Work

We are confident that the the work we have carried out in this EngD makes a major contribution towards furthering the understanding of the physical behaviour of CO_2–rich mixtures as relevant to CCS pipeline transport.

We suggest the following tasks which could be carried out, either in progression of this work, or generally for the deepening of understanding in this area. To begin with, the following important thermodynamic measurements could be conducted:

- CO_2–N_2: A range of homogeneous density–pressure measurements in the liquid phase upto a pressure of 80MPa at 303.3K and 301.3K (to complement the VLE data given in [91]), 298.15K (to complement the partial VLE data given in [104]), 293.3K (to complement the partial VLE data given in [106]), 273.15K (to complement the VLE data given in [54]), and at 270K (to complement the partial VLE data given in [98]). These should be carried out at a range of nitrogen compositions up to 50%. Also needed are the volumetric measurements to complement the currently available VLE data in which volumes are not quoted.

- CO_2–H_2: A range of homogeneous density–pressure measurements in the liquid phase upto a pressure of 80MPa at 298.15K (to complement the VLE data given in [90]), 290K, 280K, 270K, and 260K (to complement the partial VLE data given in [110]), at a range of nitrogen compositions, and the missing VLE volumes in these cases.

- CO_2–O_2: Phase boundaries at a range of temperatures between 303.22K and 283.15K to complement the homogeneous density data given in [109] and to bridge the large gap to the data at 283.15K in [112]. Also a range of homogeneous density–pressure measurements in the liquid phase upto a pressure of 80MPa at 283.15K (to complement the partial VLE data given in [112]),

273.15K (to complement the VLE data given in [54]), and 263.15K (to complement the partial VLE data given in [112]).

The above measurements are suggested as this would then give a vast increase in the amount of relevant thermodynamic data which the model parameters could be fit to. In light of the suggested measurements, this would be particularly true throughout the range of temperatures and pressures identified throughout this work as being of particular relevance. The fitted parameter values would then have been allowed to take account for describing both types of behaviour, and owing to the relatively small temperature jumps between each measurement, a suitable temperature dependence could be fit to the parameters in each case. With this having been done, it would then be possible to finalise the original aims set out at the start of this work. We highlight that the methods described in this thesis can be used to generate the full binary model descriptions.

A further potential spin–off from this project as a substitute for the suggestion of certain experimental measurements being taken would be to generate these data by using molecular simulation techniques [113]. The advantage of this would be that such methods are less costly, time–consuming, and resource intensive than acquiring laboratory equipment, setting up, and physically taking measurements, and there is seen to be a good performance of such methods. This could produce the data which would then allow for an improved fitting of our model. As a slight generalisation to this approach, we feel that another substitute to the volume estimation techniques we developed could be introduced by allowing the optimisation algorithms discussed in Chapter 2 to find values for the missing VLE volumes alongside its search for the model parameters. This would require significant computing power however, as we found that the ability of simulated annealing to find relevant optima diminished very quickly as the number of parameters grew towards ten and beyond.

Subsequently, there is then also a clear need for the equation of state to give descriptions for mixtures containing more than two components. Our work has opened the door to the generalisation to ternary mixture descriptions, and can again act as a very solid foundation for this research, in particular, the methods for developing and relating fugacity expressions would be useful in calculating the VLE properties of such systems.

As the model is developed and the number of mixture components it is able to describe grows, there is also the possibility that our model should be expanded to incorporate the other chemical impurities present in the CCS chain, such as SO_x,

NO_x, Ar, Hg, and others. Discussion with fellow researchers and experts in this field at conferences confirm there would be demand to drive this development.

Another way in which we felt our work could be continued past the conclusion of this EngD is if the beginning–to–end method we have employed using Wolfram Mathematica could be automated into a single executable programme. The ultimate aim of this expansion would be to allow the proposal of a functional form such as Equation (3.9) and some mixing rules such as equation (5.35), with supplementary homogeneous density and VLE data, of the type specified in the list above, to be processed automatically, as opposed to manually, such as in the methods used in this work, into a usable model. This would give the output of a fully–fledged equation of state much more quickly. The method would carry out fitting at all the temperature points simultaneously, as opposed to one–by–one as was done here, and could incorporate assurances that each model parameter varied smoothly with temperature by imposing high penalties in the error function for high parameter curvature with temperature.

We felt that, whereas our methods of volume estimation were suitable to our needs of creating a framework on which to build the model, that this could also be developed in order to improve accuracy. In particular, some investigation into the role and definition of the quantities ξ_{BP}, ξ_{DP}, and χ_{DP}, introduced in Chapter 5 could be carried out, as there may be applications of this method in other areas of chemistry or thermodynamics.

These are all natural steps to take in continuing the work we have conducted for this EngD.

6.6 Applications of this EngD Research Project

As discussed at length in Chapter 1, there is a pressing need for an equation of state which can simultaneously give accurate descriptions of the thermodynamic behaviour of mixtures of carbon dioxide and impurities whilst also exhibiting sufficient user–friendliness to be employed without restriction. Our project has established a new formulation which we have demonstrated has the flexibility and power to give excellent descriptions of a wide range of behaviours, whilst maintaining enough simplicity for the equation itself to be written on a single line. The requirement for this new equation of state stemmed from the lack of certainty in designing and operating carbon dioxide pipelines for Carbon Capture and Storage. It is our con-

tention that the work presented here, both as it stands and in terms of what it can be developed into has a very direct application to this task. The accuracy the model demonstrated in places where fittings had been possible was such that we feel comfortable in claiming that it can be utilised in the calculation of physical quantities with sufficient accuracy. This is especially so in light of the obvious simplicity of the model we proposed.

With this, and the possible future work highlighted in Section 6.5 as being a direct spin–off of this project, the applications could reach further perhaps than CCS pipelines. The model itself could be implemented in any process in which pressurised carbon dioxide is handled, for example in some other branches of manufacturing such as in the storage stage of CCS, or the food and beverage industry [114]. The methods will potentially have an application to the modelling of many fluid substances in many circumstances.

6.6.1 Industrial Relevance

The link between our work and its intended purpose means there is a clear industrial relevance. We feel this is a key output from this EngD project, in which there is a particular requirement for an industrial focus. Whereas there is room for development of the methods we established, the model itself could be implemented in the CCS industry under very certain conditions immediately, and for cases in which the modelling of pure carbon dioxide is required.

The industrial relevance of our work is not limited to the uses of the proposed equation itself however, as the methods presented here will facilitate investigation into other equations of state, particularly if the future work generalising our methods to ternary mixtures, and automation of the whole process, can be achieved. The clarity of the relations between different fugacity constraints in particular mean that whenever VLE is being investigated, parts of our method can be employed to allow for a more convenient appointment of the outputs required by the user.

Finally, the list of thermodynamic measurements we suggested should itself give focus to those who are in a position to carry them out in producing outputs of relevance to the CCS industry.

6.6.2 Academic Relevance

Despite the focus on industrial benefits inherent to the EngD, there are also a number of academic relevancies of our work. First and foremost, the headway made in understanding how equations of state can be developed that has come about from this work is significant. We feel that we have offered real insight into the behaviour of carbon dioxide mixtures and have pushed forward the boundaries of knowledge in this regard. Through our auxiliary methods we have also offered increased understanding in many areas surrounding that of the physical behaviour of substances.

As an EngD project, there have been, as is to be expected, many tough times in the production of the outputs presented in this thesis. Not least the struggles with manually developing a method for fitting model parameters to physical descriptions. In refining our methods to reduce these struggles and improve flexibility further, we feel that several academic projects can be created as a result. Investigation into, and improvements of our volume estimations, for example, could make for a good Undergraduate or Masters'–level research project, whilst the effect of different equation of state formulations or mixing rules could make for a good follow–up EngD or PhD project, and the automation of the whole process developed here a good and worthwhile post–doc project for someone with the correct programming expertise. All of these would have very useful industrial, commercial and academic consequences.

6.7 Final Thoughts

We set out initially to develop a new equation of state. It quickly became clear during the early days of the project that knowledge surrounding this area was low, and that equations of state which were available did not meet the specifications of CCS pipeline transport. Our aims thus expanded to include a formalisation of the method by which an equation of state can be generated from first principles, and following on from this, we made several important breakthroughs which will have a clear use in both their intended and other areas. As a result of the relative simplicity coupled with the demonstrated performance of the proposed model, we felt that the work conducted as part of this EngD represented a clear step forward in modelling the physical properties of fluid mixtures with an equation of state.

As atmospheric levels of carbon dioxide rise along with continuing dependence on fossil fuels to power the industry which has brought about phenomenal improvements in standards of living; including science and technology, agriculture, transport and

many other areas since the industrial revolution, there have been clear mandates set out, ensuring that this rise cannot do increasing long–term damage to the environment we are so dependent upon. Carbon Capture and Storage is a strategy that promises to reduce the emissions of carbon dioxide, thus minimising the environmental impacts of the methods of energy extraction that support our way of life.

Although many obstacles still stand in the way of CCS being implemented on the required scale, the many usable results presented in this thesis and the possible spin–offs should go some way to helping overcome some of these. In "Modelling CO_2 Transport and the Effect of Impurities", and through proposing "A New Equation of State for CCS Pipeline Transport", we hope that our contribution to one small part of a very large and complicated problem can be of some use.

Chapter 7

Appendices

7.1 A Summary of Literature Thermodynamic Data Used for Fitting

7.1.1 Carbon Dioxide–Nitrogen VLE Data

P (MPa)	v_{Bub} (m^3mol^{-1})	v_{Dew} (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	y_{CO_2}	y_{N_2}	Usable Data Point?
0.600	—	—	220	1.0000	0.0000	1.0000	0.0000	Vol. Est.
1.509	—	—	220	0.9868	0.0132	0.4482	0.5518	Vol. Est.
3.075	—	—	220	0.9638	0.0362	0.2577	0.7423	Vol. Est.
4.595	—	—	220	0.9399	0.0601	0.2026	0.7974	Vol. Est.
6.313	—	—	220	0.9117	0.0883	0.1786	0.8214	Vol. Est.
8.258	—	—	220	0.8791	0.1209	0.1719	0.8281	Vol. Est.
11.114	—	—	220	0.8258	0.1742	0.1835	0.8165	Vol. Est.
12.432	—	—	220	0.7984	0.2016	0.1972	0.8028	Vol. Est.
13.796	—	—	220	0.7676	0.2324	0.2131	0.7869	Vol. Est.
15.506	—	—	220	0.7229	0.2771	0.2484	0.7516	Vol. Est.
16.706	—	—	220	0.6845	0.3155	0.2785	0.7215	Vol. Est.
1.287	—	—	240	1.0000	0.0000	1.0000	0.0000	Vol. Est.
2.100	—	—	240	0.9871	0.0129	0.6688	0.3312	Vol. Est.
3.208	—	—	240	0.9693	0.0307	0.4849	0.5151	Vol. Est.
4.089	—	—	240	0.9546	0.0454	0.4110	0.5890	Vol. Est.
5.674	—	—	240	0.9266	0.0734	0.3428	0.6572	Vol. Est.
6.262	—	—	240	0.9162	0.0838	0.3290	0.6710	Vol. Est.
7.235	—	—	240	0.8978	0.1022	0.3127	0.6873	Vol. Est.
8.590	—	—	240	0.8703	0.1297	0.3019	0.6981	Vol. Est.
9.945	—	—	240	0.8408	0.1592	0.3008	0.6992	Vol. Est.
10.728	—	—	240	0.8225	0.1775	0.3040	0.6960	Vol. Est.
11.466	—	—	240	0.8042	0.1958	0.3103	0.6897	Vol. Est.
12.225	—	—	240	0.7835	0.2165	0.3194	0.6806	Vol. Est.
12.659	—	—	240	0.7704	0.2296	0.3255	0.6745	Vol. Est.
13.865	—	—	240	0.7304	0.2696	0.3483	0.6517	Vol. Est.
14.472	—	—	240	0.7056	0.2944	0.3712	0.6288	Vol. Est.
15.424	—	—	240	0.6509	0.3491	0.4071	0.5929	Vol. Est.
15.768	—	—	240	0.6184	0.3816	0.4367	0.5633	Vol. Est.
16.147	—	—	240	0.5223	0.4777	0.4798	0.5202	Vol. Est.

Data summarised from Table II of AlSahhaf83 [115]

P (MPa)	v_{Bub} (m^3mol^{-1})	v_{Dew} (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	y_{CO_2}	y_{N_2}	Usable Data Point?
6.205	—	—	230	0.9188	0.0812	0.2527	0.7473	Vol. Est.
8.619	—	—	230	0.8638	0.1362	0.2340	0.7660	Vol. Est.
9.652	—	—	230	0.8545	0.1455	0.2402	0.7598	Vol. Est.
8.963	—	—	250	0.8606	0.1394	0.3858	0.6142	Vol. Est.
10.342	—	—	250	0.8233	0.1767	0.3838	0.6162	Vol. Est.

Data summarised from TABLE 1 of AlSahhaf90 [116]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
6.88	—	—	301.3	1.0000	0.0000	1.0000	0.0000	Vol. Est.
7.22	67.2	139	301.3	0.9931	0.0069	0.9848	0.0152	Yes
7.33	68.3	132	301.3	0.9899	0.0101	0.9794	0.0206	Yes
7.61	69.6	122	301.3	0.9818	0.0182	0.9674	0.0326	Yes
7.90	74	114	301.3	0.9742	0.0258	0.9610	0.0390	Yes
8.01	81.3	106	301.3	0.9652	0.0348	0.9611	0.0389	Yes
8.05	90.7	90.7	301.3	0.9621	0.0379	0.9621	0.0379	Yes
7.27	86.2	138	303.3	0.9987	0.0013	0.9977	0.0023	Yes
7.44	74	128	303.3	0.9940	0.0060	0.9904	0.0096	Yes
7.53	75.8	125	303.3	0.9914	0.0086	0.9867	0.0133	Yes
7.54	75.7	122	303.3	0.9910	0.0090	0.9864	0.0136	Yes
7.61	77.2	118	303.3	0.9893	0.0107	0.9847	0.0153	Yes
7.73	81.9	108	303.3	0.9853	0.0147	0.9811	0.0189	Yes
7.79	90	90	303.3	0.9816	0.0184	0.9816	0.0184	Yes

Data summarised from TABLE 2 of Bian93 [91]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
2.4216675	0.000634	—	253.15	—	—	0.868	0.132	No
2.5432575	0.000647	—	253.15	—	—	0.826	0.174	No
2.9080275	0.00055	—	253.15	—	—	0.757	0.243	No
3.6375675	0.000437	—	253.15	—	—	0.653	0.347	No
4.7521425	0.000336	—	253.15	—	—	0.566	0.434	No
6.8293050	0.000223	—	253.15	—	—	0.466	0.534	No
8.8456725	—	—	253.15	—	—	0.432	0.568	No
8.9773950	0.0000445	—	253.15	0.868	0.132	—	—	No
10.6188600	0.0000459	—	253.15	0.826	0.174	—	—	No
11.5510500	—	—	253.15	—	—	0.432	0.568	No
12.7872150	0.0000496	—	253.15	0.757	0.243	—	—	No
13.1114550	—	0.0000934	253.15	—	—	0.466	0.534	No
14.3172225	0.0000572	—	253.15	0.653	0.347	—	—	No
14.3577525	—	0.0000687	253.15	—	—	0.566	0.434	No
3.4957125	—	0.000445	273.15	—	—	1.000	0.000	No
3.5058450	0.0000476	—	273.15	1.000	0.000	—	—	No
3.9111450	—	0.000396	273.15	—	—	0.929	0.071	No
4.3063125	—	0.00036	273.15	—	—	0.872	0.128	No
5.7349950	—	0.000253	273.15	—	—	0.746	0.254	No
6.6063900	—	0.000221	273.15	—	—	0.694	0.306	No
7.1130150	0.0000489	—	273.15	0.929	0.071	—	—	No
8.7544800	—	0.000155	273.15	—	—	0.633	0.367	No
9.4536225	0.0000519	—	273.15	0.872	0.128	—	—	No
10.8924375	—	0.000109	273.15	—	—	0.633	0.367	No
11.8043625	0.0000669	0.000081	273.15	0.746	0.254	0.694	0.306	No
5.0966475	—	0.000272	288.15	—	—	1.000	0.000	No
5.1169125	0.0000531	—	288.15	1.000	0.000	—	—	No
5.6944650	—	0.000239	288.15	—	—	0.940	0.060	No
6.2517525	—	0.000213	288.15	—	—	0.897	0.103	No
6.7381125	—	0.000195	288.15	—	—	0.868	0.132	No
7.1839425	—	0.000178	288.15	—	—	0.845	0.155	No
7.5892425	—	0.000166	288.15	—	—	0.827	0.173	No
7.7817600	0.0000567	—	288.15	0.940	0.060	—	—	No
8.1060000	—	0.00015	288.15	—	—	0.812	0.188	No
8.3289150	—	0.000143	288.15	—	—	0.806	0.194	No
8.5113000	—	0.000137	288.15	—	—	0.801	0.199	No
9.0685875	—	0.000118	288.15	—	—	0.798	0.202	No
9.0888525	0.0000625	—	288.15	0.897	0.103	—	—	No
9.4637550	—	0.000107	288.15	—	—	0.801	0.199	No
9.5752125	—	0.000102	288.15	—	—	0.806	0.194	No
9.6258750	0.00007	—	288.15	0.868	0.132	—	—	No
9.6664050	—	0.0000974	288.15	—	—	0.812	0.188	No
9.7575975	0.0000785	0.0000879	288.15	0.845	0.155	0.827	0.173	No

Data summarised from Table 1 of Arai71 [53]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
1.784	—	—	250	1.0000	0.0000	1.0000	0.0000	Vol. Est.
2.599	—	—	250	0.9864	0.0136	0.7439	0.2561	Vol. Est.
3.688	—	—	250	0.9669	0.0331	0.5761	0.4239	Vol. Est.
4.589	—	—	250	0.9512	0.0488	0.4999	0.5001	Vol. Est.
5.541	—	—	250	0.9336	0.0664	0.4506	0.5494	Vol. Est.
6.597	—	—	250	0.9130	0.0870	0.4151	0.5849	Vol. Est.
7.532	—	—	250	0.8931	0.1069	0.3951	0.6049	Vol. Est.
9.632	—	—	250	0.8468	0.1532	0.3777	0.6223	Vol. Est.
11.151	—	—	250	0.8069	0.1931	0.3837	0.6163	Vol. Est.
11.936	—	—	250	0.7827	0.2173	0.3937	0.6063	Vol. Est.
13.416	—	—	250	0.7292	0.2708	0.4273	0.5727	Vol. Est.
14.066	—	—	250	0.6992	0.3008	0.4563	0.5437	Vol. Est.
3.200	—	—	270	1.0000	0.0000	1.0000	0.0000	Vol. Est.
4.857	—	—	270	0.9684	0.0316	0.7577	0.2423	Vol. Est.
6.084	—	—	270	0.9439	0.0561	0.6691	0.3309	Vol. Est.
7.650	—	—	270	0.9099	0.0901	0.6058	0.3942	Vol. Est.
9.102	—	—	270	0.8721	0.1279	0.5795	0.4205	Vol. Est.

Data summarised from Table 1 of Brown89–I [95]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
0.492	—	—	220	1.0000	0.0000	1.0000	0.0000	Vol. Est.
1.012	—	—	220	—	—	0.6285	0.3715	No
1.094	—	—	220	—	—	0.5874	0.4126	No
1.195	—	—	220	—	—	0.5452	0.4548	No
1.373	—	—	220	0.9892	0.0108	0.4826	0.5174	Vol. Est.
1.675	—	—	220	—	—	0.4080	0.5920	No
1.751	—	—	220	—	—	0.3946	0.6054	No
1.795	—	—	220	—	—	0.3864	0.6136	No
2.016	—	—	220	—	—	0.3521	0.6479	No
2.363	—	—	220	—	—	0.3124	0.6876	No
2.457	—	—	220	0.9731	0.0269	0.3029	0.6971	Vol. Est.
3.444	—	—	220	—	—	0.2402	0.7598	No
3.465	—	—	220	—	—	0.2390	0.7610	No
3.775	—	—	220	—	—	0.2263	0.7737	No
4.029	—	—	220	—	—	0.2179	0.7821	No
5.207	—	—	220	—	—	0.1919	0.8081	No
5.270	—	—	220	—	—	0.1906	0.8094	No
5.313	—	—	220	—	—	0.1904	0.8096	No
5.466	—	—	220	—	—	0.1886	0.8114	No
5.985	—	—	220	—	—	0.1818	0.8182	No
5.993	—	—	220	0.9170	0.0830	0.1850	0.8150	Vol. Est.
6.746	—	—	220	—	—	0.1768	0.8232	No
7.111	—	—	220	—	—	0.1747	0.8253	No
7.143	—	—	220	—	—	0.1750	0.8250	No
7.151	—	—	220	—	—	0.1744	0.8256	No
7.281	—	—	220	—	—	0.1745	0.8255	No
7.310	—	—	220	—	—	0.1742	0.8258	No
7.485	—	—	220	0.8908	0.1092	0.1738	0.8262	Vol. Est.
7.910	—	—	220	—	—	0.1732	0.8268	No
8.625	—	—	220	—	—	0.1734	0.8266	No
9.098	—	—	220	0.8662	0.1338	0.1736	0.8264	Vol. Est.
9.198	—	—	220	—	—	0.1742	0.8258	No
10.320	—	—	220	—	—	0.1792	0.8208	No
10.460	—	—	220	—	—	0.1801	0.8199	No
10.894	—	—	220	—	—	0.1830	0.8170	No
11.311	—	—	220	—	—	0.1864	0.8136	No
11.478	—	—	220	—	—	0.1882	0.8118	No
11.968	—	—	220	—	—	0.1924	0.8076	No
11.995	—	—	220	0.8097	0.1903	0.1920	0.8080	Vol. Est.
12.677	—	—	220	—	—	0.2009	0.7991	No
12.962	—	—	220	—	—	0.2036	0.7964	Vol. Est.
3.202	—	—	270	1.0000	0.0000	0.0000	0.0000	Vol. Est.
4.334	—	—	270	—	—	0.8170	0.1830	No
4.686	—	—	270	—	—	0.7788	0.2212	No
5.074	—	—	270	—	—	0.7435	0.2565	No
5.779	—	—	270	0.9502	0.0498	0.6913	0.3087	Vol. Est.
5.860	—	—	270	—	—	0.6861	0.3139	No
6.182	—	—	270	0.9434	0.0566	0.6678	0.3322	Vol. Est.
6.436	—	—	270	—	—	0.6544	0.3456	No
7.165	—	—	270	0.9230	0.0770	0.6253	0.3747	Vol. Est.
7.289	—	—	270	—	—	0.6215	0.3785	No
7.546	—	—	270	0.9139	0.0861	0.6121	0.3879	Vol. Est.
7.766	—	—	270	—	—	0.6070	0.3930	No
8.289	—	—	270	0.8945	0.1055	0.5951	0.4049	Vol. Est.
8.476	—	—	270	0.8910	0.1090	0.5905	0.4095	Vol. Est.
9.001	—	—	270	0.8770	0.1230	0.5852	0.4148	Vol. Est.
9.283	—	—	270	—	—	0.5824	0.4176	No
9.586	—	—	270	0.8612	0.1388	0.5814	0.4186	Vol. Est.
9.618	—	—	270	—	—	0.5796	0.4204	No
10.193	—	—	270	0.8428	0.1572	0.5808	0.4192	Vol. Est.
10.393	—	—	270	—	—	0.5826	0.4174	No

Data summarised from TABLE 1 of Brown89–II [96]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
3.48530	0.00004735	0.0004505	273.15	1.0000	0.0000	1.0000	0.0000	Yes
3.79212	0.00004760	0.0004240	274.15	0.9942	0.0058	0.9470	0.0530	Yes
4.13685	0.00004788	0.0003970	275.15	0.9878	0.0122	0.8970	0.1030	Yes
4.48159	0.00004816	0.0003700	276.15	0.9810	0.0190	0.8550	0.1450	Yes
4.82633	0.00004845	0.0003430	277.15	0.9745	0.0255	0.8190	0.1810	Yes
5.17107	0.00004875	0.0003160	278.15	0.9680	0.0320	0.7905	0.2095	Yes
5.51581	0.00004805	0.0002920	279.15	0.9610	0.0390	0.7640	0.2360	Yes
5.86054	0.00004940	0.0002690	280.15	0.9540	0.0460	0.7393	0.2607	Yes
6.20528	0.00004970	0.0002520	281.15	0.9465	0.0535	0.7164	0.2836	Yes
6.55002	0.00005005	0.0002380	282.15	0.9393	0.0607	0.6962	0.3038	Yes
6.89476	0.00005040	0.0002260	283.15	0.9315	0.0685	0.6782	0.3218	Yes
7.23950	0.00005080	0.0002130	284.15	0.9236	0.0764	0.6634	0.3366	Yes
7.58423	0.00005118	0.0002020	285.15	0.9142	0.0858	0.6516	0.3484	Yes
7.92897	0.00005158	0.0001910	286.15	0.9057	0.0943	0.6412	0.3588	Yes
8.27371	0.00005200	0.0001810	287.15	0.8970	0.1030	0.6325	0.3675	Yes
8.61845	0.00005240	0.0001710	288.15	0.8885	0.1115	0.6261	0.3739	Yes
8.96318	0.00005288	0.0001620	289.15	0.8798	0.1202	0.6210	0.3790	Yes
9.30792	0.00005338	0.0001550	290.15	0.8703	0.1297	0.6175	0.3825	Yes
9.65266	0.00005395	0.0001470	291.15	0.8610	0.1390	0.6148	0.3852	Yes
9.99740	0.00005460	0.0001390	292.15	0.8508	0.1492	0.6140	0.3860	Yes
10.34214	0.00005545	0.0001310	293.15	0.8393	0.1607	0.6158	0.3842	Yes
10.68687	0.00005660	0.0001230	294.15	0.8253	0.1747	0.6200	0.3800	Yes
11.03161	0.00005820	0.0001150	295.15	0.8098	0.1902	0.6274	0.3726	Yes
11.37635	0.00006045	0.0001060	296.15	0.7905	0.2095	0.6384	0.3616	Yes
11.72109	0.00006375	0.0000960	297.15	0.7640	0.2360	0.6572	0.3428	Yes
11.89346	0.00006760	0.0000882	298.15	0.7432	0.2568	0.6776	0.3224	Yes
11.99688	0.00007750	0.0000775	299.15	0.7074	0.2926	0.7074	0.2926	Yes

Data summarised from Table III of Muirbrook64 [54]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
3.1988306	—	—	270	1.0000	0.0000	1.0000	0.0000	Vol. Est.
3.4247853	—	—	270	0.9960	0.0040	0.9528	0.0472	Vol. Est.
3.6274354	—	—	270	0.9922	0.0078	0.9150	0.0850	Vol. Est.
3.7996879	—	—	270	0.9892	0.0108	0.8860	0.1140	Vol. Est.
3.9516754	—	—	270	0.9900	0.0100	0.8669	0.1331	Vol. Est.
4.1219014	—	—	270	0.9832	0.0168	0.8402	0.1598	Vol. Est.
4.2049879	—	—	270	0.9818	0.0182	0.8317	0.1683	Vol. Est.
4.2809817	—	—	270	0.9803	0.0197	0.8217	0.1783	Vol. Est.
4.5596255	—	—	270	0.9750	0.0250	0.7885	0.2115	Vol. Est.
4.5900230	—	—	270	0.9737	0.0263	0.7844	0.2156	Vol. Est.
4.7602490	—	—	270	0.9711	0.0289	0.7677	0.2323	Vol. Est.
4.7744345	—	—	270	0.9708	0.0292	0.7675	0.2325	Vol. Est.
5.1523768	—	—	270	0.9632	0.0368	0.7326	0.2674	Vol. Est.
5.6985186	—	—	270	0.9524	0.0476	0.6931	0.3069	Vol. Est.
6.0491031	—	—	270	0.9455	0.0545	0.6720	0.3280	Vol. Est.
6.0795006	—	—	270	0.9440	0.0560	0.6710	0.3290	Vol. Est.
6.4442706	—	—	270	0.9370	0.0630	0.6530	0.3470	Vol. Est.
7.0927507	—	—	270	0.9222	0.0778	0.6230	0.3770	Vol. Est.
7.7209658	—	—	270	0.9079	0.0921	0.6039	0.3961	Vol. Est.
8.3795783	—	—	270	0.8920	0.1080	0.5874	0.4126	Vol. Est.
8.6126259	—	—	270	0.8858	0.1142	0.5861	0.4139	Vol. Est.
8.9824621	—	—	270	0.8769	0.1231	0.5810	0.4190	Vol. Est.
9.2915034	—	—	270	0.8681	0.1319	0.5827	0.4173	Vol. Est.
9.6258760	—	—	270	0.8570	0.1430	0.5790	0.4210	Vol. Est.
10.2044418	—	—	270	0.8415	0.1585	0.5812	0.4188	Vol. Est.
10.7141066	—	—	270	0.8231	0.1769	0.5866	0.4134	Vol. Est.
11.0525321	—	—	270	0.8096	0.1904	0.5906	0.4094	Vol. Est.
11.1457511	—	—	270	0.8050	0.1950	0.5920	0.4080	Vol. Est.
11.2521424	—	—	270	0.8014	0.1986	0.5939	0.4061	Vol. Est.
11.5490246	—	—	270	0.7858	0.2142	0.6014	0.3986	Vol. Est.
11.8175359	—	—	270	—	—	0.6143	0.3857	No
11.8864369	—	—	270	0.7668	0.2332	0.6200	0.3800	Vol. Est.
11.8864369	—	—	270	0.7640	0.2360	0.6192	0.3808	Vol. Est.
11.9482452	—	—	270	0.7514	0.2486	0.6238	0.3762	Vol. Est.
12.0242389	—	—	270	0.7546	0.2454	0.6280	0.3720	Vol. Est.
12.0728749	—	—	270	0.7495	0.2505	0.6336	0.3664	Vol. Est.
12.1346832	—	—	270	0.7444	0.2556	0.6360	0.3640	Vol. Est.
12.1964915	—	—	270	—	—	0.6476	0.3524	No
12.3413862	—	—	270	0.6470	0.3530	0.6470	0.3530	Vol. Est.

Data summarised from Table III, IV, V, and VIII of Somait78 [97]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
5.0	—	—	223.25	0.9327	0.0673	0.2171	0.7829	Vol. Est.
10.0	—	—	223.25	0.8444	0.1556	0.1994	0.8006	Vol. Est.
5.0	—	—	248.15	0.9425	0.0575	0.4562	0.5438	Vol. Est.
10.0	—	—	248.15	0.8384	0.1616	0.3656	0.6344	Vol. Est.
5.0	—	—	273.15	0.9709	0.0291	0.7919	0.2081	Vol. Est.
7.5	—	—	273.15	0.9168	0.0832	0.6618	0.3382	Vol. Est.

Data summarised from TABLE 5 of Weber84 [102]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
21.254	5.03423E-05	—	210.095	0.3991	0.6009	—	—	No
19.833	5.34874E-05	—	216.264	0.3991	0.6009	—	—	No
17.891	6.04522E-05	—	226.753	0.3991	0.6009	—	—	No
17.130	6.42963E-05	—	230.785	0.3991	0.6009	—	—	No
16.485	6.83995E-05	—	235.038	0.3991	0.6009	—	—	No
15.899	7.2759E-05	—	238.532	0.3991	0.6009	—	—	No
20.624	4.98853E-05	—	214.188	0.4459	0.5541	—	—	No
18.891	5.40103E-05	—	221.551	0.4459	0.5541	—	—	No
18.101	5.61892E-05	—	225.488	0.4459	0.5541	—	—	No
21.416	4.53679E-05	—	208.929	0.5037	0.4963	—	—	No
19.417	4.84426E-05	—	215.579	0.5037	0.4963	—	—	No
18.153	5.16556E-05	—	224.234	0.5037	0.4963	—	—	No
17.220	5.50297E-05	—	231.416	0.5037	0.4963	—	—	No
15.842	6.25939E-05	—	242.167	0.5037	0.4963	—	—	No
15.282	6.67958E-05	—	246.524	0.5037	0.4963	—	—	No
14.578	7.12758E-05	—	250.677	0.5037	0.4963	—	—	No
14.376	7.58783E-05	—	253.563	0.5037	0.4963	—	—	No
13.916	8.07428E-05	—	256.581	0.5037	0.4963	—	—	No
13.492	8.60511E-05	—	259.245	0.5037	0.4963	—	—	No
13.121	9.16926E-05	—	261.559	0.5037	0.4963	—	—	No
12.387	0.000102638	—	264.922	0.5037	0.4963	—	—	No
11.614	0.000114613	—	266.953	0.5037	0.4963	—	—	No
10.798	0.000128634	—	268.039	0.5037	0.4963	—	—	No

Data summarised from Table 5 of Duarte–Garza95–I [77]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
1.0009	—	—	220	0.9941	0.0059	0.6326	0.3674	Vol. Est.
1.5094	—	—	220	0.9866	0.0134	0.4417	0.5583	Vol. Est.
3.0839	—	—	220	0.9629	0.0371	0.2549	0.7451	Vol. Est.
4.5949	—	—	220	0.9381	0.0619	0.2014	0.7986	Vol. Est.
6.3075	—	—	220	0.9084	0.0916	0.1767	0.8233	Vol. Est.
6.3159	—	—	220	0.9094	0.0906	0.1760	0.8240	Vol. Est.
7.9935	—	—	220	0.8803	0.1197	0.1685	0.8315	Vol. Est.
8.2669	—	—	220	0.8802	0.1198	0.1688	0.8312	Vol. Est.
9.9974	—	—	220	0.8771	0.1229	0.1736	0.8264	Vol. Est.
10.0169	—	—	220	0.8484	0.1516	0.1742	0.8258	Vol. Est.
10.0257	—	—	220	0.8476	0.1524	0.1734	0.8266	Vol. Est.
11.9998	—	—	220	0.8092	0.1908	0.1885	0.8115	Vol. Est.
12.4303	—	—	220	0.8002	0.1998	0.1930	0.8070	Vol. Est.
13.7768	—	—	220	0.7690	0.2310	0.2108	0.7892	Vol. Est.
13.9681	—	—	220	0.7636	0.2364	0.2408	0.7592	Vol. Est.

Data summarised from Tabelle 5.4 of Trappehl87 [117]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
5.11	—	—	288.3	1.000	0.000	1.000	0.000	Vol. Est.
6.61	—	—	288.3	0.965	0.035	0.875	0.125	Vol. Est.
6.70	—	—	288.3	0.964	0.036	0.873	0.127	Vol. Est.
7.61	—	—	288.3	0.938	0.062	0.828	0.172	Vol. Est.
7.63	—	—	288.3	0.936	0.064	0.820	0.180	Vol. Est.
8.38	—	—	288.3	0.912	0.088	0.798	0.202	Vol. Est.
9.01	—	—	288.3	0.893	0.107	0.796	0.204	Vol. Est.
9.59	—	—	288.3	0.860	0.140	0.807	0.193	Vol. Est.
9.70	—	—	288.3	0.852	0.148	0.808	0.192	Vol. Est.
5.72	—	—	293.3	1.000	0.000	1.000	0.000	Vol. Est.
6.00	—	—	293.3	0.995	0.005	0.977	0.023	Vol. Est.
6.47	—	—	293.3	0.983	0.017	0.943	0.057	Vol. Est.
6.49	—	—	293.3	0.983	0.017	0.941	0.059	Vol. Est.
6.98	—	—	293.3	0.971	0.029	0.912	0.088	Vol. Est.
7.42	—	—	293.3	0.959	0.041	0.889	0.111	Vol. Est.
8.10	—	—	293.3	0.939	0.061	0.864	0.136	Vol. Est.
8.70	—	—	293.3	0.924	0.076	0.863	0.137	Vol. Est.
8.90	—	—	293.3	0.914	0.086	0.867	0.133	Vol. Est.
9.03	—	—	293.3	0.904	0.096	0.871	0.129	Vol. Est.
9.11	—	—	293.3	0.884	0.116	0.884	0.116	Vol. Est.

Data summarised from TABLE 2 of Xu92 [106]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
3.485580	—	—	273.15	1.0000	0.0000	1.0000	0.0000	Vol. Est.
4.053000	—	—	273.15	0.9850	0.0150	0.9036	0.0964	Vol. Est.
4.053000	—	—	273.15	0.9890	0.0110	0.9090	0.0910	Vol. Est.
5.066250	—	—	273.15	0.9690	0.0310	0.7850	0.2150	Vol. Est.
6.079500	—	—	273.15	0.9439	0.0561	0.7100	0.2900	Vol. Est.
6.079500	—	—	273.15	0.9490	0.0510	0.7000	0.3000	Vol. Est.
7.092750	—	—	273.15	0.9290	0.0710	0.6530	0.3470	Vol. Est.
8.106000	—	—	273.15	0.9033	0.0967	0.6300	0.3700	Vol. Est.
8.106000	—	—	273.15	0.8990	0.1010	0.6250	0.3750	Vol. Est.
9.119250	—	—	273.15	0.8740	0.1260	0.6080	0.3920	Vol. Est.
9.625875	—	—	273.15	0.8550	0.1450	0.6100	0.3900	Vol. Est.
10.132500	—	—	273.15	0.8420	0.1580	0.6030	0.3970	Vol. Est.
11.145750	—	—	273.15	0.8000	0.2000	0.6100	0.3900	Vol. Est.
11.652375	—	—	273.15	0.7490	0.2510	0.6440	0.3560	Vol. Est.
11.753700	—	—	273.15	0.7280	0.2720	0.6620	0.3380	Vol. Est.
11.824628	—	—	273.15	0.7030	0.2970	0.7030	0.2970	Vol. Est.

Data summarised from Table 1 of Yorizane70 [84]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
4.50	—	—	273.2	0.980	0.020	0.846	0.154	Vol. Est.
4.51	—	—	273.2	0.981	0.019	0.842	0.158	Vol. Est.
5.09	—	—	273.2	0.963	0.037	0.786	0.214	Vol. Est.
5.71	—	—	273.2	0.946	0.054	0.736	0.264	Vol. Est.
6.61	—	—	273.2	0.934	0.066	0.702	0.298	Vol. Est.
6.70	—	—	273.2	0.928	0.072	0.682	0.318	Vol. Est.
7.83	—	—	273.2	0.895	0.105	0.644	0.356	Vol. Est.
8.39	—	—	273.2	0.890	0.110	0.625	0.375	Vol. Est.
9.95	—	—	273.2	0.844	0.156	0.603	0.397	Vol. Est.
9.99	—	—	273.2	0.853	0.147	0.614	0.386	Vol. Est.
10.92	—	—	273.2	0.816	0.184	0.622	0.378	Vol. Est.
11.45	—	—	273.2	0.786	0.214	0.632	0.368	Vol. Est.
6.59	—	—	293.2	0.979	0.021	0.933	0.067	Vol. Est.
6.60	—	—	293.2	0.979	0.021	0.934	0.066	Vol. Est.
7.56	—	—	293.2	0.950	0.050	0.883	0.117	Vol. Est.
7.59	—	—	293.2	0.951	0.049	0.882	0.118	Vol. Est.
8.31	—	—	293.2	0.932	0.068	0.862	0.138	Vol. Est.
8.33	—	—	293.2	0.930	0.070	0.861	0.139	Vol. Est.
8.35	—	—	293.2	0.930	0.070	0.860	0.140	Vol. Est.
8.37	—	—	293.2	0.930	0.070	0.860	0.140	Vol. Est.
8.43	—	—	293.2	0.927	0.073	0.861	0.139	Vol. Est.
8.53	—	—	293.2	0.923	0.077	0.857	0.143	Vol. Est.
8.86	—	—	293.2	0.907	0.093	0.858	0.142	Vol. Est.
8.91	—	—	293.2	0.907	0.093	0.855	0.145	Vol. Est.
9.26	—	—	293.2	0.898	0.102	0.855	0.145	Vol. Est.
9.32	—	—	293.2	0.889	0.111	0.853	0.147	Vol. Est.
9.37	—	—	293.2	0.886	0.114	0.851	0.149	Vol. Est.
9.55	—	—	293.2	0.882	0.118	0.850	0.150	Vol. Est.
9.60	—	—	293.2	0.877	0.123	0.852	0.148	Vol. Est.
7.40	—	—	298.2	0.974	0.026	0.942	0.058	Vol. Est.
7.41	—	—	298.2	0.973	0.027	0.943	0.057	Vol. Est.
8.14	—	—	298.2	0.947	0.053	0.916	0.084	Vol. Est.
8.17	—	—	298.2	0.950	0.050	0.912	0.088	Vol. Est.
8.51	—	—	298.2	0.933	0.067	0.902	0.098	Vol. Est.

Data summarised from Table II of Yorizane85 [104]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
1.285	—	—	240	1.0000	0.0000	1.0000	0.0000	Vol. Est.
1.696	—	—	240	0.9906	0.0094	—	—	No
1.707	—	—	240	0.9918	0.0082	—	—	No
2	—	—	240	0.9870	0.0130	0.6814	0.3186	Vol. Est.
2.647	—	—	240	0.9735	0.0265	—	—	No
3.066	—	—	240	0.9693	0.0307	—	—	No
3.341	—	—	240	0.9675	0.0325	—	—	No
8.07	—	—	240	—	—	0.2998	0.7002	Vol. Est.
10.24	—	—	240	0.8295	0.1705	—	—	No
10.93	—	—	240	0.8170	0.1830	0.3023	0.6977	Vol. Est.
13	—	—	240	0.7533	0.2467	0.3308	0.6692	Vol. Est.
3.209	—	—	270	1.0000	0.0000	1.0000	0.0000	Vol. Est.
3.567	—	—	270	0.9936	0.0064	0.9241	0.0759	Vol. Est.
3.688	—	—	270	0.9904	0.0096	—	—	No
3.719	—	—	270	0.9912	0.0088	0.8964	0.1036	Vol. Est.
3.871	—	—	270	0.9875	0.0125	—	—	No
4.108	—	—	270	0.9836	0.0164	—	—	No
5.076	—	—	270	0.9642	0.0358	0.7371	0.2629	Vol. Est.
6	—	—	270	0.9470	0.0530	0.6750	0.3250	Vol. Est.
6.986	—	—	270	—	—	0.6272	0.3728	Vol. Est.
10.9	—	—	270	0.8150	0.1850	—	—	No
11.97	—	—	270	0.7544	0.2456	0.6178	0.3822	Vol. Est.

Data summarised from Table 3 and 6 of Yucelen99 [98]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{N_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{N_2}}$	Usable Data Point?
6.038970596	—	—	273.15	0.9479	0.0521	0.7115	0.2885	Vol. Est.
6.028838095	—	—	273.15	0.9488	0.0512	0.7080	0.2920	Vol. Est.
4.833202977	—	—	273.15	0.9735	0.0265	0.8020	0.1980	Vol. Est.
6.312548123	—	—	273.15	0.9420	0.0580	0.6900	0.3100	Vol. Est.
7.994543289	—	—	273.15	0.9048	0.0952	0.6270	0.3730	Vol. Est.
9.585345946	—	—	273.15	0.8592	0.1408	0.6040	0.3960	Vol. Est.
10.97349858	—	—	273.15	0.8077	0.1923	0.6155	0.3845	Vol. Est.
11.66250865	—	—	273.15	0.7720	0.2280	0.6460	0.3540	Vol. Est.
11.85502617	—	—	273.15	0.7025	0.2975	0.6955	0.3045	Vol. Est.
3.54637535	—	—	232.85	0.9625	0.0375	0.3720	0.6280	Vol. Est.
1.763055174	—	—	232.85	0.9792	0.0208	0.6280	0.3720	Vol. Est.
11.96648368	—	—	232.85	0.8320	0.1680	0.2600	0.7400	Vol. Est.
9.879188475	—	—	232.85	0.8590	0.1410	—	—	No
7.518315742	—	—	232.85	0.8910	0.1090	0.2600	0.7400	Vol. Est.
10.23382601	—	—	232.85	0.8435	0.1565	0.2540	0.7460	Vol. Est.
11.1052211	—	—	232.85	0.8143	0.1857	0.2470	0.7530	Vol. Est.
12.63522875	—	—	232.85	0.7810	0.2190	0.2350	0.7650	Vol. Est.
9.676538455	—	—	232.85	0.8450	0.1550	0.2440	0.7560	Vol. Est.
7.974278287	—	—	232.85	0.8790	0.1210	0.2440	0.7560	Vol. Est.
6.657053157	—	—	232.85	0.9040	0.0960	0.2620	0.7380	Vol. Est.
13.89165887	—	—	232.85	0.7320	0.2680	0.2920	0.7080	Vol. Est.
13.06079379	—	—	232.85	0.7630	0.2370	0.2530	0.7470	Vol. Est.
1.276695126	—	—	218.15	0.9910	0.0090	0.4750	0.5250	Vol. Est.
2.279812725	—	—	218.15	0.9770	0.0230	0.2900	0.7100	Vol. Est.
3.85035038	—	—	218.15	0.9520	0.0480	0.1960	0.8040	Vol. Est.
5.846453077	—	—	218.15	0.9340	0.0660	0.1640	0.8360	Vol. Est.
7.832423273	—	—	218.15	0.8830	0.1170	0.1560	0.8440	Vol. Est.
9.869055974	—	—	218.15	0.8478	0.1522	0.1530	0.8470	Vol. Est.
11.77396616	—	—	218.15	0.8108	0.1892	0.1700	0.8300	Vol. Est.
13.1621188	—	—	218.15	0.7820	0.2180	0.1850	0.8150	Vol. Est.
13.1519863	—	—	218.15	0.7818	0.2182	0.1870	0.8130	Vol. Est.

Data summarised from TABLE 2 of Zenner63 [103]

7.1.2 Carbon Dioxide–Nitrogen Density Data

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
20.474	0.000105661	323.09	0.5272	0.4728	Yes
15.179	0.000143811	323.09	0.5272	0.4728	Yes
11.500	0.000195681	323.09	0.5272	0.4728	Yes
8.743	0.000266328	323.09	0.5272	0.4728	Yes
6.625	0.00036242	323.09	0.5272	0.4728	Yes
4.994	0.000493209	323.09	0.5272	0.4728	Yes
3.748	0.000671293	323.09	0.5272	0.4728	Yes
2.801	0.000913406	323.09	0.5272	0.4728	Yes
2.087	0.001242889	323.09	0.5272	0.4728	Yes
1.547	0.001692017	323.09	0.5272	0.4728	Yes
1.144	0.002303096	323.09	0.5272	0.4728	Yes
0.845	0.003132344	323.09	0.5272	0.4728	Yes
0.623	0.004266203	323.09	0.5272	0.4728	Yes
0.459	0.005808069	323.09	0.5272	0.4728	Yes
0.338	0.007903979	323.09	0.5272	0.4728	Yes
20.329	7.94959E-05	323.14	0.7650	0.2350	Yes
15.134	0.000109625	323.14	0.7650	0.2350	Yes
12.065	0.000147219	323.14	0.7650	0.2350	Yes
9.685	0.000200347	323.14	0.7650	0.2350	Yes
7.680	0.000272627	323.14	0.7650	0.2350	Yes
5.999	0.000384491	323.14	0.7650	0.2350	Yes
4.621	0.000504962	323.14	0.7650	0.2350	Yes
3.519	0.000687145	323.14	0.7650	0.2350	Yes
2.657	0.000935049	323.14	0.7650	0.2350	Yes
1.996	0.00127243	323.14	0.7650	0.2350	Yes
1.486	0.001732275	323.14	0.7650	0.2350	Yes
1.104	0.002356004	323.14	0.7650	0.2350	Yes
0.819	0.003206696	323.14	0.7650	0.2350	Yes
0.606	0.004363506	323.14	0.7650	0.2350	Yes
0.448	0.005935406	323.14	0.7650	0.2350	Yes
20.332	0.000130918	323.15	0.2150	0.7850	Yes
14.677	0.000178175	323.15	0.2150	0.7850	Yes
10.766	0.000242253	323.15	0.2150	0.7850	Yes
7.924	0.000329986	323.15	0.2150	0.7850	Yes
5.851	0.000449058	323.15	0.2150	0.7850	Yes
4.320	0.000611002	323.15	0.2150	0.7850	Yes
3.188	0.000831498	323.15	0.2150	0.7850	Yes
2.350	0.001131779	323.15	0.2150	0.7850	Yes
1.731	0.00154038	323.15	0.2150	0.7850	Yes
1.275	0.002095508	323.15	0.2150	0.7850	Yes
0.938	0.002940945	333.15	0.2150	0.7850	Yes
0.690	0.004002396	333.15	0.2150	0.7850	Yes
0.508	0.005440687	333.15	0.2150	0.7850	Yes
0.373	0.007415778	333.15	0.2150	0.7850	Yes
20.164	0.000117947	333.15	0.4565	0.5435	Yes
14.929	0.000160513	333.15	0.4565	0.5435	Yes
11.222	0.000218447	333.15	0.4565	0.5435	Yes
8.456	0.000297306	333.15	0.4565	0.5435	Yes
6.356	0.000404556	333.15	0.4565	0.5435	Yes
4.758	0.000550558	333.15	0.4565	0.5435	Yes
3.547	0.000749225	333.15	0.4565	0.5435	Yes
2.635	0.001019578	333.15	0.4565	0.5435	Yes
1.952	0.001387536	333.15	0.4565	0.5435	Yes
1.443	0.001888297	333.15	0.4565	0.5435	Yes
1.065	0.002569173	333.15	0.4565	0.5435	Yes
0.785	0.003496505	333.15	0.4565	0.5435	Yes
0.578	0.004759257	333.15	0.4565	0.5435	Yes
0.425	0.006481714	333.15	0.4565	0.5435	Yes
4.872	0.000508213	333.18	0.6925	0.3075	Yes
3.771	0.000674078	333.18	0.6925	0.3075	Yes
2.838	0.000917157	333.18	0.6925	0.3075	Yes
2.122	0.001248162	333.18	0.6925	0.3075	Yes
1.579	0.001698795	333.18	0.6925	0.3075	Yes
1.170	0.002312062	333.18	0.6925	0.3075	Yes
0.865	0.003147474	333.18	0.6925	0.3075	Yes
0.639	0.004280607	333.18	0.6925	0.3075	Yes
0.471	0.005827445	333.18	0.6925	0.3075	Yes
0.347	0.007925841	333.18	0.6925	0.3075	Yes
20.110	0.000140412	343.11	0.2510	0.7490	Yes
14.537	0.000191081	343.11	0.2510	0.7490	Yes
10.647	0.000260064	343.11	0.2510	0.7490	Yes
7.844	0.000353906	343.11	0.2510	0.7490	Yes
5.787	0.000481575	343.11	0.2510	0.7490	Yes
4.270	0.00065547	343.11	0.2510	0.7490	Yes
3.149	0.000891979	343.11	0.2510	0.7490	Yes
2.320	0.001214028	343.11	0.2510	0.7490	Yes
1.710	0.00165144	343.11	0.2510	0.7490	Yes
1.258	0.002248658	343.11	0.2510	0.7490	Yes
0.926	0.003059802	343.11	0.2510	0.7490	Yes
0.682	0.004159948	343.11	0.2510	0.7490	Yes
0.501	0.005670816	343.11	0.2510	0.7490	Yes

Data summarised from Table 1 of Altunin72 [118]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
20.072	0.000123665	343.11	0.4738	0.5262	Yes
14.857	0.000168302	343.11	0.4738	0.5262	Yes
11.149	0.000229061	343.11	0.4738	0.5262	Yes
8.384	0.000311716	343.11	0.4738	0.5262	Yes
6.289	0.000424174	343.11	0.4738	0.5262	Yes
4.699	0.000577294	343.11	0.4738	0.5262	Yes
3.498	0.000785614	343.11	0.4738	0.5262	Yes
2.596	0.001069021	343.11	0.4738	0.5262	Yes
1.922	0.001453847	343.11	0.4738	0.5262	Yes
1.419	0.001980658	343.11	0.4738	0.5262	Yes
1.047	0.002692289	343.11	0.4738	0.5262	Yes
0.772	0.003665742	343.11	0.4738	0.5262	Yes
0.568	0.004992356	343.11	0.4738	0.5262	Yes
0.418	0.006793427	343.11	0.4738	0.5262	Yes
20.072	9.70586E-05	343.11	0.7195	0.2805	Yes
15.335	0.0001321	343.11	0.7195	0.2805	Yes
12.011	0.000179774	343.11	0.7195	0.2805	Yes
9.403	0.000244654	343.11	0.7195	0.2805	Yes
7.286	0.00033285	343.11	0.7195	0.2805	Yes
5.585	0.000453073	343.11	0.7195	0.2805	Yes
4.236	0.000616754	343.11	0.7195	0.2805	Yes
3.188	0.000839099	343.11	0.7195	0.2805	Yes
2.384	0.001142067	343.11	0.7195	0.2805	Yes
1.774	0.001554232	343.11	0.7195	0.2805	Yes
1.316	0.002114435	343.11	0.7195	0.2805	Yes
0.973	0.00287799	343.11	0.7195	0.2805	Yes
0.718	0.003918791	343.11	0.7195	0.2805	Yes
0.529	0.005339381	343.11	0.7195	0.2805	Yes
0.390	0.007252632	343.11	0.7195	0.2805	Yes

Continued: Data summarised from Table 1 of Altunin72 [118]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
2.4115350	0.000754	273.15	1.000	0.000	Yes
2.5837875	0.000692	273.15	1.000	0.000	Yes
2.9688225	0.000573	273.15	1.000	0.000	Yes
3.1613400	0.000522	273.15	1.000	0.000	Yes
3.3538575	0.000476	273.15	1.000	0.000	Yes
4.9041300	0.0000451	273.15	1.000	0.000	Yes
7.4980500	0.0000442	273.15	1.000	0.000	Yes
9.0584550	0.0000438	273.15	1.000	0.000	Yes
11.3787975	0.0000431	273.15	1.000	0.000	Yes
12.1590000	0.0000425	273.15	1.000	0.000	Yes
14.5097400	0.000042	273.15	1.000	0.000	Yes
7.4980500	0.0000483	273.15	0.929	0.071	Yes
9.0584550	0.0000471	273.15	0.929	0.071	Yes
11.3889300	0.0000463	273.15	0.929	0.071	Yes
12.1691325	0.0000457	273.15	0.929	0.071	Yes
12.9493350	0.0000454	273.15	0.929	0.071	Yes
14.5097400	0.0000445	273.15	0.929	0.071	Yes
9.8386575	0.0000511	273.15	0.872	0.128	Yes
10.2338250	0.0000506	273.15	0.872	0.128	Yes
10.6087275	0.0000504	273.15	0.872	0.128	Yes
11.3889300	0.0000498	273.15	0.872	0.128	Yes
12.5541675	0.0000489	273.15	0.872	0.128	Yes
14.5097400	0.0000472	273.15	0.872	0.128	Yes
2.4216675	0.000811	273.15	0.786	0.214	Yes
2.9789550	0.000635	273.15	0.786	0.214	Yes
3.3639900	0.000545	273.15	0.786	0.214	Yes
4.1340600	0.000414	273.15	0.786	0.214	Yes
4.9142625	0.000321	273.15	0.786	0.214	Yes
12.0171450	0.000066	273.15	0.746	0.254	Yes
12.1691325	0.000065	273.15	0.746	0.254	Yes
12.9493350	0.0000622	273.15	0.746	0.254	Yes
13.7295375	0.0000587	273.15	0.746	0.254	Yes
14.5097400	0.0000585	273.15	0.746	0.254	Yes
2.4216675	0.000827	273.15	0.702	0.298	Yes
3.3639900	0.000565	273.15	0.702	0.298	Yes
4.1441925	0.000437	273.15	0.702	0.298	Yes
4.9243950	0.000348	273.15	0.702	0.298	Yes
5.6944650	0.000281	273.15	0.702	0.298	Yes
6.2416200	0.000244	273.15	0.702	0.298	Yes
6.4746675	0.000227	273.15	0.702	0.298	Yes
12.0171450	0.0000791	273.15	0.694	0.306	Yes
12.1691325	0.0000783	273.15	0.694	0.306	Yes
12.9493350	0.0000731	273.15	0.694	0.306	Yes
13.7295375	0.0000696	273.15	0.694	0.306	Yes
14.5097400	0.0000667	273.15	0.694	0.306	Yes
11.3889300	0.000102	273.15	0.633	0.367	Yes
12.1691325	0.0000937	273.15	0.633	0.367	Yes
12.9594675	0.000087	273.15	0.633	0.367	Yes
13.7396700	0.0000812	273.15	0.633	0.367	Yes
14.5198725	0.0000773	273.15	0.633	0.367	Yes

Data summarised from Table 2 and 4 of Arai71 [53]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
2.6749800	0.000756	273.15	0.626	0.374	Yes
3.3639900	0.000579	273.15	0.626	0.374	Yes
4.1441925	0.000453	273.15	0.626	0.374	Yes
4.9142625	0.000366	273.15	0.626	0.374	Yes
6.7178475	0.000239	273.15	0.626	0.374	Yes
7.4980500	0.000203	273.15	0.626	0.374	Yes
8.6734200	0.00016	273.15	0.626	0.374	Yes
9.0584550	0.000149	273.15	0.626	0.374	Yes
2.9890875	0.000675	273.15	0.576	0.424	Yes
3.3741225	0.000587	273.15	0.576	0.424	Yes
4.1441925	0.000462	273.15	0.576	0.424	Yes
4.9243950	0.000376	273.15	0.576	0.424	Yes
6.7279800	0.000251	273.15	0.576	0.424	Yes
8.6734200	0.000175	273.15	0.576	0.424	Yes
10.6087275	0.000129	273.15	0.576	0.424	Yes
12.1691325	0.000106	273.15	0.576	0.424	Yes
12.9493350	0.000098	273.15	0.576	0.424	Yes
2.4318000	0.000869	273.15	0.492	0.508	Yes
3.3639900	0.000607	273.15	0.492	0.508	Yes
4.1441925	0.000481	273.15	0.492	0.508	Yes
4.9243950	0.000395	273.15	0.492	0.508	Yes
6.7279800	0.00027	273.15	0.492	0.508	Yes
8.6734200	0.000195	273.15	0.492	0.508	Yes
10.6087275	0.000151	273.15	0.492	0.508	Yes
11.3889300	0.000138	273.15	0.492	0.508	Yes
12.9493350	0.000117	273.15	0.492	0.508	Yes
14.5097400	0.000102	273.15	0.492	0.508	Yes
2.4318000	0.000821	288.15	1.000	0.000	Yes
2.9890875	0.000634	288.15	1.000	0.000	Yes
3.7692900	0.000461	288.15	1.000	0.000	Yes
4.3873725	0.000361	288.15	1.000	0.000	Yes
4.5596250	0.000344	288.15	1.000	0.000	Yes
4.7217450	0.000323	288.15	1.000	0.000	Yes
4.8737325	0.000302	288.15	1.000	0.000	Yes
4.9243950	0.000288	288.15	1.000	0.000	Yes
5.4208875	0.0000525	288.15	1.000	0.000	Yes
6.7279800	0.000051	288.15	1.000	0.000	Yes
10.6188600	0.0000486	288.15	1.000	0.000	Yes
12.1792650	0.0000478	288.15	1.000	0.000	Yes
14.5198725	0.0000468	288.15	1.000	0.000	Yes
8.2579875	0.0000552	288.15	0.940	0.060	Yes
9.0685875	0.0000538	288.15	0.940	0.060	Yes
9.8386575	0.0000527	288.15	0.940	0.060	Yes
10.6188600	0.0000517	288.15	0.940	0.060	Yes
11.7840975	0.0000507	288.15	0.940	0.060	Yes
13.3445025	0.0000496	288.15	0.940	0.060	Yes
13.7396700	0.0000492	288.15	0.940	0.060	Yes
2.4318000	0.000838	288.15	0.918	0.082	Yes
2.9890875	0.000653	288.15	0.918	0.082	Yes
3.7692900	0.000485	288.15	0.918	0.082	Yes
4.5393600	0.00037	288.15	0.918	0.082	Yes
5.9984400	0.000221	288.15	0.918	0.082	Yes
2.4419325	0.00085	288.15	0.897	0.103	Yes
3.7692900	0.000495	288.15	0.897	0.103	Yes
4.9345275	0.000335	288.15	0.897	0.103	Yes
5.7147300	0.000259	288.15	0.897	0.103	Yes
9.4637550	0.0000606	288.15	0.897	0.103	Yes
9.8589225	0.0000593	288.15	0.897	0.103	Yes
10.2439575	0.000058	288.15	0.897	0.103	Yes
10.6188600	0.0000572	288.15	0.897	0.103	Yes
12.1792650	0.0000544	288.15	0.897	0.103	Yes
13.7396700	0.0000526	288.15	0.897	0.103	Yes
14.5198725	0.0000518	288.15	0.897	0.103	Yes
9.8589225	0.000068	288.15	0.868	0.132	Yes
10.2439575	0.0000654	288.15	0.868	0.132	Yes
10.6188600	0.0000634	288.15	0.868	0.132	Yes
11.3990625	0.0000605	288.15	0.868	0.132	Yes
12.1792650	0.0000586	288.15	0.868	0.132	Yes
13.3546350	0.0000563	288.15	0.868	0.132	Yes
14.5198725	0.0000547	288.15	0.868	0.132	Yes
10.0919700	0.0000744	288.15	0.845	0.155	Yes
10.2439575	0.0000729	288.15	0.845	0.155	Yes
10.6188600	0.0000696	288.15	0.845	0.155	Yes
11.3990625	0.0000659	288.15	0.845	0.155	Yes
10.6188600	0.0000757	288.15	0.827	0.173	Yes
11.3990625	0.0000697	288.15	0.827	0.173	Yes
12.1792650	0.0000656	288.15	0.827	0.173	Yes
12.9594675	0.000062	288.15	0.827	0.173	Yes
13.7396700	0.0000604	288.15	0.827	0.173	Yes
2.4419325	0.000869	288.15	0.813	0.187	Yes
4.9345275	0.000362	288.15	0.813	0.187	Yes
6.7381125	0.00022	288.15	0.813	0.187	Yes
7.5183150	0.000177	288.15	0.813	0.187	Yes
10.1426325	0.0000861	288.15	0.812	0.188	Yes
10.4567400	0.0000819	288.15	0.812	0.188	Yes
11.2977375	0.0000743	288.15	0.812	0.188	Yes

Continued: Data summarised from Table 2 and 4 of Arai71 [53]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
12.0779400	0.0000691	288.15	0.812	0.188	Yes
12.8581425	0.0000657	288.15	0.812	0.188	Yes
13.6383450	0.0000629	288.15	0.812	0.188	Yes
9.8589225	0.0000978	288.15	0.801	0.199	Yes
10.2540900	0.0000909	288.15	0.801	0.199	Yes
10.6188600	0.0000855	288.15	0.801	0.199	Yes
11.3585325	0.0000773	288.15	0.801	0.199	Yes
12.1792650	0.0000716	288.15	0.801	0.199	Yes
13.3546350	0.0000661	288.15	0.801	0.199	Yes
14.5198725	0.0000625	288.15	0.801	0.199	Yes
2.6141850	0.000816	288.15	0.736	0.264	Yes
4.9345275	0.000379	288.15	0.736	0.264	Yes
6.7381125	0.000245	288.15	0.736	0.264	Yes
8.6835525	0.00016	288.15	0.736	0.264	Yes
10.6188600	0.00011	288.15	0.736	0.264	Yes
12.5643000	0.0000848	288.15	0.736	0.264	Yes
14.5198725	0.0000722	288.15	0.736	0.264	Yes
2.7661725	0.000769	288.15	0.702	0.298	Yes
5.0966475	0.000371	288.15	0.702	0.298	Yes
6.7381125	0.000253	288.15	0.702	0.298	Yes
10.6188600	0.000121	288.15	0.702	0.298	Yes
14.5198725	0.0000785	288.15	0.702	0.298	Yes

Continued: Data summarised from Table 2 and 4 of Arai71 [53]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
41.00439	6.06487E-05	300.019	0.447	0.553	Yes
38.54936	6.18204E-05	300.132	0.447	0.553	Yes
27.63501	7.61707E-05	300.030	0.447	0.553	Yes
21.86764	9.12959E-05	300.023	0.447	0.553	Yes
21.09454	9.31159E-05	299.992	0.447	0.553	Yes
17.16298	0.000114686	300.000	0.447	0.553	Yes
15.50388	0.000127456	300.006	0.447	0.553	Yes
14.46641	0.000137469	300.014	0.447	0.553	Yes
14.06685	0.000140289	299.978	0.447	0.553	Yes
11.80328	0.000172697	300.013	0.447	0.553	Yes
10.75626	0.000191912	299.975	0.447	0.553	Yes
10.07421	0.00020701	300.025	0.447	0.553	Yes
9.82850	0.000211375	299.978	0.447	0.553	Yes
8.25051	0.000260064	300.011	0.447	0.553	Yes
7.51655	0.00028897	300.000	0.447	0.553	Yes
7.02829	0.00031174	300.018	0.447	0.553	Yes
6.86538	0.000318493	299.919	0.447	0.553	Yes
5.72708	0.000391642	300.027	0.447	0.553	Yes
5.20380	0.0004351	299.999	0.447	0.553	Yes
4.85458	0.000469473	300.024	0.447	0.553	Yes
4.74645	0.000479904	299.983	0.447	0.553	Yes
3.93098	0.00058981	300.024	0.447	0.553	Yes
3.56291	0.000655128	299.984	0.447	0.553	Yes
3.31707	0.000707024	300.020	0.447	0.553	Yes
3.24311	0.000723134	299.914	0.447	0.553	Yes
2.91424	0.000810806	299.999	0.447	0.553	Yes
2.67210	0.000888265	299.995	0.447	0.553	Yes
2.41732	0.000986563	299.990	0.447	0.553	Yes
2.19764	0.001089645	299.970	0.447	0.553	Yes
1.95959	0.00120636	300.010	0.447	0.553	Yes
1.80350	0.001337739	300.005	0.447	0.553	Yes
1.62900	0.001485685	299.988	0.447	0.553	Yes
1.51258	0.001603618	300.016	0.447	0.553	Yes
1.47509	0.001641928	299.998	0.447	0.553	Yes
1.32364	0.001839013	300.008	0.447	0.553	Yes
1.21087	0.002014707	300.026	0.447	0.553	Yes
1.09235	0.002237737	299.976	0.447	0.553	Yes
1.01292	0.002415109	299.809	0.447	0.553	Yes
0.98849	0.002474206	299.977	0.447	0.553	Yes
0.88603	0.002769623	300.009	0.447	0.553	Yes
0.80990	0.003034257	300.026	0.447	0.553	Yes
0.67763	0.003637289	300.160	0.447	0.553	Yes
0.66029	0.003728283	299.978	0.447	0.553	Yes
0.59158	0.004171185	300.011	0.447	0.553	Yes
0.54047	0.004569757	300.017	0.447	0.553	Yes
0.45180	0.005477951	300.155	0.447	0.553	Yes
0.44023	0.005617978	299.985	0.447	0.553	Yes
0.39416	0.006282196	300.005	0.447	0.553	Yes
0.36004	0.006882312	300.017	0.447	0.553	Yes
0.30090	0.008250144	300.149	0.447	0.553	Yes
0.29313	0.008465967	299.991	0.447	0.553	Yes
0.26238	0.009460738	300.003	0.447	0.553	Yes
0.23963	0.010364842	300.019	0.447	0.553	Yes
0.20011	0.012425447	300.148	0.447	0.553	Yes
0.19507	0.012756729	299.997	0.447	0.553	Yes
0.17449	0.014249074	300.011	0.447	0.553	Yes
0.15934	0.015610365	300.010	0.447	0.553	Yes
0.13301	0.018712575	300.145	0.447	0.553	Yes
0.12961	0.019223376	300.006	0.447	0.553	Yes
0.11596	0.021459227	300.013	0.447	0.553	Yes
0.10590	0.023512814	300.011	0.447	0.553	Yes
0.08840	0.028184893	300.145	0.447	0.553	Yes

Data summarised from Table VIII of Bailey89 [82]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
9.27379	0.0002622	300	0.10560	0.89440	Yes
7.83286	0.0003107	300	0.10560	0.89440	Yes
6.14139	0.0003973	300	0.10560	0.89440	Yes
5.19435	0.0004707	300	0.10560	0.89440	Yes
4.07540	0.0006018	300	0.10560	0.89440	Yes
3.44681	0.0007130	300	0.10560	0.89440	Yes
2.70338	0.0009115	300	0.10560	0.89440	Yes
2.28539	0.0010800	300	0.10560	0.89440	Yes
1.79084	0.0013811	300	0.10560	0.89440	Yes
1.51331	0.0016363	300	0.10560	0.89440	Yes
1.18531	0.0020922	300	0.10560	0.89440	Yes
1.00124	0.0024789	300	0.10560	0.89440	Yes
0.78389	0.0031695	300	0.10560	0.89440	Yes
0.66198	0.0037554	300	0.10560	0.89440	Yes
0.51809	0.0048017	300	0.10560	0.89440	Yes
0.43745	0.0056890	300	0.10560	0.89440	Yes
0.34229	0.0072741	300	0.10560	0.89440	Yes
0.28896	0.0086188	300	0.10560	0.89440	Yes
0.22607	0.0110198	300	0.10560	0.89440	Yes
9.86634	0.000234078	300	0.25147	0.74853	Yes
8.42048	0.000276255	300	0.25147	0.74853	Yes
6.63406	0.00035458	300	0.25147	0.74853	Yes
5.66125	0.000418444	300	0.25147	0.74853	Yes
4.45281	0.000537127	300	0.25147	0.74853	Yes
3.79423	0.00063392	300	0.25147	0.74853	Yes
2.97716	0.000813768	300	0.25147	0.74853	Yes
2.53320	0.000960333	300	0.25147	0.74853	Yes
1.98351	0.001232833	300	0.25147	0.74853	Yes
1.68560	0.001454904	300	0.25147	0.74853	Yes
1.31779	0.001867703	300	0.25147	0.74853	Yes
1.11883	0.002204166	300	0.25147	0.74853	Yes
0.87366	0.002829597	300	0.25147	0.74853	Yes
0.74129	0.0033393	300	0.25147	0.74853	Yes
0.57839	0.004286794	300	0.25147	0.74853	Yes
0.49054	0.005059051	300	0.25147	0.74853	Yes
0.38254	0.006494403	300	0.25147	0.74853	Yes
0.32434	0.007664304	300	0.25147	0.74853	Yes
0.25283	0.009839264	300	0.25147	0.74853	Yes
0.21432	0.011611728	300	0.25147	0.74853	Yes
9.53694	0.000212203	300	0.50365	0.49635	Yes
8.64623	0.000238431	300	0.50365	0.49635	Yes
6.69079	0.000321595	300	0.50365	0.49635	Yes
6.04314	0.000361286	300	0.50365	0.49635	Yes
4.62709	0.000487176	300	0.50365	0.49635	Yes
4.16204	0.000547312	300	0.50365	0.49635	Yes
3.15653	0.00073807	300	0.50365	0.49635	Yes
2.83087	0.000828953	300	0.50365	0.49635	Yes
2.13134	0.00111809	300	0.50365	0.49635	Yes
1.90686	0.001255837	300	0.50365	0.49635	Yes
1.42852	0.001693842	300	0.50365	0.49635	Yes
1.27583	0.001902764	300	0.50365	0.49635	Yes
0.95265	0.002566058	300	0.50365	0.49635	Yes
0.84990	0.002882508	300	0.50365	0.49635	Yes
0.63313	0.00388734	300	0.50365	0.49635	Yes
0.56442	0.004366873	300	0.50365	0.49635	Yes
0.41982	0.00588909	300	0.50365	0.49635	Yes
0.37407	0.006615614	300	0.50365	0.49635	Yes
0.27794	0.008921975	300	0.50365	0.49635	Yes
0.24757	0.010022535	300	0.50365	0.49635	Yes
8.90956	0.000191352	300	0.71105	0.28895	Yes
7.95354	0.000225637	300	0.71105	0.28895	Yes
6.62487	0.000289938	300	0.71105	0.28895	Yes
5.83538	0.000341839	300	0.71105	0.28895	Yes
4.76488	0.00043924	300	0.71105	0.28895	Yes
4.14835	0.00051783	300	0.71105	0.28895	Yes
3.33496	0.000665497	300	0.71105	0.28895	Yes
2.87919	0.000784464	300	0.71105	0.28895	Yes
2.29002	0.001008083	300	0.71105	0.28895	Yes
1.96530	0.001188433	300	0.71105	0.28895	Yes
1.55174	0.001527188	300	0.71105	0.28895	Yes
1.32645	0.001800463	300	0.71105	0.28895	Yes
1.04221	0.002313622	300	0.71105	0.28895	Yes
0.88855	0.002727658	300	0.71105	0.28895	Yes
0.69589	0.003505079	300	0.71105	0.28895	Yes
0.59227	0.004132288	300	0.71105	0.28895	Yes
0.46284	0.005310094	300	0.71105	0.28895	Yes
0.39347	0.00626031	300	0.71105	0.28895	Yes
0.30704	0.008044892	300	0.71105	0.28895	Yes
0.26083	0.009484287	300	0.71105	0.28895	Yes

Data summarised from Table I and II of Brugge89 [85]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
5.50863	0.000320691	300	0.90921	0.09079	Yes
5.21854	0.000348	300	0.90921	0.09079	Yes
4.09677	0.000485818	300	0.90921	0.09079	Yes
3.84375	0.000527199	300	0.90921	0.09079	Yes
2.92334	0.000735894	300	0.90921	0.09079	Yes
2.72538	0.000798667	300	0.90921	0.09079	Yes
2.03001	0.001114977	300	0.90921	0.09079	Yes
1.88511	0.001209941	300	0.90921	0.09079	Yes
1.38528	0.001689132	300	0.90921	0.09079	Yes
1.28301	0.001832996	300	0.90921	0.09079	Yes
0.93460	0.002558914	300	0.90921	0.09079	Yes
0.86408	0.002776954	300	0.90921	0.09079	Yes
0.62584	0.003876602	300	0.90921	0.09079	Yes
0.57793	0.004207079	300	0.90921	0.09079	Yes
0.41703	0.005872872	300	0.90921	0.09079	Yes
0.38482	0.006373517	300	0.90921	0.09079	Yes
0.27699	0.008897268	300	0.90921	0.09079	Yes
0.25547	0.009655699	300	0.90921	0.09079	Yes
9.81270	0.000268453	320	0.10560	0.89440	Yes
8.23109	0.000319592	320	0.10560	0.89440	Yes
6.46611	0.000406735	320	0.10560	0.89440	Yes
5.43492	0.000484169	320	0.10560	0.89440	Yes
4.27577	0.000616159	320	0.10560	0.89440	Yes
3.59568	0.000733446	320	0.10560	0.89440	Yes
2.82923	0.000933416	320	0.10560	0.89440	Yes
2.37918	0.001111026	320	0.10560	0.89440	Yes
1.87154	0.001414031	320	0.10560	0.89440	Yes
1.57337	0.001683244	320	0.10560	0.89440	Yes
1.23738	0.002142152	320	0.10560	0.89440	Yes
1.04001	0.002550072	320	0.10560	0.89440	Yes
0.81772	0.003245337	320	0.10560	0.89440	Yes
0.68719	0.003863213	320	0.10560	0.89440	Yes
0.54019	0.004916632	320	0.10560	0.89440	Yes
0.45392	0.005852497	320	0.10560	0.89440	Yes
0.35678	0.007448273	320	0.10560	0.89440	Yes
0.29977	0.008866239	320	0.10560	0.89440	Yes
0.23559	0.011283887	320	0.10560	0.89440	Yes
10.59715	0.00023813	320	0.25147	0.74853	Yes
9.01444	0.000281026	320	0.25147	0.74853	Yes
7.07010	0.000360801	320	0.25147	0.74853	Yes
6.01957	0.000425738	320	0.25147	0.74853	Yes
4.71948	0.000546628	320	0.25147	0.74853	Yes
4.01581	0.000644936	320	0.25147	0.74853	Yes
3.14400	0.000828091	320	0.25147	0.74853	Yes
2.67268	0.000977032	320	0.25147	0.74853	Yes
2.08949	0.001254527	320	0.25147	0.74853	Yes
1.77468	0.001480173	320	0.25147	0.74853	Yes
1.38583	0.001900575	320	0.25147	0.74853	Yes
1.17630	0.002242412	320	0.25147	0.74853	Yes
0.91777	0.002879406	320	0.25147	0.74853	Yes
0.77864	0.003397259	320	0.25147	0.74853	Yes
0.60715	0.004362207	320	0.25147	0.74853	Yes
0.51493	0.005146906	320	0.25147	0.74853	Yes
0.34033	0.007797486	320	0.25147	0.74853	Yes
0.30137	0.008801516	320	0.25147	0.74853	Yes
0.26519	0.010012375	320	0.25147	0.74853	Yes
0.22483	0.01181317	320	0.25147	0.74853	Yes
10.20113	0.000222635	320	0.50365	0.49635	Yes
9.20586	0.000249926	320	0.50365	0.49635	Yes
7.03706	0.000337371	320	0.50365	0.49635	Yes
6.34060	0.000378417	320	0.50365	0.49635	Yes
4.80926	0.00051124	320	0.50365	0.49635	Yes
4.32407	0.000573058	320	0.50365	0.49635	Yes
3.25577	0.000774537	320	0.50365	0.49635	Yes
2.92123	0.000867984	320	0.50365	0.49635	Yes
2.18700	0.001173513	320	0.50365	0.49635	Yes
1.95904	0.001314915	320	0.50365	0.49635	Yes
1.46056	0.00177834	320	0.50365	0.49635	Yes
1.30719	0.001991992	320	0.50365	0.49635	Yes
0.97179	0.002694408	320	0.50365	0.49635	Yes
0.86918	0.003017791	320	0.50365	0.49635	Yes
0.64489	0.004082168	320	0.50365	0.49635	Yes
0.57649	0.00457181	320	0.50365	0.49635	Yes
0.42718	0.006184578	320	0.50365	0.49635	Yes
0.38174	0.006926234	320	0.50365	0.49635	Yes
0.28263	0.00936993	320	0.50365	0.49635	Yes
0.25251	0.010493088	320	0.50365	0.49635	Yes

Continued: Data summarised from Table I and II of Brugge89 [85]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
9.71988	0.000204633	320	0.71105	0.28895	Yes
8.25659	0.000252739	320	0.71105	0.28895	Yes
7.01148	0.000309987	320	0.71105	0.28895	Yes
5.88416	0.00038291	320	0.71105	0.28895	Yes
4.94061	0.000469565	320	0.71105	0.28895	Yes
4.10141	0.000580061	320	0.71105	0.28895	Yes
3.41246	0.000711332	320	0.71105	0.28895	Yes
2.81027	0.00087867	320	0.71105	0.28895	Yes
2.32297	0.001077517	320	0.71105	0.28895	Yes
1.90218	0.001331084	320	0.71105	0.28895	Yes
1.56509	0.00163249	320	0.71105	0.28895	Yes
1.27672	0.002016586	320	0.71105	0.28895	Yes
1.04735	0.002473111	320	0.71105	0.28895	Yes
0.85216	0.003055051	320	0.71105	0.28895	Yes
0.69765	0.003746606	320	0.71105	0.28895	Yes
0.56666	0.004628266	320	0.71105	0.28895	Yes
0.46331	0.005675658	320	0.71105	0.28895	Yes
0.37588	0.007011371	320	0.71105	0.28895	Yes
0.30705	0.008598182	320	0.71105	0.28895	Yes
0.24891	0.010622171	320	0.71105	0.28895	Yes
7.30279	0.000254944	320	0.90921	0.09079	Yes
6.52578	0.000300779	320	0.90921	0.09079	Yes
5.43121	0.000386191	320	0.90921	0.09079	Yes
4.77261	0.000455571	320	0.90921	0.09079	Yes
3.88549	0.000585075	320	0.90921	0.09079	Yes
3.37337	0.00069021	320	0.90921	0.09079	Yes
2.70577	0.000886289	320	0.90921	0.09079	Yes
2.33018	0.001045593	320	0.90921	0.09079	Yes
1.85038	0.001342674	320	0.90921	0.09079	Yes
1.58500	0.001583887	320	0.90921	0.09079	Yes
1.25019	0.00203411	320	0.90921	0.09079	Yes
1.06716	0.002399456	320	0.90921	0.09079	Yes
0.83807	0.003081399	320	0.90921	0.09079	Yes
0.71366	0.003635051	320	0.90921	0.09079	Yes
0.55886	0.004668018	320	0.90921	0.09079	Yes
0.47514	0.005506977	320	0.90921	0.09079	Yes
0.37137	0.007071863	320	0.90921	0.09079	Yes
0.31543	0.008342531	320	0.90921	0.09079	Yes
0.24622	0.010713609	320	0.90921	0.09079	Yes
0.20900	0.012638261	320	0.90921	0.09079	Yes

Continued: Data summarised from Table I and II of Brugge89 [85]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
68.759	0.0000456162759	225	0.10560	0.89440	Yes
62.510	0.0000469792352	225	0.10560	0.89440	Yes
57.402	0.0000482951801	225	0.10560	0.89440	Yes
51.819	0.0000500250125	225	0.10560	0.89440	Yes
45.955	0.0000522575251	225	0.10560	0.89440	Yes
40.271	0.0000550721445	225	0.10560	0.89440	Yes
34.553	0.0000588997526	225	0.10560	0.89440	Yes
28.832	0.0000645036445	225	0.10560	0.89440	Yes
23.073	0.0000737408746	225	0.10560	0.89440	Yes
17.334	0.0000914996798	225	0.10560	0.89440	Yes
11.565	0.0001350438893	225	0.10560	0.89440	Yes
5.789	0.0002881844380	225	0.10560	0.89440	Yes
68.723	0.0000432806752	225	0.25147	0.74853	Yes
63.995	0.0000440703363	225	0.25147	0.74853	Yes
59.486	0.0000449155587	225	0.25147	0.74853	Yes
54.635	0.0000459643317	225	0.25147	0.74853	Yes
50.028	0.0000471164719	225	0.25147	0.74853	Yes
45.559	0.0000484449181	225	0.25147	0.74853	Yes
40.832	0.0000501353655	225	0.25147	0.74853	Yes
36.052	0.0000522821143	225	0.25147	0.74853	Yes
31.521	0.0000549571334	225	0.25147	0.74853	Yes
26.560	0.0000590841950	225	0.25147	0.74853	Yes
22.097	0.0000648256191	225	0.25147	0.74853	Yes
17.324	0.0000758265089	225	0.25147	0.74853	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
68.757	0.0000396589332	225	0.50365	0.49635	Yes
64.284	0.0000401026628	225	0.50365	0.49635	Yes
59.971	0.0000405695971	225	0.50365	0.49635	Yes
55.490	0.0000411048997	225	0.50365	0.49635	Yes
51.251	0.0000416736123	225	0.50365	0.49635	Yes
47.029	0.0000423047635	225	0.50365	0.49635	Yes
42.734	0.0000430366672	225	0.50365	0.49635	Yes
38.334	0.0000439039382	225	0.50365	0.49635	Yes
33.940	0.0000449337228	225	0.50365	0.49635	Yes
29.435	0.0000462384982	225	0.50365	0.49635	Yes
25.084	0.0000478858402	225	0.50365	0.49635	Yes
68.765	0.0000373203956	225	0.71105	0.28895	Yes
63.528	0.0000376477675	225	0.71105	0.28895	Yes
58.351	0.0000379996960	225	0.71105	0.28895	Yes
52.872	0.0000384054075	225	0.71105	0.28895	Yes
47.575	0.0000388424937	225	0.71105	0.28895	Yes
42.444	0.0000393112666	225	0.71105	0.28895	Yes
37.012	0.0000398708185	225	0.71105	0.28895	Yes
31.663	0.0000405022276	225	0.71105	0.28895	Yes
26.429	0.0000412354130	225	0.71105	0.28895	Yes
20.934	0.0000421798549	225	0.71105	0.28895	Yes
68.831	0.0000356239535	225	0.90921	0.09079	Yes
63.930	0.0000358140534	225	0.90921	0.09079	Yes
59.307	0.0000360074896	225	0.90921	0.09079	Yes
54.341	0.0000362253215	225	0.90921	0.09079	Yes
49.927	0.0000364351818	225	0.90921	0.09079	Yes
44.731	0.0000366945545	225	0.90921	0.09079	Yes
40.095	0.0000369398988	225	0.90921	0.09079	Yes
34.971	0.0000372328543	225	0.90921	0.09079	Yes
30.735	0.0000374925015	225	0.90921	0.09079	Yes
25.841	0.0000378143316	225	0.90921	0.09079	Yes
23.482	0.0000379852617	225	0.90921	0.09079	Yes
15.997	0.0000385757821	225	0.90921	0.09079	Yes
11.238	0.0000390076455	225	0.90921	0.09079	Yes
68.953	0.0000481904487	245	0.10560	0.89440	Yes
57.208	0.0000515596803	245	0.10560	0.89440	Yes
49.629	0.0000545702592	245	0.10560	0.89440	Yes
40.517	0.0000597550045	245	0.10560	0.89440	Yes
34.424	0.0000649603742	245	0.10560	0.89440	Yes
29.447	0.0000710934167	245	0.10560	0.89440	Yes
25.196	0.0000787277594	245	0.10560	0.89440	Yes
21.643	0.0000880591758	245	0.10560	0.89440	Yes
18.586	0.0000997804829	245	0.10560	0.89440	Yes
15.875	0.0001149689584	245	0.10560	0.89440	Yes
13.324	0.0001362212233	245	0.10560	0.89440	Yes
10.939	0.0001665556296	245	0.10560	0.89440	Yes
8.579	0.0002151925974	245	0.10560	0.89440	Yes
6.223	0.0003028467595	245	0.10560	0.89440	Yes
3.806	0.0005083884087	245	0.10560	0.89440	Yes
1.265	0.0015847860539	245	0.10560	0.89440	Yes
68.896	0.0000456975735	245	0.25147	0.74853	Yes
55.480	0.0000488376636	245	0.25147	0.74853	Yes
45.088	0.0000524851729	245	0.25147	0.74853	Yes
37.041	0.0000567633536	245	0.25147	0.74853	Yes
30.934	0.0000616979269	245	0.25147	0.74853	Yes
26.204	0.0000675128274	245	0.25147	0.74853	Yes
22.498	0.0000743936914	245	0.25147	0.74853	Yes
19.130	0.0000838785439	245	0.25147	0.74853	Yes
16.575	0.0000949126803	245	0.25147	0.74853	Yes
14.379	0.0001089087345	245	0.25147	0.74853	Yes
12.171	0.0001299714063	245	0.25147	0.74853	Yes
10.182	0.0001591596371	245	0.25147	0.74853	Yes

Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
8.167	0.0002058460272	245	0.25147	0.74853	Yes
6.059	0.0002907822041	245	0.25147	0.74853	Yes
3.737	0.0004987531172	245	0.25147	0.74853	Yes
1.182	0.0016835016835	245	0.25147	0.74853	Yes
69.031	0.0000417414534	245	0.50365	0.49635	Yes
64.442	0.0000423172951	245	0.50365	0.49635	Yes
59.470	0.0000430089028	245	0.50365	0.49635	Yes
54.654	0.0000437847541	245	0.50365	0.49635	Yes
49.798	0.0000446747677	245	0.50365	0.49635	Yes
44.823	0.0000457498399	245	0.50365	0.49635	Yes
40.137	0.0000469527655	245	0.50365	0.49635	Yes
35.095	0.0000485625486	245	0.50365	0.49635	Yes
30.213	0.0000505970451	245	0.50365	0.49635	Yes
25.376	0.0000534016875	245	0.50365	0.49635	Yes
20.573	0.0000577800890	245	0.50365	0.49635	Yes
69.042	0.0000390976268	245	0.71105	0.28895	Yes
64.182	0.0000394835551	245	0.71105	0.28895	Yes
58.841	0.0000399456739	245	0.71105	0.28895	Yes
54.941	0.0000403193291	245	0.71105	0.28895	Yes
49.385	0.0000409148562	245	0.71105	0.28895	Yes
44.239	0.0000415385893	245	0.71105	0.28895	Yes
39.256	0.0000422279465	245	0.71105	0.28895	Yes
34.043	0.0000430718870	245	0.71105	0.28895	Yes
29.624	0.0000439309406	245	0.71105	0.28895	Yes
24.157	0.0000452570601	245	0.71105	0.28895	Yes
18.997	0.0000469682025	245	0.71105	0.28895	Yes
68.926	0.0000371388249	245	0.90921	0.09079	Yes
63.374	0.0000374223486	245	0.90921	0.09079	Yes
57.687	0.0000377287304	245	0.90921	0.09079	Yes
52.013	0.0000380691335	245	0.90921	0.09079	Yes
46.110	0.0000384511862	245	0.90921	0.09079	Yes
40.397	0.0000388681592	245	0.90921	0.09079	Yes
34.971	0.0000392989075	245	0.90921	0.09079	Yes
29.357	0.0000398009950	245	0.90921	0.09079	Yes
23.315	0.0000404236397	245	0.90921	0.09079	Yes
17.497	0.0000411336432	245	0.90921	0.09079	Yes
11.846	0.0000419691946	245	0.90921	0.09079	Yes
68.418	0.0000429516365	255	0.50365	0.49635	Yes
63.922	0.0000435995814	255	0.50365	0.49635	Yes
59.345	0.0000443360674	255	0.50365	0.49635	Yes
55.723	0.0000449923513	255	0.50365	0.49635	Yes
50.245	0.0000461254613	255	0.50365	0.49635	Yes
45.746	0.0000472076665	255	0.50365	0.49635	Yes
41.210	0.0000485342652	255	0.50365	0.49635	Yes
36.441	0.0000502462064	255	0.50365	0.49635	Yes
32.023	0.0000522793810	255	0.50365	0.49635	Yes
27.634	0.0000550024751	255	0.50365	0.49635	Yes
22.818	0.0000594707107	255	0.50365	0.49635	Yes
18.165	0.0000671005838	255	0.50365	0.49635	Yes
68.980	0.0000508750509	265	0.10560	0.89440	Yes
59.626	0.0000539170755	265	0.10560	0.89440	Yes
51.662	0.0000574118728	265	0.10560	0.89440	Yes
45.014	0.0000613346418	265	0.10560	0.89440	Yes
39.419	0.0000657721652	265	0.10560	0.89440	Yes
34.460	0.0000710782572	265	0.10560	0.89440	Yes
30.257	0.0000771843161	265	0.10560	0.89440	Yes
26.580	0.0000844737287	265	0.10560	0.89440	Yes
23.281	0.0000933881210	265	0.10560	0.89440	Yes
20.372	0.0001041775185	265	0.10560	0.89440	Yes
17.697	0.0001178689298	265	0.10560	0.89440	Yes
15.189	0.0001359434475	265	0.10560	0.89440	Yes
12.832	0.0001602564103	265	0.10560	0.89440	Yes
10.538	0.0001953888238	265	0.10560	0.89440	Yes
8.288	0.0002502502503	265	0.10560	0.89440	Yes
6.015	0.0003487966516	265	0.10560	0.89440	Yes
3.740	0.0005701254276	265	0.10560	0.89440	Yes
1.408	0.0015455950541	265	0.10560	0.89440	Yes
68.657	0.0000483675937	265	0.25147	0.74853	Yes
58.009	0.0000513109959	265	0.25147	0.74853	Yes
49.373	0.0000546179475	265	0.25147	0.74853	Yes
42.394	0.0000583260426	265	0.25147	0.74853	Yes
36.542	0.0000626841346	265	0.25147	0.74853	Yes
31.649	0.0000677874187	265	0.25147	0.74853	Yes
27.743	0.0000734969866	265	0.25147	0.74853	Yes
24.334	0.0000804569957	265	0.25147	0.74853	Yes
21.323	0.0000890551251	265	0.25147	0.74853	Yes
18.758	0.0000993048659	265	0.25147	0.74853	Yes
16.383	0.0001125999324	265	0.25147	0.74853	Yes
14.202	0.0001299545159	265	0.25147	0.74853	Yes
12.108	0.0001538698261	265	0.25147	0.74853	Yes
10.055	0.0001884303750	265	0.25147	0.74853	Yes
8.034	0.0002414875634	265	0.25147	0.74853	Yes
5.906	0.0003385240352	265	0.25147	0.74853	Yes
3.669	0.0005643340858	265	0.25147	0.74853	Yes
1.242	0.0017361111111	265	0.25147	0.74853	Yes
69.001	0.0000439966563	265	0.50365	0.49635	Yes
55.649	0.0000463994061	265	0.50365	0.49635	Yes
43.359	0.0000497240316	265	0.50365	0.49635	Yes
35.192	0.0000531603849	265	0.50365	0.49635	Yes
29.030	0.0000571265353	265	0.50365	0.49635	Yes
24.410	0.0000617627077	265	0.50365	0.49635	Yes
20.995	0.0000670555891	265	0.50365	0.49635	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
18.245	0.0000736105999	265	0.50365	0.49635	Yes
16.080	0.0000815328170	265	0.50365	0.49635	Yes
14.235	0.0000917010546	265	0.50365	0.49635	Yes
12.784	0.0001034447088	265	0.50365	0.49635	Yes
11.373	0.0001198897015	265	0.50365	0.49635	Yes
10.049	0.0001418842225	265	0.50365	0.49635	Yes
8.649	0.0001744896179	265	0.50365	0.49635	Yes
7.181	0.0002258355917	265	0.50365	0.49635	Yes
5.511	0.0003192848020	265	0.50365	0.49635	Yes
3.500	0.0005506607930	265	0.50365	0.49635	Yes
1.140	0.0018587360595	265	0.50365	0.49635	Yes
68.931	0.0000410441635	265	0.71105	0.28895	Yes
57.785	0.0000422725736	265	0.71105	0.28895	Yes
48.415	0.0000435938794	265	0.71105	0.28895	Yes
40.590	0.0000449984251	265	0.71105	0.28895	Yes
34.035	0.0000465354367	265	0.71105	0.28895	Yes
28.869	0.0000481185641	265	0.71105	0.28895	Yes
24.672	0.0000498206457	265	0.71105	0.28895	Yes
21.376	0.0000516129032	265	0.71105	0.28895	Yes
18.559	0.0000536682230	265	0.71105	0.28895	Yes
16.504	0.0000557506829	265	0.71105	0.28895	Yes
14.781	0.0000581598232	265	0.71105	0.28895	Yes
13.579	0.0000605070491	265	0.71105	0.28895	Yes
13.579	0.0000605070491	265	0.71105	0.28895	Yes
68.251	0.0000388440025	265	0.90921	0.09079	Yes
61.833	0.0000392680437	265	0.90921	0.09079	Yes
56.018	0.0000396998690	265	0.90921	0.09079	Yes
50.756	0.0000401300213	265	0.90921	0.09079	Yes
45.612	0.0000405959485	265	0.90921	0.09079	Yes
41.002	0.0000410509031	265	0.90921	0.09079	Yes
36.809	0.0000415092773	265	0.90921	0.09079	Yes
32.721	0.0000420150414	265	0.90921	0.09079	Yes
29.107	0.0000425115844	265	0.90921	0.09079	Yes
25.874	0.0000430107527	265	0.90921	0.09079	Yes
22.907	0.0000435198886	265	0.90921	0.09079	Yes
20.145	0.0000440606274	265	0.90921	0.09079	Yes
17.673	0.0000446030330	265	0.90921	0.09079	Yes
15.450	0.0000451528424	265	0.90921	0.09079	Yes
13.391	0.0000457414692	265	0.90921	0.09079	Yes
11.756	0.0000462727315	265	0.90921	0.09079	Yes
9.953	0.0000469461528	265	0.90921	0.09079	Yes
8.547	0.0000475511175	265	0.90921	0.09079	Yes
69.014	0.0000451691585	275	0.50365	0.49635	Yes
55.386	0.0000479363405	275	0.50365	0.49635	Yes
45.081	0.0000510334269	275	0.50365	0.49635	Yes
37.149	0.0000545791944	275	0.50365	0.49635	Yes
31.129	0.0000586372698	275	0.50365	0.49635	Yes
26.449	0.0000633793890	275	0.50365	0.49635	Yes
22.837	0.0000689369916	275	0.50365	0.49635	Yes
19.987	0.0000755229968	275	0.50365	0.49635	Yes
17.566	0.0000838855801	275	0.50365	0.49635	Yes
15.661	0.0000935278713	275	0.50365	0.49635	Yes
13.921	0.0001062022090	275	0.50365	0.49635	Yes
12.286	0.0001234872808	275	0.50365	0.49635	Yes
10.850	0.0001451589490	275	0.50365	0.49635	Yes
9.299	0.0001781895937	275	0.50365	0.49635	Yes
7.643	0.0002308402585	275	0.50365	0.49635	Yes
5.790	0.0003264773098	275	0.50365	0.49635	Yes
3.684	0.0005534034311	275	0.50365	0.49635	Yes
1.152	0.0019157088123	275	0.50365	0.49635	Yes
68.988	0.0000420751462	275	0.71105	0.28895	Yes
56.724	0.0000436338249	275	0.71105	0.28895	Yes
46.572	0.0000453576450	275	0.71105	0.28895	Yes
38.614	0.0000471809389	275	0.71105	0.28895	Yes
32.303	0.0000491424640	275	0.71105	0.28895	Yes
27.197	0.0000513267977	275	0.71105	0.28895	Yes
23.293	0.0000536682230	275	0.71105	0.28895	Yes
20.170	0.0000563126478	275	0.71105	0.28895	Yes
17.915	0.0000590179415	275	0.71105	0.28895	Yes
16.008	0.0000622703780	275	0.71105	0.28895	Yes
14.525	0.0000658978583	275	0.71105	0.28895	Yes
13.428	0.0000697058413	275	0.71105	0.28895	Yes
12.490	0.0000742115028	275	0.71105	0.28895	Yes
12.490	0.0000742115028	275	0.71105	0.28895	Yes
69.124	0.0000536020583	285	0.10560	0.89440	Yes
61.286	0.0000564812200	285	0.10560	0.89440	Yes
54.492	0.0000596801146	285	0.10560	0.89440	Yes
48.534	0.0000632671138	285	0.10560	0.89440	Yes
43.343	0.0000673038094	285	0.10560	0.89440	Yes
38.736	0.0000718597298	285	0.10560	0.89440	Yes
34.711	0.0000769882208	285	0.10560	0.89440	Yes
30.952	0.0000831462543	285	0.10560	0.89440	Yes
27.610	0.0000903260771	285	0.10560	0.89440	Yes
24.590	0.0000987751877	285	0.10560	0.89440	Yes
21.802	0.0001090393632	285	0.10560	0.89440	Yes
19.227	0.0001215509906	285	0.10560	0.89440	Yes
16.819	0.0001372495196	285	0.10560	0.89440	Yes
14.481	0.0001580777743	285	0.10560	0.89440	Yes
12.256	0.0001859427296	285	0.10560	0.89440	Yes
10.090	0.0002255808707	285	0.10560	0.89440	Yes
7.932	0.0002880184332	285	0.10560	0.89440	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
5.792	0.0003961965135	285	0.10560	0.89440	Yes
3.650	0.0006345177665	285	0.10560	0.89440	Yes
1.477	0.0015873015873	285	0.10560	0.89440	Yes
69.088	0.0000509580106	285	0.25147	0.74853	Yes
60.329	0.0000537056928	285	0.25147	0.74853	Yes
52.977	0.0000567472478	285	0.25147	0.74853	Yes
46.679	0.0000601503759	285	0.25147	0.74853	Yes
41.260	0.0000640286849	285	0.25147	0.74853	Yes
36.619	0.0000684041316	285	0.25147	0.74853	Yes
32.596	0.0000734052705	285	0.25147	0.74853	Yes
29.030	0.0000792958528	285	0.25147	0.74853	Yes
25.912	0.0000861029792	285	0.25147	0.74853	Yes
23.106	0.0000942418245	285	0.25147	0.74853	Yes
20.577	0.0001039609107	285	0.25147	0.74853	Yes
18.220	0.0001160766106	285	0.25147	0.74853	Yes
15.997	0.0001314924392	285	0.25147	0.74853	Yes
13.903	0.0001513546239	285	0.25147	0.74853	Yes
11.843	0.0001787629603	285	0.25147	0.74853	Yes
9.840	0.0002174858634	285	0.25147	0.74853	Yes
7.824	0.0002776235425	285	0.25147	0.74853	Yes
5.730	0.0003862495172	285	0.25147	0.74853	Yes
3.582	0.0006325110689	285	0.25147	0.74853	Yes
1.354	0.0017123287671	285	0.25147	0.74853	Yes
69.189	0.0000463800380	285	0.50365	0.49635	Yes
57.633	0.0000488997555	285	0.50365	0.49635	Yes
48.491	0.0000516982888	285	0.50365	0.49635	Yes
41.194	0.0000548305735	285	0.50365	0.49635	Yes
35.359	0.0000583532707	285	0.50365	0.49635	Yes
30.659	0.0000623908161	285	0.50365	0.49635	Yes
26.842	0.0000670376081	285	0.50365	0.49635	Yes
23.732	0.0000723903287	285	0.50365	0.49635	Yes
21.142	0.0000787091696	285	0.50365	0.49635	Yes
18.932	0.0000862143288	285	0.50365	0.49635	Yes
16.990	0.0000954289531	285	0.50365	0.49635	Yes
15.270	0.0001066666667	285	0.50365	0.49635	Yes
13.678	0.0001208751360	285	0.50365	0.49635	Yes
12.150	0.0001394116827	285	0.50365	0.49635	Yes
10.616	0.0001651527663	285	0.50365	0.49635	Yes
9.050	0.0002021018593	285	0.50365	0.49635	Yes
7.376	0.0002606202763	285	0.50365	0.49635	Yes
5.543	0.0003660322108	285	0.50365	0.49635	Yes
3.502	0.0006146281500	285	0.50365	0.49635	Yes
1.192	0.0019157088123	285	0.50365	0.49635	Yes
69.080	0.0000431276146	285	0.71105	0.28895	Yes
55.607	0.0000451019304	285	0.71105	0.28895	Yes
44.919	0.0000473014522	285	0.71105	0.28895	Yes
35.358	0.0000502008032	285	0.71105	0.28895	Yes
26.656	0.0000546060176	285	0.71105	0.28895	Yes
21.011	0.0000598479861	285	0.71105	0.28895	Yes
17.501	0.0000658197854	285	0.71105	0.28895	Yes
15.302	0.0000722804481	285	0.71105	0.28895	Yes
13.685	0.0000799808046	285	0.71105	0.28895	Yes
12.389	0.0000897263347	285	0.71105	0.28895	Yes
11.337	0.0001015640869	285	0.71105	0.28895	Yes
10.346	0.0001179662616	285	0.71105	0.28895	Yes
9.405	0.0001399188471	285	0.71105	0.28895	Yes
8.387	0.0001721170396	285	0.71105	0.28895	Yes
7.189	0.0002226675573	285	0.71105	0.28895	Yes
5.658	0.0003166561115	285	0.71105	0.28895	Yes
3.656	0.0005515719801	285	0.71105	0.28895	Yes
1.088	0.0020833333333	285	0.71105	0.28895	Yes
69.019	0.0000406140850	285	0.90921	0.09079	Yes
57.355	0.0000416597234	285	0.90921	0.09079	Yes
47.721	0.0000427386956	285	0.90921	0.09079	Yes
39.762	0.0000438461876	285	0.90921	0.09079	Yes
32.843	0.0000450511330	285	0.90921	0.09079	Yes
27.142	0.0000463177397	285	0.90921	0.09079	Yes
22.447	0.0000476621705	285	0.90921	0.09079	Yes
18.648	0.0000490966222	285	0.90921	0.09079	Yes
15.654	0.0000505996053	285	0.90921	0.09079	Yes
13.219	0.0000522356874	285	0.90921	0.09079	Yes
11.374	0.0000539723661	285	0.90921	0.09079	Yes
10.034	0.0000557444674	285	0.90921	0.09079	Yes
9.013	0.0000576568266	285	0.90921	0.09079	Yes
69.055	0.0000557537913	300	0.10560	0.89440	Yes
61.675	0.0000587130108	300	0.10560	0.89440	Yes
55.165	0.0000620424370	300	0.10560	0.89440	Yes
49.506	0.0000657073395	300	0.10560	0.89440	Yes
44.370	0.0000699007409	300	0.10560	0.89440	Yes
39.817	0.0000746491490	300	0.10560	0.89440	Yes
35.681	0.0000801538955	300	0.10560	0.89440	Yes
31.967	0.0000864453665	300	0.10560	0.89440	Yes
28.534	0.0000940026321	300	0.10560	0.89440	Yes
25.493	0.0001026377912	300	0.10560	0.89440	Yes
22.642	0.0001131221719	300	0.10560	0.89440	Yes
19.933	0.0001262785705	300	0.10560	0.89440	Yes
17.400	0.0001427144284	300	0.10560	0.89440	Yes
14.971	0.0001642575558	300	0.10560	0.89440	Yes
12.682	0.0001927525058	300	0.10560	0.89440	Yes
10.413	0.0002340823970	300	0.10560	0.89440	Yes
8.196	0.0002973535534	300	0.10560	0.89440	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
5.999	0.0004071661238	300	0.10560	0.89440	Yes
3.767	0.0006518904824	300	0.10560	0.89440	Yes
1.537	0.0016129032258	300	0.10560	0.89440	Yes
69.107	0.0000533646406	300	0.25147	0.74853	Yes
60.931	0.0000562619557	300	0.25147	0.74853	Yes
54.037	0.0000594247682	300	0.25147	0.74853	Yes
48.072	0.0000629485081	300	0.25147	0.74853	Yes
42.827	0.0000669792364	300	0.25147	0.74853	Yes
38.228	0.0000715409930	300	0.25147	0.74853	Yes
34.097	0.0000768875903	300	0.25147	0.74853	Yes
30.514	0.0000829600133	300	0.25147	0.74853	Yes
27.295	0.0000900576369	300	0.25147	0.74853	Yes
24.350	0.0000985998817	300	0.25147	0.74853	Yes
21.667	0.0001088257699	300	0.25147	0.74853	Yes
19.169	0.0001214771623	300	0.25147	0.74853	Yes
16.816	0.0001374381528	300	0.25147	0.74853	Yes
14.565	0.0001582528881	300	0.25147	0.74853	Yes
12.396	0.0001862891207	300	0.25147	0.74853	Yes
10.244	0.0002268602541	300	0.25147	0.74853	Yes
8.099	0.0002900232019	300	0.25147	0.74853	Yes
5.937	0.0004006410256	300	0.25147	0.74853	Yes
3.713	0.0006523157208	300	0.25147	0.74853	Yes
1.436	0.0017211703959	300	0.25147	0.74853	Yes
69.028	0.0000483863163	300	0.50365	0.49635	Yes
58.681	0.0000510021931	300	0.50365	0.49635	Yes
50.230	0.0000539345235	300	0.50365	0.49635	Yes
43.426	0.0000571820677	300	0.50365	0.49635	Yes
37.763	0.0000608828006	300	0.50365	0.49635	Yes
33.118	0.0000650702759	300	0.50365	0.49635	Yes
29.248	0.0000699202909	300	0.50365	0.49635	Yes
26.056	0.0000754204691	300	0.50365	0.49635	Yes
23.267	0.0000820008200	300	0.50365	0.49635	Yes
20.829	0.0000899038029	300	0.50365	0.49635	Yes
18.707	0.0000993147284	300	0.50365	0.49635	Yes
16.744	0.0001110247585	300	0.50365	0.49635	Yes
14.914	0.0001259128683	300	0.50365	0.49635	Yes
13.165	0.0001451800232	300	0.50365	0.49635	Yes
11.413	0.0001718803713	300	0.50365	0.49635	Yes
9.643	0.0002101723413	300	0.50365	0.49635	Yes
7.789	0.0002706359946	300	0.50365	0.49635	Yes
5.819	0.0003780718336	300	0.50365	0.49635	Yes
3.652	0.0006333122229	300	0.50365	0.49635	Yes
1.262	0.0019379844961	300	0.50365	0.49635	Yes
69.024	0.0000448651801	300	0.71105	0.28895	Yes
55.166	0.0000473036897	300	0.71105	0.28895	Yes
44.719	0.0000500175061	300	0.71105	0.28895	Yes
36.720	0.0000530701056	300	0.71105	0.28895	Yes
30.675	0.0000565418975	300	0.71105	0.28895	Yes
26.095	0.0000604741171	300	0.71105	0.28895	Yes
22.632	0.0000649814803	300	0.71105	0.28895	Yes
19.974	0.0000701360640	300	0.71105	0.28895	Yes
17.845	0.0000763883584	300	0.71105	0.28895	Yes
16.111	0.0000838855801	300	0.71105	0.28895	Yes
14.704	0.0000927213723	300	0.71105	0.28895	Yes
13.465	0.0001034661148	300	0.71105	0.28895	Yes
12.271	0.0001177163037	300	0.71105	0.28895	Yes
11.181	0.0001354646437	300	0.71105	0.28895	Yes
9.989	0.0001611084260	300	0.71105	0.28895	Yes
8.735	0.0001972775695	300	0.71105	0.28895	Yes
7.292	0.0002551020408	300	0.71105	0.28895	Yes
5.602	0.0003602305476	300	0.71105	0.28895	Yes
3.567	0.0006172839506	300	0.71105	0.28895	Yes
1.147	0.0021052631579	300	0.71105	0.28895	Yes
69.020	0.0000420486082	300	0.90921	0.09079	Yes
55.550	0.0000435521101	300	0.90921	0.09079	Yes
43.810	0.0000453370812	300	0.90921	0.09079	Yes
34.664	0.0000472656804	300	0.90921	0.09079	Yes
26.591	0.0000497784857	300	0.90921	0.09079	Yes
19.704	0.0000533049041	300	0.90921	0.09079	Yes
14.523	0.0000586235198	300	0.90921	0.09079	Yes
11.758	0.0000652869361	300	0.90921	0.09079	Yes
10.406	0.0000732118017	300	0.90921	0.09079	Yes
9.571	0.0000844880027	300	0.90921	0.09079	Yes
9.037	0.0000984736583	300	0.90921	0.09079	Yes
8.608	0.0001160900859	300	0.90921	0.09079	Yes
8.212	0.0001374381528	300	0.90921	0.09079	Yes
7.677	0.0001683501684	300	0.90921	0.09079	Yes
6.831	0.0002203613927	300	0.90921	0.09079	Yes
5.587	0.0003135779241	300	0.90921	0.09079	Yes
3.708	0.0005509641873	300	0.90921	0.09079	Yes
1.031	0.0023094688222	300	0.90921	0.09079	Yes
34.747	0.0000878657411	320	0.10560	0.89440	Yes
30.700	0.0000961076406	320	0.10560	0.89440	Yes
27.037	0.0001060670344	320	0.10560	0.89440	Yes
23.668	0.0001183291918	320	0.10560	0.89440	Yes
20.550	0.0001336183859	320	0.10560	0.89440	Yes
17.649	0.0001533272002	320	0.10560	0.89440	Yes
14.819	0.0001804402743	320	0.10560	0.89440	Yes
12.114	0.0002189621196	320	0.10560	0.89440	Yes
9.397	0.0002810567735	320	0.10560	0.89440	Yes
6.805	0.0003875968992	320	0.10560	0.89440	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
4.181	0.0006317119394	320	0.10560	0.89440	Yes
1.740	0.0015197568389	320	0.10560	0.89440	Yes
69.011	0.0000559002739	320	0.25147	0.74853	Yes
61.506	0.0000588754784	320	0.25147	0.74853	Yes
54.928	0.0000622432466	320	0.25147	0.74853	Yes
50.951	0.0000647081662	320	0.25147	0.74853	Yes
45.125	0.0000692376930	320	0.25147	0.74853	Yes
39.687	0.0000748727164	320	0.25147	0.74853	Yes
35.619	0.0000804052424	320	0.25147	0.74853	Yes
32.020	0.0000865875833	320	0.25147	0.74853	Yes
28.675	0.0000940733772	320	0.25147	0.74853	Yes
25.733	0.0001025956705	320	0.25147	0.74853	Yes
22.962	0.0001129943503	320	0.25147	0.74853	Yes
20.261	0.0001263743207	320	0.25147	0.74853	Yes
17.748	0.0001428979708	320	0.25147	0.74853	Yes
15.405	0.0001638538424	320	0.25147	0.74853	Yes
13.081	0.0001926411096	320	0.25147	0.74853	Yes
10.804	0.0002339181287	320	0.25147	0.74853	Yes
8.566	0.0002965599051	320	0.25147	0.74853	Yes
6.308	0.0004061738424	320	0.25147	0.74853	Yes
3.923	0.0006605019815	320	0.25147	0.74853	Yes
1.554	0.0016977928693	320	0.25147	0.74853	Yes
69.044	0.0000510334269	320	0.50365	0.49635	Yes
59.508	0.0000538502962	320	0.50365	0.49635	Yes
51.900	0.0000569281567	320	0.50365	0.49635	Yes
45.580	0.0000603463883	320	0.50365	0.49635	Yes
40.180	0.0000642590927	320	0.50365	0.49635	Yes
35.685	0.0000686436024	320	0.50365	0.49635	Yes
31.758	0.0000737463127	320	0.50365	0.49635	Yes
28.435	0.0000795861520	320	0.50365	0.49635	Yes
25.458	0.0000865875833	320	0.50365	0.49635	Yes
22.859	0.0000947777462	320	0.50365	0.49635	Yes
20.472	0.0001047449461	320	0.50365	0.49635	Yes
18.276	0.0001172058134	320	0.50365	0.49635	Yes
16.233	0.0001325205407	320	0.50365	0.49635	Yes
14.233	0.0001528584531	320	0.50365	0.49635	Yes
12.261	0.0001806032147	320	0.50365	0.49635	Yes
10.290	0.0002205071665	320	0.50365	0.49635	Yes
8.230	0.0002836879433	320	0.50365	0.49635	Yes
6.074	0.0003971405878	320	0.50365	0.49635	Yes
3.800	0.0006587615283	320	0.50365	0.49635	Yes
1.353	0.0019305019305	320	0.50365	0.49635	Yes
68.951	0.0000472902677	320	0.71105	0.28895	Yes
56.959	0.0000498902415	320	0.71105	0.28895	Yes
47.500	0.0000528345749	320	0.71105	0.28895	Yes
40.063	0.0000561671534	320	0.71105	0.28895	Yes
34.288	0.0000598945855	320	0.71105	0.28895	Yes
29.742	0.0000641972138	320	0.71105	0.28895	Yes
26.138	0.0000691323885	320	0.71105	0.28895	Yes
23.221	0.0000748727164	320	0.71105	0.28895	Yes
20.797	0.0000816459830	320	0.71105	0.28895	Yes
18.747	0.0000898311175	320	0.71105	0.28895	Yes
16.988	0.0000997506234	320	0.71105	0.28895	Yes
15.338	0.0001122838536	320	0.71105	0.28895	Yes
13.797	0.0001283532281	320	0.71105	0.28895	Yes
12.287	0.0001496110114	320	0.71105	0.28895	Yes
10.719	0.0001796299623	320	0.71105	0.28895	Yes
9.068	0.0002242152466	320	0.71105	0.28895	Yes
7.231	0.0002991325157	320	0.71105	0.28895	Yes
5.144	0.0004488330341	320	0.71105	0.28895	Yes
2.761	0.0008984725966	320	0.71105	0.28895	Yes
1.224	0.0021186440678	320	0.71105	0.28895	Yes
69.065	0.0000441423148	320	0.90921	0.09079	Yes
55.533	0.0000460935699	320	0.90921	0.09079	Yes
41.924	0.0000490148025	320	0.90921	0.09079	Yes
31.439	0.0000527398344	320	0.90921	0.09079	Yes
24.524	0.0000570353049	320	0.90921	0.09079	Yes
19.987	0.0000620770998	320	0.90921	0.09079	Yes
17.288	0.0000673763644	320	0.90921	0.09079	Yes
15.306	0.0000741125028	320	0.90921	0.09079	Yes
13.907	0.0000821287779	320	0.90921	0.09079	Yes
12.841	0.0000918779860	320	0.90921	0.09079	Yes
11.919	0.0001044277360	320	0.90921	0.09079	Yes
11.058	0.0001208605270	320	0.90921	0.09079	Yes
10.159	0.0001433691756	320	0.90921	0.09079	Yes
9.113	0.0001764602082	320	0.90921	0.09079	Yes
7.881	0.0002263980077	320	0.90921	0.09079	Yes
6.126	0.0003286230693	320	0.90921	0.09079	Yes
3.955	0.0005727376861	320	0.90921	0.09079	Yes
1.111	0.0022988505747	320	0.90921	0.09079	Yes
69.189	0.0000627667587	350	0.10560	0.89440	Yes
62.799	0.0000660938533	350	0.10560	0.89440	Yes
57.018	0.0000697982830	350	0.10560	0.89440	Yes
51.735	0.0000739644970	350	0.10560	0.89440	Yes
46.821	0.0000787401575	350	0.10560	0.89440	Yes
42.587	0.0000838433806	350	0.10560	0.89440	Yes
38.449	0.0000899928006	350	0.10560	0.89440	Yes
34.625	0.0000971062342	350	0.10560	0.89440	Yes
31.132	0.0001052742394	350	0.10560	0.89440	Yes
27.855	0.0001150350857	350	0.10560	0.89440	Yes
24.756	0.0001268391679	350	0.10560	0.89440	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
21.856	0.0001412229911	350	0.10560	0.89440	Yes
19.062	0.0001594642003	350	0.10560	0.89440	Yes
16.417	0.0001827819411	350	0.10560	0.89440	Yes
13.867	0.0002141327623	350	0.10560	0.89440	Yes
11.366	0.0002592688618	350	0.10560	0.89440	Yes
8.925	0.0003281916639	350	0.10560	0.89440	Yes
6.550	0.0004452359751	350	0.10560	0.89440	Yes
4.182	0.0006949270327	350	0.10560	0.89440	Yes
1.840	0.0015748031496	350	0.10560	0.89440	Yes
69.195	0.0000600925425	350	0.25147	0.74853	Yes
62.429	0.0000632871337	350	0.25147	0.74853	Yes
56.348	0.0000668538575	350	0.25147	0.74853	Yes
50.943	0.0000708315625	350	0.25147	0.74853	Yes
46.046	0.0000753579503	350	0.25147	0.74853	Yes
41.551	0.0000805542130	350	0.25147	0.74853	Yes
37.578	0.0000862887221	350	0.25147	0.74853	Yes
33.822	0.0000931532371	350	0.25147	0.74853	Yes
30.428	0.0001010611420	350	0.25147	0.74853	Yes
27.254	0.0001105094486	350	0.25147	0.74853	Yes
24.223	0.0001221150324	350	0.25147	0.74853	Yes
21.446	0.0001359804188	350	0.25147	0.74853	Yes
18.790	0.0001535390757	350	0.25147	0.74853	Yes
16.208	0.0001766472355	350	0.25147	0.74853	Yes
13.711	0.0002077274616	350	0.25147	0.74853	Yes
8.875	0.0003206155819	350	0.25147	0.74853	Yes
6.486	0.0004395604396	350	0.25147	0.74853	Yes
4.097	0.0006993006993	350	0.25147	0.74853	Yes
1.687	0.0017064846416	350	0.25147	0.74853	Yes
69.156	0.0000551571980	350	0.50365	0.49635	Yes
61.236	0.0000581057525	350	0.50365	0.49635	Yes
54.438	0.0000613986615	350	0.50365	0.49635	Yes
48.458	0.0000651805501	350	0.50365	0.49635	Yes
43.405	0.0000693000693	350	0.50365	0.49635	Yes
38.917	0.0000740795614	350	0.50365	0.49635	Yes
34.980	0.0000794975753	350	0.50365	0.49635	Yes
31.453	0.0000858369099	350	0.50365	0.49635	Yes
28.285	0.0000932835821	350	0.50365	0.49635	Yes
25.426	0.0001020304051	350	0.50365	0.49635	Yes
22.752	0.0001127268628	350	0.50365	0.49635	Yes
20.228	0.0001261034048	350	0.50365	0.49635	Yes
17.857	0.0001427551749	350	0.50365	0.49635	Yes
15.571	0.0001643925695	350	0.50365	0.49635	Yes
13.325	0.0001939111887	350	0.50365	0.49635	Yes
11.077	0.0002364625207	350	0.50365	0.49635	Yes
8.801	0.0003029385035	350	0.50365	0.49635	Yes
6.454	0.0004219409283	350	0.50365	0.49635	Yes
4.034	0.0006915629322	350	0.50365	0.49635	Yes
1.476	0.0019531250000	350	0.50365	0.49635	Yes
69.088	0.0000511325868	350	0.71105	0.28895	Yes
59.363	0.0000539199827	350	0.71105	0.28895	Yes
51.469	0.0000569930468	350	0.71105	0.28895	Yes
45.039	0.0000603937674	350	0.71105	0.28895	Yes
39.580	0.0000643459237	350	0.71105	0.28895	Yes
35.089	0.0000687757909	350	0.71105	0.28895	Yes
31.309	0.0000738552437	350	0.71105	0.28895	Yes
28.076	0.0000797575371	350	0.71105	0.28895	Yes
25.267	0.0000867302689	350	0.71105	0.28895	Yes
22.802	0.0000949667616	350	0.71105	0.28895	Yes
20.562	0.0001049979000	350	0.71105	0.28895	Yes
18.453	0.0001176885960	350	0.71105	0.28895	Yes
16.502	0.0001333333333	350	0.71105	0.28895	Yes
14.597	0.0001537042730	350	0.71105	0.28895	Yes
12.664	0.0001818843216	350	0.71105	0.28895	Yes
10.712	0.0002221728505	350	0.71105	0.28895	Yes
8.374	0.0002968239834	350	0.71105	0.28895	Yes
6.421	0.0004016064257	350	0.71105	0.28895	Yes
3.980	0.0006784260516	350	0.71105	0.28895	Yes
1.333	0.0021321961620	350	0.71105	0.28895	Yes
69.093	0.0000476122459	350	0.90921	0.09079	Yes
56.576	0.0000501806503	350	0.90921	0.09079	Yes
46.868	0.0000530532124	350	0.90921	0.09079	Yes
39.302	0.0000563253351	350	0.90921	0.09079	Yes
33.571	0.0000599628230	350	0.90921	0.09079	Yes
29.105	0.0000641395677	350	0.90921	0.09079	Yes
25.639	0.0000689179876	350	0.90921	0.09079	Yes
22.896	0.0000745267551	350	0.90921	0.09079	Yes
20.684	0.0000810635538	350	0.90921	0.09079	Yes
18.865	0.0000887705282	350	0.90921	0.09079	Yes
17.249	0.0000982607841	350	0.90921	0.09079	Yes
15.798	0.0001099263493	350	0.90921	0.09079	Yes
14.396	0.0001249531426	350	0.90921	0.09079	Yes
13.019	0.0001446340758	350	0.90921	0.09079	Yes
11.601	0.0001709693965	350	0.90921	0.09079	Yes
10.053	0.0002095118374	350	0.90921	0.09079	Yes
8.306	0.0002711496746	350	0.90921	0.09079	Yes
6.290	0.0003849114704	350	0.90921	0.09079	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
3.957	0.0006591957811	350	0.90921	0.09079	Yes
1.220	0.0023041474654	350	0.90921	0.09079	Yes
68.655	0.0000701557458	400	0.10560	0.89440	Yes
63.076	0.0000737517516	400	0.10560	0.89440	Yes
57.528	0.0000780822987	400	0.10560	0.89440	Yes
51.633	0.0000837591088	400	0.10560	0.89440	Yes
45.922	0.0000907605736	400	0.10560	0.89440	Yes
40.264	0.0000997506234	400	0.10560	0.89440	Yes
34.122	0.0001131605749	400	0.10560	0.89440	Yes
28.750	0.0001299038711	400	0.10560	0.89440	Yes
22.860	0.0001579529300	400	0.10560	0.89440	Yes
17.385	0.0002020202020	400	0.10560	0.89440	Yes
11.889	0.0002887669651	400	0.10560	0.89440	Yes
5.747	0.0005854800937	400	0.10560	0.89440	Yes
68.727	0.0000675858340	400	0.25147	0.74853	Yes
63.061	0.0000709975151	400	0.25147	0.74853	Yes
57.436	0.0000750976269	400	0.25147	0.74853	Yes
51.693	0.0000802954874	400	0.25147	0.74853	Yes
45.922	0.0000869489610	400	0.25147	0.74853	Yes
40.281	0.0000955109838	400	0.25147	0.74853	Yes
34.456	0.0001075384450	400	0.25147	0.74853	Yes
28.669	0.0001249063203	400	0.25147	0.74853	Yes
23.064	0.0001507386192	400	0.25147	0.74853	Yes
16.675	0.0002033346889	400	0.25147	0.74853	Yes
11.547	0.0002894356006	400	0.25147	0.74853	Yes
5.867	0.0005659309564	400	0.25147	0.74853	Yes
68.619	0.0000627234523	400	0.50365	0.49635	Yes
63.139	0.0000654835964	400	0.50365	0.49635	Yes
57.289	0.0000690941754	400	0.50365	0.49635	Yes
51.725	0.0000733944954	400	0.50365	0.49635	Yes
45.830	0.0000792707095	400	0.50365	0.49635	Yes
40.049	0.0000870322019	400	0.50365	0.49635	Yes
34.424	0.0000975419430	400	0.50365	0.49635	Yes
28.635	0.0001135460429	400	0.50365	0.49635	Yes
22.930	0.0001386577926	400	0.50365	0.49635	Yes
17.447	0.0001805380032	400	0.50365	0.49635	Yes
11.530	0.0002746498215	400	0.50365	0.49635	Yes
6.060	0.0005307855626	400	0.50365	0.49635	Yes
68.723	0.0000584043920	400	0.71105	0.28895	Yes
63.024	0.0000607348922	400	0.71105	0.28895	Yes
57.544	0.0000634880325	400	0.71105	0.28895	Yes
51.834	0.0000670735797	400	0.71105	0.28895	Yes
45.987	0.0000718648940	400	0.71105	0.28895	Yes
40.123	0.0000784375245	400	0.71105	0.28895	Yes
34.480	0.0000874737579	400	0.71105	0.28895	Yes
28.678	0.0001016983627	400	0.71105	0.28895	Yes
22.998	0.0001247972045	400	0.71105	0.28895	Yes
17.097	0.0001691474966	400	0.71105	0.28895	Yes
11.537	0.0002586652871	400	0.71105	0.28895	Yes
5.890	0.0005316321106	400	0.71105	0.28895	Yes
68.626	0.0000543507799	400	0.90921	0.09079	Yes
63.073	0.0000560915414	400	0.90921	0.09079	Yes
57.472	0.0000582207732	400	0.90921	0.09079	Yes
51.935	0.0000608383525	400	0.90921	0.09079	Yes
45.955	0.0000645327827	400	0.90921	0.09079	Yes
40.612	0.0000689940665	400	0.90921	0.09079	Yes
34.588	0.0000763358779	400	0.90921	0.09079	Yes
28.277	0.0000891186169	400	0.90921	0.09079	Yes
23.033	0.0001080730574	400	0.90921	0.09079	Yes
17.344	0.0001478415139	400	0.90921	0.09079	Yes
11.728	0.0002345765893	400	0.90921	0.09079	Yes
6.627	0.0004508566276	400	0.90921	0.09079	Yes
68.588	0.0000773455024	450	0.10560	0.89440	Yes
57.394	0.0000867829558	450	0.10560	0.89440	Yes
51.431	0.0000935891437	450	0.10560	0.89440	Yes
45.745	0.0001018433649	450	0.10560	0.89440	Yes
40.044	0.0001125619090	450	0.10560	0.89440	Yes
34.451	0.0001266624446	450	0.10560	0.89440	Yes
28.416	0.0001485001485	450	0.10560	0.89440	Yes
22.867	0.0001791472590	450	0.10560	0.89440	Yes
17.279	0.0002306273063	450	0.10560	0.89440	Yes
11.263	0.0003447087211	450	0.10560	0.89440	Yes
5.828	0.0006527415144	450	0.10560	0.89440	Yes
68.690	0.0000749232037	450	0.25147	0.74853	Yes
63.105	0.0000789639924	450	0.25147	0.74853	Yes
57.351	0.0000840406757	450	0.25147	0.74853	Yes
51.698	0.0000901875902	450	0.25147	0.74853	Yes
45.871	0.0000982511299	450	0.25147	0.74853	Yes
40.112	0.0001086838387	450	0.25147	0.74853	Yes
34.454	0.0001225490196	450	0.25147	0.74853	Yes
28.331	0.0001443001443	450	0.25147	0.74853	Yes
23.239	0.0001717032967	450	0.25147	0.74853	Yes
17.196	0.0002262443439	450	0.25147	0.74853	Yes
11.652	0.0003278688525	450	0.25147	0.74853	Yes
5.613	0.0006711409396	450	0.25147	0.74853	Yes
68.770	0.0000702197879	450	0.50365	0.49635	Yes
63.009	0.0000739262216	450	0.50365	0.49635	Yes
57.446	0.0000782840144	450	0.50365	0.49635	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
51.741	0.0000838926174	450	0.50365	0.49635	Yes
45.854	0.0000913242009	450	0.50365	0.49635	Yes
40.196	0.0001007759750	450	0.50365	0.49635	Yes
34.390	0.0001141552511	450	0.50365	0.49635	Yes
28.731	0.0001331026221	450	0.50365	0.49635	Yes
23.022	0.0001626545218	450	0.50365	0.49635	Yes
17.215	0.0002146383344	450	0.50365	0.49635	Yes
11.855	0.0003104625893	450	0.50365	0.49635	Yes
5.842	0.0006325110689	450	0.50365	0.49635	Yes
68.603	0.0000661157025	450	0.71105	0.28895	Yes
62.976	0.0000692712663	450	0.71105	0.28895	Yes
57.406	0.0000731101038	450	0.71105	0.28895	Yes
51.741	0.0000780274657	450	0.71105	0.28895	Yes
45.928	0.0000845522956	450	0.71105	0.28895	Yes
40.166	0.0000932835821	450	0.71105	0.28895	Yes
34.452	0.0001054296257	450	0.71105	0.28895	Yes
28.755	0.0001233654083	450	0.71105	0.28895	Yes
23.164	0.0001510345869	450	0.71105	0.28895	Yes
17.260	0.0002024701357	450	0.71105	0.28895	Yes
11.587	0.0003053435115	450	0.71105	0.28895	Yes
5.867	0.0006165228113	450	0.71105	0.28895	Yes
68.731	0.0000617932398	450	0.90921	0.09079	Yes
62.897	0.0000645078054	450	0.90921	0.09079	Yes
57.367	0.0000676910580	450	0.90921	0.09079	Yes
51.720	0.0000717978173	450	0.90921	0.09079	Yes
45.919	0.0000773514851	450	0.90921	0.09079	Yes
40.171	0.0000848824378	450	0.90921	0.09079	Yes
34.466	0.0000956480153	450	0.90921	0.09079	Yes
28.330	0.0001136880400	450	0.90921	0.09079	Yes
22.817	0.0001406271973	450	0.90921	0.09079	Yes
17.241	0.0001890001890	450	0.90921	0.09079	Yes
11.920	0.0002823263693	450	0.90921	0.09079	Yes
5.856	0.0006045949214	450	0.90921	0.09079	Yes

Continued: Data summarised from Table 1 of Brugge97 [86]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
69.031	5.03956E-05	300	0.3991	0.6009	Yes
65.422	5.12952E-05	300	0.3991	0.6009	Yes
62.028	5.22794E-05	300	0.3991	0.6009	Yes
58.63	5.33874E-05	300	0.3991	0.6009	Yes
55.214	5.46717E-05	300	0.3991	0.6009	Yes
51.775	5.61293E-05	300	0.3991	0.6009	Yes
48.387	5.77868E-05	300	0.3991	0.6009	Yes
43.634	6.06134E-05	300	0.3991	0.6009	Yes
39.295	6.38814E-05	300	0.3991	0.6009	Yes
34.539	6.85965E-05	300	0.3991	0.6009	Yes
30.092	7.25689E-05	300	0.3991	0.6009	Yes
69.189	4.638E-05	285	0.5037	0.4963	Yes
57.633	4.88998E-05	285	0.5037	0.4963	Yes
48.491	5.16983E-05	285	0.5037	0.4963	Yes
41.194	5.48306E-05	285	0.5037	0.4963	Yes
35.359	5.83533E-05	285	0.5037	0.4963	Yes
30.659	6.23908E-05	285	0.5037	0.4963	Yes
26.842	6.70376E-05	285	0.5037	0.4963	Yes
23.732	7.23903E-05	285	0.5037	0.4963	Yes
21.142	7.87092E-05	285	0.5037	0.4963	Yes
18.932	8.62143E-05	285	0.5037	0.4963	Yes
16.99	9.5429E-05	285	0.5037	0.4963	Yes
15.27	0.000106667	285	0.5037	0.4963	Yes
13.678	0.000120875	285	0.5037	0.4963	Yes
12.15	0.000139412	285	0.5037	0.4963	Yes
10.616	0.000165153	285	0.5037	0.4963	Yes
9.05	0.000202102	285	0.5037	0.4963	Yes
7.376	0.00026062	285	0.5037	0.4963	Yes
5.543	0.000366032	285	0.5037	0.4963	Yes
3.502	0.000614628	285	0.5037	0.4963	Yes
1.192	0.001915709	285	0.5037	0.4963	Yes
69.028	4.83863E-05	300	0.5037	0.4963	Yes
58.681	5.10022E-05	300	0.5037	0.4963	Yes
50.23	5.39345E-05	300	0.5037	0.4963	Yes
43.426	5.71821E-05	300	0.5037	0.4963	Yes
37.763	6.08828E-05	300	0.5037	0.4963	Yes
33.118	6.50703E-05	300	0.5037	0.4963	Yes
29.248	6.99203E-05	300	0.5037	0.4963	Yes
26.056	7.54205E-05	300	0.5037	0.4963	Yes
23.267	8.20008E-05	300	0.5037	0.4963	Yes
20.829	8.99038E-05	300	0.5037	0.4963	Yes
18.707	9.93147E-05	300	0.5037	0.4963	Yes
16.744	0.000111025	300	0.5037	0.4963	Yes
14.914	0.000125913	300	0.5037	0.4963	Yes
13.165	0.00014518	300	0.5037	0.4963	Yes
11.413	0.00017188	300	0.5037	0.4963	Yes
9.643	0.000210172	300	0.5037	0.4963	Yes

Data summarised from Table 1 of Duarte–Garza95–I [77]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
68.759	4.56163E-05	225	0.10560	0.89440	Yes
62.510	4.69792E-05	225	0.10560	0.89440	Yes
57.402	4.82952E-05	225	0.10560	0.89440	Yes
51.819	5.0025E-05	225	0.10560	0.89440	Yes
45.955	5.22575E-05	225	0.10560	0.89440	Yes
40.271	5.50721E-05	225	0.10560	0.89440	Yes
34.533	5.88998E-05	225	0.10560	0.89440	Yes
28.832	6.45036E-05	225	0.10560	0.89440	Yes
23.073	7.37409E-05	225	0.10560	0.89440	Yes
17.334	9.14997E-05	225	0.10560	0.89440	Yes
11.565	0.000135044	225	0.10560	0.89440	Yes
5.789	0.000288184	225	0.10560	0.89440	Yes
68.723	4.32807E-05	225	0.25147	0.74853	Yes
63.995	4.40703E-05	225	0.25147	0.74853	Yes
59.486	4.49156E-05	225	0.25147	0.74853	Yes
54.635	4.59643E-05	225	0.25147	0.74853	Yes
50.028	4.71165E-05	225	0.25147	0.74853	Yes
45.559	4.84449E-05	225	0.25147	0.74853	Yes
40.832	5.01354E-05	225	0.25147	0.74853	Yes
36.052	5.22821E-05	225	0.25147	0.74853	Yes
31.521	5.49571E-05	225	0.25147	0.74853	Yes
26.560	5.90842E-05	225	0.25147	0.74853	Yes
22.097	6.48256E-05	225	0.25147	0.74853	Yes
17.324	7.58265E-05	225	0.25147	0.74853	Yes

Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
68.757	3.96589E-05	225	0.50365	0.49635	Yes
64.284	4.01027E-05	225	0.50365	0.49635	Yes
59.971	4.05696E-05	225	0.50365	0.49635	Yes
55.490	4.11049E-05	225	0.50365	0.49635	Yes
51.251	4.16736E-05	225	0.50365	0.49635	Yes
47.029	4.23048E-05	225	0.50365	0.49635	Yes
42.734	4.30367E-05	225	0.50365	0.49635	Yes
38.334	4.39039E-05	225	0.50365	0.49635	Yes
33.940	4.49337E-05	225	0.50365	0.49635	Yes
29.435	4.62385E-05	225	0.50365	0.49635	Yes
25.084	4.78858E-05	225	0.50365	0.49635	Yes
68.765	3.73204E-05	225	0.71105	0.28895	Yes
63.528	3.76478E-05	225	0.71105	0.28895	Yes
58.351	3.79997E-05	225	0.71105	0.28895	Yes
52.872	3.84054E-05	225	0.71105	0.28895	Yes
47.575	3.88425E-05	225	0.71105	0.28895	Yes
42.444	3.93113E-05	225	0.71105	0.28895	Yes
37.012	3.98708E-05	225	0.71105	0.28895	Yes
31.663	4.05022E-05	225	0.71105	0.28895	Yes
26.429	4.12354E-05	225	0.71105	0.28895	Yes
20.934	4.21799E-05	225	0.71105	0.28895	Yes
68.831	3.5624E-05	225	0.90921	0.09079	Yes
63.930	3.58141E-05	225	0.90921	0.09079	Yes
59.307	3.60075E-05	225	0.90921	0.09079	Yes
54.341	3.62253E-05	225	0.90921	0.09079	Yes
49.927	3.64352E-05	225	0.90921	0.09079	Yes
44.731	3.66946E-05	225	0.90921	0.09079	Yes
40.095	3.69399E-05	225	0.90921	0.09079	Yes
34.971	3.72329E-05	225	0.90921	0.09079	Yes
30.735	3.74925E-05	225	0.90921	0.09079	Yes
25.841	3.78143E-05	225	0.90921	0.09079	Yes
23.482	3.79853E-05	225	0.90921	0.09079	Yes
15.997	3.85758E-05	225	0.90921	0.09079	Yes
11.238	3.90076E-05	225	0.90921	0.09079	Yes
68.953	4.81904E-05	245	0.10560	0.89440	Yes
57.208	5.15597E-05	245	0.10560	0.89440	Yes
49.629	5.45703E-05	245	0.10560	0.89440	Yes
40.517	5.97514E-05	245	0.10560	0.89440	Yes
34.424	6.49604E-05	245	0.10560	0.89440	Yes
29.447	7.10934E-05	245	0.10560	0.89440	Yes
25.196	7.87278E-05	245	0.10560	0.89440	Yes
21.643	8.80592E-05	245	0.10560	0.89440	Yes
18.586	9.97805E-05	245	0.10560	0.89440	Yes
15.875	0.000114969	245	0.10560	0.89440	Yes
13.324	0.000136221	245	0.10560	0.89440	Yes
10.939	0.000166556	245	0.10560	0.89440	Yes
8.579	0.000215193	245	0.10560	0.89440	Yes
6.223	0.000302847	245	0.10560	0.89440	Yes
3.806	0.000508388	245	0.10560	0.89440	Yes
1.265	0.001584786	245	0.10560	0.89440	Yes
68.896	4.56976E-05	245	0.25147	0.74853	Yes
55.480	4.88377E-05	245	0.25147	0.74853	Yes
45.088	5.24852E-05	245	0.25147	0.74853	Yes
37.041	5.67634E-05	245	0.25147	0.74853	Yes
30.934	6.16979E-05	245	0.25147	0.74853	Yes
26.204	6.75128E-05	245	0.25147	0.74853	Yes
22.498	7.43937E-05	245	0.25147	0.74853	Yes
19.130	8.38785E-05	245	0.25147	0.74853	Yes
16.575	9.49127E-05	245	0.25147	0.74853	Yes
14.379	0.000108909	245	0.25147	0.74853	Yes
12.171	0.000129971	245	0.25147	0.74853	Yes
10.182	0.00015916	245	0.25147	0.74853	Yes
8.167	0.000205846	245	0.25147	0.74853	Yes
6.057	0.000290782	245	0.25147	0.74853	Yes
3.737	0.000498753	245	0.25147	0.74853	Yes
1.182	0.001683502	245	0.25147	0.74853	Yes
69.031	4.17415E-05	245	0.50365	0.49635	Yes
64.442	4.23173E-05	245	0.50365	0.49635	Yes
59.570	4.30089E-05	245	0.50365	0.49635	Yes
54.654	4.37848E-05	245	0.50365	0.49635	Yes
49.798	4.46748E-05	245	0.50365	0.49635	Yes
44.823	4.57498E-05	245	0.50365	0.49635	Yes
40.137	4.69528E-05	245	0.50365	0.49635	Yes
35.095	4.85625E-05	245	0.50365	0.49635	Yes
30.213	5.0597E-05	245	0.50365	0.49635	Yes
25.376	5.34017E-05	245	0.50365	0.49635	Yes
20.573	5.77801E-05	245	0.50365	0.49635	Yes
20.573	5.77801E-05	245	0.50365	0.49635	Yes
69.042	3.90976E-05	245	0.71105	0.28895	Yes
64.182	3.94836E-05	245	0.71105	0.28895	Yes
58.841	3.99457E-05	245	0.71105	0.28895	Yes
56.941	4.03193E-05	245	0.71105	0.28895	Yes
49.385	4.09149E-05	245	0.71105	0.28895	Yes
44.239	4.15386E-05	245	0.71105	0.28895	Yes
39.256	4.22279E-05	245	0.71105	0.28895	Yes
34.043	4.30719E-05	245	0.71105	0.28895	Yes
29.624	4.39309E-05	245	0.71105	0.28895	Yes
24.157	4.52571E-05	245	0.71105	0.28895	Yes
18.997	4.69682E-05	245	0.71105	0.28895	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
68.926	3.71388E-05	245	0.90921	0.09079	Yes
63.374	3.74223E-05	245	0.90921	0.09079	Yes
57.687	3.77287E-05	245	0.90921	0.09079	Yes
52.013	3.80691E-05	245	0.90921	0.09079	Yes
46.110	3.84512E-05	245	0.90921	0.09079	Yes
40.397	3.88682E-05	245	0.90921	0.09079	Yes
34.971	3.92989E-05	245	0.90921	0.09079	Yes
29.357	3.9801E-05	245	0.90921	0.09079	Yes
23.315	4.04236E-05	245	0.90921	0.09079	Yes
17.497	4.11336E-05	245	0.90921	0.09079	Yes
11.846	4.19692E-05	245	0.90921	0.09079	Yes
68.418	4.29516E-05	255	0.50365	0.49635	Yes
63.922	4.35996E-05	255	0.50365	0.49635	Yes
59.345	4.43361E-05	255	0.50365	0.49635	Yes
55.723	4.49924E-05	255	0.50365	0.49635	Yes
50.245	4.61255E-05	255	0.50365	0.49635	Yes
45.746	4.72077E-05	255	0.50365	0.49635	Yes
41.210	4.85343E-05	255	0.50365	0.49635	Yes
36.441	5.02462E-05	255	0.50365	0.49635	Yes
32.023	5.22794E-05	255	0.50365	0.49635	Yes
27.634	5.50025E-05	255	0.50365	0.49635	Yes
22.818	5.94707E-05	255	0.50365	0.49635	Yes
18.165	6.71006E-05	255	0.50365	0.49635	Yes
68.980	5.08751E-05	265	0.10560	0.89440	Yes
59.626	5.39171E-05	265	0.10560	0.89440	Yes
51.662	5.74119E-05	265	0.10560	0.89440	Yes
45.014	6.13346E-05	265	0.10560	0.89440	Yes
39.419	6.57722E-05	265	0.10560	0.89440	Yes
34.460	7.10783E-05	265	0.10560	0.89440	Yes
30.257	7.71843E-05	265	0.10560	0.89440	Yes
26.580	8.44737E-05	265	0.10560	0.89440	Yes
23.281	9.33881E-05	265	0.10560	0.89440	Yes
20.372	0.000104178	265	0.10560	0.89440	Yes
17.697	0.000117869	265	0.10560	0.89440	Yes
15.189	0.000135943	265	0.10560	0.89440	Yes
12.832	0.000160256	265	0.10560	0.89440	Yes
10.538	0.000195427	265	0.10560	0.89440	Yes
8.288	0.00025025	265	0.10560	0.89440	Yes
6.015	0.000348797	265	0.10560	0.89440	Yes
3.740	0.000570125	265	0.10560	0.89440	Yes
1.408	0.001545595	265	0.10560	0.89440	Yes
68.657	4.83676E-05	265	0.25147	0.74853	Yes
58.009	5.1311E-05	265	0.25147	0.74853	Yes
49.373	5.46179E-05	265	0.25147	0.74853	Yes
42.394	5.8326E-05	265	0.25147	0.74853	Yes
36.542	6.26841E-05	265	0.25147	0.74853	Yes
31.649	6.77874E-05	265	0.25147	0.74853	Yes
27.743	7.3497E-05	265	0.25147	0.74853	Yes
24.334	8.0457E-05	265	0.25147	0.74853	Yes
21.323	8.90551E-05	265	0.25147	0.74853	Yes
18.758	9.93049E-05	265	0.25147	0.74853	Yes
16.383	0.0001126	265	0.25147	0.74853	Yes
14.202	0.000129955	265	0.25147	0.74853	Yes
12.108	0.00015387	265	0.25147	0.74853	Yes
10.005	0.00018843	265	0.25147	0.74853	Yes
8.034	0.000241488	265	0.25147	0.74853	Yes
5.906	0.000338524	265	0.25147	0.74853	Yes
3.669	0.000564334	265	0.25147	0.74853	Yes
1.242	0.001736111	265	0.25147	0.74853	Yes
69.001	4.39967E-05	265	0.50365	0.49635	Yes
55.649	4.63994E-05	265	0.50365	0.49635	Yes
43.359	4.9724E-05	265	0.50365	0.49635	Yes
35.192	5.31604E-05	265	0.50365	0.49635	Yes
29.030	5.71265E-05	265	0.50365	0.49635	Yes
24.410	6.17627E-05	265	0.50365	0.49635	Yes
20.995	6.70556E-05	265	0.50365	0.49635	Yes
18.245	7.36106E-05	265	0.50365	0.49635	Yes
16.080	8.15328E-05	265	0.50365	0.49635	Yes
14.235	9.17011E-05	265	0.50365	0.49635	Yes
12.784	0.000103445	265	0.50365	0.49635	Yes
11.373	0.00011989	265	0.50365	0.49635	Yes
10.049	0.000141884	265	0.50365	0.49635	Yes
8.649	0.00017449	265	0.50365	0.49635	Yes
7.181	0.000225836	265	0.50365	0.49635	Yes
5.511	0.000319285	265	0.50365	0.49635	Yes
3.500	0.000550661	265	0.50365	0.49635	Yes
1.140	0.001858736	265	0.50365	0.49635	Yes
68.931	4.10442E-05	265	0.71105	0.28895	Yes
57.785	4.22726E-05	265	0.71105	0.28895	Yes
48.415	4.35939E-05	265	0.71105	0.28895	Yes
40.580	4.49984E-05	265	0.71105	0.28895	Yes
34.035	4.65354E-05	265	0.71105	0.28895	Yes
28.869	4.81186E-05	265	0.71105	0.28895	Yes
24.672	4.98206E-05	265	0.71105	0.28895	Yes
21.376	5.16129E-05	265	0.71105	0.28895	Yes
18.559	5.36682E-05	265	0.71105	0.28895	Yes
16.504	5.57507E-05	265	0.71105	0.28895	Yes
14.781	5.81598E-05	265	0.71105	0.28895	Yes
13.579	6.0507E-05	265	0.71105	0.28895	Yes
13.579	6.0507E-05	265	0.71105	0.28895	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
68.251	3.8844E-05	265	0.90921	0.09079	Yes
61.833	3.9268E-05	265	0.90921	0.09079	Yes
56.018	3.96999E-05	265	0.90921	0.09079	Yes
50.756	4.013E-05	265	0.90921	0.09079	Yes
45.612	4.05959E-05	265	0.90921	0.09079	Yes
41.002	4.10509E-05	265	0.90921	0.09079	Yes
36.809	4.15093E-05	265	0.90921	0.09079	Yes
32.721	4.2015E-05	265	0.90921	0.09079	Yes
29.107	4.25116E-05	265	0.90921	0.09079	Yes
25.874	4.30108E-05	265	0.90921	0.09079	Yes
22.907	4.35199E-05	265	0.90921	0.09079	Yes
20.145	4.40606E-05	265	0.90921	0.09079	Yes
17.673	4.4603E-05	265	0.90921	0.09079	Yes
15.450	4.51528E-05	265	0.90921	0.09079	Yes
13.391	4.57415E-05	265	0.90921	0.09079	Yes
11.756	4.62727E-05	265	0.90921	0.09079	Yes
9.953	4.69462E-05	265	0.90921	0.09079	Yes
8.547	4.75511E-05	265	0.90921	0.09079	Yes
69.014	4.51692E-05	275	0.50365	0.49635	Yes
55.386	4.79363E-05	275	0.50365	0.49635	Yes
45.081	5.10334E-05	275	0.50365	0.49635	Yes
37.149	5.45792E-05	275	0.50365	0.49635	Yes
31.129	5.86373E-05	275	0.50365	0.49635	Yes
26.449	6.33794E-05	275	0.50365	0.49635	Yes
22.837	6.8937E-05	275	0.50365	0.49635	Yes
19.987	7.5523E-05	275	0.50365	0.49635	Yes
17.566	8.38856E-05	275	0.50365	0.49635	Yes
15.661	9.35279E-05	275	0.50365	0.49635	Yes
13.921	0.000106202	275	0.50365	0.49635	Yes
12.286	0.000123487	275	0.50365	0.49635	Yes
10.850	0.000145159	275	0.50365	0.49635	Yes
9.299	0.00017819	275	0.50365	0.49635	Yes
7.643	0.00023084	275	0.50365	0.49635	Yes
5.790	0.000326477	275	0.50365	0.49635	Yes
3.684	0.000553403	275	0.50365	0.49635	Yes
1.152	0.001915709	275	0.50365	0.49635	Yes
68.988	4.20751E-05	275	0.71105	0.28895	Yes
56.724	4.36338E-05	275	0.71105	0.28895	Yes
46.572	4.53576E-05	275	0.71105	0.28895	Yes
38.614	4.71809E-05	275	0.71105	0.28895	Yes
32.303	4.91425E-05	275	0.71105	0.28895	Yes
27.197	5.13268E-05	275	0.71105	0.28895	Yes
23.293	5.36682E-05	275	0.71105	0.28895	Yes
20.170	5.63126E-05	275	0.71105	0.28895	Yes
17.915	5.90179E-05	275	0.71105	0.28895	Yes
16.008	6.22704E-05	275	0.71105	0.28895	Yes
14.525	6.58979E-05	275	0.71105	0.28895	Yes
13.428	6.97058E-05	275	0.71105	0.28895	Yes
12.490	7.42115E-05	275	0.71105	0.28895	Yes
12.490	7.42115E-05	275	0.71105	0.28895	Yes
69.124	5.36021E-05	285	0.10560	0.89440	Yes
61.286	5.64812E-05	285	0.10560	0.89440	Yes
54.492	5.96801E-05	285	0.10560	0.89440	Yes
48.534	6.32671E-05	285	0.10560	0.89440	Yes
43.343	6.73038E-05	285	0.10560	0.89440	Yes
38.736	7.18597E-05	285	0.10560	0.89440	Yes
34.711	7.69882E-05	285	0.10560	0.89440	Yes
30.952	8.31463E-05	285	0.10560	0.89440	Yes
27.610	9.03261E-05	285	0.10560	0.89440	Yes
24.590	9.87752E-05	285	0.10560	0.89440	Yes
21.802	0.000109039	285	0.10560	0.89440	Yes
19.227	0.000121551	285	0.10560	0.89440	Yes
16.819	0.00013725	285	0.10560	0.89440	Yes
14.481	0.000158078	285	0.10560	0.89440	Yes
12.256	0.000185943	285	0.10560	0.89440	Yes
10.090	0.000225581	285	0.10560	0.89440	Yes
7.932	0.000288018	285	0.10560	0.89440	Yes
5.792	0.000396197	285	0.10560	0.89440	Yes
3.650	0.000634518	285	0.10560	0.89440	Yes
1.477	0.001587302	285	0.10560	0.89440	Yes
69.088	5.0958E-05	285	0.25147	0.74853	Yes
60.329	5.37057E-05	285	0.25147	0.74853	Yes
52.977	5.67472E-05	285	0.25147	0.74853	Yes
46.679	6.01504E-05	285	0.25147	0.74853	Yes
41.260	6.40287E-05	285	0.25147	0.74853	Yes
36.619	6.84041E-05	285	0.25147	0.74853	Yes
32.596	7.34053E-05	285	0.25147	0.74853	Yes
29.030	7.92959E-05	285	0.25147	0.74853	Yes
25.912	8.6103E-05	285	0.25147	0.74853	Yes
23.106	9.42418E-05	285	0.25147	0.74853	Yes
20.577	0.000103961	285	0.25147	0.74853	Yes
18.220	0.000116077	285	0.25147	0.74853	Yes
15.997	0.000131492	285	0.25147	0.74853	Yes
13.903	0.000151355	285	0.25147	0.74853	Yes
11.845	0.000178763	285	0.25147	0.74853	Yes
9.840	0.000217486	285	0.25147	0.74853	Yes
7.824	0.000277624	285	0.25147	0.74853	Yes
5.730	0.00038625	285	0.25147	0.74853	Yes
3.582	0.000632511	285	0.25147	0.74853	Yes
1.354	0.001712329	285	0.25147	0.74853	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
69.189	4.638E-05	285	0.50365	0.49635	Yes
57.633	4.88998E-05	285	0.50365	0.49635	Yes
48.491	5.16983E-05	285	0.50365	0.49635	Yes
41.194	5.48306E-05	285	0.50365	0.49635	Yes
35.359	5.83533E-05	285	0.50365	0.49635	Yes
30.659	6.23908E-05	285	0.50365	0.49635	Yes
26.842	6.70376E-05	285	0.50365	0.49635	Yes
23.732	7.23903E-05	285	0.50365	0.49635	Yes
21.142	7.87092E-05	285	0.50365	0.49635	Yes
18.932	8.62143E-05	285	0.50365	0.49635	Yes
16.990	9.5429E-05	285	0.50365	0.49635	Yes
15.270	0.000106667	285	0.50365	0.49635	Yes
13.678	0.000120875	285	0.50365	0.49635	Yes
12.150	0.000139412	285	0.50365	0.49635	Yes
10.616	0.000165153	285	0.50365	0.49635	Yes
9.050	0.000202102	285	0.50365	0.49635	Yes
7.376	0.00026062	285	0.50365	0.49635	Yes
5.543	0.000366032	285	0.50365	0.49635	Yes
3.502	0.000614628	285	0.50365	0.49635	Yes
1.192	0.001915709	285	0.50365	0.49635	Yes
69.080	4.31276E-05	285	0.71105	0.28895	Yes
55.607	4.51019E-05	285	0.71105	0.28895	Yes
44.919	4.73015E-05	285	0.71105	0.28895	Yes
35.358	5.02008E-05	285	0.71105	0.28895	Yes
26.656	5.4606E-05	285	0.71105	0.28895	Yes
21.011	5.9848E-05	285	0.71105	0.28895	Yes
17.501	6.58198E-05	285	0.71105	0.28895	Yes
15.302	7.22804E-05	285	0.71105	0.28895	Yes
13.685	7.99808E-05	285	0.71105	0.28895	Yes
12.389	8.97263E-05	285	0.71105	0.28895	Yes
11.377	0.000101564	285	0.71105	0.28895	Yes
10.346	0.000117966	285	0.71105	0.28895	Yes
9.405	0.000139919	285	0.71105	0.28895	Yes
8.387	0.000172117	285	0.71105	0.28895	Yes
7.189	0.000222668	285	0.71105	0.28895	Yes
5.658	0.000316656	285	0.71105	0.28895	Yes
3.656	0.000551572	285	0.71105	0.28895	Yes
1.088	0.002083333	285	0.71105	0.28895	Yes
69.019	4.06141E-05	285	0.90921	0.09079	Yes
57.355	4.16597E-05	285	0.90921	0.09079	Yes
47.721	4.27387E-05	285	0.90921	0.09079	Yes
39.762	4.38462E-05	285	0.90921	0.09079	Yes
32.843	4.50511E-05	285	0.90921	0.09079	Yes
27.142	4.63177E-05	285	0.90921	0.09079	Yes
22.447	4.76622E-05	285	0.90921	0.09079	Yes
18.648	4.90966E-05	285	0.90921	0.09079	Yes
15.654	5.05996E-05	285	0.90921	0.09079	Yes
13.219	5.22357E-05	285	0.90921	0.09079	Yes
11.374	5.39724E-05	285	0.90921	0.09079	Yes
10.034	5.57445E-05	285	0.90921	0.09079	Yes
9.013	5.76568E-05	285	0.90921	0.09079	Yes
69.055	5.57538E-05	300	0.10560	0.89440	Yes
61.675	5.8713E-05	300	0.10560	0.89440	Yes
55.165	6.20424E-05	300	0.10560	0.89440	Yes
49.506	6.57073E-05	300	0.10560	0.89440	Yes
44.370	6.99007E-05	300	0.10560	0.89440	Yes
39.817	7.46491E-05	300	0.10560	0.89440	Yes
35.681	8.01539E-05	300	0.10560	0.89440	Yes
31.967	8.64454E-05	300	0.10560	0.89440	Yes
28.534	9.40026E-05	300	0.10560	0.89440	Yes
25.493	0.000102638	300	0.10560	0.89440	Yes
22.642	0.000113122	300	0.10560	0.89440	Yes
19.933	0.000126279	300	0.10560	0.89440	Yes
17.400	0.000142714	300	0.10560	0.89440	Yes
14.971	0.000164258	300	0.10560	0.89440	Yes
12.682	0.000192753	300	0.10560	0.89440	Yes
10.413	0.000234082	300	0.10560	0.89440	Yes
8.196	0.000297354	300	0.10560	0.89440	Yes
5.999	0.000407166	300	0.10560	0.89440	Yes
3.767	0.00065189	300	0.10560	0.89440	Yes
1.537	0.001612903	300	0.10560	0.89440	Yes
69.107	5.33646E-05	300	0.25147	0.74853	Yes
60.931	5.6262E-05	300	0.25147	0.74853	Yes
54.037	5.94248E-05	300	0.25147	0.74853	Yes
48.072	6.29485E-05	300	0.25147	0.74853	Yes
42.827	6.69792E-05	300	0.25147	0.74853	Yes
38.228	7.1541E-05	300	0.25147	0.74853	Yes
34.097	7.68876E-05	300	0.25147	0.74853	Yes
30.514	8.296E-05	300	0.25147	0.74853	Yes
27.285	9.00576E-05	300	0.25147	0.74853	Yes
24.350	9.85999E-05	300	0.25147	0.74853	Yes
21.667	0.000108826	300	0.25147	0.74853	Yes
19.169	0.000121477	300	0.25147	0.74853	Yes
16.816	0.000137438	300	0.25147	0.74853	Yes
14.565	0.000158253	300	0.25147	0.74853	Yes
12.396	0.000186289	300	0.25147	0.74853	Yes
10.244	0.00022686	300	0.25147	0.74853	Yes
8.099	0.000290023	300	0.25147	0.74853	Yes
5.937	0.000400641	300	0.25147	0.74853	Yes
3.713	0.000652316	300	0.25147	0.74853	Yes
1.436	0.00172117	300	0.25147	0.74853	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
69.028	4.83863E-05	300	0.50365	0.49635	Yes
58.681	5.10022E-05	300	0.50365	0.49635	Yes
50.230	5.39345E-05	300	0.50365	0.49635	Yes
43.426	5.71821E-05	300	0.50365	0.49635	Yes
37.763	6.08828E-05	300	0.50365	0.49635	Yes
33.118	6.50703E-05	300	0.50365	0.49635	Yes
29.248	6.99203E-05	300	0.50365	0.49635	Yes
26.056	7.54205E-05	300	0.50365	0.49635	Yes
23.267	8.20008E-05	300	0.50365	0.49635	Yes
20.829	8.99038E-05	300	0.50365	0.49635	Yes
18.707	9.93147E-05	300	0.50365	0.49635	Yes
16.744	0.000111025	300	0.50365	0.49635	Yes
14.914	0.000125913	300	0.50365	0.49635	Yes
13.165	0.00014518	300	0.50365	0.49635	Yes
11.413	0.00017188	300	0.50365	0.49635	Yes
9.643	0.000210172	300	0.50365	0.49635	Yes
7.789	0.000270636	300	0.50365	0.49635	Yes
5.819	0.000378072	300	0.50365	0.49635	Yes
3.652	0.000633312	300	0.50365	0.49635	Yes
1.262	0.001937984	300	0.50365	0.49635	Yes
69.024	4.48652E-05	300	0.71105	0.28895	Yes
55.166	4.73037E-05	300	0.71105	0.28895	Yes
44.719	5.00175E-05	300	0.71105	0.28895	Yes
36.720	5.30701E-05	300	0.71105	0.28895	Yes
30.675	5.65419E-05	300	0.71105	0.28895	Yes
26.095	6.04741E-05	300	0.71105	0.28895	Yes
22.632	6.49815E-05	300	0.71105	0.28895	Yes
19.974	7.01361E-05	300	0.71105	0.28895	Yes
17.845	7.63884E-05	300	0.71105	0.28895	Yes
16.111	8.38856E-05	300	0.71105	0.28895	Yes
14.704	9.27214E-05	300	0.71105	0.28895	Yes
13.465	0.000103466	300	0.71105	0.28895	Yes
12.271	0.000117716	300	0.71105	0.28895	Yes
11.181	0.000135465	300	0.71105	0.28895	Yes
9.989	0.000161108	300	0.71105	0.28895	Yes
8.735	0.000197278	300	0.71105	0.28895	Yes
7.292	0.000255102	300	0.71105	0.28895	Yes
5.602	0.000360231	300	0.71105	0.28895	Yes
3.567	0.000617284	300	0.71105	0.28895	Yes
1.147	0.002105263	300	0.71105	0.28895	Yes
69.020	4.20486E-05	300	0.90921	0.09079	Yes
55.550	4.35521E-05	300	0.90921	0.09079	Yes
43.810	4.53371E-05	300	0.90921	0.09079	Yes
34.664	4.72657E-05	300	0.90921	0.09079	Yes
26.591	4.97785E-05	300	0.90921	0.09079	Yes
19.704	5.33049E-05	300	0.90921	0.09079	Yes
14.523	5.86235E-05	300	0.90921	0.09079	Yes
11.758	6.52869E-05	300	0.90921	0.09079	Yes
10.406	7.32118E-05	300	0.90921	0.09079	Yes
9.571	8.4488E-05	300	0.90921	0.09079	Yes
9.037	9.84737E-05	300	0.90921	0.09079	Yes
8.608	0.00011609	300	0.90921	0.09079	Yes
8.212	0.000137438	300	0.90921	0.09079	Yes
7.677	0.00016835	300	0.90921	0.09079	Yes
6.831	0.000220361	300	0.90921	0.09079	Yes
5.587	0.000313578	300	0.90921	0.09079	Yes
3.708	0.000550964	300	0.90921	0.09079	Yes
1.031	0.002309469	300	0.90921	0.09079	Yes
34.747	8.78657E-05	320	0.10560	0.89440	Yes
30.700	9.61076E-05	320	0.10560	0.89440	Yes
27.037	0.000106067	320	0.10560	0.89440	Yes
23.668	0.000118329	320	0.10560	0.89440	Yes
20.550	0.000133618	320	0.10560	0.89440	Yes
17.649	0.000153327	320	0.10560	0.89440	Yes
14.819	0.00018044	320	0.10560	0.89440	Yes
12.114	0.000218962	320	0.10560	0.89440	Yes
9.397	0.000281057	320	0.10560	0.89440	Yes
6.805	0.000387597	320	0.10560	0.89440	Yes
4.181	0.000631712	320	0.10560	0.89440	Yes
1.740	0.001519757	320	0.10560	0.89440	Yes
69.011	5.59003E-05	320	0.25147	0.74853	Yes
61.506	5.88755E-05	320	0.25147	0.74853	Yes
54.928	6.22432E-05	320	0.25147	0.74853	Yes
50.951	6.47082E-05	320	0.25147	0.74853	Yes
45.125	6.92377E-05	320	0.25147	0.74853	Yes
39.687	7.48727E-05	320	0.25147	0.74853	Yes
35.619	8.04052E-05	320	0.25147	0.74853	Yes
32.020	8.65876E-05	320	0.25147	0.74853	Yes
28.675	9.40734E-05	320	0.25147	0.74853	Yes
25.733	0.000102596	320	0.25147	0.74853	Yes
22.962	0.000112994	320	0.25147	0.74853	Yes
20.261	0.000126374	320	0.25147	0.74853	Yes
17.748	0.000142898	320	0.25147	0.74853	Yes
15.405	0.000163854	320	0.25147	0.74853	Yes
13.081	0.000192641	320	0.25147	0.74853	Yes
10.804	0.000233918	320	0.25147	0.74853	Yes
8.566	0.00029656	320	0.25147	0.74853	Yes
6.308	0.000406174	320	0.25147	0.74853	Yes
3.923	0.000660502	320	0.25147	0.74853	Yes
1.554	0.001697793	320	0.25147	0.74853	Yes
69.044	5.10334E-05	320	0.50365	0.49635	Yes
59.508	5.38503E-05	320	0.50365	0.49635	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
51.900	5.69282E-05	320	0.50365	0.49635	Yes
45.580	6.03464E-05	320	0.50365	0.49635	Yes
40.180	6.42591E-05	320	0.50365	0.49635	Yes
35.685	6.86436E-05	320	0.50365	0.49635	Yes
31.758	7.37463E-05	320	0.50365	0.49635	Yes
28.435	7.95862E-05	320	0.50365	0.49635	Yes
25.458	8.65876E-05	320	0.50365	0.49635	Yes
22.859	9.47777E-05	320	0.50365	0.49635	Yes
20.472	0.000104745	320	0.50365	0.49635	Yes
18.276	0.000117206	320	0.50365	0.49635	Yes
16.233	0.000132521	320	0.50365	0.49635	Yes
14.233	0.000152858	320	0.50365	0.49635	Yes
12.261	0.000180603	320	0.50365	0.49635	Yes
10.290	0.000220507	320	0.50365	0.49635	Yes
8.230	0.000283688	320	0.50365	0.49635	Yes
6.074	0.000397141	320	0.50365	0.49635	Yes
3.800	0.000658762	320	0.50365	0.49635	Yes
1.353	0.001930502	320	0.50365	0.49635	Yes
68.951	4.72903E-05	320	0.71105	0.28895	Yes
56.959	4.98902E-05	320	0.71105	0.28895	Yes
47.500	5.28346E-05	320	0.71105	0.28895	Yes
40.063	5.61672E-05	320	0.71105	0.28895	Yes
34.288	5.98946E-05	320	0.71105	0.28895	Yes
29.742	6.41972E-05	320	0.71105	0.28895	Yes
26.138	6.91324E-05	320	0.71105	0.28895	Yes
23.221	7.48727E-05	320	0.71105	0.28895	Yes
20.797	8.1646E-05	320	0.71105	0.28895	Yes
18.747	8.98311E-05	320	0.71105	0.28895	Yes
16.988	9.97506E-05	320	0.71105	0.28895	Yes
15.338	0.000112284	320	0.71105	0.28895	Yes
13.797	0.000128353	320	0.71105	0.28895	Yes
12.287	0.000149611	320	0.71105	0.28895	Yes
10.719	0.00017963	320	0.71105	0.28895	Yes
9.068	0.000224215	320	0.71105	0.28895	Yes
7.231	0.000299133	320	0.71105	0.28895	Yes
5.144	0.000448833	320	0.71105	0.28895	Yes
2.761	0.000898473	320	0.71105	0.28895	Yes
1.224	0.002118644	320	0.71105	0.28895	Yes
69.065	4.41423E-05	320	0.90921	0.09079	Yes
55.533	4.60936E-05	320	0.90921	0.09079	Yes
41.924	4.90148E-05	320	0.90921	0.09079	Yes
31.439	5.27398E-05	320	0.90921	0.09079	Yes
24.524	5.70353E-05	320	0.90921	0.09079	Yes
19.987	6.20771E-05	320	0.90921	0.09079	Yes
17.288	6.73764E-05	320	0.90921	0.09079	Yes
15.306	7.41125E-05	320	0.90921	0.09079	Yes
13.907	8.21288E-05	320	0.90921	0.09079	Yes
12.841	9.1878E-05	320	0.90921	0.09079	Yes
11.919	0.000104428	320	0.90921	0.09079	Yes
11.058	0.000120861	320	0.90921	0.09079	Yes
10.159	0.000143369	320	0.90921	0.09079	Yes
9.113	0.00017646	320	0.90921	0.09079	Yes
7.881	0.000226398	320	0.90921	0.09079	Yes
6.126	0.000328623	320	0.90921	0.09079	Yes
3.955	0.000572738	320	0.90921	0.09079	Yes
1.111	0.002298851	320	0.90921	0.09079	Yes
69.189	6.27668E-05	350	0.10560	0.89440	Yes
62.799	6.60939E-05	350	0.10560	0.89440	Yes
57.018	6.97983E-05	350	0.10560	0.89440	Yes
51.735	7.39645E-05	350	0.10560	0.89440	Yes
46.821	7.87402E-05	350	0.10560	0.89440	Yes
42.587	8.38434E-05	350	0.10560	0.89440	Yes
38.449	8.99928E-05	350	0.10560	0.89440	Yes
34.625	9.71062E-05	350	0.10560	0.89440	Yes
31.132	0.000105274	350	0.10560	0.89440	Yes
27.855	0.000115035	350	0.10560	0.89440	Yes
24.756	0.000126839	350	0.10560	0.89440	Yes
21.856	0.000141223	350	0.10560	0.89440	Yes
19.062	0.000159464	350	0.10560	0.89440	Yes
16.417	0.000182782	350	0.10560	0.89440	Yes
13.867	0.000214133	350	0.10560	0.89440	Yes
11.366	0.000259269	350	0.10560	0.89440	Yes
8.925	0.000328192	350	0.10560	0.89440	Yes
6.550	0.000445236	350	0.10560	0.89440	Yes
4.182	0.000694927	350	0.10560	0.89440	Yes
1.840	0.001574803	350	0.10560	0.89440	Yes
69.195	6.00925E-05	350	0.25147	0.74853	Yes
62.429	6.32871E-05	350	0.25147	0.74853	Yes
56.348	6.68539E-05	350	0.25147	0.74853	Yes
50.943	7.08316E-05	350	0.25147	0.74853	Yes
46.046	7.5358E-05	350	0.25147	0.74853	Yes
41.551	8.05542E-05	350	0.25147	0.74853	Yes
37.578	8.62887E-05	350	0.25147	0.74853	Yes
33.822	9.31532E-05	350	0.25147	0.74853	Yes
30.428	0.000101061	350	0.25147	0.74853	Yes
27.254	0.000110509	350	0.25147	0.74853	Yes
24.223	0.000122115	350	0.25147	0.74853	Yes
21.446	0.00013598	350	0.25147	0.74853	Yes
18.790	0.000153539	350	0.25147	0.74853	Yes
16.208	0.000176647	350	0.25147	0.74853	Yes
13.711	0.000207727	350	0.25147	0.74853	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
11.296	0.000251572	350	0.25147	0.74853	Yes
8.875	0.000320616	350	0.25147	0.74853	Yes
6.486	0.00043956	350	0.25147	0.74853	Yes
4.097	0.000699301	350	0.25147	0.74853	Yes
1.687	0.001706485	350	0.25147	0.74853	Yes
69.156	5.51572E-05	350	0.50365	0.49635	Yes
61.236	5.81058E-05	350	0.50365	0.49635	Yes
54.438	6.13987E-05	350	0.50365	0.49635	Yes
48.458	6.51806E-05	350	0.50365	0.49635	Yes
43.405	6.93001E-05	350	0.50365	0.49635	Yes
38.918	7.40796E-05	350	0.50365	0.49635	Yes
34.980	7.94976E-05	350	0.50365	0.49635	Yes
31.453	8.58369E-05	350	0.50365	0.49635	Yes
28.285	9.32836E-05	350	0.50365	0.49635	Yes
25.426	0.00010203	350	0.50365	0.49635	Yes
22.752	0.000112727	350	0.50365	0.49635	Yes
20.228	0.000126103	350	0.50365	0.49635	Yes
17.857	0.000142755	350	0.50365	0.49635	Yes
15.571	0.000164393	350	0.50365	0.49635	Yes
13.325	0.000193911	350	0.50365	0.49635	Yes
11.077	0.000236463	350	0.50365	0.49635	Yes
8.801	0.000302939	350	0.50365	0.49635	Yes
6.454	0.000421941	350	0.50365	0.49635	Yes
4.034	0.000691563	350	0.50365	0.49635	Yes
1.476	0.001953125	350	0.50365	0.49635	Yes
69.088	5.11326E-05	350	0.71105	0.28895	Yes
59.363	5.392E-05	350	0.71105	0.28895	Yes
51.469	5.6993E-05	350	0.71105	0.28895	Yes
45.039	6.03938E-05	350	0.71105	0.28895	Yes
39.580	6.43459E-05	350	0.71105	0.28895	Yes
35.089	6.87758E-05	350	0.71105	0.28895	Yes
31.309	7.38552E-05	350	0.71105	0.28895	Yes
28.076	7.97575E-05	350	0.71105	0.28895	Yes
25.267	8.67303E-05	350	0.71105	0.28895	Yes
22.802	9.49668E-05	350	0.71105	0.28895	Yes
20.562	0.000104998	350	0.71105	0.28895	Yes
18.453	0.000117689	350	0.71105	0.28895	Yes
16.502	0.000133333	350	0.71105	0.28895	Yes
14.597	0.000153704	350	0.71105	0.28895	Yes
12.664	0.000181884	350	0.71105	0.28895	Yes
10.712	0.000222173	350	0.71105	0.28895	Yes
8.374	0.000296824	350	0.71105	0.28895	Yes
6.421	0.000401606	350	0.71105	0.28895	Yes
3.980	0.000678426	350	0.71105	0.28895	Yes
1.333	0.002132196	350	0.71105	0.28895	Yes
69.093	4.76122E-05	350	0.90921	0.09079	Yes
56.576	5.01807E-05	350	0.90921	0.09079	Yes
46.868	5.30532E-05	350	0.90921	0.09079	Yes
39.302	5.63253E-05	350	0.90921	0.09079	Yes
33.571	5.99628E-05	350	0.90921	0.09079	Yes
29.105	6.41396E-05	350	0.90921	0.09079	Yes
25.639	6.8918E-05	350	0.90921	0.09079	Yes
22.896	7.45268E-05	350	0.90921	0.09079	Yes
20.684	8.10636E-05	350	0.90921	0.09079	Yes
18.865	8.87705E-05	350	0.90921	0.09079	Yes
17.249	9.82608E-05	350	0.90921	0.09079	Yes
15.798	0.000109926	350	0.90921	0.09079	Yes
14.396	0.000124953	350	0.90921	0.09079	Yes
13.019	0.000144634	350	0.90921	0.09079	Yes
11.601	0.000170969	350	0.90921	0.09079	Yes
10.053	0.000209512	350	0.90921	0.09079	Yes
8.306	0.00027115	350	0.90921	0.09079	Yes
6.290	0.000384911	350	0.90921	0.09079	Yes
3.957	0.000659196	350	0.90921	0.09079	Yes
1.220	0.002304147	350	0.90921	0.09079	Yes
68.655	7.01557E-05	400	0.10560	0.89440	Yes
63.076	7.37518E-05	400	0.10560	0.89440	Yes
57.528	7.80823E-05	400	0.10560	0.89440	Yes
51.633	8.37591E-05	400	0.10560	0.89440	Yes
45.922	9.07606E-05	400	0.10560	0.89440	Yes
40.264	9.97506E-05	400	0.10560	0.89440	Yes
34.122	0.000113161	400	0.10560	0.89440	Yes
28.750	0.000129904	400	0.10560	0.89440	Yes
22.860	0.000157953	400	0.10560	0.89440	Yes
17.385	0.00020202	400	0.10560	0.89440	Yes
11.889	0.000288767	400	0.10560	0.89440	Yes
5.747	0.00058548	400	0.10560	0.89440	Yes
68.727	6.75858E-05	400	0.25147	0.74853	Yes
63.061	7.09975E-05	400	0.25147	0.74853	Yes
57.436	7.50976E-05	400	0.25147	0.74853	Yes
51.693	8.02955E-05	400	0.25147	0.74853	Yes
45.922	8.6949E-05	400	0.25147	0.74853	Yes
40.281	9.5511E-05	400	0.25147	0.74853	Yes
34.456	0.000107538	400	0.25147	0.74853	Yes
28.669	0.000124906	400	0.25147	0.74853	Yes
23.064	0.000150739	400	0.25147	0.74853	Yes
16.675	0.000203335	400	0.25147	0.74853	Yes
11.547	0.000289436	400	0.25147	0.74853	Yes
5.867	0.000565931	400	0.25147	0.74853	Yes
68.619	6.27235E-05	400	0.50365	0.49635	Yes
63.139	6.54836E-05	400	0.50365	0.49635	Yes
57.289	6.90942E-05	400	0.50365	0.49635	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
51.725	7.33945E-05	400	0.50365	0.49635	Yes
45.830	7.92707E-05	400	0.50365	0.49635	Yes
40.049	8.70322E-05	400	0.50365	0.49635	Yes
34.424	9.75419E-05	400	0.50365	0.49635	Yes
28.635	0.000113546	400	0.50365	0.49635	Yes
22.930	0.000138658	400	0.50365	0.49635	Yes
17.447	0.000180538	400	0.50365	0.49635	Yes
11.530	0.00027465	400	0.50365	0.49635	Yes
6.060	0.000530786	400	0.50365	0.49635	Yes
68.723	5.84044E-05	400	0.71105	0.28895	Yes
63.024	6.07349E-05	400	0.71105	0.28895	Yes
57.544	6.3488E-05	400	0.71105	0.28895	Yes
51.834	6.70736E-05	400	0.71105	0.28895	Yes
45.987	7.18649E-05	400	0.71105	0.28895	Yes
40.123	7.84375E-05	400	0.71105	0.28895	Yes
34.480	8.74738E-05	400	0.71105	0.28895	Yes
28.678	0.000101698	400	0.71105	0.28895	Yes
22.998	0.000124797	400	0.71105	0.28895	Yes
17.097	0.000169147	400	0.71105	0.28895	Yes
11.537	0.000258665	400	0.71105	0.28895	Yes
5.890	0.000531632	400	0.71105	0.28895	Yes
68.626	5.43508E-05	400	0.90921	0.09079	Yes
63.073	5.60915E-05	400	0.90921	0.09079	Yes
57.472	5.82208E-05	400	0.90921	0.09079	Yes
51.935	6.08384E-05	400	0.90921	0.09079	Yes
45.955	6.45328E-05	400	0.90921	0.09079	Yes
40.612	6.89845E-05	400	0.90921	0.09079	Yes
34.588	7.63359E-05	400	0.90921	0.09079	Yes
28.277	8.91186E-05	400	0.90921	0.09079	Yes
23.033	0.000108073	400	0.90921	0.09079	Yes
17.344	0.000147842	400	0.90921	0.09079	Yes
11.728	0.000234577	400	0.90921	0.09079	Yes
6.627	0.000450857	400	0.90921	0.09079	Yes
68.588	7.73455E-05	450	0.10560	0.89440	Yes
57.394	8.6783E-05	450	0.10560	0.89440	Yes
51.431	9.35891E-05	450	0.10560	0.89440	Yes
45.745	0.000101843	450	0.10560	0.89440	Yes
40.044	0.000112562	450	0.10560	0.89440	Yes
34.451	0.000126662	450	0.10560	0.89440	Yes
28.416	0.0001485	450	0.10560	0.89440	Yes
22.867	0.000179147	450	0.10560	0.89440	Yes
17.279	0.000230627	450	0.10560	0.89440	Yes
11.263	0.000344709	450	0.10560	0.89440	Yes
5.828	0.000652742	450	0.10560	0.89440	Yes
68.690	7.49232E-05	450	0.25147	0.74853	Yes
63.105	7.8964E-05	450	0.25147	0.74853	Yes
57.351	8.40407E-05	450	0.25147	0.74853	Yes
51.698	9.01876E-05	450	0.25147	0.74853	Yes
45.871	9.82511E-05	450	0.25147	0.74853	Yes
40.112	0.000108684	450	0.25147	0.74853	Yes
34.454	0.000122549	450	0.25147	0.74853	Yes
28.331	0.0001443	450	0.25147	0.74853	Yes
23.239	0.000171703	450	0.25147	0.74853	Yes
17.196	0.000226244	450	0.25147	0.74853	Yes
11.652	0.000327869	450	0.25147	0.74853	Yes
5.613	0.000671141	450	0.25147	0.74853	Yes
68.770	7.02198E-05	450	0.50365	0.49635	Yes
63.009	7.39262E-05	450	0.50365	0.49635	Yes
57.446	7.8284E-05	450	0.50365	0.49635	Yes
51.741	8.38926E-05	450	0.50365	0.49635	Yes
45.854	9.13242E-05	450	0.50365	0.49635	Yes
40.196	0.000100776	450	0.50365	0.49635	Yes
34.390	0.000114155	450	0.50365	0.49635	Yes
28.731	0.000133103	450	0.50365	0.49635	Yes
23.022	0.000162655	450	0.50365	0.49635	Yes
17.215	0.000214638	450	0.50365	0.49635	Yes
11.855	0.000310463	450	0.50365	0.49635	Yes
5.842	0.000632511	450	0.50365	0.49635	Yes
68.603	6.61157E-05	450	0.71105	0.28895	Yes
62.976	6.92713E-05	450	0.71105	0.28895	Yes
57.406	7.31101E-05	450	0.71105	0.28895	Yes
51.741	7.80275E-05	450	0.71105	0.28895	Yes
45.928	8.45523E-05	450	0.71105	0.28895	Yes
40.166	9.32836E-05	450	0.71105	0.28895	Yes
34.452	0.00010543	450	0.71105	0.28895	Yes
28.755	0.000123365	450	0.71105	0.28895	Yes
23.164	0.000151035	450	0.71105	0.28895	Yes
17.260	0.00020247	450	0.71105	0.28895	Yes
11.587	0.000305344	450	0.71105	0.28895	Yes
5.867	0.000616523	450	0.71105	0.28895	Yes
68.731	6.17932E-05	450	0.90921	0.09079	Yes
62.897	6.45078E-05	450	0.90921	0.09079	Yes
57.367	6.76911E-05	450	0.90921	0.09079	Yes
51.720	7.17978E-05	450	0.90921	0.09079	Yes
45.919	7.73515E-05	450	0.90921	0.09079	Yes
40.171	8.48824E-05	450	0.90921	0.09079	Yes
34.466	9.5648E-05	450	0.90921	0.09079	Yes
28.330	0.000113688	450	0.90921	0.09079	Yes
22.817	0.000140627	450	0.90921	0.09079	Yes
17.241	0.000189	450	0.90921	0.09079	Yes
11.920	0.000282326	450	0.90921	0.09079	Yes
5.856	0.000604595	450	0.90921	0.09079	Yes

Continued: Data summarised from Table III of Duarte–Garza95–II [83]

P (MPa)	v ($m^3 mol^{-1}$)	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
7.5075386	4.163419E-05	250	0.982	0.018	Yes
16.8021364	4.191016E-05	260	0.982	0.018	Yes
8.6841811	4.551281E-05	270	0.982	0.018	Yes
26.9498034	4.201476E-05	270	0.982	0.018	Yes
32.0556331	4.205123E-05	275	0.982	0.018	Yes
16.0366138	4.579484E-05	280	0.982	0.018	Yes
9.1347922	4.994448E-05	285	0.982	0.018	Yes
12.0067428	5.009951E-05	290	0.982	0.018	Yes
23.8272641	4.591001E-05	290	0.982	0.018	Yes
8.7895674	5.540408E-05	295	0.982	0.018	Yes
5.1465335	3.329160E-04	300	0.982	0.018	Yes
11.0317251	5.554229E-05	300	0.982	0.018	Yes
17.9089753	5.031430E-05	300	0.982	0.018	Yes
31.6712158	4.598582E-05	300	0.982	0.018	Yes
2.2563767	1.001295E-03	305	0.982	0.018	Yes
6.9332505	1.994778E-04	305	0.982	0.018	Yes
6.9344043	1.995055E-04	305	0.982	0.018	Yes
7.6234034	1.427596E-04	305	0.982	0.018	Yes
9.7177665	6.281127E-05	305	0.982	0.018	Yes
13.2691923	5.568125E-05	305	0.982	0.018	Yes
2.3030787	1.001845E-03	310	0.982	0.018	Yes
5.4990380	3.334137E-04	310	0.982	0.018	Yes
7.2767758	1.996719E-04	310	0.982	0.018	Yes
7.2784895	1.996996E-04	310	0.982	0.018	Yes
8.1559388	1.429245E-04	310	0.982	0.018	Yes
8.4027714	1.258409E-04	310	0.982	0.018	Yes
8.6037832	1.119534E-04	310	0.982	0.018	Yes
8.7748915	1.007028E-04	310	0.982	0.018	Yes
8.9505344	9.142770E-05	310	0.982	0.018	Yes
9.1510023	8.369819E-05	310	0.982	0.018	Yes
9.4131032	7.737188E-05	310	0.982	0.018	Yes
9.8060106	7.196761E-05	310	0.982	0.018	Yes
11.3995553	6.296163E-05	310	0.982	0.018	Yes
15.5331725	5.581194E-05	310	0.982	0.018	Yes
15.5459561	5.578811E-05	310	0.982	0.018	Yes
23.8315070	5.041402E-05	310	0.982	0.018	Yes
9.0117425	1.260071E-04	315	0.982	0.018	Yes
9.3045870	1.121102E-04	315	0.982	0.018	Yes
9.5713644	1.008523E-04	315	0.982	0.018	Yes
9.8485366	9.157197E-05	315	0.982	0.018	Yes
10.1636378	8.384112E-05	315	0.982	0.018	Yes
10.5555296	7.751614E-05	315	0.982	0.018	Yes
11.1010267	7.212122E-05	315	0.982	0.018	Yes
13.0922670	6.312050E-05	315	0.982	0.018	Yes
17.8357655	5.588562E-05	315	0.982	0.018	Yes
17.8576940	5.585414E-05	315	0.982	0.018	Yes
26.9949116	5.045537E-05	315	0.982	0.018	Yes
2.3954203	1.002953E-03	320	0.982	0.018	Yes
5.8424573	3.339247E-04	320	0.982	0.018	Yes
7.9446804	2.000773E-04	320	0.982	0.018	Yes
7.9463864	2.001047E-04	320	0.982	0.018	Yes
9.1854392	1.432882E-04	320	0.982	0.018	Yes
9.6104091	1.261898E-04	320	0.982	0.018	Yes
9.9980651	1.122872E-04	320	0.982	0.018	Yes
10.3631781	1.010250E-04	320	0.982	0.018	Yes
10.7486806	9.174282E-05	320	0.982	0.018	Yes
11.1825192	8.401268E-05	320	0.982	0.018	Yes
11.7078025	7.768306E-05	320	0.982	0.018	Yes
12.4064600	7.229140E-05	320	0.982	0.018	Yes
14.8072431	6.323965E-05	320	0.982	0.018	Yes
20.1535098	5.594284E-05	320	0.982	0.018	Yes
20.1726324	5.591106E-05	320	0.982	0.018	Yes
30.0249795	5.049208E-05	320	0.982	0.018	Yes
33.0510853	5.052643E-05	325	0.982	0.018	Yes
2.4871487	1.004076E-03	330	0.982	0.018	Yes
6.1782653	3.344536E-04	330	0.982	0.018	Yes
8.5922178	2.005131E-04	330	0.982	0.018	Yes
8.5942598	2.005400E-04	330	0.982	0.018	Yes
10.1820483	1.437140E-04	330	0.982	0.018	Yes
10.7838284	1.266147E-04	330	0.982	0.018	Yes
11.3624320	1.127037E-04	330	0.982	0.018	Yes
11.9329135	1.014280E-04	330	0.982	0.018	Yes
12.5417041	9.212397E-05	330	0.982	0.018	Yes
13.2369688	8.436464E-05	330	0.982	0.018	Yes
14.0287225	7.799266E-05	330	0.982	0.018	Yes
15.0469659	7.255003E-05	330	0.982	0.018	Yes
18.2752200	6.339305E-05	330	0.982	0.018	Yes
24.8029975	5.603500E-05	330	0.982	0.018	Yes
24.8365755	5.600308E-05	330	0.982	0.018	Yes

Data summarised from Table 31 of Ely87 [75]

P (MPa)	v ($m^3 mol^{-1}$)	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
7.5075386	4.163419E-05	250	0.982	0.018	Yes
16.8021364	4.191016E-05	260	0.982	0.018	Yes
8.6841811	4.551281E-05	270	0.982	0.018	Yes
26.9498034	4.201476E-05	270	0.982	0.018	Yes
32.0556331	4.205123E-05	275	0.982	0.018	Yes
16.0366138	4.579484E-05	280	0.982	0.018	Yes
9.1347922	4.994448E-05	285	0.982	0.018	Yes
12.0067428	5.009951E-05	290	0.982	0.018	Yes
23.8272641	4.591001E-05	290	0.982	0.018	Yes
8.7895674	5.540408E-05	295	0.982	0.018	Yes
5.1465335	3.329160E-04	300	0.982	0.018	Yes
11.0317251	5.554229E-05	300	0.982	0.018	Yes
17.9089753	5.031430E-05	300	0.982	0.018	Yes
31.6712158	4.598582E-05	300	0.982	0.018	Yes
2.2563767	1.001295E-03	305	0.982	0.018	Yes
6.9332505	1.994778E-04	305	0.982	0.018	Yes
6.9344043	1.995055E-04	305	0.982	0.018	Yes
7.6234034	1.427596E-04	305	0.982	0.018	Yes
9.7177665	6.281127E-05	305	0.982	0.018	Yes
13.2691923	5.568125E-05	305	0.982	0.018	Yes
2.3030787	1.001845E-03	310	0.982	0.018	Yes
5.4990380	3.334137E-04	310	0.982	0.018	Yes
7.2767758	1.996719E-04	310	0.982	0.018	Yes
7.2784895	1.996996E-04	310	0.982	0.018	Yes
8.1559388	1.429245E-04	310	0.982	0.018	Yes
8.4027714	1.258409E-04	310	0.982	0.018	Yes
8.6037832	1.119534E-04	310	0.982	0.018	Yes
8.7748915	1.007028E-04	310	0.982	0.018	Yes
8.9505344	9.142770E-05	310	0.982	0.018	Yes
9.1510023	8.369819E-05	310	0.982	0.018	Yes
9.4131032	7.737188E-05	310	0.982	0.018	Yes
9.8060106	7.196761E-05	310	0.982	0.018	Yes
11.3995553	6.296163E-05	310	0.982	0.018	Yes
15.5331725	5.581194E-05	310	0.982	0.018	Yes
15.5459561	5.578811E-05	310	0.982	0.018	Yes
23.8315070	5.041402E-05	310	0.982	0.018	Yes
9.0117425	1.260071E-04	315	0.982	0.018	Yes
9.3045870	1.121102E-04	315	0.982	0.018	Yes
9.5713644	1.008523E-04	315	0.982	0.018	Yes
9.8485366	9.157197E-05	315	0.982	0.018	Yes
10.1636378	8.384112E-05	315	0.982	0.018	Yes
10.5555296	7.751614E-05	315	0.982	0.018	Yes
11.1010267	7.212122E-05	315	0.982	0.018	Yes
13.0922670	6.312050E-05	315	0.982	0.018	Yes
17.8357655	5.588562E-05	315	0.982	0.018	Yes
17.8576940	5.585414E-05	315	0.982	0.018	Yes
26.9949116	5.045537E-05	315	0.982	0.018	Yes
2.3954203	1.002953E-03	320	0.982	0.018	Yes
5.8424573	3.339247E-04	320	0.982	0.018	Yes
7.9446804	2.000773E-04	320	0.982	0.018	Yes
7.9463864	2.001047E-04	320	0.982	0.018	Yes
9.1854392	1.432882E-04	320	0.982	0.018	Yes
9.6104091	1.261898E-04	320	0.982	0.018	Yes
9.9980651	1.122872E-04	320	0.982	0.018	Yes
10.3631781	1.010250E-04	320	0.982	0.018	Yes
10.7486806	9.174282E-05	320	0.982	0.018	Yes
11.1825192	8.401268E-05	320	0.982	0.018	Yes
11.7078025	7.768306E-05	320	0.982	0.018	Yes
12.4064600	7.229140E-05	320	0.982	0.018	Yes
14.8072431	6.323965E-05	320	0.982	0.018	Yes
20.1535098	5.594284E-05	320	0.982	0.018	Yes
20.1726324	5.591106E-05	320	0.982	0.018	Yes
30.0249795	5.049208E-05	320	0.982	0.018	Yes
33.0510853	5.052643E-05	325	0.982	0.018	Yes
2.4871487	1.004076E-03	330	0.982	0.018	Yes
6.1782653	3.344536E-04	330	0.982	0.018	Yes
8.5922178	2.005131E-04	330	0.982	0.018	Yes
8.5942598	2.005400E-04	330	0.982	0.018	Yes
10.1820483	1.437140E-04	330	0.982	0.018	Yes
10.7838284	1.266147E-04	330	0.982	0.018	Yes
11.3624320	1.127037E-04	330	0.982	0.018	Yes
11.9329135	1.014280E-04	330	0.982	0.018	Yes
12.5417041	9.212397E-05	330	0.982	0.018	Yes
13.2369688	8.436464E-05	330	0.982	0.018	Yes
14.0287225	7.799266E-05	330	0.982	0.018	Yes
15.0469659	7.255003E-05	330	0.982	0.018	Yes
18.2752200	6.339305E-05	330	0.982	0.018	Yes
24.8029975	5.603500E-05	330	0.982	0.018	Yes
24.8365755	5.600308E-05	330	0.982	0.018	Yes

Data summarised from TABLE 1 of Ely89 [88]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
41.0044	6.06493E-05	300	0.44696	0.55304	Yes
27.6350	7.61709E-05	300	0.44696	0.55304	Yes
21.8676	9.1297E-05	300	0.44696	0.55304	Yes
17.1630	0.000114686	300	0.44696	0.55304	Yes
15.5039	0.000127457	300	0.44696	0.55304	Yes
14.4664	0.000137471	300	0.44696	0.55304	Yes
11.8033	0.000172698	300	0.44696	0.55304	Yes
10.7563	0.000191915	300	0.44696	0.55304	Yes
10.0742	0.000207011	300	0.44696	0.55304	Yes
8.2505	0.000260067	300	0.44696	0.55304	Yes
7.5166	0.000288968	300	0.44696	0.55304	Yes
7.0283	0.000311741	300	0.44696	0.55304	Yes
5.7271	0.000391646	300	0.44696	0.55304	Yes
5.1038	0.000443626	300	0.44696	0.55304	Yes
4.8546	0.000469476	300	0.44696	0.55304	Yes
3.9310	0.000589814	300	0.44696	0.55304	Yes
3.5629	0.000655139	300	0.44696	0.55304	Yes
3.3171	0.000707027	300	0.44696	0.55304	Yes
2.9142	0.000810839	300	0.44696	0.55304	Yes
2.6721	0.000888271	300	0.44696	0.55304	Yes
2.4173	0.000986571	300	0.44696	0.55304	Yes
1.9696	0.001221077	300	0.44696	0.55304	Yes
1.8035	0.001337754	300	0.44696	0.55304	Yes
1.6290	0.001485687	300	0.44696	0.55304	Yes
1.5126	0.001603617	300	0.44696	0.55304	Yes
1.3236	0.001839026	300	0.44696	0.55304	Yes
1.2109	0.002014708	300	0.44696	0.55304	Yes
1.0923	0.002237747	300	0.44696	0.55304	Yes
1.0157	0.00241038	300	0.44696	0.55304	Yes
1.0129	0.002415132	300	0.44696	0.55304	Yes
0.8860	0.002810681	300	0.44696	0.55304	Yes
0.8099	0.003034246	300	0.44696	0.55304	Yes
0.6776	0.003637306	300	0.44696	0.55304	Yes
0.5916	0.004171228	300	0.44696	0.55304	Yes
0.5405	0.004569744	300	0.44696	0.55304	Yes
0.4518	0.005477952	300	0.44696	0.55304	Yes
0.3942	0.006282211	300	0.44696	0.55304	Yes
0.3600	0.006882337	300	0.44696	0.55304	Yes
0.3009	0.008250169	300	0.44696	0.55304	Yes
0.2624	0.009460841	300	0.44696	0.55304	Yes
0.2396	0.01036523	300	0.44696	0.55304	Yes
0.2001	0.012425343	300	0.44696	0.55304	Yes
0.1745	0.01424923	300	0.44696	0.55304	Yes
0.1593	0.015610252	300	0.44696	0.55304	Yes
0.1330	0.018713486	300	0.44696	0.55304	Yes
0.1160	0.021455726	300	0.44696	0.55304	Yes
0.1059	0.023511005	300	0.44696	0.55304	Yes
0.0884	0.028184405	300	0.44696	0.55304	Yes

Data summarised from Table 2 of Esper89 [78]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
49.0	6.75395E-05	323	0.2515	0.7485	Yes
50.0	6.68629E-05	323	0.2515	0.7485	Yes
51.0	6.6186E-05	323	0.2515	0.7485	Yes
52.0	6.55092E-05	323	0.2515	0.7485	Yes
53.1	6.48199E-05	323	0.2515	0.7485	Yes
54.1	6.4145E-05	323	0.2515	0.7485	Yes
55.2	6.34714E-05	323	0.2515	0.7485	Yes
56.4	6.27995E-05	323	0.2515	0.7485	Yes
57.6	6.21175E-05	323	0.2515	0.7485	Yes
58.9	6.14384E-05	323	0.2515	0.7485	Yes
60.3	6.07625E-05	323	0.2515	0.7485	Yes
61.6	6.00788E-05	323	0.2515	0.7485	Yes
63.1	5.94102E-05	323	0.2515	0.7485	Yes
64.7	5.87241E-05	323	0.2515	0.7485	Yes
66.3	5.80536E-05	323	0.2515	0.7485	Yes
68.0	5.73778E-05	323	0.2515	0.7485	Yes
69.9	5.66973E-05	323	0.2515	0.7485	Yes
71.7	5.60231E-05	323	0.2515	0.7485	Yes
72.8	5.56823E-05	323	0.2515	0.7485	Yes
73.7	5.54317E-05	323	0.2515	0.7485	Yes
75.5	5.48621E-05	323	0.2515	0.7485	Yes
77.4	5.43041E-05	323	0.2515	0.7485	Yes
79.4	5.37393E-05	323	0.2515	0.7485	Yes
81.5	5.31773E-05	323	0.2515	0.7485	Yes
83.6	5.26183E-05	323	0.2515	0.7485	Yes
86.0	5.20539E-05	323	0.2515	0.7485	Yes
88.4	5.14933E-05	323	0.2515	0.7485	Yes
90.9	5.09366E-05	323	0.2515	0.7485	Yes
93.6	5.03679E-05	323	0.2515	0.7485	Yes
96.5	4.98118E-05	323	0.2515	0.7485	Yes
99.2	4.92452E-05	323	0.2515	0.7485	Yes
102.4	4.86839E-05	323	0.2515	0.7485	Yes
113.2	4.69982E-05	323	0.2515	0.7485	Yes
117.3	4.64395E-05	323	0.2515	0.7485	Yes
119.5	4.61585E-05	323	0.2515	0.7485	Yes
121.7	4.56976E-05	323	0.2515	0.7485	Yes
125.4	4.5233E-05	323	0.2515	0.7485	Yes

Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [119]

P (MPa)	v ($m^3 mol^{-1}$)	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
129.5	4.47715E-05	323	0.2515	0.7485	Yes
133.8	4.43071E-05	323	0.2515	0.7485	Yes
138.2	4.38462E-05	323	0.2515	0.7485	Yes
142.9	4.3383E-05	323	0.2515	0.7485	Yes
147.8	4.2918E-05	323	0.2515	0.7485	Yes
152.9	4.24516E-05	323	0.2515	0.7485	Yes
158.4	4.19898E-05	323	0.2515	0.7485	Yes
164.7	4.15271E-05	323	0.2515	0.7485	Yes
170.9	4.1064E-05	323	0.2515	0.7485	Yes
177.4	4.06008E-05	323	0.2515	0.7485	Yes
184.3	4.01378E-05	323	0.2515	0.7485	Yes
192.1	3.96706E-05	323	0.2515	0.7485	Yes
200.0	3.92141E-05	323	0.2515	0.7485	Yes
208.6	3.87492E-05	323	0.2515	0.7485	Yes
217.8	3.82861E-05	323	0.2515	0.7485	Yes
222.3	3.80542E-05	323	0.2515	0.7485	Yes
51.1	7.06528E-05	348	0.2515	0.7485	Yes
52.0	6.99432E-05	348	0.2515	0.7485	Yes
53.0	6.92328E-05	348	0.2515	0.7485	Yes
54.0	6.85219E-05	348	0.2515	0.7485	Yes
55.1	6.78112E-05	348	0.2515	0.7485	Yes
56.1	6.7101E-05	348	0.2515	0.7485	Yes
57.2	6.63917E-05	348	0.2515	0.7485	Yes
58.3	6.56838E-05	348	0.2515	0.7485	Yes
59.6	6.49777E-05	348	0.2515	0.7485	Yes
60.8	6.42737E-05	348	0.2515	0.7485	Yes
62.1	6.35595E-05	348	0.2515	0.7485	Yes
63.4	6.28487E-05	348	0.2515	0.7485	Yes
64.8	6.21416E-05	348	0.2515	0.7485	Yes
66.3	6.14384E-05	348	0.2515	0.7485	Yes
67.9	6.0728E-05	348	0.2515	0.7485	Yes
69.5	6.00112E-05	348	0.2515	0.7485	Yes
71.1	5.93112E-05	348	0.2515	0.7485	Yes
73.0	5.85952E-05	348	0.2515	0.7485	Yes
74.0	5.82436E-05	348	0.2515	0.7485	Yes
75.9	5.75013E-05	348	0.2515	0.7485	Yes
77.5	5.6919E-05	348	0.2515	0.7485	Yes
79.3	5.63384E-05	348	0.2515	0.7485	Yes
81.4	5.57598E-05	348	0.2515	0.7485	Yes
83.5	5.5174E-05	348	0.2515	0.7485	Yes
85.5	5.4591E-05	348	0.2515	0.7485	Yes
87.8	5.40111E-05	348	0.2515	0.7485	Yes
90.1	5.34256E-05	348	0.2515	0.7485	Yes
92.7	5.28439E-05	348	0.2515	0.7485	Yes
95.2	5.22577E-05	348	0.2515	0.7485	Yes
98.0	5.16761E-05	348	0.2515	0.7485	Yes
100.8	5.10991E-05	348	0.2515	0.7485	Yes
103.8	5.05109E-05	348	0.2515	0.7485	Yes
107.2	4.99283E-05	348	0.2515	0.7485	Yes
110.8	4.93438E-05	348	0.2515	0.7485	Yes
114.3	4.87654E-05	348	0.2515	0.7485	Yes
118.2	4.81787E-05	348	0.2515	0.7485	Yes
120.2	4.78906E-05	348	0.2515	0.7485	Yes
122.5	4.74086E-05	348	0.2515	0.7485	Yes
126.0	4.69294E-05	348	0.2515	0.7485	Yes
129.9	4.64463E-05	348	0.2515	0.7485	Yes
134.0	4.59664E-05	348	0.2515	0.7485	Yes
138.2	4.54899E-05	348	0.2515	0.7485	Yes
142.7	4.50105E-05	348	0.2515	0.7485	Yes
147.4	4.45288E-05	348	0.2515	0.7485	Yes
152.5	4.40451E-05	348	0.2515	0.7485	Yes
157.7	4.35659E-05	348	0.2515	0.7485	Yes
163.5	4.30854E-05	348	0.2515	0.7485	Yes
169.4	4.26041E-05	348	0.2515	0.7485	Yes
175.5	4.21278E-05	348	0.2515	0.7485	Yes
182.4	4.16459E-05	348	0.2515	0.7485	Yes
189.6	4.11642E-05	348	0.2515	0.7485	Yes
197.3	4.06833E-05	348	0.2515	0.7485	Yes
205.3	4.01983E-05	348	0.2515	0.7485	Yes
214.0	3.97247E-05	348	0.2515	0.7485	Yes
218.8	3.94848E-05	348	0.2515	0.7485	Yes
63.3	5.72977E-05	323	0.5685	0.4315	Yes
64.8	5.67197E-05	323	0.5685	0.4315	Yes
66.4	5.61447E-05	323	0.5685	0.4315	Yes
68.2	5.55729E-05	323	0.5685	0.4315	Yes
70.0	5.49963E-05	323	0.5685	0.4315	Yes
72.0	5.44236E-05	323	0.5685	0.4315	Yes
74.1	5.38549E-05	323	0.5685	0.4315	Yes
76.3	5.32749E-05	323	0.5685	0.4315	Yes
78.7	5.26999E-05	323	0.5685	0.4315	Yes
81.2	5.21225E-05	323	0.5685	0.4315	Yes
83.9	5.15504E-05	323	0.5685	0.4315	Yes
86.8	5.09768E-05	323	0.5685	0.4315	Yes
89.7	5.04021E-05	323	0.5685	0.4315	Yes
92.9	4.98268E-05	323	0.5685	0.4315	Yes
96.1	4.92514E-05	323	0.5685	0.4315	Yes
103.7	4.81022E-05	323	0.5685	0.4315	Yes
107.8	4.75291E-05	323	0.5685	0.4315	Yes
109.8	4.72387E-05	323	0.5685	0.4315	Yes
113.2	4.67624E-05	323	0.5685	0.4315	Yes
117.2	4.62899E-05	323	0.5685	0.4315	Yes

Continued: Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [119]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
121.3	4.58212E-05	323	0.5685	0.4315	Yes
125.8	4.53397E-05	323	0.5685	0.4315	Yes
130.6	4.48736E-05	323	0.5685	0.4315	Yes
135.7	4.43958E-05	323	0.5685	0.4315	Yes
141.1	4.39228E-05	323	0.5685	0.4315	Yes
146.7	4.34496E-05	323	0.5685	0.4315	Yes
152.8	4.29766E-05	323	0.5685	0.4315	Yes
159.3	4.24991E-05	323	0.5685	0.4315	Yes
166.2	4.20274E-05	323	0.5685	0.4315	Yes
173.5	4.15521E-05	323	0.5685	0.4315	Yes
181.3	4.10783E-05	323	0.5685	0.4315	Yes
189.7	4.01319E-05	323	0.5685	0.4315	Yes
208.2	3.96559E-05	323	0.5685	0.4315	Yes
218.6	3.91827E-05	323	0.5685	0.4315	Yes
224.2	3.89483E-05	323	0.5685	0.4315	Yes
65.6	6.03448E-05	348	0.5685	0.4315	Yes
67.1	5.97328E-05	348	0.5685	0.4315	Yes
68.8	5.91331E-05	348	0.5685	0.4315	Yes
70.6	5.85268E-05	348	0.5685	0.4315	Yes
72.4	5.79238E-05	348	0.5685	0.4315	Yes
74.3	5.73154E-05	348	0.5685	0.4315	Yes
76.3	5.6711E-05	348	0.5685	0.4315	Yes
78.4	5.61022E-05	348	0.5685	0.4315	Yes
80.6	5.54981E-05	348	0.5685	0.4315	Yes
83.1	5.48905E-05	348	0.5685	0.4315	Yes
85.6	5.42882E-05	348	0.5685	0.4315	Yes
88.2	5.36834E-05	348	0.5685	0.4315	Yes
91.0	5.30768E-05	348	0.5685	0.4315	Yes
94.0	5.24689E-05	348	0.5685	0.4315	Yes
97.1	5.18675E-05	348	0.5685	0.4315	Yes
100.5	5.12585E-05	348	0.5685	0.4315	Yes
104.1	5.06567E-05	348	0.5685	0.4315	Yes
107.9	5.00553E-05	348	0.5685	0.4315	Yes
109.8	4.97466E-05	348	0.5685	0.4315	Yes
113.0	4.92514E-05	348	0.5685	0.4315	Yes
115.4	4.87531E-05	348	0.5685	0.4315	Yes
120.4	4.82523E-05	348	0.5685	0.4315	Yes
124.4	4.77493E-05	348	0.5685	0.4315	Yes
128.8	4.72507E-05	348	0.5685	0.4315	Yes
133.4	4.67566E-05	348	0.5685	0.4315	Yes
138.3	4.62553E-05	348	0.5685	0.4315	Yes
143.3	4.5759E-05	348	0.5685	0.4315	Yes
148.7	4.52567E-05	348	0.5685	0.4315	Yes
154.5	4.476E-05	348	0.5685	0.4315	Yes
160.8	4.42581E-05	348	0.5685	0.4315	Yes
167.3	4.37622E-05	348	0.5685	0.4315	Yes
174.3	4.32622E-05	348	0.5685	0.4315	Yes
181.6	4.27587E-05	348	0.5685	0.4315	Yes
189.7	4.2262E-05	348	0.5685	0.4315	Yes
198.2	4.17625E-05	348	0.5685	0.4315	Yes
207.2	4.12656E-05	348	0.5685	0.4315	Yes
212.2	4.10147E-05	348	0.5685	0.4315	Yes
56.4	5.29927E-05	323	0.7450	0.2550	Yes
58.5	5.24566E-05	323	0.7450	0.2550	Yes
60.3	5.24566E-05	323	0.7450	0.2550	Yes
62.3	5.13966E-05	323	0.7450	0.2550	Yes
64.6	5.08662E-05	323	0.7450	0.2550	Yes
66.8	5.0334E-05	323	0.7450	0.2550	Yes
69.2	4.98004E-05	323	0.7450	0.2550	Yes
71.8	4.9272E-05	323	0.7450	0.2550	Yes
74.6	4.87367E-05	323	0.7450	0.2550	Yes
77.5	4.82072E-05	323	0.7450	0.2550	Yes
80.7	4.76719E-05	323	0.7450	0.2550	Yes
84.2	4.71429E-05	323	0.7450	0.2550	Yes
87.9	4.66091E-05	323	0.7450	0.2550	Yes
91.8	4.60766E-05	323	0.7450	0.2550	Yes
96.0	4.55458E-05	323	0.7450	0.2550	Yes
100.5	4.50169E-05	323	0.7450	0.2550	Yes
105.5	4.44853E-05	323	0.7450	0.2550	Yes
111.0	4.39516E-05	323	0.7450	0.2550	Yes
113.9	4.36871E-05	323	0.7450	0.2550	Yes
119.0	4.32517E-05	323	0.7450	0.2550	Yes
124.1	4.28112E-05	323	0.7450	0.2550	Yes
129.7	4.2375E-05	323	0.7450	0.2550	Yes
135.9	4.19345E-05	323	0.7450	0.2550	Yes
142.3	4.14943E-05	323	0.7450	0.2550	Yes
149.2	4.10591E-05	323	0.7450	0.2550	Yes
156.6	4.06205E-05	323	0.7450	0.2550	Yes
164.5	4.01832E-05	323	0.7450	0.2550	Yes
173.0	3.97432E-05	323	0.7450	0.2550	Yes
182.2	3.9305E-05	323	0.7450	0.2550	Yes
191.8	3.88651E-05	323	0.7450	0.2550	Yes
202.3	3.84275E-05	323	0.7450	0.2550	Yes
213.5	3.79888E-05	323	0.7450	0.2550	Yes
224.1	3.75529E-05	323	0.7450	0.2550	Yes
237.0	3.71131E-05	323	0.7450	0.2550	Yes
250.8	3.66768E-05	323	0.7450	0.2550	Yes
265.8	3.62374E-05	323	0.7450	0.2550	Yes
273.7	3.60184E-05	323	0.7450	0.2550	Yes
60.6	5.52741E-05	348	0.7450	0.2550	Yes
62.4	5.47211E-05	348	0.7450	0.2550	Yes
64.3	5.41718E-05	348	0.7450	0.2550	Yes

Continued: Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [119]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
66.3	5.36117E-05	348	0.7450	0.2550	Yes
68.2	5.30631E-05	348	0.7450	0.2550	Yes
70.4	5.25049E-05	348	0.7450	0.2550	Yes
72.3	5.19516E-05	348	0.7450	0.2550	Yes
75.2	5.13966E-05	348	0.7450	0.2550	Yes
77.9	5.08403E-05	348	0.7450	0.2550	Yes
80.7	5.02897E-05	348	0.7450	0.2550	Yes
83.8	4.97322E-05	348	0.7450	0.2550	Yes
86.8	4.91809E-05	348	0.7450	0.2550	Yes
90.3	4.8624E-05	348	0.7450	0.2550	Yes
94.1	4.80679E-05	348	0.7450	0.2550	Yes
97.9	4.75131E-05	348	0.7450	0.2550	Yes
102.0	4.69599E-05	348	0.7450	0.2550	Yes
106.6	4.64086E-05	348	0.7450	0.2550	Yes
111.3	4.58491E-05	348	0.7450	0.2550	Yes
113.9	4.55718E-05	348	0.7450	0.2550	Yes
118.0	4.51186E-05	348	0.7450	0.2550	Yes
122.7	4.46594E-05	348	0.7450	0.2550	Yes
127.7	4.42046E-05	348	0.7450	0.2550	Yes
132.9	4.37445E-05	348	0.7450	0.2550	Yes
138.7	4.32892E-05	348	0.7450	0.2550	Yes
144.7	4.28296E-05	348	0.7450	0.2550	Yes
151.2	4.2375E-05	348	0.7450	0.2550	Yes
158.0	4.19169E-05	348	0.7450	0.2550	Yes
165.5	4.14599E-05	348	0.7450	0.2550	Yes
173.3	4.10001E-05	348	0.7450	0.2550	Yes
181.7	4.05463E-05	348	0.7450	0.2550	Yes
190.7	4.00863E-05	348	0.7450	0.2550	Yes
200.2	3.96288E-05	348	0.7450	0.2550	Yes
210.7	3.91739E-05	348	0.7450	0.2550	Yes
221.9	3.87181E-05	348	0.7450	0.2550	Yes
233.8	3.82581E-05	348	0.7450	0.2550	Yes
246.3	3.78018E-05	348	0.7450	0.2550	Yes
252.7	3.75741E-05	348	0.7450	0.2550	Yes

Continued: Data summarised from Table I, II, III, IV, V, and VI of Hacura88 [108]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
3.03975	0.000760956	298.15	0.5048	0.4952	Yes
5.06625	0.000435631	298.15	0.5048	0.4952	Yes
7.59938	0.00027411	298.15	0.5048	0.4952	Yes
10.13250	0.000194842	298.15	0.5048	0.4952	Yes
12.66563	0.000149219	298.15	0.5048	0.4952	Yes
15.19875	0.000120908	298.15	0.5048	0.4952	Yes
17.73188	0.000102615	298.15	0.5048	0.4952	Yes
20.26500	9.05587E-05	298.15	0.5048	0.4952	Yes
22.79813	8.19102E-05	298.15	0.5048	0.4952	Yes
25.33125	7.55002E-05	298.15	0.5048	0.4952	Yes
30.39750	6.74348E-05	298.15	0.5048	0.4952	Yes
35.46375	6.20582E-05	298.15	0.5048	0.4952	Yes
40.53000	5.82949E-05	298.15	0.5048	0.4952	Yes
45.59625	5.54767E-05	298.15	0.5048	0.4952	Yes
50.66250	5.32416E-05	298.15	0.5048	0.4952	Yes
3.03975	0.000790722	298.15	0.2513	0.7487	Yes
5.06625	0.000466017	298.15	0.2513	0.7487	Yes
7.59938	0.000304969	298.15	0.2513	0.7487	Yes
10.13250	0.00022562	298.15	0.2513	0.7487	Yes
12.66563	0.000179067	298.15	0.2513	0.7487	Yes
15.19875	0.000149761	298.15	0.2513	0.7487	Yes
17.73188	0.000128255	298.15	0.2513	0.7487	Yes
20.26500	0.000113385	298.15	0.2513	0.7487	Yes
22.79813	0.000102309	298.15	0.2513	0.7487	Yes
25.33125	9.37808E-05	298.15	0.2513	0.7487	Yes
30.39750	8.1641E-05	298.15	0.2513	0.7487	Yes
35.46375	7.37178E-05	298.15	0.2513	0.7487	Yes
40.53000	6.81361E-05	298.15	0.2513	0.7487	Yes
45.59625	6.38384E-05	298.15	0.2513	0.7487	Yes
50.66250	6.05372E-05	298.15	0.2513	0.7487	Yes
3.03975	0.000711345	273.15	0.5048	0.4952	Yes
5.06625	0.000413583	273.15	0.5048	0.4952	Yes
7.59938	0.00026562	273.15	0.5048	0.4952	Yes
10.13250	0.000192603	273.15	0.5048	0.4952	Yes
12.66563	0.000149905	273.15	0.5048	0.4952	Yes
15.19875	0.000122545	273.15	0.5048	0.4952	Yes
17.73188	0.000104142	273.15	0.5048	0.4952	Yes
20.26500	9.13481E-05	273.15	0.5048	0.4952	Yes
22.79813	8.19654E-05	273.15	0.5048	0.4952	Yes
25.33125	7.49523E-05	273.15	0.5048	0.4952	Yes
30.39750	6.52844E-05	273.15	0.5048	0.4952	Yes
35.46375	5.92113E-05	273.15	0.5048	0.4952	Yes
40.53000	5.48414E-05	273.15	0.5048	0.4952	Yes
45.59625	5.16517E-05	273.15	0.5048	0.4952	Yes
50.66250	4.93152E-05	273.15	0.5048	0.4952	Yes

Data summarised from TABLE II of Haney44 [108]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
3.03975	0.000732563	273.15	0.2513	0.7487	Yes
5.06625	0.000434741	273.15	0.2513	0.7487	Yes
7.59938	0.00028669	273.15	0.2513	0.7487	Yes
10.13250	0.000213538	273.15	0.2513	0.7487	Yes
12.66563	0.000170292	273.15	0.2513	0.7487	Yes
15.19875	0.00014206	273.15	0.2513	0.7487	Yes
17.73188	0.00012247	273.15	0.2513	0.7487	Yes
20.26500	0.000107161	273.15	0.2513	0.7487	Yes
22.79813	9.74858E-05	273.15	0.2513	0.7487	Yes
25.33125	8.91538E-05	273.15	0.2513	0.7487	Yes
30.39750	7.71041E-05	273.15	0.2513	0.7487	Yes
35.46375	6.89198E-05	273.15	0.2513	0.7487	Yes
40.53000	6.31345E-05	273.15	0.2513	0.7487	Yes
45.59625	5.89388E-05	273.15	0.2513	0.7487	Yes
50.66250	5.54656E-05	273.15	0.2513	0.7487	Yes
3.03975	0.000721431	273.15	0.5048	0.4952	Yes
5.06625	0.000423445	273.15	0.5048	0.4952	Yes
7.59938	0.000275244	273.15	0.5048	0.4952	Yes
10.13250	0.000201995	273.15	0.5048	0.4952	Yes
12.66563	0.00015887	273.15	0.5048	0.4952	Yes
15.19875	0.000130927	273.15	0.5048	0.4952	Yes
17.73188	0.000111711	273.15	0.5048	0.4952	Yes
20.26500	9.77921E-05	273.15	0.5048	0.4952	Yes
22.79813	8.74244E-05	273.15	0.5048	0.4952	Yes
25.33125	7.95337E-05	273.15	0.5048	0.4952	Yes
30.39750	6.85419E-05	273.15	0.5048	0.4952	Yes
35.46375	6.13502E-05	273.15	0.5048	0.4952	Yes
40.53000	5.62535E-05	273.15	0.5048	0.4952	Yes
45.59625	5.25383E-05	273.15	0.5048	0.4952	Yes
50.66250	4.98487E-05	273.15	0.5048	0.4952	Yes
3.03975	0.000737718	273.15	0.2513	0.7487	Yes
5.06625	0.000439941	273.15	0.2513	0.7487	Yes
7.59938	0.000291591	273.15	0.2513	0.7487	Yes
10.13250	0.000218178	273.15	0.2513	0.7487	Yes
12.66563	0.000174703	273.15	0.2513	0.7487	Yes
15.19875	0.000146169	273.15	0.2513	0.7487	Yes
17.73188	0.000126197	273.15	0.2513	0.7487	Yes
20.26500	0.000111532	273.15	0.2513	0.7487	Yes
22.79813	0.000100325	273.15	0.2513	0.7487	Yes
25.33125	9.15207E-05	273.15	0.2513	0.7487	Yes
30.39750	7.88225E-05	273.15	0.2513	0.7487	Yes
35.46375	7.00597E-05	273.15	0.2513	0.7487	Yes
40.53000	6.38014E-05	273.15	0.2513	0.7487	Yes
45.59625	5.9133E-05	273.15	0.2513	0.7487	Yes
50.66250	5.55104E-05	273.15	0.2513	0.7487	Yes
3.03975	0.000728305	273.15	0.5048	0.4952	Yes
5.06625	0.000430348	273.15	0.5048	0.4952	Yes
7.59938	0.000282117	273.15	0.5048	0.4952	Yes
10.13250	0.000208652	273.15	0.5048	0.4952	Yes
12.66563	0.000165182	273.15	0.5048	0.4952	Yes
15.19875	0.00013668	273.15	0.5048	0.4952	Yes
17.73188	0.000116847	273.15	0.5048	0.4952	Yes
20.26500	0.000102465	273.15	0.5048	0.4952	Yes
22.79813	9.17279E-05	273.15	0.5048	0.4952	Yes
25.33125	8.32993E-05	273.15	0.5048	0.4952	Yes
30.39750	7.13437E-05	273.15	0.5048	0.4952	Yes
35.46375	6.32714E-05	273.15	0.5048	0.4952	Yes
40.53000	5.75311E-05	273.15	0.5048	0.4952	Yes
45.59625	5.34747E-05	273.15	0.5048	0.4952	Yes
50.66250	5.02611E-05	273.15	0.5048	0.4952	Yes
3.03975	0.000741529	273.15	0.2513	0.7487	Yes
5.06625	0.000443572	273.15	0.2513	0.7487	Yes
7.59938	0.000295267	273.15	0.2513	0.7487	Yes
10.13250	0.000221652	273.15	0.2513	0.7487	Yes
12.66563	0.000177895	273.15	0.2513	0.7487	Yes
15.19875	0.000149053	273.15	0.2513	0.7487	Yes
17.73188	0.000128759	273.15	0.2513	0.7487	Yes
20.26500	0.000113807	273.15	0.2513	0.7487	Yes
22.79813	0.000102317	273.15	0.2513	0.7487	Yes
25.33125	9.33228E-05	273.15	0.2513	0.7487	Yes
30.39750	8.00776E-05	273.15	0.2513	0.7487	Yes
35.46375	7.09434E-05	273.15	0.2513	0.7487	Yes
40.53000	6.43729E-05	273.15	0.2513	0.7487	Yes
45.59625	5.9407E-05	273.15	0.2513	0.7487	Yes
50.66250	5.54925E-05	273.15	0.2513	0.7487	Yes
3.03975	0.000734207	273.15	0.5048	0.4952	Yes
5.06625	0.000435952	273.15	0.5048	0.4952	Yes
7.59938	0.000287347	273.15	0.5048	0.4952	Yes
10.13250	0.000213605	273.15	0.5048	0.4952	Yes
12.66563	0.000169898	273.15	0.5048	0.4952	Yes
15.19875	0.000141118	273.15	0.5048	0.4952	Yes
17.73188	0.000120959	273.15	0.5048	0.4952	Yes
20.26500	0.000106186	273.15	0.5048	0.4952	Yes
22.79813	9.50153E-05	273.15	0.5048	0.4952	Yes
25.33125	8.624E-05	273.15	0.5048	0.4952	Yes
30.39750	7.35776E-05	273.15	0.5048	0.4952	Yes
35.46375	6.50005E-05	273.15	0.5048	0.4952	Yes
40.53000	5.88591E-05	273.15	0.5048	0.4952	Yes
45.59625	5.43862E-05	273.15	0.5048	0.4952	Yes
50.66250	5.07138E-05	273.15	0.5048	0.4952	Yes

Continued: Data summarised from TABLE II of Haney44 [108]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
3.03975	0.000744368	273.15	0.2513	0.7487	Yes
5.06625	0.000446352	273.15	0.2513	0.7487	Yes
7.59938	0.000297897	273.15	0.2513	0.7487	Yes
10.13250	0.00022414	273.15	0.2513	0.7487	Yes
12.66563	0.000180226	273.15	0.2513	0.7487	Yes
15.19875	0.000151205	273.15	0.2513	0.7487	Yes
17.73188	0.000130693	273.15	0.2513	0.7487	Yes
20.26500	0.00011551	273.15	0.2513	0.7487	Yes
22.79813	0.000103841	273.15	0.2513	0.7487	Yes
25.33125	9.46138E-05	273.15	0.2513	0.7487	Yes
30.39750	8.10489E-05	273.15	0.2513	0.7487	Yes
35.46375	7.16158E-05	273.15	0.2513	0.7487	Yes
40.53000	6.53087E-05	273.15	0.2513	0.7487	Yes
45.59625	5.95763E-05	273.15	0.2513	0.7487	Yes
50.66250	5.54701E-05	273.15	0.2513	0.7487	Yes
4.69758	0.000430097	293.2	0.702400	0.297600	Yes
4.28804	0.000480128	293.2	0.702400	0.297600	Yes
4.00226	0.000521057	293.2	0.702400	0.297600	Yes
3.50269	0.000608533	293.2	0.702400	0.297600	Yes
3.00310	0.000724882	293.2	0.702400	0.297600	Yes
2.50368	0.000887384	293.2	0.702400	0.297600	Yes
2.00442	0.001130487	293.2	0.702400	0.297600	Yes
1.50699	0.001532498	293.2	0.702400	0.297600	Yes
1.00550	0.002339860	293.2	0.702400	0.297600	Yes
0.80569	0.002941322	293.2	0.702400	0.297600	Yes
0.60615	0.003937615	293.2	0.702400	0.297600	Yes
5.18106	0.000409518	293.2	0.539900	0.460100	Yes
4.18809	0.000520861	293.2	0.539900	0.460100	Yes
3.70248	0.000597156	293.2	0.539900	0.460100	Yes
3.20700	0.000698819	293.2	0.539900	0.460100	Yes
2.69969	0.000841641	293.2	0.539900	0.460100	Yes
2.20817	0.001042639	293.2	0.539900	0.460100	Yes
1.71058	0.001363788	293.2	0.539900	0.460100	Yes
1.44089	0.001630535	293.2	0.539900	0.460100	Yes
1.00646	0.002360839	293.2	0.539900	0.460100	Yes
0.80573	0.002964268	293.2	0.539900	0.460100	Yes
0.60297	0.003981678	293.2	0.539900	0.460100	Yes
4.05769	0.000549598	293.2	0.468600	0.531400	Yes
3.50024	0.000644900	293.2	0.468600	0.531400	Yes
3.00078	0.000760485	293.2	0.468600	0.531400	Yes
2.50151	0.000922334	293.2	0.468600	0.531400	Yes
2.00001	0.001166443	293.2	0.468600	0.531400	Yes
1.50165	0.001570698	293.2	0.468600	0.531400	Yes
1.00236	0.002379108	293.2	0.468600	0.531400	Yes
0.80172	0.002987644	293.2	0.468600	0.531400	Yes
0.60197	0.003996519	293.2	0.468600	0.531400	Yes

Data summarised from TABLE 1 of Jiang90 [107]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
4.53762	0.000510150	293.2	0.271200	0.728800	Yes
4.01826	0.000579211	293.2	0.271200	0.728800	Yes
3.51901	0.000664932	293.2	0.271200	0.728800	Yes
3.00972	0.000781806	293.2	0.271200	0.728800	Yes
2.50625	0.000944190	293.2	0.271200	0.728800	Yes
2.00715	0.001185738	293.2	0.271200	0.728800	Yes
1.51140	0.001583796	293.2	0.271200	0.728800	Yes
1.00979	0.002384688	293.2	0.271200	0.728800	Yes
0.80509	0.002998340	293.2	0.271200	0.728800	Yes
0.60840	0.003977091	293.2	0.271200	0.728800	Yes
5.950	0.000355641	313.05	0.6772	0.3228	Yes
8.825	0.000214003	313.05	0.6772	0.3228	Yes
10.863	0.000160437	313.05	0.6772	0.3228	Yes
17.698	0.000085872	313.05	0.6772	0.3228	Yes
20.619	0.000074995	313.05	0.6772	0.3228	Yes
23.548	0.000068275	313.05	0.6772	0.3228	Yes
26.480	0.000063762	313.05	0.6772	0.3228	Yes
29.414	0.000060437	313.05	0.6772	0.3228	Yes
32.350	0.000057937	313.05	0.6772	0.3228	Yes
35.287	0.000055940	313.05	0.6772	0.3228	Yes
38.224	0.000054304	313.05	0.6772	0.3228	Yes
41.162	0.000052894	313.05	0.6772	0.3228	Yes
44.101	0.000051694	313.05	0.6772	0.3228	Yes
47.037	0.000050665	313.05	0.6772	0.3228	Yes
49.978	0.000049756	313.05	0.6772	0.3228	Yes
52.917	0.000048940	313.05	0.6772	0.3228	Yes
55.858	0.000048181	313.05	0.6772	0.3228	Yes
58.795	0.000047509	313.05	0.6772	0.3228	Yes

Data summarised from TABLE 2 of Kosov75 [120]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
5.960	0.000391413	313.05	0.4706	0.5294	Yes
8.838	0.000251556	313.05	0.4706	0.5294	Yes
12.174	0.000174883	313.05	0.4706	0.5294	Yes
18.708	0.000110033	313.05	0.4706	0.5294	Yes
20.652	0.000100091	313.05	0.4706	0.5294	Yes
23.574	0.000089065	313.05	0.4706	0.5294	Yes
26.501	0.000081173	313.05	0.4706	0.5294	Yes
29.432	0.000075273	313.05	0.4706	0.5294	Yes
32.365	0.000070776	313.05	0.4706	0.5294	Yes
35.299	0.000067186	313.05	0.4706	0.5294	Yes
38.234	0.000064268	313.05	0.4706	0.5294	Yes
41.171	0.000061884	313.05	0.4706	0.5294	Yes
44.108	0.000059864	313.05	0.4706	0.5294	Yes
47.046	0.000058100	313.05	0.4706	0.5294	Yes
49.983	0.000056597	313.05	0.4706	0.5294	Yes
52.921	0.000055255	313.05	0.4706	0.5294	Yes
55.889	0.000054095	313.05	0.4706	0.5294	Yes
58.798	0.000053035	313.05	0.4706	0.5294	Yes
5.945	0.000420057	313.05	0.2329	0.7671	Yes
8.831	0.000279038	313.05	0.2329	0.7671	Yes
11.846	0.000206722	313.05	0.2329	0.7671	Yes
14.751	0.000166064	313.05	0.2329	0.7671	Yes
19.687	0.000126054	313.05	0.2329	0.7671	Yes
23.580	0.000107538	313.05	0.2329	0.7671	Yes
26.506	0.000097602	313.05	0.2329	0.7671	Yes
29.436	0.000089964	313.05	0.2329	0.7671	Yes
32.368	0.000083938	313.05	0.2329	0.7671	Yes
35.301	0.000079050	313.05	0.2329	0.7671	Yes
38.235	0.000075026	313.05	0.2329	0.7671	Yes
41.171	0.000071661	313.05	0.2329	0.7671	Yes
44.107	0.000068744	313.05	0.2329	0.7671	Yes
47.044	0.000066278	313.05	0.2329	0.7671	Yes
49.981	0.000064154	313.05	0.2329	0.7671	Yes
52.919	0.000062259	313.05	0.2329	0.7671	Yes
55.857	0.000060587	313.05	0.2329	0.7671	Yes
58.795	0.000059140	313.05	0.2329	0.7671	Yes
23.589	0.000091114	353.15	0.6772	0.3228	Yes
26.513	0.000082893	353.15	0.6772	0.3228	Yes
29.443	0.000076578	353.15	0.6772	0.3228	Yes
32.374	0.000071759	353.15	0.6772	0.3228	Yes
35.308	0.000067983	353.15	0.6772	0.3228	Yes
38.243	0.000064992	353.15	0.6772	0.3228	Yes
41.179	0.000062526	353.15	0.6772	0.3228	Yes
44.116	0.000060460	353.15	0.6772	0.3228	Yes
47.053	0.000058720	353.15	0.6772	0.3228	Yes
49.991	0.000057184	353.15	0.6772	0.3228	Yes
52.929	0.000055851	353.15	0.6772	0.3228	Yes
55.867	0.000054664	353.15	0.6772	0.3228	Yes
58.805	0.000053611	353.15	0.6772	0.3228	Yes
23.687	0.000110630	353.15	0.4706	0.5294	Yes
26.532	0.000100206	353.15	0.4706	0.5294	Yes
29.459	0.000091934	353.15	0.4706	0.5294	Yes
32.389	0.000085448	353.15	0.4706	0.5294	Yes
35.320	0.000080261	353.15	0.4706	0.5294	Yes
38.254	0.000076039	353.15	0.4706	0.5294	Yes
41.188	0.000072548	353.15	0.4706	0.5294	Yes
44.124	0.000069577	353.15	0.4706	0.5294	Yes
47.030	0.000067088	353.15	0.4706	0.5294	Yes
49.996	0.000064864	353.15	0.4706	0.5294	Yes
52.934	0.000062972	353.15	0.4706	0.5294	Yes
55.871	0.000061291	353.15	0.4706	0.5294	Yes
58.809	0.000059792	353.15	0.4706	0.5294	Yes
23.608	0.000126592	353.15	0.2329	0.7671	Yes
26.531	0.000114283	353.15	0.2329	0.7671	Yes
29.458	0.000105190	353.15	0.2329	0.7671	Yes
32.387	0.000097626	353.15	0.2329	0.7671	Yes
35.318	0.000091453	353.15	0.2329	0.7671	Yes
38.251	0.000086328	353.15	0.2329	0.7671	Yes
41.185	0.000082003	353.15	0.2329	0.7671	Yes
44.121	0.000078377	353.15	0.2329	0.7671	Yes
47.056	0.000075210	353.15	0.2329	0.7671	Yes
49.993	0.000072483	353.15	0.2329	0.7671	Yes
52.930	0.000070070	353.15	0.2329	0.7671	Yes
55.867	0.000067931	353.15	0.2329	0.7671	Yes
55.804	0.000069570	353.15	0.2329	0.7671	Yes

Continued: Data summarised from TABLE 2 of Kosov75 [120]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
5.06625	0.00046508	323.15	0.473	0.527	Yes
10.13250	0.00022219	323.15	0.473	0.527	Yes
20.26500	0.00011109	323.15	0.473	0.527	Yes
30.39750	0.00007994	323.15	0.473	0.527	Yes
40.53000	0.00006671	323.15	0.473	0.527	Yes
50.66250	0.00005914	323.15	0.473	0.527	Yes
5.06625	0.00055557	373.15	0.473	0.527	Yes
10.13250	0.00027779	373.15	0.473	0.527	Yes
20.26500	0.00013829	373.15	0.473	0.527	Yes
30.39750	0.00009770	373.15	0.473	0.527	Yes
40.53000	0.00007962	373.15	0.473	0.527	Yes
50.66250	0.00006916	373.15	0.473	0.527	Yes
5.06625	0.00063787	423.15	0.473	0.527	Yes
10.13250	0.00033328	423.15	0.473	0.527	Yes
20.26500	0.00016889	423.15	0.473	0.527	Yes
30.39750	0.00011639	423.15	0.473	0.527	Yes
40.53000	0.00009302	423.15	0.473	0.527	Yes
50.66250	0.00007955	423.15	0.473	0.527	Yes
5.06625	0.00074626	473.15	0.473	0.527	Yes
10.13250	0.00037878	473.15	0.473	0.527	Yes
20.26500	0.00019489	473.15	0.473	0.527	Yes
30.39750	0.00013589	473.15	0.473	0.527	Yes
40.53000	0.00010809	473.15	0.473	0.527	Yes
50.66250	0.00009200	473.15	0.473	0.527	Yes
5.06625	0.00038757	273.15	0.242	0.758	Yes
10.13250	0.00019208	273.15	0.242	0.758	Yes
20.26500	0.00009666	273.15	0.242	0.758	Yes
30.39750	0.00007183	273.15	0.242	0.758	Yes
40.53000	0.00006135	273.15	0.242	0.758	Yes
50.66250	0.00005507	273.15	0.242	0.758	Yes
5.06625	0.00050246	323.15	0.242	0.758	Yes
10.13250	0.00024838	323.15	0.242	0.758	Yes
20.26500	0.00012719	323.15	0.242	0.758	Yes
30.39750	0.00009061	323.15	0.242	0.758	Yes
40.53000	0.00007428	323.15	0.242	0.758	Yes
50.66250	0.00006514	323.15	0.242	0.758	Yes
5.06625	0.00058815	373.15	0.242	0.758	Yes
10.13250	0.00029938	373.15	0.242	0.758	Yes
20.26500	0.00015309	373.15	0.242	0.758	Yes
30.39750	0.00010889	373.15	0.242	0.758	Yes
40.53000	0.00008759	373.15	0.242	0.758	Yes
50.66250	0.00007512	373.15	0.242	0.758	Yes
5.06625	0.00068484	423.15	0.242	0.758	Yes
10.13250	0.00034717	423.15	0.242	0.758	Yes
20.26500	0.00017919	423.15	0.242	0.758	Yes
30.39750	0.00012529	423.15	0.242	0.758	Yes
40.53000	0.00009999	423.15	0.242	0.758	Yes
50.66250	0.00008524	423.15	0.242	0.758	Yes
5.06625	0.00076334	473.15	0.242	0.758	Yes
10.13250	0.00038607	473.15	0.242	0.758	Yes
20.26500	0.00020258	473.15	0.242	0.758	Yes
30.39750	0.00014269	473.15	0.242	0.758	Yes
40.53000	0.00011349	473.15	0.242	0.758	Yes
50.66250	0.00009582	473.15	0.242	0.758	Yes

Data summarised from Table 1 of Kritschewsky40 [99]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
1.001	0.002420212	303.22	0.9585	0.0415	Yes
2.000	0.001148238	303.22	0.9585	0.0415	Yes
3.001	0.000720991	303.22	0.9585	0.0415	Yes
4.001	0.000506083	303.22	0.9585	0.0415	Yes
5.001	0.000372452	303.22	0.9585	0.0415	Yes
6.000	0.000277912	303.22	0.9585	0.0415	Yes
7.001	0.000203226	303.22	0.9585	0.0415	Yes
8.001	0.000130986	303.22	0.9585	0.0415	Yes
9.001	7.96011E-05	303.22	0.9585	0.0415	Yes
10.002	6.82915E-05	303.22	0.9585	0.0415	Yes
11.001	6.34539E-05	303.22	0.9585	0.0415	Yes
12.001	6.0567E-05	303.22	0.9585	0.0415	Yes
13.001	5.8548E-05	303.22	0.9585	0.0415	Yes
14.002	5.70853E-05	303.22	0.9585	0.0415	Yes
15.004	5.59527E-05	303.22	0.9585	0.0415	Yes
16.001	5.49637E-05	303.22	0.9585	0.0415	Yes
17.003	5.4077E-05	303.22	0.9585	0.0415	Yes
18.001	5.32827E-05	303.22	0.9585	0.0415	Yes
19.005	5.25776E-05	303.22	0.9585	0.0415	Yes
20.001	5.19998E-05	303.22	0.9585	0.0415	Yes
1.001	0.002581656	323.18	0.9585	0.0415	Yes
2.004	0.001240229	323.18	0.9585	0.0415	Yes
3.000	0.000792142	323.18	0.9585	0.0415	Yes
4.001	0.000566985	323.18	0.9585	0.0415	Yes
5.003	0.00043002	323.18	0.9585	0.0415	Yes
6.001	0.000337323	323.18	0.9585	0.0415	Yes
7.001	0.000269247	323.18	0.9585	0.0415	Yes
8.001	0.000216287	323.18	0.9585	0.0415	Yes
9.001	0.000173571	323.18	0.9585	0.0415	Yes
10.001	0.00013857	323.18	0.9585	0.0415	Yes
11.002	0.000111249	323.18	0.9585	0.0415	Yes
12.001	9.27524E-05	323.18	0.9585	0.0415	Yes
13.001	8.14376E-05	323.18	0.9585	0.0415	Yes
14.001	7.43767E-05	323.18	0.9585	0.0415	Yes
15.002	6.99298E-05	323.18	0.9585	0.0415	Yes
16.001	6.67437E-05	323.18	0.9585	0.0415	Yes
17.001	6.43717E-05	323.18	0.9585	0.0415	Yes
18.003	6.24861E-05	323.18	0.9585	0.0415	Yes
19.002	6.08938E-05	323.18	0.9585	0.0415	Yes
20.001	5.95281E-05	323.18	0.9585	0.0415	Yes
1.003	0.002851711	343.15	0.9585	0.0415	Yes
2.001	0.001344896	343.15	0.9585	0.0415	Yes
3.001	0.000864844	343.15	0.9585	0.0415	Yes
4.002	0.000632604	343.15	0.9585	0.0415	Yes
5.003	0.000485235	343.15	0.9585	0.0415	Yes
6.002	0.000387052	343.15	0.9585	0.0415	Yes
7.000	0.000317414	343.15	0.9585	0.0415	Yes
8.001	0.000264773	343.15	0.9585	0.0415	Yes
9.000	0.000223721	343.15	0.9585	0.0415	Yes

Data summarised from Table 4 and 5 of Mantovani12 [109]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
10.001	0.000190758	343.15	0.9585	0.0415	Yes
11.002	0.000163891	343.15	0.9585	0.0415	Yes
12.000	0.000142002	343.15	0.9585	0.0415	Yes
13.000	0.00012429	343.15	0.9585	0.0415	Yes
14.000	0.000110295	343.15	0.9585	0.0415	Yes
15.001	9.94288E-05	343.15	0.9585	0.0415	Yes
16.001	9.11185E-05	343.15	0.9585	0.0415	Yes
17.003	8.48375E-05	343.15	0.9585	0.0415	Yes
18.001	7.9986E-05	343.15	0.9585	0.0415	Yes
19.002	7.61231E-05	343.15	0.9585	0.0415	Yes
20.004	7.30075E-05	343.15	0.9585	0.0415	Yes
1.002	0.003089522	363.15	0.9585	0.0415	Yes
2.002	0.001426324	363.15	0.9585	0.0415	Yes
3.000	0.000930771	363.15	0.9585	0.0415	Yes
4.002	0.000680151	363.15	0.9585	0.0415	Yes
5.001	0.000529708	363.15	0.9585	0.0415	Yes
6.001	0.00042832	363.15	0.9585	0.0415	Yes
7.002	0.000356464	363.15	0.9585	0.0415	Yes
8.005	0.000302105	363.15	0.9585	0.0415	Yes
9.003	0.000260118	363.15	0.9585	0.0415	Yes
10.001	0.000226492	363.15	0.9585	0.0415	Yes
11.002	0.00019899	363.15	0.9585	0.0415	Yes
12.002	0.000176304	363.15	0.9585	0.0415	Yes
13.001	0.000157582	363.15	0.9585	0.0415	Yes
14.000	0.000141881	363.15	0.9585	0.0415	Yes
15.001	0.000128795	363.15	0.9585	0.0415	Yes
16.002	0.000117907	363.15	0.9585	0.0415	Yes
17.001	0.000108959	363.15	0.9585	0.0415	Yes
18.001	0.000101527	363.15	0.9585	0.0415	Yes
19.001	9.5354E-05	363.15	0.9585	0.0415	Yes
20.002	9.01445E-05	363.15	0.9585	0.0415	Yes
1.002	0.003313914	383.14	0.9585	0.0415	Yes
2.001	0.001573358	383.14	0.9585	0.0415	Yes
3.000	0.001013942	383.14	0.9585	0.0415	Yes
4.003	0.000739693	383.14	0.9585	0.0415	Yes
5.003	0.000578332	383.14	0.9585	0.0415	Yes
6.000	0.000470641	383.14	0.9585	0.0415	Yes
7.003	0.00039427	383.14	0.9585	0.0415	Yes
8.001	0.000337087	383.14	0.9585	0.0415	Yes
9.002	0.000292562	383.14	0.9585	0.0415	Yes
10.001	0.000257216	383.14	0.9585	0.0415	Yes
11.002	0.000228197	383.14	0.9585	0.0415	Yes
12.002	0.000204347	383.14	0.9585	0.0415	Yes
13.002	0.000184585	383.14	0.9585	0.0415	Yes
14.002	0.000167767	383.14	0.9585	0.0415	Yes
15.002	0.000153524	383.14	0.9585	0.0415	Yes
16.001	0.000141349	383.14	0.9585	0.0415	Yes
17.001	0.000130947	383.14	0.9585	0.0415	Yes
1.000	0.002436487	303.22	0.9021	0.0979	Yes
2.000	0.001159028	303.22	0.9021	0.0979	Yes
3.001	0.000731282	303.22	0.9021	0.0979	Yes
4.001	0.000516849	303.22	0.9021	0.0979	Yes
5.000	0.00038543	303.22	0.9021	0.0979	Yes
6.002	0.000294747	303.22	0.9021	0.0979	Yes
7.000	0.000226789	303.22	0.9021	0.0979	Yes
8.001	0.000170621	303.22	0.9021	0.0979	Yes
9.000	0.000124126	303.22	0.9021	0.0979	Yes
10.003	9.35046E-05	303.22	0.9021	0.0979	Yes
11.002	7.84076E-05	303.22	0.9021	0.0979	Yes
12.003	7.08078E-05	303.22	0.9021	0.0979	Yes
13.000	6.62922E-05	303.22	0.9021	0.0979	Yes
14.002	6.32137E-05	303.22	0.9021	0.0979	Yes
15.002	6.10655E-05	303.22	0.9021	0.0979	Yes
16.001	5.93584E-05	303.22	0.9021	0.0979	Yes
17.005	5.79846E-05	303.22	0.9021	0.0979	Yes
18.001	5.67542E-05	303.22	0.9021	0.0979	Yes
19.003	5.57185E-05	303.22	0.9021	0.0979	Yes
20.001	5.48757E-05	303.22	0.9021	0.0979	Yes
1.002	0.002628087	323.18	0.9021	0.0979	Yes
2.000	0.001264331	323.18	0.9021	0.0979	Yes
3.003	0.000805687	323.18	0.9021	0.0979	Yes
4.001	0.000578882	323.18	0.9021	0.0979	Yes
5.001	0.000442813	323.18	0.9021	0.0979	Yes
6.000	0.000350658	323.18	0.9021	0.0979	Yes
7.002	0.000283543	323.18	0.9021	0.0979	Yes
8.001	0.000232682	323.18	0.9021	0.0979	Yes
9.000	0.000192322	323.18	0.9021	0.0979	Yes
10.001	0.000159911	323.18	0.9021	0.0979	Yes
11.002	0.000134175	323.18	0.9021	0.0979	Yes
12.001	0.000114169	323.18	0.9021	0.0979	Yes
13.000	9.96048E-05	323.18	0.9021	0.0979	Yes
14.002	8.91728E-05	323.18	0.9021	0.0979	Yes
15.001	8.17559E-05	323.18	0.9021	0.0979	Yes
16.000	7.65425E-05	323.18	0.9021	0.0979	Yes
17.001	7.26413E-05	323.18	0.9021	0.0979	Yes
18.000	6.95763E-05	323.18	0.9021	0.0979	Yes
19.001	6.70738E-05	323.18	0.9021	0.0979	Yes
20.001	6.50008E-05	323.18	0.9021	0.0979	Yes

Continued: Data summarised from Table 4 and 5 of Mantovani12 [109]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
1.001	0.002970161	343.15	0.9021	0.0979	Yes
2.003	0.001383429	343.15	0.9021	0.0979	Yes
3.001	0.000892422	343.15	0.9021	0.0979	Yes
4.001	0.000641821	343.15	0.9021	0.0979	Yes
5.003	0.000493702	343.15	0.9021	0.0979	Yes
6.003	0.000396188	343.15	0.9021	0.0979	Yes
7.003	0.00032659	343.15	0.9021	0.0979	Yes
8.001	0.00027484	343.15	0.9021	0.0979	Yes
9.002	0.000234236	343.15	0.9021	0.0979	Yes
10.000	0.000201987	343.15	0.9021	0.0979	Yes
11.001	0.000175721	343.15	0.9021	0.0979	Yes
12.002	0.000154206	343.15	0.9021	0.0979	Yes
13.001	0.000136668	343.15	0.9021	0.0979	Yes
14.001	0.000122397	343.15	0.9021	0.0979	Yes
15.001	0.000110894	343.15	0.9021	0.0979	Yes
16.000	0.00010163	343.15	0.9021	0.0979	Yes
17.002	9.43044E-05	343.15	0.9021	0.0979	Yes
18.002	8.84113E-05	343.15	0.9021	0.0979	Yes
19.001	8.35965E-05	343.15	0.9021	0.0979	Yes
20.002	7.96719E-05	343.15	0.9021	0.0979	Yes
1.001	0.003160357	363.15	0.9021	0.0979	Yes
2.001	0.0014856	363.15	0.9021	0.0979	Yes
3.000	0.000958528	363.15	0.9021	0.0979	Yes
4.003	0.000686013	363.15	0.9021	0.0979	Yes
5.003	0.00053631	363.15	0.9021	0.0979	Yes
6.001	0.000435051	363.15	0.9021	0.0979	Yes
7.001	0.000363045	363.15	0.9021	0.0979	Yes
8.004	0.000309423	363.15	0.9021	0.0979	Yes
9.002	0.000267732	363.15	0.9021	0.0979	Yes
10.001	0.000234301	363.15	0.9021	0.0979	Yes
11.001	0.000207173	363.15	0.9021	0.0979	Yes
12.000	0.000184794	363.15	0.9021	0.0979	Yes
13.002	0.0001661	363.15	0.9021	0.0979	Yes
14.000	0.000150488	363.15	0.9021	0.0979	Yes
15.001	0.000137358	363.15	0.9021	0.0979	Yes
16.001	0.000126309	363.15	0.9021	0.0979	Yes
17.003	0.000117002	363.15	0.9021	0.0979	Yes
18.000	0.000109199	363.15	0.9021	0.0979	Yes
19.001	0.000102622	363.15	0.9021	0.0979	Yes
20.001	9.68988E-05	363.15	0.9021	0.0979	Yes
1.000	0.003400929	383.14	0.9021	0.0979	Yes
2.003	0.00159084	383.14	0.9021	0.0979	Yes
3.001	0.001022737	383.14	0.9021	0.0979	Yes
4.001	0.000746064	383.14	0.9021	0.0979	Yes
5.002	0.000584542	383.14	0.9021	0.0979	Yes
6.001	0.000477055	383.14	0.9021	0.0979	Yes
7.000	0.000400411	383.14	0.9021	0.0979	Yes
8.003	0.000343145	383.14	0.9021	0.0979	Yes
9.001	0.000298835	383.14	0.9021	0.0979	Yes
10.000	0.00026333	383.14	0.9021	0.0979	Yes
11.001	0.000234625	383.14	0.9021	0.0979	Yes
12.002	0.000210942	383.14	0.9021	0.0979	Yes
13.000	0.000191179	383.14	0.9021	0.0979	Yes
14.002	0.000174414	383.14	0.9021	0.0979	Yes
15.001	0.000160189	383.14	0.9021	0.0979	Yes
16.001	0.000148026	383.14	0.9021	0.0979	Yes
17.001	0.00013746	383.14	0.9021	0.0979	Yes
18.001	0.000128318	383.14	0.9021	0.0979	Yes
19.002	0.000120524	383.14	0.9021	0.0979	Yes
20.002	0.000113775	383.14	0.9021	0.0979	Yes

Continued: Data summarised from Table 4 and 5 of Mantovani12 [109]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
19.86622	9.78254E-05	250.044	0.10	0.90	Yes
18.04077	0.000106271	250.044	0.10	0.90	Yes
16.02422	0.000118332	250.044	0.10	0.90	Yes
14.01532	0.000134471	250.044	0.10	0.90	Yes
12.01104	0.000156813	250.045	0.10	0.90	Yes
10.00715	0.000189166	250.046	0.10	0.90	Yes
8.00002	0.000239157	250.047	0.10	0.90	Yes
5.99883	0.000323925	250.048	0.10	0.90	Yes
3.99732	0.000495706	250.047	0.10	0.90	Yes
1.98511	0.001021034	250.046	0.10	0.90	Yes
19.84087	0.000112825	275.019	0.10	0.90	Yes
18.05655	0.000122635	275.019	0.10	0.90	Yes
16.02186	0.000136874	275.018	0.10	0.90	Yes
14.01343	0.000155488	275.016	0.10	0.90	Yes
12.00866	0.000180904	275.017	0.10	0.90	Yes
10.00450	0.000217257	275.016	0.10	0.90	Yes
7.99787	0.000272891	275.012	0.10	0.90	Yes
6.00199	0.000366347	275.009	0.10	0.90	Yes
3.99710	0.000555785	275.019	0.10	0.90	Yes

Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
19.16513	0.000130961	299.963	0.10	0.90	Yes
17.86924	0.000139509	299.966	0.10	0.90	Yes
16.01378	0.000154356	299.967	0.10	0.90	Yes
14.00977	0.000175181	299.966	0.10	0.90	Yes
12.00591	0.000203435	299.966	0.10	0.90	Yes
10.00204	0.000243597	299.967	0.10	0.90	Yes
7.99970	0.000304586	299.967	0.10	0.90	Yes
5.99638	0.000407335	299.967	0.10	0.90	Yes
3.99646	0.000614061	299.968	0.10	0.90	Yes
1.99790	0.001236584	299.967	0.10	0.90	Yes
19.62110	0.00014211	324.979	0.10	0.90	Yes
18.00085	0.000153587	324.980	0.10	0.90	Yes
16.00130	0.000171185	324.979	0.10	0.90	Yes
13.98251	0.000194374	324.979	0.10	0.90	Yes
11.99919	0.000225128	324.979	0.10	0.90	Yes
9.99890	0.000268969	324.978	0.10	0.90	Yes
8.01923	0.000334497	324.978	0.10	0.90	Yes
5.99183	0.000447274	324.978	0.10	0.90	Yes
3.99616	0.000671261	324.978	0.10	0.90	Yes
1.99599	0.001347195	324.980	0.10	0.90	Yes
19.37788	0.000157217	349.967	0.10	0.90	Yes
17.99350	0.000168117	349.967	0.10	0.90	Yes
15.99987	0.000187305	349.966	0.10	0.90	Yes
13.99498	0.000212372	349.966	0.10	0.90	Yes
11.99755	0.000245985	349.966	0.10	0.90	Yes
9.99755	0.000293482	349.966	0.10	0.90	Yes
7.99575	0.000365326	349.966	0.10	0.90	Yes
5.99670	0.000485585	349.965	0.10	0.90	Yes
3.99656	0.000727358	349.964	0.10	0.90	Yes
1.99606	0.001455752	349.964	0.10	0.90	Yes
18.71878	0.000175779	374.975	0.10	0.90	Yes
17.96004	0.000182511	374.975	0.10	0.90	Yes
15.96599	0.000203384	374.974	0.10	0.90	Yes
13.97204	0.000230421	374.974	0.10	0.90	Yes
11.98120	0.000266651	374.974	0.10	0.90	Yes
9.98248	0.000317881	374.973	0.10	0.90	Yes
7.98995	0.00039489	374.973	0.10	0.90	Yes
5.99454	0.000523904	374.973	0.10	0.90	Yes
3.96223	0.000789726	374.970	0.10	0.90	Yes
1.97464	0.001580633	374.969	0.10	0.90	Yes
18.90806	0.000187244	400.038	0.10	0.90	Yes
17.81457	0.000197669	400.037	0.10	0.90	Yes
15.98414	0.000218408	400.035	0.10	0.90	Yes
13.99217	0.000247317	400.036	0.10	0.90	Yes
11.98674	0.000286355	400.035	0.10	0.90	Yes
9.99291	0.000340956	400.034	0.10	0.90	Yes
7.98095	0.000424103	400.035	0.10	0.90	Yes
5.99205	0.000561646	400.036	0.10	0.90	Yes
3.99487	0.000838311	400.034	0.10	0.90	Yes
1.99589	0.001670805	400.037	0.10	0.90	Yes
19.99666	9.32179E-05	250.059	0.15	0.85	Yes
18.01935	0.000101924	250.063	0.15	0.85	Yes
16.01636	0.000113523	250.064	0.15	0.85	Yes
14.01375	0.000129235	250.066	0.15	0.85	Yes
12.00577	0.000151284	250.066	0.15	0.85	Yes
10.00316	0.000183374	250.066	0.15	0.85	Yes
7.99621	0.000233229	250.064	0.15	0.85	Yes
5.98407	0.000318626	250.064	0.15	0.85	Yes
3.98271	0.000491443	250.061	0.15	0.85	Yes
1.94406	0.001036575	250.061	0.15	0.85	Yes
19.98318	0.000108524	275.028	0.15	0.85	Yes
17.99374	0.000119165	275.027	0.15	0.85	Yes
15.98143	0.00013309	275.027	0.15	0.85	Yes
14.00115	0.000151278	275.026	0.15	0.85	Yes
12.00000	0.000176479	275.026	0.15	0.85	Yes
9.99554	0.000212729	275.026	0.15	0.85	Yes
7.99430	0.000268154	275.025	0.15	0.85	Yes
5.99802	0.000361645	275.022	0.15	0.85	Yes
4.00063	0.000550357	275.019	0.15	0.85	Yes
1.98846	0.00112663	275.019	0.15	0.85	Yes
19.97735	0.000123058	299.963	0.15	0.85	Yes
17.99426	0.000135285	299.965	0.15	0.85	Yes
15.96936	0.000151242	299.968	0.15	0.85	Yes
13.99130	0.000171721	299.967	0.15	0.85	Yes
12.00779	0.000199568	299.968	0.15	0.85	Yes
10.00322	0.000239598	299.966	0.15	0.85	Yes
8.00779	0.000300197	299.966	0.15	0.85	Yes
5.99919	0.000402958	299.966	0.15	0.85	Yes
3.98234	0.00061197	299.967	0.15	0.85	Yes
1.99212	0.001235426	299.969	0.15	0.85	Yes
19.97825	0.000137045	324.980	0.15	0.85	Yes
18.01598	0.000150539	324.980	0.15	0.85	Yes
16.00631	0.000168073	324.981	0.15	0.85	Yes
14.01385	0.000190772	324.981	0.15	0.85	Yes
11.99115	0.000221968	324.981	0.15	0.85	Yes
9.99694	0.000265601	324.981	0.15	0.85	Yes
19.98296	0.000150419	349.967	0.15	0.85	Yes

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
18.00779	0.00016536	349.967	0.15	0.85	Yes
16.00783	0.00018448	349.967	0.15	0.85	Yes
14.00355	0.000209405	349.967	0.15	0.85	Yes
11.99797	0.000243033	349.967	0.15	0.85	Yes
9.99946	0.000290382	349.967	0.15	0.85	Yes
7.99535	0.000362201	349.967	0.15	0.85	Yes
5.99688	0.000482323	349.967	0.15	0.85	Yes
3.99534	0.000724168	349.967	0.15	0.85	Yes
1.99594	0.001451759	349.967	0.15	0.85	Yes
19.97235	0.00016352	374.956	0.15	0.85	Yes
17.99229	0.000179833	374.956	0.15	0.85	Yes
15.99852	0.000200533	374.956	0.15	0.85	Yes
13.98957	0.000227594	374.956	0.15	0.85	Yes
11.94535	0.000264776	374.955	0.15	0.85	Yes
9.98626	0.000315041	374.954	0.15	0.85	Yes
7.99726	0.000391745	374.954	0.15	0.85	Yes
5.99557	0.000520915	374.954	0.15	0.85	Yes
3.95365	0.000788416	374.953	0.15	0.85	Yes
1.96362	0.001586167	374.955	0.15	0.85	Yes
17.81821	0.000195515	400.023	0.15	0.85	Yes
15.97720	0.000216313	400.022	0.15	0.85	Yes
13.98802	0.000245135	400.022	0.15	0.85	Yes
11.98638	0.000284033	400.020	0.15	0.85	Yes
9.99083	0.000338626	400.020	0.15	0.85	Yes
7.99123	0.00042108	400.021	0.15	0.85	Yes
5.99535	0.000558761	400.019	0.15	0.85	Yes
3.99567	0.000835508	400.020	0.15	0.85	Yes
1.99535	0.00166877	400.019	0.15	0.85	Yes
19.63290	9.02991E-05	250.020	0.20	0.80	Yes
18.03870	9.70916E-05	250.020	0.20	0.80	Yes
17.63930	9.90853E-05	250.047	0.20	0.80	Yes
17.01160	0.000102396	250.046	0.20	0.80	Yes
16.02670	0.000108223	250.019	0.20	0.80	Yes
15.00850	0.000115374	250.047	0.20	0.80	Yes
14.01750	0.000123486	250.020	0.20	0.80	Yes
13.00490	0.000133454	250.046	0.20	0.80	Yes
12.01020	0.000145095	250.020	0.20	0.80	Yes
11.00090	0.000159536	250.049	0.20	0.80	Yes
10.00410	0.000176926	250.020	0.20	0.80	Yes
8.99881	0.000198925	250.046	0.20	0.80	Yes
8.00094	0.000226512	250.020	0.20	0.80	Yes
6.99772	0.000262783	250.048	0.20	0.80	Yes
6.01320	0.000310414	250.019	0.20	0.80	Yes
4.99748	0.000379943	250.044	0.20	0.80	Yes
4.03244	0.000478652	250.018	0.20	0.80	Yes
2.99627	0.000656238	250.044	0.20	0.80	Yes
1.97928	0.001012424	250.018	0.20	0.80	Yes
0.99791	0.002044948	250.046	0.20	0.80	Yes
0.99448	0.00205194	250.015	0.20	0.80	Yes
0.48824	0.004219278	250.046	0.20	0.80	Yes
19.42970	0.000107292	274.985	0.20	0.80	Yes
18.04310	0.000114724	274.986	0.20	0.80	Yes
16.00910	0.00012843	274.988	0.20	0.80	Yes
14.00570	0.000146519	274.989	0.20	0.80	Yes
12.00480	0.000171468	274.989	0.20	0.80	Yes
10.00030	0.000207508	274.991	0.20	0.80	Yes
7.99888	0.000262772	274.990	0.20	0.80	Yes
5.99721	0.000356429	274.991	0.20	0.80	Yes
3.99564	0.00054582	274.991	0.20	0.80	Yes
1.98781	0.0011225	274.989	0.20	0.80	Yes
0.99823	0.002261594	274.987	0.20	0.80	Yes
18.15090	0.000130668	299.954	0.20	0.80	Yes
17.07680	0.000138373	299.953	0.20	0.80	Yes
15.00170	0.000156717	299.951	0.20	0.80	Yes
13.03690	0.000180028	299.951	0.20	0.80	Yes
11.03220	0.000213038	299.950	0.20	0.80	Yes
8.99761	0.000262476	299.951	0.20	0.80	Yes
6.99712	0.000340141	299.951	0.20	0.80	Yes
4.99627	0.000481391	299.951	0.20	0.80	Yes
2.99620	0.000813057	299.953	0.20	0.80	Yes
0.98474	0.002512276	299.956	0.20	0.80	Yes
0.49288	0.005039561	299.957	0.20	0.80	Yes
19.96380	0.000134216	324.963	0.20	0.80	Yes
18.00200	0.000147592	324.962	0.20	0.80	Yes
16.00360	0.000164915	324.962	0.20	0.80	Yes
14.00150	0.000187624	324.961	0.20	0.80	Yes
12.00130	0.000218368	324.961	0.20	0.80	Yes
9.99931	0.000262035	324.960	0.20	0.80	Yes
7.99747	0.000328312	324.959	0.20	0.80	Yes
5.99710	0.000439664	324.960	0.20	0.80	Yes
3.97658	0.000667237	324.960	0.20	0.80	Yes
1.99409	0.0013415	324.960	0.20	0.80	Yes
1.99404	0.0013415	324.959	0.20	0.80	Yes
19.82050	0.000148952	349.948	0.20	0.80	Yes
17.99340	0.000162811	349.948	0.20	0.80	Yes
15.99920	0.000181802	349.948	0.20	0.80	Yes
13.99520	0.000206663	349.948	0.20	0.80	Yes
11.99640	0.000240121	349.948	0.20	0.80	Yes
9.97881	0.000287966	349.948	0.20	0.80	Yes
7.99624	0.000359107	349.949	0.20	0.80	Yes

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
5.99652	0.000479291	349.947	0.20	0.80	Yes
3.99594	0.000721068	349.948	0.20	0.80	Yes
1.99547	0.001450077	349.949	0.20	0.80	Yes
19.90270	0.000161719	374.942	0.20	0.80	Yes
17.84660	0.000178778	374.941	0.20	0.80	Yes
16.02340	0.000197761	374.942	0.20	0.80	Yes
13.98810	0.000225057	374.940	0.20	0.80	Yes
11.99000	0.000261196	374.941	0.20	0.80	Yes
9.99297	0.000312141	374.942	0.20	0.80	Yes
7.99534	0.00038907	374.941	0.20	0.80	Yes
5.99514	0.000518129	374.941	0.20	0.80	Yes
3.99570	0.000777238	374.940	0.20	0.80	Yes
1.99240	0.00156089	374.941	0.20	0.80	Yes
0.98192	0.003170137	374.940	0.20	0.80	Yes
19.97900	0.000174041	400.011	0.20	0.80	Yes
17.97910	0.000191741	400.012	0.20	0.80	Yes
15.98120	0.00021403	400.011	0.20	0.80	Yes
13.98660	0.000242857	400.012	0.20	0.80	Yes
11.98990	0.00028159	400.012	0.20	0.80	Yes
9.99056	0.00033622	400.012	0.20	0.80	Yes
7.99379	0.000418499	400.012	0.20	0.80	Yes
5.99466	0.000556358	400.012	0.20	0.80	Yes
3.99403	0.000833333	400.012	0.20	0.80	Yes
1.97816	0.001680668	400.010	0.20	0.80	Yes
0.99668	0.003335827	400.008	0.20	0.80	Yes
17.56300	8.44439E-05	275.039	0.50	0.50	Yes
17.02700	8.68477E-05	275.037	0.50	0.50	Yes
15.92570	9.26169E-05	275.029	0.50	0.50	Yes
15.03210	9.83165E-05	275.027	0.50	0.50	Yes
14.03160	0.000106097	275.027	0.50	0.50	Yes
13.02530	0.000115819	275.025	0.50	0.50	Yes
12.02510	0.000127903	275.025	0.50	0.50	Yes
11.01830	0.000143168	275.024	0.50	0.50	Yes
10.02880	0.000162084	275.023	0.50	0.50	Yes
9.12550	0.000183649	275.023	0.50	0.50	Yes
8.00600	0.000217945	275.023	0.50	0.50	Yes
7.00335	0.000258548	275.023	0.50	0.50	Yes
5.99952	0.000313185	275.023	0.50	0.50	Yes
4.99873	0.000389672	275.023	0.50	0.50	Yes
3.99739	0.000504525	275.024	0.50	0.50	Yes
2.99662	0.000695792	275.024	0.50	0.50	Yes
1.99331	0.001080635	275.023	0.50	0.50	Yes
0.99658	0.002228066	275.023	0.50	0.50	Yes
19.96960	9.34696E-05	299.971	0.50	0.50	Yes
19.02040	9.78291E-05	299.969	0.50	0.50	Yes
17.99720	0.000103247	299.969	0.50	0.50	Yes
16.99580	0.00010944	299.971	0.50	0.50	Yes
15.99850	0.000116666	299.965	0.50	0.50	Yes
14.99570	0.00012524	299.968	0.50	0.50	Yes
13.99620	0.000135376	299.968	0.50	0.50	Yes
12.99820	0.000147456	299.966	0.50	0.50	Yes
11.99480	0.00016205	299.968	0.50	0.50	Yes
10.99650	0.000179629	299.969	0.50	0.50	Yes
9.99650	0.000201219	299.973	0.50	0.50	Yes
9.99330	0.00020121	299.973	0.50	0.50	Yes
9.01433	0.000227481	299.970	0.50	0.50	Yes
8.00905	0.000261435	299.969	0.50	0.50	Yes
7.00490	0.000305428	299.969	0.50	0.50	Yes
6.02374	0.000362945	299.966	0.50	0.50	Yes
5.01581	0.000445751	299.967	0.50	0.50	Yes
4.00017	0.000571651	299.966	0.50	0.50	Yes
2.99882	0.000779522	299.966	0.50	0.50	Yes
1.99512	0.001197898	299.966	0.50	0.50	Yes
0.99587	0.002451995	299.964	0.50	0.50	Yes
19.43570	0.000114163	324.980	0.50	0.50	Yes
19.02310	0.000116608	324.980	0.50	0.50	Yes
18.01810	0.000123152	324.980	0.50	0.50	Yes
17.01240	0.000130659	324.980	0.50	0.50	Yes
16.01750	0.000139218	324.981	0.50	0.50	Yes
14.99080	0.000149467	324.981	0.50	0.50	Yes
14.01090	0.000160884	324.981	0.50	0.50	Yes
13.00840	0.000174594	324.982	0.50	0.50	Yes
12.00510	0.00019087	324.981	0.50	0.50	Yes
11.00120	0.000210385	324.980	0.50	0.50	Yes
10.00360	0.000233971	324.980	0.50	0.50	Yes
9.00191	0.000263181	324.981	0.50	0.50	Yes
7.99825	0.000300078	324.981	0.50	0.50	Yes
6.99807	0.000347644	324.981	0.50	0.50	Yes
5.99509	0.000411613	324.982	0.50	0.50	Yes
4.99725	0.00050103	324.982	0.50	0.50	Yes
3.99531	0.000636051	324.982	0.50	0.50	Yes
2.99643	0.000860865	324.983	0.50	0.50	Yes
1.99147	0.001315818	324.984	0.50	0.50	Yes
0.97407	0.002732999	324.983	0.50	0.50	Yes

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
19.97710	0.000127896	349.961	0.50	0.50	Yes
18.99730	0.000134393	349.962	0.50	0.50	Yes
17.99570	0.000141889	349.961	0.50	0.50	Yes
16.99630	0.000150384	349.961	0.50	0.50	Yes
15.99460	0.00016011	349.962	0.50	0.50	Yes
14.99750	0.00017124	349.962	0.50	0.50	Yes
14.00010	0.000184126	349.961	0.50	0.50	Yes
12.99820	0.000199235	349.961	0.50	0.50	Yes
11.99720	0.000217044	349.962	0.50	0.50	Yes
10.99770	0.000238232	349.961	0.50	0.50	Yes
9.99633	0.000263962	349.961	0.50	0.50	Yes
9.99633	0.000263962	349.961	0.50	0.50	Yes
8.99622	0.000295576	349.960	0.50	0.50	Yes
7.99547	0.000335354	349.960	0.50	0.50	Yes
6.99592	0.000386668	349.961	0.50	0.50	Yes
5.99622	0.000455396	349.961	0.50	0.50	Yes
4.99593	0.000551962	349.962	0.50	0.50	Yes
3.99702	0.000696963	349.962	0.50	0.50	Yes
2.99638	0.000939571	349.961	0.50	0.50	Yes
1.98830	0.001431695	349.962	0.50	0.50	Yes
0.98348	0.002926928	349.962	0.50	0.50	Yes
19.94080	0.000143787	374.953	0.50	0.50	Yes
19.11920	0.000149821	374.951	0.50	0.50	Yes
17.98780	0.000159158	374.953	0.50	0.50	Yes
16.99010	0.000168525	374.953	0.50	0.50	Yes
15.98960	0.000179206	374.953	0.50	0.50	Yes
14.99370	0.000191367	374.953	0.50	0.50	Yes
13.99470	0.000205437	374.954	0.50	0.50	Yes
12.99150	0.000221881	374.954	0.50	0.50	Yes
11.99250	0.000241136	374.953	0.50	0.50	Yes
10.99520	0.000263972	374.954	0.50	0.50	Yes
9.99586	0.000291647	374.953	0.50	0.50	Yes
9.99586	0.000291647	374.953	0.50	0.50	Yes
8.96527	0.000326811	374.953	0.50	0.50	Yes
8.05362	0.000365587	374.954	0.50	0.50	Yes
6.99503	0.000423493	374.952	0.50	0.50	Yes
5.99458	0.000497273	374.953	0.50	0.50	Yes
4.99326	0.000600988	374.952	0.50	0.50	Yes
3.99475	0.000756465	374.952	0.50	0.50	Yes
2.99568	0.001016112	374.953	0.50	0.50	Yes
1.98785	0.001543572	374.951	0.50	0.50	Yes
0.98706	0.003133484	374.954	0.50	0.50	Yes
19.96030	0.000158532	400.020	0.50	0.50	Yes
18.98310	0.000166446	400.018	0.50	0.50	Yes
17.96470	0.000175684	400.020	0.50	0.50	Yes
16.98380	0.00018572	400.018	0.50	0.50	Yes
15.98500	0.000197287	400.018	0.50	0.50	Yes
14.98390	0.000210523	400.019	0.50	0.50	Yes
13.98590	0.000225704	400.018	0.50	0.50	Yes
12.98370	0.000243403	400.019	0.50	0.50	Yes
11.98640	0.000264082	400.018	0.50	0.50	Yes
10.98740	0.000288655	400.019	0.50	0.50	Yes
9.97978	0.000318622	400.019	0.50	0.50	Yes
9.97978	0.000318622	400.019	0.50	0.50	Yes
8.99459	0.00035453	400.017	0.50	0.50	Yes
7.99241	0.000400307	400.018	0.50	0.50	Yes
6.99141	0.000459282	400.019	0.50	0.50	Yes
5.99420	0.000537864	400.020	0.50	0.50	Yes
4.99316	0.000648513	400.020	0.50	0.50	Yes
3.98088	0.000817332	400.019	0.50	0.50	Yes
2.99564	0.001091477	400.018	0.50	0.50	Yes
1.98761	0.001654339	400.019	0.50	0.50	Yes
0.97589	0.003388858	400.018	0.50	0.50	Yes

Continued: Data summarised from Appendix A.1., A.2., A.3., and A.4. of Mondejar12 [105]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{N_2}	Usable Data Point?
19.94	0.00028586	673.15	0.9	0.1	Yes
29.94	0.00019486	673.15	0.9	0.1	Yes
39.94	0.00015053	673.15	0.9	0.1	Yes
79.93	0.00008816	673.15	0.9	0.1	Yes
19.94	0.00028796	673.15	0.8	0.2	Yes
29.94	0.00019706	673.15	0.8	0.2	Yes
39.94	0.00015290	673.15	0.8	0.2	Yes
59.93	0.00010985	673.15	0.8	0.2	Yes
79.93	0.00008948	673.15	0.8	0.2	Yes
99.93	0.00007760	673.15	0.8	0.2	Yes
19.94	0.00029161	673.15	0.7	0.3	Yes
29.94	0.00019967	673.15	0.7	0.3	Yes
39.94	0.00015471	673.15	0.7	0.3	Yes
59.93	0.00011156	673.15	0.7	0.3	Yes
79.93	0.00009073	673.15	0.7	0.3	Yes
99.93	0.00007862	673.15	0.7	0.3	Yes
19.94	0.00029426	673.15	0.6	0.4	Yes
29.94	0.00020190	673.15	0.6	0.4	Yes
39.94	0.00015677	673.15	0.6	0.4	Yes
59.93	0.00011306	673.15	0.6	0.4	Yes
79.93	0.00009197	673.15	0.6	0.4	Yes
99.93	0.00007953	673.15	0.6	0.4	Yes
19.94	0.00029657	673.15	0.5	0.5	Yes
29.94	0.00020376	673.15	0.5	0.5	Yes
39.94	0.00015852	673.15	0.5	0.5	Yes
59.93	0.00011451	673.15	0.5	0.5	Yes
79.93	0.00009310	673.15	0.5	0.5	Yes
99.93	0.00008047	673.15	0.5	0.5	Yes
19.94	0.00029940	673.15	0.4	0.6	Yes
29.94	0.00020592	673.15	0.4	0.6	Yes
39.94	0.00016034	673.15	0.4	0.6	Yes
59.93	0.00011598	673.15	0.4	0.6	Yes
79.93	0.00009416	673.15	0.4	0.6	Yes
99.93	0.00008130	673.15	0.4	0.6	Yes
19.94	0.00030134	673.15	0.3	0.7	Yes
29.94	0.00020768	673.15	0.3	0.7	Yes
39.94	0.00016214	673.15	0.3	0.7	Yes
59.93	0.00011724	673.15	0.3	0.7	Yes
79.93	0.00009520	673.15	0.3	0.7	Yes
99.93	0.00008204	673.15	0.3	0.7	Yes
19.94	0.00030325	673.15	0.2	0.8	Yes
29.94	0.00020911	673.15	0.2	0.8	Yes
39.94	0.00016343	673.15	0.2	0.8	Yes
59.93	0.00011837	673.15	0.2	0.8	Yes
79.93	0.00009609	673.15	0.2	0.8	Yes
99.93	0.00008274	673.15	0.2	0.8	Yes
19.94	0.00030523	673.15	0.1	0.9	Yes
29.94	0.00021085	673.15	0.1	0.9	Yes
59.93	0.00011940	673.15	0.1	0.9	Yes
79.93	0.00009701	673.15	0.1	0.9	Yes
99.93	0.00008333	673.15	0.1	0.9	Yes

Data summarised from TABLE 3 of Seitz96 [81]

7.1.3 Carbon Dioxide–Hydrogen VLE Data

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{H_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{H_2}}$	Usable Data Point?
4.805	7.29286E-05	—	278.15	0.9912	0.0088	0.8861	0.1139	Vol. Est.
5.864	7.06064E-05	—	278.15	0.9798	0.0202	0.8158	0.1842	Vol. Est.
6.933	7.16311E-05	—	278.15	0.9751	0.0249	0.7467	0.2533	Vol. Est.
7.722	8.58936E-05	—	278.15	0.971	0.029	0.7211	0.2789	Vol. Est.
8.671	8.08698E-05	—	278.15	0.9555	0.0445	0.6963	0.3037	Vol. Est.
9.961	7.8573E-05	—	278.15	0.9386	0.0614	0.6589	0.3411	Vol. Est.
10.86	7.56868E-05	—	278.15	0.9339	0.0661	0.6419	0.3581	Vol. Est.
11.4	7.74803E-05	—	278.15	0.9282	0.0718	0.6238	0.3762	Vol. Est.
11.77	7.48026E-05	—	278.15	0.9251	0.0749	0.6182	0.3818	Vol. Est.
12.6	7.73807E-05	—	278.15	0.9181	0.0819	0.5898	0.4102	Vol. Est.
13.688	7.74632E-05	—	278.15	0.9088	0.0912	0.5669	0.4331	Vol. Est.
14.487	7.5925E-05	—	278.15	0.903	0.097	0.5493	0.4507	Vol. Est.
15.367	7.51067E-05	—	278.15	0.8974	0.1026	0.5204	0.4796	Vol. Est.
16.985	7.37238E-05	—	278.15	0.8821	0.1179	0.4962	0.5038	Vol. Est.
18.68	7.21551E-05	—	278.15	0.8709	0.1291	0.4958	0.5042	Vol. Est.
19.253	7.22321E-05	—	278.15	0.8693	0.1307	0.4945	0.5055	Vol. Est.
6.174	7.68363E-05	—	290.15	0.9887	0.0113	0.9505	0.0495	Vol. Est.
7.1	7.5917E-05	—	290.15	0.9772	0.0228	0.9021	0.0979	Vol. Est.
8.392	8.51229E-05	—	290.15	0.9651	0.0349	0.8444	0.1556	Vol. Est.
9.23	8.3795E-05	—	290.15	0.9477	0.0523	0.7944	0.2056	Vol. Est.
9.31	8.02502E-05	—	290.15	0.9459	0.0541	0.7811	0.2189	Vol. Est.
9.79	8.01922E-05	—	290.15	0.9427	0.0573	0.7611	0.2389	Vol. Est.
9.93	7.34361E-05	—	290.15	0.9395	0.0605	—	—	No
10.37	7.35931E-05	—	290.15	0.9339	0.0661	—	—	No
10.93	7.78437E-05	—	290.15	0.9287	0.0713	—	—	No
11.62	7.78023E-05	—	290.15	0.9204	0.0796	0.7265	0.2735	Vol. Est.
12.38	7.85079E-05	—	290.15	0.9103	0.0897	0.718	0.282	Vol. Est.
13.29	7.69746E-05	—	290.15	0.8969	0.1031	0.7082	0.2918	Vol. Est.
13.558	7.51758E-05	—	290.15	0.8963	0.1037	—	—	No
14.547	7.46894E-05	—	290.15	0.8861	0.1139	—	—	No
14.997	7.58879E-05	—	290.15	0.8785	0.1215	—	—	No
16.026	7.61376E-05	—	290.15	0.8636	0.1364	0.6799	0.3201	Vol. Est.
17.565	7.49539E-05	—	290.15	0.8455	0.1545	0.6638	0.3362	Vol. Est.
18.394	7.38506E-05	—	290.15	0.8429	0.1571	0.6771	0.3229	Vol. Est.
7.193	7.84861E-05	—	298.15	0.9904	0.0096	0.9575	0.0425	Vol. Est.
8.02	7.66238E-05	—	298.15	0.9716	0.0284	0.9257	0.0743	Vol. Est.
8.592	7.97702E-05	—	298.15	0.9618	0.0382	0.8994	0.1006	Vol. Est.
9.061	7.79605E-05	—	298.15	0.9556	0.0444	0.8667	0.1333	Vol. Est.
9.57	7.86966E-05	—	298.15	0.9439	0.0561	0.8391	0.1609	Vol. Est.
11.09	7.94229E-05	—	298.15	0.9192	0.0808	0.8062	0.1938	Vol. Est.
11.39	8.0662E-05	—	298.15	0.9122	0.0878	—	—	No
11.59	7.92922E-05	—	298.15	0.911	0.089	—	—	No

Data summarised from Table 4 of Bezanehtak02 [90]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{H_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{H_2}}$	Usable Data Point?
6.909	—	0.000278	258.15	—	—	0.448	0.552	No
6.915	0.0000439	0.000286	258.15	0.976	0.024	0.449	0.551	Vol. Est.
13.789	0.0000432	0.000154	258.15	0.9405	0.0595	0.299	0.701	Vol. Est.
27.558	0.000042	0.0000847	258.15	0.868	0.132	0.242	0.758	Vol. Est.
6.895	0.0000474	0.000258	273.15	0.9734	0.0266	0.6385	0.3615	Vol. Est.
13.796	0.0000467	0.000145	273.15	0.9201	0.0799	0.45	0.55	Vol. Est.
27.607	0.0000457	0.0000806	273.15	0.807	0.193	0.39	0.61	Vol. Est.

Data summarised from TABLE 1 and 2 of Freitag86 [92]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{H_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{H_2}}$	Usable Data Point?
2.04	—	—	252.80	—	—	0.9699	0.0301	No
8	—	—	252.80	0.9699	0.0301	—	—	No
7.96	—	—	257.82	0.9699	0.0301	—	—	No
2.38	—	—	257.83	—	—	0.9699	0.0301	No
2.76	—	—	262.79	—	—	0.9699	0.0301	No
7.76	—	—	262.81	0.9699	0.0301	—	—	No
3.17	—	—	267.76	—	—	0.9699	0.0301	No
7.75	—	—	267.78	0.9699	0.0301	—	—	No
3.63	—	—	272.74	—	—	0.9699	0.0301	No
7.76	—	—	272.74	0.9699	0.0301	—	—	No
10.56	—	—	272.97	0.9501	0.0499	—	—	No
3.76	—	—	273.00	—	—	0.9501	0.0499	No
10.48	—	—	274.00	0.9501	0.0499	—	—	No
10.34	—	—	275.89	0.9501	0.0499	—	—	No
4.19	—	—	276.98	—	—	0.9501	0.0499	No
7.78	—	—	277.79	0.9699	0.0301	—	—	No
4.16	—	—	277.81	—	—	0.9699	0.0301	No
10.35	—	—	277.95	0.9501	0.0499	—	—	No
10.25	—	—	280.95	0.9501	0.0499	—	—	No
4.66	—	—	280.98	—	—	0.9501	0.0499	No
7.98	—	—	282.78	0.9699	0.0301	—	—	No
4.75	—	—	282.86	—	—	0.9699	0.0301	No
10.26	—	—	282.95	0.9501	0.0499	—	—	No
5.18	—	—	284.97	—	—	0.9501	0.0499	No
10.21	—	—	284.97	0.9501	0.0499	—	—	No
7.98	—	—	285.32	0.9699	0.0301	—	—	No
5.32	—	—	285.98	—	—	0.9501	0.0499	No
8.18	—	—	287.82	0.9699	0.0301	—	—	No
5.38	—	—	287.83	—	—	0.9699	0.0301	No
10.18	—	—	287.96	0.9501	0.0499	—	—	No
5.75	—	—	288.97	—	—	0.9501	0.0499	No
10.06	—	—	289.94	0.9501	0.0499	—	—	No
5.73	—	—	290.30	—	—	0.9699	0.0301	No
8.26	—	—	290.35	0.9699	0.0301	—	—	No
8.36	—	—	292.80	0.9699	0.0301	—	—	No
6.08	—	—	292.81	—	—	0.9699	0.0301	No
10.1	—	—	292.97	0.9501	0.0499	—	—	No
6.39	—	—	292.98	—	—	0.9501	0.0499	No
10.03	—	—	294.96	0.9501	0.0499	—	—	No
6.47	—	—	295.34	—	—	0.9699	0.0301	No
8.47	—	—	295.34	0.9699	0.0301	—	—	No
6.84	—	—	295.49	—	—	0.9501	0.0499	No
8.57	—	—	296.36	0.9699	0.0301	—	—	No
9.99	—	—	296.42	0.9501	0.0499	—	—	No
8.6	—	—	297.83	0.9699	0.0301	—	—	No
6.91	—	—	297.84	—	—	0.9699	0.0301	No
7.35	—	—	297.99	—	—	0.9501	0.0499	No
9.92	—	—	297.99	0.9501	0.0499	—	—	No
7.08	—	—	298.83	—	—	0.9699	0.0301	No
8.72	—	—	298.83	0.9699	0.0301	—	—	No
9.88	—	—	299.00	0.9501	0.0499	—	—	No
7.7	—	—	299.49	—	—	0.9501	0.0499	No
7.29	—	—	299.86	—	—	0.9699	0.0301	No
9.73	—	—	299.98	0.9501	0.0499	—	—	No
8.68	—	—	300.34	0.9699	0.0301	—	—	No
7.43	—	—	300.40	—	—	0.9699	0.0301	No
7.99	—	—	300.48	—	—	0.9501	0.0499	No
7.53	—	—	300.86	—	—	0.9699	0.0301	No
8.12	—	—	300.98	—	—	0.9501	0.0499	No
9.59	—	—	300.98	0.9501	0.0499	—	—	No
7.63	—	—	301.38	—	—	0.9699	0.0301	No
8.21	—	—	301.48	—	—	0.9501	0.0499	No
9.39	—	—	301.48	0.9501	0.0499	—	—	No
8.62	—	—	301.86	0.9699	0.0301	—	—	No
7.76	—	—	301.88	—	—	0.9699	0.0301	No
8.36	—	—	301.96	—	—	0.9501	0.0499	No
9.19	—	—	301.99	0.9501	0.0499	—	—	No
8.59	—	—	302.11	0.9699	0.0301	—	—	No
8.54	—	—	302.22	—	—	0.9501	0.0499	No
8.96	—	—	302.23	0.9501	0.0499	—	—	No
8.81	—	—	302.41	—	—	0.9501	0.0499	No
7.88	—	—	302.42	—	—	0.9699	0.0301	No
8.32	—	—	302.87	—	—	—	—	No

Data summarised from Table 1 and 2 of Parrott13 [121]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{H_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{H_2}}$	Usable Data Point?
0.93	—	—	220	0.9985	0.0015	0.7102	0.2898	Vol. Est.
1.00	—	—	220	—	—	0.6555	0.3445	No
1.07	—	—	220	0.9972	0.0028	0.6129	0.3871	Vol. Est.
1.18	—	—	220	—	—	0.5691	0.4309	No
1.27	—	—	220	0.9968	0.0032	0.5358	0.4642	Vol. Est.
1.35	—	—	220	0.9965	0.0035	0.4975	0.5025	Vol. Est.
2.23	—	—	220	0.9933	0.0067	0.3245	0.6755	Vol. Est.
3.51	—	—	220	0.9888	0.0112	0.2190	0.7810	Vol. Est.
5.13	—	—	220	0.9841	0.0159	0.1631	0.8369	Vol. Est.
7.13	—	—	220	0.9782	0.0218	0.1263	0.8737	Vol. Est.
11.01	—	—	220	0.9703	0.0297	0.0945	0.9055	Vol. Est.
14.00	—	—	220	0.9639	0.0361	0.0838	0.9162	Vol. Est.
15.46	—	—	220	0.9606	0.0394	0.0811	0.9189	Vol. Est.
16.93	—	—	220	0.9573	0.0427	0.0787	0.9213	Vol. Est.
18.79	—	—	220	0.9537	0.0463	0.0791	0.9209	Vol. Est.
20.99	—	—	220	0.9486	0.0514	0.0740	0.9260	Vol. Est.
24.34	—	—	220	0.9407	0.0593	0.0701	0.9299	Vol. Est.
26.44	—	—	220	0.9353	0.0647	0.0693	0.9307	Vol. Est.
27.59	—	—	220	0.9337	0.0663	0.0697	0.9303	Vol. Est.
31.50	—	—	220	0.9279	0.0721	0.0693	0.9307	Vol. Est.
35.40	—	—	220	0.9162	0.0838	0.0685	0.9315	Vol. Est.
1.18	—	—	225	0.9977	0.0023	0.6898	0.3102	Vol. Est.
1.47	—	—	225	0.9961	0.0039	0.5628	0.4372	Vol. Est.
1.49	—	—	225	0.9961	0.0039	0.7873	0.2127	Vol. Est.
2.14	—	—	225	0.9931	0.0069	0.5772	0.4228	Vol. Est.
2.16	—	—	225	0.9932	0.0068	0.4003	0.5997	Vol. Est.
2.78	—	—	225	0.9911	0.0089	0.3243	0.6757	Vol. Est.
3.38	—	—	225	0.9879	0.0121	0.3912	0.6088	Vol. Est.
3.56	—	—	225	0.9883	0.0117	0.2591	0.7409	Vol. Est.
4.85	—	—	225	0.9841	0.0159	0.2035	0.7965	Vol. Est.
5.22	—	—	225	0.9815	0.0185	0.2714	0.7286	Vol. Est.
7.00	—	—	225	0.9782	0.0218	0.1493	0.8507	Vol. Est.
7.06	—	—	225	0.9757	0.0243	0.2194	0.7806	Vol. Est.
10.46	—	—	225	0.9658	0.0342	0.1678	0.8322	Vol. Est.
10.65	—	—	225	0.9688	0.0312	0.1110	0.8890	Vol. Est.
14.03	—	—	225	0.9550	0.0450	0.1438	0.8562	Vol. Est.
14.22	—	—	225	0.9607	0.0393	0.0964	0.9036	Vol. Est.
20.73	—	—	225	0.9341	0.0659	0.1245	0.8755	Vol. Est.
21.15	—	—	225	0.9433	0.0567	0.0822	0.9178	Vol. Est.
27.71	—	—	225	0.9119	0.0881	0.3172	0.6828	Vol. Est.
27.88	—	—	225	0.9260	0.0740	0.0775	0.9225	Vol. Est.
34.69	—	—	225	0.9086	0.0914	0.0768	0.9232	Vol. Est.
35.22	—	—	225	0.8877	0.1123	0.1132	0.8868	Vol. Est.
41.38	—	—	225	0.8693	0.1307	0.1136	0.8864	Vol. Est.
41.44	—	—	225	0.8927	0.1073	0.0760	0.9240	Vol. Est.
48.37	—	—	225	0.8765	0.1235	0.0772	0.9228	Vol. Est.
55.17	—	—	225	0.8293	0.1707	0.1187	0.8813	Vol. Est.
55.35	—	—	225	0.8610	0.1390	0.0791	0.9209	Vol. Est.
69.99	—	—	225	0.8310	0.1690	0.0869	0.9131	Vol. Est.
73.10	—	—	225	0.7816	0.2184	0.1296	0.8704	Vol. Est.
79.48	—	—	225	0.8123	0.1877	0.0930	0.9070	Vol. Est.
91.26	—	—	225	0.7888	0.2112	0.0964	0.9036	Vol. Est.
93.03	—	—	225	0.7272	0.2728	0.1438	0.8562	Vol. Est.
117.61	—	—	225	0.6629	0.3371	0.1657	0.8343	Vol. Est.
137.35	—	—	225	0.6072	0.3928	0.1898	0.8102	Vol. Est.
152.00	—	—	225	0.5635	0.4365	0.2123	0.7877	Vol. Est.
165.58	—	—	225	0.5116	0.4884	0.2444	0.7556	Vol. Est.
168.96	—	—	225	0.4938	0.5062	0.2545	0.7455	Vol. Est.
171.79	—	—	225	0.4736	0.5264	0.2672	0.7328	Vol. Est.
132.08	—	—	237	0.5933	0.4067	0.2051	0.7949	Vol. Est.
138.00	—	—	237	0.5719	0.4281	0.2163	0.7837	Vol. Est.
144.90	—	—	237	0.5470	0.4530	0.2302	0.7698	Vol. Est.
148.35	—	—	237	0.5269	0.4731	0.2476	0.7524	Vol. Est.
150.28	—	—	237	0.5211	0.4789	0.2514	0.7486	Vol. Est.
152.07	—	—	237	0.5092	0.4908	0.2610	0.7390	Vol. Est.
154.90	—	—	237	0.4951	0.5049	0.2700	0.7300	Vol. Est.
156.97	—	—	237	0.4762	0.5238	0.2810	0.7190	Vol. Est.
158.83	—	—	237	0.4599	0.5401	0.2954	0.7046	Vol. Est.
160.41	—	—	237	0.4434	0.5566	0.3079	0.6921	Vol. Est.
83.68	—	—	245	0.6749	0.3251	0.2082	0.7918	Vol. Est.
89.58	—	—	245	0.6479	0.3521	0.2224	0.7776	Vol. Est.
96.65	—	—	245	0.6118	0.3882	0.2400	0.7600	Vol. Est.
101.54	—	—	245	0.5845	0.4155	0.2559	0.7441	Vol. Est.
105.06	—	—	245	0.5621	0.4379	0.2697	0.7303	Vol. Est.
108.51	—	—	245	0.5343	0.4657	0.2906	0.7094	Vol. Est.
111.83	—	—	245	0.4990	0.5010	0.3211	0.6789	Vol. Est.
113.23	—	—	245	0.4738	0.5262	0.3397	0.6603	Vol. Est.

Data summarised from Table 1 of Tsang81 [110]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{H_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{H_2}}$	Usable Data Point?
2.31	—	—	250	0.9956	0.0044	0.8411	0.1589	Vol. Est.
3.04	—	—	250	0.9914	0.0086	0.6804	0.3196	Vol. Est.
3.63	—	—	250	0.9876	0.0124	0.5910	0.4090	Vol. Est.
5.20	—	—	250	0.9814	0.0186	0.4499	0.5501	Vol. Est.
6.90	—	—	250	0.9738	0.0262	0.3629	0.6371	Vol. Est.
10.29	—	—	250	0.9604	0.0396	0.2821	0.7179	Vol. Est.
13.85	—	—	250	0.9455	0.0545	0.2415	0.7585	Vol. Est.
17.28	—	—	250	0.9305	0.0695	0.2178	0.7822	Vol. Est.
25.44	—	—	250	0.8942	0.1058	0.1956	0.8044	Vol. Est.
31.54	—	—	250	0.8668	0.1332	0.1895	0.8105	Vol. Est.
35.34	—	—	250	0.8512	0.1488	0.1884	0.8116	Vol. Est.
49.66	—	—	250	0.7879	0.2121	0.1940	0.8060	Vol. Est.
62.81	—	—	250	0.7276	0.2724	0.2166	0.7834	Vol. Est.
75.88	—	—	250	0.6588	0.3412	0.2459	0.7541	Vol. Est.
83.22	—	—	250	0.6113	0.3887	0.2700	0.7300	Vol. Est.
86.54	—	—	250	0.5853	0.4147	0.2874	0.7126	Vol. Est.
88.39	—	—	250	0.5683	0.4317	0.2970	0.7030	Vol. Est.
91.61	—	—	250	0.5320	0.4680	—	—	No
3.37	—	—	260	0.9919	0.0081	0.7917	0.2083	Vol. Est.
4.38	—	—	260	0.9882	0.0118	0.8232	0.1768	Vol. Est.
5.31	—	—	260	0.9809	0.0191	0.7251	0.2749	Vol. Est.
5.58	—	—	260	0.9792	0.0208	0.5489	0.4511	Vol. Est.
7.08	—	—	260	0.9699	0.0301	0.6029	0.3971	Vol. Est.
7.23	—	—	260	0.9716	0.0284	0.4618	0.5382	Vol. Est.
10.53	—	—	260	0.9550	0.0450	0.3652	0.6348	Vol. Est.
10.62	—	—	260	0.9436	0.0564	0.4718	0.5282	Vol. Est.
13.49	—	—	260	0.9404	0.0596	0.3213	0.6787	Vol. Est.
13.86	—	—	260	0.9183	0.0817	0.4148	0.5852	Vol. Est.
17.44	—	—	260	0.8905	0.1095	0.3799	0.6201	Vol. Est.
21.62	—	—	260	0.8956	0.1044	0.2658	0.7342	Vol. Est.
21.93	—	—	260	0.8612	0.1388	0.3560	0.6440	Vol. Est.
25.26	—	—	260	0.8294	0.1706	0.3504	0.6496	Vol. Est.
27.97	—	—	260	0.8044	0.1956	0.3525	0.6475	Vol. Est.
28.15	—	—	260	0.8586	0.1414	0.2517	0.7483	Vol. Est.
34.70	—	—	260	0.8223	0.1777	0.2517	0.7483	Vol. Est.
34.76	—	—	260	0.7543	0.2457	0.3601	0.6399	Vol. Est.
39.99	—	—	260	0.7050	0.2950	0.3843	0.6157	Vol. Est.
41.71	—	—	260	0.7803	0.2197	0.2630	0.7370	Vol. Est.
44.14	—	—	260	0.6440	0.3560	0.4249	0.5751	Vol. Est.
45.69	—	—	260	0.6033	0.3967	0.4668	0.5332	Vol. Est.
48.44	—	—	260	0.7360	0.2640	0.2783	0.7217	Vol. Est.
55.59	—	—	260	0.6801	0.3199	0.3035	0.6965	Vol. Est.
62.04	—	—	260	0.6092	0.3908	0.3529	0.6471	Vol. Est.
65.64	—	—	260	0.5232	0.4768	0.4227	0.5773	Vol. Est.
7.44	—	—	280	—	—	0.7109	0.2891	No
9.15	—	—	280	—	—	0.6388	0.3612	No
11.27	—	—	280	—	—	0.5749	0.4251	No
13.80	—	—	280	0.8900	0.1100	0.5269	0.4731	Vol. Est.
18.35	—	—	280	0.8420	0.1580	0.4834	0.5166	Vol. Est.
20.30	—	—	280	0.8209	0.1791	0.4745	0.5255	Vol. Est.
22.62	—	—	280	0.8000	0.2000	0.4736	0.5264	Vol. Est.
24.56	—	—	280	0.7805	0.2195	—	—	No
26.01	—	—	280	0.7642	0.2358	0.4806	0.5194	Vol. Est.
27.45	—	—	280	0.7464	0.2536	0.4867	0.5133	Vol. Est.
29.25	—	—	280	0.7255	0.2745	0.4961	0.5039	Vol. Est.
31.19	—	—	280	0.6957	0.3043	0.5260	0.4740	Vol. Est.
31.96	—	—	280	0.6730	0.3270	0.5528	0.4472	Vol. Est.
8.53	—	—	290	0.9595	0.0405	0.8012	0.1988	Vol. Est.
9.49	—	—	290	0.9472	0.0528	0.7658	0.2342	Vol. Est.
11.29	—	—	290	0.9196	0.0804	0.7133	0.2867	Vol. Est.
11.72	—	—	290	—	—	0.7031	0.2969	No
13.88	—	—	290	0.8774	0.1226	0.6704	0.3296	Vol. Est.
15.65	—	—	290	0.8551	0.1449	0.6540	0.3460	Vol. Est.
17.27	—	—	290	0.8330	0.1670	0.6475	0.3525	Vol. Est.
18.95	—	—	290	0.8080	0.1920	0.6673	0.3327	Vol. Est.
19.71	—	—	290	0.7935	0.2065	0.6759	0.3241	Vol. Est.

Continued: Data summarised from Table 1 of Tsang81 [110]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{H_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{H_2}}$	Usable Data Point?
6.079500	—	—	273.15	—	—	0.7170	0.2830	No
10.436475	—	—	273.15	0.9530	0.0470	0.5260	0.4740	Vol. Est.
13.881525	—	—	273.15	0.9211	0.0789	0.4370	0.5630	Vol. Est.
18.339825	—	—	273.15	0.8960	0.1040	0.4040	0.5960	Vol. Est.
23.304750	—	—	273.15	0.8440	0.1560	0.3750	0.6250	Vol. Est.
27.763050	—	—	273.15	0.8200	0.1800	0.3510	0.6490	Vol. Est.
30.296175	—	—	273.15	0.7860	0.2140	0.3490	0.6510	Vol. Est.
31.309425	—	—	273.15	0.7770	0.2230	—	—	No
34.045200	—	—	273.15	0.7140	0.2860	0.3960	0.6040	Vol. Est.
35.463750	—	—	273.15	0.6830	0.3170	0.4200	0.5800	Vol. Est.
36.274350	—	—	273.15	0.6790	0.3210	0.4660	0.5340	Vol. Est.
37.490250	—	—	273.15	0.5280	0.4720	0.5220	0.4780	Vol. Est.

Data summarised from Table 2 of Yorizane70 [84]

7.1.4 Carbon Dioxide–Hydrogen Density Data

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
5.06625	0.00048430	323.15	0.527	0.473	Yes
10.13250	0.00024100	323.15	0.527	0.473	Yes
20.26500	0.00011790	323.15	0.527	0.473	Yes
30.39750	0.00008247	323.15	0.527	0.473	Yes
40.53000	0.00006618	323.15	0.527	0.473	Yes
50.66250	0.00005692	323.15	0.527	0.473	Yes
5.06625	0.00058820	373.15	0.527	0.473	Yes
10.13250	0.00029370	373.15	0.527	0.473	Yes
20.26500	0.00014620	373.15	0.527	0.473	Yes
30.39750	0.00010150	373.15	0.527	0.473	Yes
40.53000	0.00007943	373.15	0.527	0.473	Yes
50.66250	0.00006689	373.15	0.527	0.473	Yes
5.06625	0.00068710	423.15	0.527	0.473	Yes
10.13250	0.00034160	423.15	0.527	0.473	Yes
20.26500	0.00017120	423.15	0.527	0.473	Yes
30.39750	0.00011810	423.15	0.527	0.473	Yes
40.53000	0.00009276	423.15	0.527	0.473	Yes
50.66250	0.00007806	423.15	0.527	0.473	Yes
5.06625	0.00075760	473.15	0.527	0.473	Yes
10.13250	0.00037450	473.15	0.527	0.473	Yes
20.26500	0.00019690	473.15	0.527	0.473	Yes
30.39750	0.00013610	473.15	0.527	0.473	Yes
40.53000	0.00010700	473.15	0.527	0.473	Yes
50.66250	0.00008985	473.15	0.527	0.473	Yes
5.06625	0.00043880	273.15	0.264	0.736	Yes
10.13250	0.00021830	273.15	0.264	0.736	Yes
20.26500	0.00011330	273.15	0.264	0.736	Yes
30.39750	0.00008006	273.15	0.264	0.736	Yes
40.53000	0.00006412	273.15	0.264	0.736	Yes
50.66250	0.00005488	273.15	0.264	0.736	Yes
5.06625	0.00052360	323.15	0.264	0.736	Yes
10.13250	0.00026600	323.15	0.264	0.736	Yes
20.26500	0.00013770	323.15	0.264	0.736	Yes
30.39750	0.00009553	323.15	0.264	0.736	Yes
40.53000	0.00007680	323.15	0.264	0.736	Yes
50.66250	0.00006452	323.15	0.264	0.736	Yes
5.06625	0.00061350	373.15	0.264	0.736	Yes
10.13250	0.00030960	373.15	0.264	0.736	Yes
20.26500	0.00016040	373.15	0.264	0.736	Yes
30.39750	0.00011220	373.15	0.264	0.736	Yes
40.53000	0.00008842	373.15	0.264	0.736	Yes
50.66250	0.00007413	373.15	0.264	0.736	Yes
5.06625	0.00069930	423.15	0.264	0.736	Yes
10.13250	0.00035460	423.15	0.264	0.736	Yes
20.26500	0.00018350	423.15	0.264	0.736	Yes
30.39750	0.00012780	423.15	0.264	0.736	Yes
40.53000	0.00009881	423.15	0.264	0.736	Yes
50.66250	0.00008361	423.15	0.264	0.736	Yes
5.06625	0.00076920	473.15	0.264	0.736	Yes
10.13250	0.00039220	473.15	0.264	0.736	Yes
20.26500	0.00020470	473.15	0.264	0.736	Yes
30.39750	0.00014200	473.15	0.264	0.736	Yes
40.53000	0.00011090	473.15	0.264	0.736	Yes
50.66250	0.00009234	473.15	0.264	0.736	Yes

Data summarised from Table 1 of Kritschewsky40 [99]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
0.1000	0.026881618	323.15	0.1367	0.8633	Yes
0.5000	0.005386534	323.15	0.1367	0.8633	Yes
1.0000	0.002699984	323.15	0.1367	0.8633	Yes
1.5000	0.001927344	323.15	0.1367	0.8633	Yes
2.0000	0.001357112	323.15	0.1367	0.8633	Yes
2.5000	0.001088591	323.15	0.1367	0.8633	Yes
3.0000	0.000909488	323.15	0.1367	0.8633	Yes
3.5000	0.00078148	323.15	0.1367	0.8633	Yes
4.0000	0.00068534	323.15	0.1367	0.8633	Yes
4.5000	0.000610445	323.15	0.1367	0.8633	Yes
5.0000	0.000550422	323.15	0.1367	0.8633	Yes
5.5000	0.000501116	323.15	0.1367	0.8633	Yes
6.0000	0.000459849	323.15	0.1367	0.8633	Yes
0.1000	0.028961273	348.15	0.1367	0.8633	Yes
0.5000	0.005803254	348.15	0.1367	0.8633	Yes
1.0000	0.002908864	348.15	0.1367	0.8633	Yes
1.5000	0.00194426	348.15	0.1367	0.8633	Yes
2.0000	0.001461958	348.15	0.1367	0.8633	Yes
2.5000	0.001172693	348.15	0.1367	0.8633	Yes
3.0000	0.000979849	348.15	0.1367	0.8633	Yes

Data summarised from TABLE 1 of Mallu90 [122]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
3.5000	0.000842104	348.15	0.1367	0.8633	Yes
4.0000	0.000738722	348.15	0.1367	0.8633	Yes
4.5000	0.00065825	348.15	0.1367	0.8633	Yes
5.0000	0.000593815	348.15	0.1367	0.8633	Yes
5.5000	0.000540937	348.15	0.1367	0.8633	Yes
6.0000	0.000496824	348.15	0.1367	0.8633	Yes
0.1000	0.031040928	373.15	0.1367	0.8633	Yes
0.5000	0.006219355	373.15	0.1367	0.8633	Yes
1.0000	0.003117434	373.15	0.1367	0.8633	Yes
1.5000	0.002083667	373.15	0.1367	0.8633	Yes
2.0000	0.001566783	373.15	0.1367	0.8633	Yes
2.5000	0.001256902	373.15	0.1367	0.8633	Yes
3.0000	0.00105021	373.15	0.1367	0.8633	Yes
3.5000	0.000902662	373.15	0.1367	0.8633	Yes
4.0000	0.000791924	373.15	0.1367	0.8633	Yes
4.5000	0.000705725	373.15	0.1367	0.8633	Yes
5.0000	0.000636766	373.15	0.1367	0.8633	Yes
5.5000	0.000580288	373.15	0.1367	0.8633	Yes
6.0000	0.00053312	373.15	0.1367	0.8633	Yes
0.1000	0.033120583	398.15	0.1367	0.8633	Yes
0.5000	0.006636034	398.15	0.1367	0.8633	Yes
1.0000	0.003326293	398.15	0.1367	0.8633	Yes
1.5000	0.002223046	398.15	0.1367	0.8633	Yes
2.0000	0.001671754	398.15	0.1367	0.8633	Yes
2.5000	0.001340978	398.15	0.1367	0.8633	Yes
3.0000	0.001120461	398.15	0.1367	0.8633	Yes
3.5000	0.000963044	398.15	0.1367	0.8633	Yes
4.0000	0.000844898	398.15	0.1367	0.8633	Yes
4.5000	0.000753006	398.15	0.1367	0.8633	Yes
5.0000	0.000679427	398.15	0.1367	0.8633	Yes
5.5000	0.000619226	398.15	0.1367	0.8633	Yes
6.0000	0.000568948	398.15	0.1367	0.8633	Yes
0.1000	0.035200238	423.15	0.1367	0.8633	Yes
0.5000	0.007052713	423.15	0.1367	0.8633	Yes
1.0000	0.003535152	423.15	0.1367	0.8633	Yes
1.5000	0.002362632	423.15	0.1367	0.8633	Yes
2.0000	0.001776548	423.15	0.1367	0.8633	Yes
2.5000	0.001425038	423.15	0.1367	0.8633	Yes
3.0000	0.001190698	423.15	0.1367	0.8633	Yes
3.5000	0.001023312	423.15	0.1367	0.8633	Yes
4.0000	0.000897773	423.15	0.1367	0.8633	Yes
4.5000	0.000800053	423.15	0.1367	0.8633	Yes
5.0000	0.000721878	423.15	0.1367	0.8633	Yes
5.5000	0.000657788	423.15	0.1367	0.8633	Yes
6.0000	0.000604321	423.15	0.1367	0.8633	Yes
0.1000	0.026814448	323.15	0.7659	0.2341	Yes
0.5000	0.005319363	323.15	0.7659	0.2341	Yes
1.0000	0.002632545	323.15	0.7659	0.2341	Yes
1.5000	0.001736939	323.15	0.7659	0.2341	Yes
2.0000	0.001289135	323.15	0.7659	0.2341	Yes
2.5000	0.001020561	323.15	0.7659	0.2341	Yes
3.0000	0.000841422	323.15	0.7659	0.2341	Yes
3.5000	0.000713542	323.15	0.7659	0.2341	Yes
4.0000	0.000617565	323.15	0.7659	0.2341	Yes
4.5000	0.000542916	323.15	0.7659	0.2341	Yes
5.0000	0.000483197	323.15	0.7659	0.2341	Yes
5.5000	0.000434385	323.15	0.7659	0.2341	Yes
6.0000	0.000393708	323.15	0.7659	0.2341	Yes
0.1000	0.02890338	348.15	0.7659	0.2341	Yes
0.5000	0.005744782	348.15	0.7659	0.2341	Yes
1.0000	0.002850391	348.15	0.7659	0.2341	Yes
1.5000	0.001885788	348.15	0.7659	0.2341	Yes
2.0000	0.001403486	348.15	0.7659	0.2341	Yes
2.5000	0.00111422	348.15	0.7659	0.2341	Yes
3.0000	0.000921473	348.15	0.7659	0.2341	Yes
3.5000	0.000783797	348.15	0.7659	0.2341	Yes
4.0000	0.000680612	348.15	0.7659	0.2341	Yes
4.5000	0.000600357	348.15	0.7659	0.2341	Yes
5.0000	0.000536153	348.15	0.7659	0.2341	Yes
5.5000	0.000483622	348.15	0.7659	0.2341	Yes
6.0000	0.000439895	348.15	0.7659	0.2341	Yes
0.1000	0.030988185	373.15	0.7659	0.2341	Yes
0.5000	0.006169094	373.15	0.7659	0.2341	Yes
1.0000	0.003066862	373.15	0.7659	0.2341	Yes
1.5000	0.002032992	373.15	0.7659	0.2341	Yes
2.0000	0.001516212	373.15	0.7659	0.2341	Yes
2.5000	0.001206268	373.15	0.7659	0.2341	Yes
3.0000	0.000999639	373.15	0.7659	0.2341	Yes
3.5000	0.000852224	373.15	0.7659	0.2341	Yes
4.0000	0.000741663	373.15	0.7659	0.2341	Yes
4.5000	0.00065567	373.15	0.7659	0.2341	Yes
5.0000	0.000586939	373.15	0.7659	0.2341	Yes
5.5000	0.000530704	373.15	0.7659	0.2341	Yes
6.0000	0.000483893	373.15	0.7659	0.2341	Yes

Continued: Data summarised from TABLE 1 of Mallu90 [122]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
0.1000	0.033074237	398.15	0.7659	0.2341	Yes
0.5000	0.006592337	398.15	0.7659	0.2341	Yes
1.0000	0.003282265	398.15	0.7659	0.2341	Yes
1.5000	0.002178907	398.15	0.7659	0.2341	Yes
2.0000	0.00162756	398.15	0.7659	0.2341	Yes
2.5000	0.001296884	398.15	0.7659	0.2341	Yes
3.0000	0.001076433	398.15	0.7659	0.2341	Yes
3.5000	0.000919062	398.15	0.7659	0.2341	Yes
4.0000	0.000801035	398.15	0.7659	0.2341	Yes
4.5000	0.000709309	398.15	0.7659	0.2341	Yes
5.0000	0.000635995	398.15	0.7659	0.2341	Yes
5.5000	0.00057601	398.15	0.7659	0.2341	Yes
6.0000	0.000526078	398.15	0.7659	0.2341	Yes
0.1000	0.035161537	423.15	0.7659	0.2341	Yes
0.5000	0.007014716	423.15	0.7659	0.2341	Yes
1.0000	0.003496451	423.15	0.7659	0.2341	Yes
1.5000	0.002324166	423.15	0.7659	0.2341	Yes
2.0000	0.001737847	423.15	0.7659	0.2341	Yes
2.5000	0.001386337	423.15	0.7659	0.2341	Yes
3.0000	0.001151997	423.15	0.7659	0.2341	Yes
3.5000	0.000984611	423.15	0.7659	0.2341	Yes
4.0000	0.00085916	423.15	0.7659	0.2341	Yes
4.5000	0.000761587	423.15	0.7659	0.2341	Yes
5.0000	0.000683669	423.15	0.7659	0.2341	Yes
5.5000	0.000619854	423.15	0.7659	0.2341	Yes
6.0000	0.000566734	423.15	0.7659	0.2341	Yes

Continued: Data summarised from TABLE 1 of Mallu90 [122]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
19.80	0.0000498164	288.15	0.9003	0.0997	Yes
18.56	0.0000506270	288.15	0.9003	0.0997	Yes
17.45	0.0000514578	288.15	0.9003	0.0997	Yes
16.52	0.0000522820	288.15	0.9003	0.0997	Yes
15.74	0.0000530764	288.15	0.9003	0.0997	Yes
15.06	0.0000538588	288.15	0.9003	0.0997	Yes
14.53	0.0000545748	288.15	0.9003	0.0997	Yes
20.75	0.0000480527	288.15	0.9252	0.0748	Yes
19.35	0.0000486940	288.15	0.9252	0.0748	Yes
17.88	0.0000494242	288.15	0.9252	0.0748	Yes
17.65	0.0000495560	288.15	0.9252	0.0748	Yes
16.46	0.0000502816	288.15	0.9252	0.0748	Yes
15.49	0.0000509650	288.15	0.9252	0.0748	Yes
14.56	0.0000517262	288.15	0.9252	0.0748	Yes
13.79	0.0000524700	288.15	0.9252	0.0748	Yes
13.14	0.0000531731	288.15	0.9252	0.0748	Yes
12.60	0.0000538386	288.15	0.9252	0.0748	Yes
22.26	0.0000457929	288.15	0.9803	0.0197	Yes
20.08	0.0000463782	288.15	0.9803	0.0197	Yes
18.21	0.0000469377	288.15	0.9803	0.0197	Yes
16.55	0.0000475057	288.15	0.9803	0.0197	Yes
15.07	0.0000480716	288.15	0.9803	0.0197	Yes
13.75	0.0000486456	288.15	0.9803	0.0197	Yes
12.59	0.0000492167	288.15	0.9803	0.0197	Yes
11.58	0.0000497783	288.15	0.9803	0.0197	Yes
10.70	0.0000503354	288.15	0.9803	0.0197	Yes
9.93	0.0000508870	288.15	0.9803	0.0197	Yes
9.27	0.0000514264	288.15	0.9803	0.0197	Yes
8.69	0.0000519523	288.15	0.9803	0.0197	Yes
8.20	0.0000524508	288.15	0.9803	0.0197	Yes
7.77	0.0000529395	288.15	0.9803	0.0197	Yes
19.16	0.0000521081	293.15	0.9000	0.1000	Yes
18.24	0.0000528904	293.15	0.9000	0.1000	Yes
17.47	0.0000536459	293.15	0.9000	0.1000	Yes
16.78	0.0000544009	293.15	0.9000	0.1000	Yes
16.17	0.0000551546	293.15	0.9000	0.1000	Yes
15.63	0.0000559138	293.15	0.9000	0.1000	Yes
15.15	0.0000566699	293.15	0.9000	0.1000	Yes
14.72	0.0000574302	293.15	0.9000	0.1000	Yes
14.33	0.0000581856	293.15	0.9000	0.1000	Yes
14.00	0.0000589263	293.15	0.9000	0.1000	Yes
21.72	0.0000490707	293.15	0.9249	0.0751	Yes
20.31	0.0000497883	293.15	0.9249	0.0751	Yes
19.13	0.0000504710	293.15	0.9249	0.0751	Yes
19.08	0.0000504959	293.15	0.9249	0.0751	Yes
18.06	0.0000511662	293.15	0.9249	0.0751	Yes
17.11	0.0000518744	293.15	0.9249	0.0751	Yes
16.27	0.0000525753	293.15	0.9249	0.0751	Yes
15.30	0.0000535258	293.15	0.9249	0.0751	Yes
15.03	0.0000538220	293.15	0.9249	0.0751	Yes
14.20	0.0000548332	293.15	0.9249	0.0751	Yes
13.48	0.0000558680	293.15	0.9249	0.0751	Yes
12.85	0.0000569504	293.15	0.9249	0.0751	Yes
12.69	0.0000572698	293.15	0.9249	0.0751	Yes

Data summarised from Table S1 of Sanchez–Vicente13 [111]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
22.71	0.0000467417	293.15	0.9799	0.0201	Yes
20.78	0.0000473207	293.15	0.9799	0.0201	Yes
19.09	0.0000479036	293.15	0.9799	0.0201	Yes
17.56	0.0000484847	293.15	0.9799	0.0201	Yes
16.21	0.0000490689	293.15	0.9799	0.0201	Yes
15.00	0.0000496502	293.15	0.9799	0.0201	Yes
13.91	0.0000502455	293.15	0.9799	0.0201	Yes
12.93	0.0000508492	293.15	0.9799	0.0201	Yes
12.06	0.0000514615	293.15	0.9799	0.0201	Yes
11.31	0.0000520636	293.15	0.9799	0.0201	Yes
10.39	0.0000529513	293.15	0.9799	0.0201	Yes
9.78	0.0000536156	293.15	0.9799	0.0201	Yes
9.23	0.0000543173	293.15	0.9799	0.0201	Yes
8.75	0.0000550305	293.15	0.9799	0.0201	Yes
8.07	0.0000562496	293.15	0.9799	0.0201	Yes
22.07	0.0000536314	303.15	0.9000	0.1000	Yes
20.96	0.0000546249	303.15	0.9000	0.1000	Yes
20.02	0.0000555859	303.15	0.9000	0.1000	Yes
19.18	0.0000565893	303.15	0.9000	0.1000	Yes
18.39	0.0000576631	303.15	0.9000	0.1000	Yes
17.74	0.0000586399	303.15	0.9000	0.1000	Yes
17.72	0.0000586917	303.15	0.9000	0.1000	Yes
17.14	0.0000596950	303.15	0.9000	0.1000	Yes
16.57	0.0000608632	303.15	0.9000	0.1000	Yes
16.08	0.0000619717	303.15	0.9000	0.1000	Yes
15.62	0.0000631614	303.15	0.9000	0.1000	Yes
15.22	0.0000643456	303.15	0.9000	0.1000	Yes
14.85	0.0000655426	303.15	0.9000	0.1000	Yes
14.51	0.0000667739	303.15	0.9000	0.1000	Yes
14.21	0.0000680407	303.15	0.9000	0.1000	Yes
13.92	0.0000693685	303.15	0.9000	0.1000	Yes
13.65	0.0000707115	303.15	0.9000	0.1000	Yes
13.01	0.0000746355	303.15	0.9000	0.1000	Yes
12.41	0.0000797169	303.15	0.9000	0.1000	Yes
11.85	0.0000855590	303.15	0.9000	0.1000	Yes
11.30	0.0000936279	303.15	0.9000	0.1000	Yes
10.75	0.0001066165	303.15	0.9000	0.1000	Yes
10.20	0.0001204192	303.15	0.9000	0.1000	Yes
9.66	0.0001361512	303.15	0.9000	0.1000	Yes
9.12	0.0001541851	303.15	0.9000	0.1000	Yes
8.57	0.0001752999	303.15	0.9000	0.1000	Yes
8.04	0.0001976693	303.15	0.9000	0.1000	Yes
7.52	0.0002224056	303.15	0.9000	0.1000	Yes
7.03	0.0002486608	303.15	0.9000	0.1000	Yes
6.61	0.0002741777	303.15	0.9000	0.1000	Yes
5.94	0.0003205362	303.15	0.9000	0.1000	Yes
5.41	0.0003655702	303.15	0.9000	0.1000	Yes
4.87	0.0004203865	303.15	0.9000	0.1000	Yes
4.33	0.0004872778	303.15	0.9000	0.1000	Yes
3.81	0.0005711707	303.15	0.9000	0.1000	Yes
3.28	0.0006805231	303.15	0.9000	0.1000	Yes
2.80	0.0008191481	303.15	0.9000	0.1000	Yes
2.29	0.0010286977	303.15	0.9000	0.1000	Yes
1.78	0.0013495119	303.15	0.9000	0.1000	Yes
22.17	0.0000519573	303.15	0.9246	0.0754	Yes
20.81	0.0000529131	303.15	0.9246	0.0754	Yes
19.67	0.0000538337	303.15	0.9246	0.0754	Yes
18.68	0.0000547722	303.15	0.9246	0.0754	Yes
17.81	0.0000557060	303.15	0.9246	0.0754	Yes
17.04	0.0000566565	303.15	0.9246	0.0754	Yes
16.36	0.0000576237	303.15	0.9246	0.0754	Yes
15.76	0.0000586076	303.15	0.9246	0.0754	Yes
15.20	0.0000596693	303.15	0.9246	0.0754	Yes
14.72	0.0000606799	303.15	0.9246	0.0754	Yes
14.30	0.0000617253	303.15	0.9246	0.0754	Yes
13.92	0.0000627881	303.15	0.9246	0.0754	Yes
13.57	0.0000638581	303.15	0.9246	0.0754	Yes
13.27	0.0000649446	303.15	0.9246	0.0754	Yes
12.99	0.0000660794	303.15	0.9246	0.0754	Yes
12.73	0.0000672434	303.15	0.9246	0.0754	Yes
12.11	0.0000709831	303.15	0.9246	0.0754	Yes
11.52	0.0000759882	303.15	0.9246	0.0754	Yes
10.97	0.0000828136	303.15	0.9246	0.0754	Yes
10.42	0.0000920109	303.15	0.9246	0.0754	Yes
9.92	0.0001079663	303.15	0.9246	0.0754	Yes
9.41	0.0001246754	303.15	0.9246	0.0754	Yes
8.89	0.0001450929	303.15	0.9246	0.0754	Yes
8.37	0.0001673920	303.15	0.9246	0.0754	Yes
7.85	0.0001916643	303.15	0.9246	0.0754	Yes
7.36	0.0002174848	303.15	0.9246	0.0754	Yes
6.91	0.0002434067	303.15	0.9246	0.0754	Yes
6.45	0.0002733846	303.15	0.9246	0.0754	Yes
5.87	0.0003156387	303.15	0.9246	0.0754	Yes
5.33	0.0003620891	303.15	0.9246	0.0754	Yes
4.81	0.0004171977	303.15	0.9246	0.0754	Yes
4.28	0.0004856558	303.15	0.9246	0.0754	Yes
3.75	0.0005720399	303.15	0.9246	0.0754	Yes
3.25	0.0006807275	303.15	0.9246	0.0754	Yes
2.73	0.0008335439	303.15	0.9246	0.0754	Yes
2.22	0.0010526715	303.15	0.9246	0.0754	Yes
1.71	0.0013987552	303.15	0.9246	0.0754	Yes

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
22.73	0.0000490928	303.15	0.9797	0.0203	Yes
20.81	0.0000498931	303.15	0.9797	0.0203	Yes
19.17	0.0000506901	303.15	0.9797	0.0203	Yes
17.75	0.0000514761	303.15	0.9797	0.0203	Yes
16.55	0.0000522488	303.15	0.9797	0.0203	Yes
15.50	0.0000530256	303.15	0.9797	0.0203	Yes
14.60	0.0000537922	303.15	0.9797	0.0203	Yes
13.82	0.0000545469	303.15	0.9797	0.0203	Yes
13.14	0.0000553018	303.15	0.9797	0.0203	Yes
12.55	0.0000560560	303.15	0.9797	0.0203	Yes
12.04	0.0000568012	303.15	0.9797	0.0203	Yes
11.59	0.0000575894	303.15	0.9797	0.0203	Yes
11.21	0.0000583446	303.15	0.9797	0.0203	Yes
10.87	0.0000590875	303.15	0.9797	0.0203	Yes
10.60	0.0000597667	303.15	0.9797	0.0203	Yes
10.34	0.0000604871	303.15	0.9797	0.0203	Yes
9.77	0.0000625200	303.15	0.9797	0.0203	Yes
9.25	0.0000652518	303.15	0.9797	0.0203	Yes
8.76	0.0000692626	303.15	0.9797	0.0203	Yes
6.24	0.0002510618	303.15	0.9797	0.0203	Yes
6.18	0.0002559758	303.15	0.9797	0.0203	Yes
5.64	0.0003011690	303.15	0.9797	0.0203	Yes
5.10	0.0003537502	303.15	0.9797	0.0203	Yes
4.57	0.0004169809	303.15	0.9797	0.0203	Yes
4.03	0.0004943588	303.15	0.9797	0.0203	Yes
3.50	0.0005928231	303.15	0.9797	0.0203	Yes
2.99	0.0007192920	303.15	0.9797	0.0203	Yes
2.48	0.0008991150	303.15	0.9797	0.0203	Yes
1.97	0.0011664195	303.15	0.9797	0.0203	Yes
21.75	0.0000582793	313.15	0.9000	0.1000	Yes
20.73	0.0000596235	313.15	0.9000	0.1000	Yes
19.84	0.0000609844	313.15	0.9000	0.1000	Yes
19.04	0.0000623893	313.15	0.9000	0.1000	Yes
18.33	0.0000638195	313.15	0.9000	0.1000	Yes
17.68	0.0000652954	313.15	0.9000	0.1000	Yes
17.11	0.0000667963	313.15	0.9000	0.1000	Yes
16.60	0.0000683326	313.15	0.9000	0.1000	Yes
16.14	0.0000698677	313.15	0.9000	0.1000	Yes
15.72	0.0000714732	313.15	0.9000	0.1000	Yes
15.32	0.0000730604	313.15	0.9000	0.1000	Yes
14.96	0.0000747898	313.15	0.9000	0.1000	Yes
14.64	0.0000764559	313.15	0.9000	0.1000	Yes
14.34	0.0000781826	313.15	0.9000	0.1000	Yes
14.06	0.0000799249	313.15	0.9000	0.1000	Yes
13.41	0.0000847756	313.15	0.9000	0.1000	Yes
12.79	0.0000904992	313.15	0.9000	0.1000	Yes
12.20	0.0000975272	313.15	0.9000	0.1000	Yes
11.62	0.0001062466	313.15	0.9000	0.1000	Yes
11.08	0.0001162353	313.15	0.9000	0.1000	Yes
10.53	0.0001293392	313.15	0.9000	0.1000	Yes
9.98	0.0001436687	313.15	0.9000	0.1000	Yes
9.43	0.0001602681	313.15	0.9000	0.1000	Yes
8.88	0.0001807108	313.15	0.9000	0.1000	Yes
8.34	0.0002017770	313.15	0.9000	0.1000	Yes
7.81	0.0002261966	313.15	0.9000	0.1000	Yes
7.30	0.0002518065	313.15	0.9000	0.1000	Yes
6.81	0.0002787857	313.15	0.9000	0.1000	Yes
6.37	0.0003060000	313.15	0.9000	0.1000	Yes
5.73	0.0003541868	313.15	0.9000	0.1000	Yes
5.19	0.0004029413	313.15	0.9000	0.1000	Yes
4.65	0.0004623763	313.15	0.9000	0.1000	Yes
4.12	0.0005365310	313.15	0.9000	0.1000	Yes
3.59	0.0006309128	313.15	0.9000	0.1000	Yes
3.08	0.0007539886	313.15	0.9000	0.1000	Yes
2.56	0.0009279860	313.15	0.9000	0.1000	Yes
2.05	0.0011848393	313.15	0.9000	0.1000	Yes
1.55	0.0015988193	313.15	0.9000	0.1000	Yes
21.49	0.0000563769	313.15	0.9245	0.0755	Yes
20.35	0.0000576340	313.15	0.9245	0.0755	Yes
19.35	0.0000589144	313.15	0.9245	0.0755	Yes
18.49	0.0000602085	313.15	0.9245	0.0755	Yes
17.70	0.0000615608	313.15	0.9245	0.0755	Yes
17.01	0.0000629461	313.15	0.9245	0.0755	Yes
16.41	0.0000643648	313.15	0.9245	0.0755	Yes
15.88	0.0000657640	313.15	0.9245	0.0755	Yes
15.40	0.0000672476	313.15	0.9245	0.0755	Yes
14.96	0.0000687880	313.15	0.9245	0.0755	Yes
14.56	0.0000703886	313.15	0.9245	0.0755	Yes
14.20	0.0000719384	313.15	0.9245	0.0755	Yes
13.87	0.0000736377	313.15	0.9245	0.0755	Yes
13.57	0.0000752940	313.15	0.9245	0.0755	Yes
13.30	0.0000770410	313.15	0.9245	0.0755	Yes
12.64	0.0000820564	313.15	0.9245	0.0755	Yes
12.03	0.0000883971	313.15	0.9245	0.0755	Yes
10.89	0.0001063804	313.15	0.9245	0.0755	Yes
10.34	0.0001203284	313.15	0.9245	0.0755	Yes
9.84	0.0001341197	313.15	0.9245	0.0755	Yes
9.32	0.0001511453	313.15	0.9245	0.0755	Yes
8.79	0.0001705196	313.15	0.9245	0.0755	Yes

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
8.27	0.0001941962	313.15	0.9245	0.0755	Yes
7.75	0.0002181595	313.15	0.9245	0.0755	Yes
7.27	0.0002430920	313.15	0.9245	0.0755	Yes
6.83	0.0002681514	313.15	0.9245	0.0755	Yes
6.22	0.0003079898	313.15	0.9245	0.0755	Yes
5.70	0.0003487571	313.15	0.9245	0.0755	Yes
5.16	0.0003980454	313.15	0.9245	0.0755	Yes
4.63	0.0004578414	313.15	0.9245	0.0755	Yes
4.10	0.0005324570	313.15	0.9245	0.0755	Yes
3.58	0.0006282993	313.15	0.9245	0.0755	Yes
3.06	0.0007534954	313.15	0.9245	0.0755	Yes
2.55	0.0009281694	313.15	0.9245	0.0755	Yes
2.06	0.0011769295	313.15	0.9245	0.0755	Yes
1.56	0.0015890838	313.15	0.9245	0.0755	Yes
21.17	0.0000528373	313.15	0.9797	0.0203	Yes
19.18	0.0000542180	313.15	0.9797	0.0203	Yes
17.49	0.0000556871	313.15	0.9797	0.0203	Yes
15.74	0.0000577204	313.15	0.9797	0.0203	Yes
15.40	0.0000581951	313.15	0.9797	0.0203	Yes
13.88	0.0000608367	313.15	0.9797	0.0203	Yes
13.65	0.0000613381	313.15	0.9797	0.0203	Yes
12.62	0.0000640795	313.15	0.9797	0.0203	Yes
11.77	0.0000673915	313.15	0.9797	0.0203	Yes
11.56	0.0000683954	313.15	0.9797	0.0203	Yes
10.81	0.0000735472	313.15	0.9797	0.0203	Yes
10.24	0.0000801291	313.15	0.9797	0.0203	Yes
9.74	0.0000900616	313.15	0.9797	0.0203	Yes
9.35	0.0001028540	313.15	0.9797	0.0203	Yes
8.99	0.0001198820	313.15	0.9797	0.0203	Yes
8.62	0.0001405325	313.15	0.9797	0.0203	Yes
8.36	0.0001536402	313.15	0.9797	0.0203	Yes
8.26	0.0001594883	313.15	0.9797	0.0203	Yes
7.65	0.0001943157	313.15	0.9797	0.0203	Yes
6.83	0.0002442418	313.15	0.9797	0.0203	Yes
6.35	0.0002771838	313.15	0.9797	0.0203	Yes
5.82	0.0003180363	313.15	0.9797	0.0203	Yes
5.32	0.0003626683	313.15	0.9797	0.0203	Yes
4.81	0.0004181930	313.15	0.9797	0.0203	Yes
4.29	0.0004865561	313.15	0.9797	0.0203	Yes
3.77	0.0005723809	313.15	0.9797	0.0203	Yes
3.26	0.0006839544	313.15	0.9797	0.0203	Yes
2.75	0.0008363861	313.15	0.9797	0.0203	Yes
2.24	0.0010526225	313.15	0.9797	0.0203	Yes
1.75	0.0013877017	313.15	0.9797	0.0203	Yes
20.23	0.0000664437	323.15	0.8999	0.1001	Yes
19.07	0.0000691924	323.15	0.8999	0.1001	Yes
18.08	0.0000721784	323.15	0.8999	0.1001	Yes
17.22	0.0000752484	323.15	0.8999	0.1001	Yes
17.21	0.0000752911	323.15	0.8999	0.1001	Yes
16.45	0.0000786222	323.15	0.8999	0.1001	Yes
15.84	0.0000818052	323.15	0.8999	0.1001	Yes
15.23	0.0000854581	323.15	0.8999	0.1001	Yes
14.78	0.0000887150	323.15	0.8999	0.1001	Yes
14.34	0.0000921444	323.15	0.8999	0.1001	Yes
14.00	0.0000951851	323.15	0.8999	0.1001	Yes
13.66	0.0000986039	323.15	0.8999	0.1001	Yes
13.39	0.0001016507	323.15	0.8999	0.1001	Yes
13.13	0.0001048365	323.15	0.8999	0.1001	Yes
12.42	0.0001149809	323.15	0.8999	0.1001	Yes
11.79	0.0001250594	323.15	0.8999	0.1001	Yes
11.17	0.0001368858	323.15	0.8999	0.1001	Yes
10.51	0.0001518749	323.15	0.8999	0.1001	Yes
9.96	0.0001665540	323.15	0.8999	0.1001	Yes
9.38	0.0001842889	323.15	0.8999	0.1001	Yes
8.82	0.0002037175	323.15	0.8999	0.1001	Yes
8.29	0.0002247679	323.15	0.8999	0.1001	Yes
7.76	0.0002487900	323.15	0.8999	0.1001	Yes
7.24	0.0002754768	323.15	0.8999	0.1001	Yes
6.76	0.0003036339	323.15	0.8999	0.1001	Yes
6.29	0.0003347889	323.15	0.8999	0.1001	Yes
5.77	0.0003755321	323.15	0.8999	0.1001	Yes
5.23	0.0004257369	323.15	0.8999	0.1001	Yes
4.69	0.0004860366	323.15	0.8999	0.1001	Yes
4.16	0.0005614443	323.15	0.8999	0.1001	Yes
3.63	0.0006579570	323.15	0.8999	0.1001	Yes
3.11	0.0007851361	323.15	0.8999	0.1001	Yes
2.59	0.0009638354	323.15	0.8999	0.1001	Yes
2.08	0.0012248123	323.15	0.8999	0.1001	Yes
1.58	0.0016381235	323.15	0.8999	0.1001	Yes
21.48	0.0000613360	323.15	0.9246	0.0754	Yes
19.92	0.0000639381	323.15	0.9246	0.0754	Yes
18.63	0.0000666944	323.15	0.9246	0.0754	Yes
18.43	0.0000671771	323.15	0.9246	0.0754	Yes
17.53	0.0000696872	323.15	0.9246	0.0754	Yes
16.74	0.0000723922	323.15	0.9246	0.0754	Yes
16.57	0.0000730264	323.15	0.9246	0.0754	Yes
15.73	0.0000767161	323.15	0.9246	0.0754	Yes

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
15.00	0.0000807666	323.15	0.9246	0.0754	Yes
14.45	0.0000843180	323.15	0.9246	0.0754	Yes
13.96	0.0000883488	323.15	0.9246	0.0754	Yes
13.53	0.0000925321	323.15	0.9246	0.0754	Yes
13.09	0.0000970389	323.15	0.9246	0.0754	Yes
12.73	0.0001019053	323.15	0.9246	0.0754	Yes
12.48	0.0001054030	323.15	0.9246	0.0754	Yes
12.31	0.0001073421	323.15	0.9246	0.0754	Yes
11.70	0.0001177390	323.15	0.9246	0.0754	Yes
11.06	0.0001308253	323.15	0.9246	0.0754	Yes
10.44	0.0001457141	323.15	0.9246	0.0754	Yes
9.87	0.0001613098	323.15	0.9246	0.0754	Yes
9.31	0.0001785905	323.15	0.9246	0.0754	Yes
8.75	0.0001984628	323.15	0.9246	0.0754	Yes
8.24	0.0002193537	323.15	0.9246	0.0754	Yes
7.73	0.0002428279	323.15	0.9246	0.0754	Yes
7.24	0.0002685316	323.15	0.9246	0.0754	Yes
6.72	0.0002990018	323.15	0.9246	0.0754	Yes
6.24	0.0003323324	323.15	0.9246	0.0754	Yes
5.69	0.0003760926	323.15	0.9246	0.0754	Yes
5.15	0.0004272349	323.15	0.9246	0.0754	Yes
4.62	0.0004891455	323.15	0.9246	0.0754	Yes
4.09	0.0005672730	323.15	0.9246	0.0754	Yes
3.57	0.0006652061	323.15	0.9246	0.0754	Yes
3.06	0.0007930806	323.15	0.9246	0.0754	Yes
2.54	0.0009747888	323.15	0.9246	0.0754	Yes
2.03	0.0012452333	323.15	0.9246	0.0754	Yes
1.53	0.0016877542	323.15	0.9246	0.0754	Yes
22.63	0.0000552842	323.15	0.9799	0.0201	Yes
20.78	0.0000569622	323.15	0.9799	0.0201	Yes
19.41	0.0000584508	323.15	0.9799	0.0201	Yes
18.02	0.0000602792	323.15	0.9799	0.0201	Yes
16.78	0.0000623965	323.15	0.9799	0.0201	Yes
16.68	0.0000626047	323.15	0.9799	0.0201	Yes
15.63	0.0000649698	323.15	0.9799	0.0201	Yes
14.69	0.0000677644	323.15	0.9799	0.0201	Yes
13.85	0.0000711253	323.15	0.9799	0.0201	Yes
13.10	0.0000753069	323.15	0.9799	0.0201	Yes
12.38	0.0000809563	323.15	0.9799	0.0201	Yes
12.43	0.0000805485	323.15	0.9799	0.0201	Yes
11.94	0.0000858511	323.15	0.9799	0.0201	Yes
11.45	0.0000931304	323.15	0.9799	0.0201	Yes
11.04	0.0001009729	323.15	0.9799	0.0201	Yes
10.65	0.0001102296	323.15	0.9799	0.0201	Yes
10.19	0.0001238620	323.15	0.9799	0.0201	Yes
9.85	0.0001351046	323.15	0.9799	0.0201	Yes
9.53	0.0001466234	323.15	0.9799	0.0201	Yes
9.19	0.0001599923	323.15	0.9799	0.0201	Yes
8.85	0.0001737059	323.15	0.9799	0.0201	Yes
8.54	0.0001866231	323.15	0.9799	0.0201	Yes
8.24	0.0001999348	323.15	0.9799	0.0201	Yes
7.95	0.0002132704	323.15	0.9799	0.0201	Yes
7.66	0.0002273087	323.15	0.9799	0.0201	Yes
7.25	0.0002492259	323.15	0.9799	0.0201	Yes
6.70	0.0002826845	323.15	0.9799	0.0201	Yes
6.23	0.0003148499	323.15	0.9799	0.0201	Yes
5.75	0.0003529511	323.15	0.9799	0.0201	Yes
5.23	0.0004019173	323.15	0.9799	0.0201	Yes
4.74	0.0004577510	323.15	0.9799	0.0201	Yes
4.22	0.0005296432	323.15	0.9799	0.0201	Yes
3.70	0.0006202000	323.15	0.9799	0.0201	Yes
3.19	0.0007378790	323.15	0.9799	0.0201	Yes
2.68	0.0009011674	323.15	0.9799	0.0201	Yes
2.20	0.0011241125	323.15	0.9799	0.0201	Yes
21.04	0.0000712731	333.15	0.9004	0.0996	Yes
19.98	0.0000742079	333.15	0.9004	0.0996	Yes
19.05	0.0000773047	333.15	0.9004	0.0996	Yes
18.16	0.0000807694	333.15	0.9004	0.0996	Yes
17.41	0.0000843801	333.15	0.9004	0.0996	Yes
16.74	0.0000880747	333.15	0.9004	0.0996	Yes
16.66	0.0000884267	333.15	0.9004	0.0996	Yes
16.06	0.0000923641	333.15	0.9004	0.0996	Yes
15.50	0.0000964344	333.15	0.9004	0.0996	Yes
14.97	0.0001008289	333.15	0.9004	0.0996	Yes
14.51	0.0001052243	333.15	0.9004	0.0996	Yes
14.10	0.0001095363	333.15	0.9004	0.0996	Yes
13.72	0.0001139554	333.15	0.9004	0.0996	Yes
13.44	0.0001175543	333.15	0.9004	0.0996	Yes
13.15	0.0001213510	333.15	0.9004	0.0996	Yes
12.51	0.0001311406	333.15	0.9004	0.0996	Yes
11.85	0.0001425462	333.15	0.9004	0.0996	Yes
11.25	0.0001541905	333.15	0.9004	0.0996	Yes
10.73	0.0001663634	333.15	0.9004	0.0996	Yes
10.16	0.0001805412	333.15	0.9004	0.0996	Yes
9.59	0.0001974586	333.15	0.9004	0.0996	Yes
9.04	0.0002156329	333.15	0.9004	0.0996	Yes
8.53	0.0002348314	333.15	0.9004	0.0996	Yes
8.00	0.0002574492	333.15	0.9004	0.0996	Yes
7.48	0.0002828650	333.15	0.9004	0.0996	Yes
6.99	0.0003106661	333.15	0.9004	0.0996	Yes
6.49	0.0003421598	333.15	0.9004	0.0996	Yes

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{H_2}	Usable Data Point?
5.96	0.0003818542	333.15	0.9004	0.0996	Yes
5.42	0.0004291745	333.15	0.9004	0.0996	Yes
4.89	0.0004862930	333.15	0.9004	0.0996	Yes
4.36	0.0005570265	333.15	0.9004	0.0996	Yes
3.84	0.0006465487	333.15	0.9004	0.0996	Yes
3.32	0.0007600648	333.15	0.9004	0.0996	Yes
2.84	0.0009051681	333.15	0.9004	0.0996	Yes
2.32	0.0011282549	333.15	0.9004	0.0996	Yes
1.82	0.0014642426	333.15	0.9004	0.0996	Yes
21.79	0.0000666400	333.15	0.9246	0.0754	Yes
20.59	0.0000692383	333.15	0.9246	0.0754	Yes
19.60	0.0000718320	333.15	0.9246	0.0754	Yes
18.63	0.0000749287	333.15	0.9246	0.0754	Yes
18.42	0.0000757065	333.15	0.9246	0.0754	Yes
17.36	0.0000801327	333.15	0.9246	0.0754	Yes
16.45	0.0000849847	333.15	0.9246	0.0754	Yes
16.24	0.0000861862	333.15	0.9246	0.0754	Yes
15.42	0.0000919074	333.15	0.9246	0.0754	Yes
14.82	0.0000969007	333.15	0.9246	0.0754	Yes
14.65	0.0000985372	333.15	0.9246	0.0754	Yes
14.11	0.0001040868	333.15	0.9246	0.0754	Yes
13.61	0.0001102095	333.15	0.9246	0.0754	Yes
13.15	0.0001163968	333.15	0.9246	0.0754	Yes
12.73	0.0001229860	333.15	0.9246	0.0754	Yes
12.35	0.0001295390	333.15	0.9246	0.0754	Yes
12.04	0.0001336507	333.15	0.9246	0.0754	Yes
11.89	0.0001363273	333.15	0.9246	0.0754	Yes
11.29	0.0001484684	333.15	0.9246	0.0754	Yes
10.70	0.0001620780	333.15	0.9246	0.0754	Yes
10.12	0.0001768123	333.15	0.9246	0.0754	Yes
9.55	0.0001932970	333.15	0.9246	0.0754	Yes
8.98	0.0002122851	333.15	0.9246	0.0754	Yes
8.42	0.0002331259	333.15	0.9246	0.0754	Yes
7.89	0.0002560731	333.15	0.9246	0.0754	Yes
7.37	0.0002816804	333.15	0.9246	0.0754	Yes
6.87	0.0003105981	333.15	0.9246	0.0754	Yes
6.38	0.0003420741	333.15	0.9246	0.0754	Yes
5.96	0.0003750565	333.15	0.9246	0.0754	Yes
5.43	0.0004223749	333.15	0.9246	0.0754	Yes
4.89	0.0004805136	333.15	0.9246	0.0754	Yes
4.36	0.0005519412	333.15	0.9246	0.0754	Yes
3.84	0.0006401826	333.15	0.9246	0.0754	Yes
3.33	0.0007535729	333.15	0.9246	0.0754	Yes
2.81	0.0009096582	333.15	0.9246	0.0754	Yes
2.30	0.0011345459	333.15	0.9246	0.0754	Yes
1.80	0.0014798425	333.15	0.9246	0.0754	Yes
20.76	0.0000619402	333.15	0.9802	0.0198	Yes
18.97	0.0000649790	333.15	0.9802	0.0198	Yes
17.44	0.0000685700	333.15	0.9802	0.0198	Yes
16.14	0.0000729490	333.15	0.9802	0.0198	Yes
16.12	0.0000730230	333.15	0.9802	0.0198	Yes
15.01	0.0000784208	333.15	0.9802	0.0198	Yes
14.05	0.0000850976	333.15	0.9802	0.0198	Yes
13.15	0.0000940913	333.15	0.9802	0.0198	Yes
12.40	0.0001046245	333.15	0.9802	0.0198	Yes
11.72	0.0001173011	333.15	0.9802	0.0198	Yes
10.87	0.0001369008	333.15	0.9802	0.0198	Yes
10.26	0.0001541539	333.15	0.9802	0.0198	Yes
9.59	0.0001750954	333.15	0.9802	0.0198	Yes
9.05	0.0001938865	333.15	0.9802	0.0198	Yes
8.95	0.0001976134	333.15	0.9802	0.0198	Yes
8.36	0.0002215419	333.15	0.9802	0.0198	Yes
7.69	0.0002519167	333.15	0.9802	0.0198	Yes
7.37	0.0002686902	333.15	0.9802	0.0198	Yes
7.17	0.0002800163	333.15	0.9802	0.0198	Yes
6.70	0.0003084180	333.15	0.9802	0.0198	Yes
6.19	0.0003437780	333.15	0.9802	0.0198	Yes
5.71	0.0003824492	333.15	0.9802	0.0198	Yes
5.26	0.0004262440	333.15	0.9802	0.0198	Yes
4.73	0.0004867928	333.15	0.9802	0.0198	Yes
4.21	0.0005614892	333.15	0.9802	0.0198	Yes
3.69	0.0006552127	333.15	0.9802	0.0198	Yes
3.18	0.0007793956	333.15	0.9802	0.0198	Yes
2.66	0.0009510687	333.15	0.9802	0.0198	Yes
2.16	0.0011994033	333.15	0.9802	0.0198	Yes
1.66	0.0015933033	333.15	0.9802	0.0198	Yes

Continued: Data summarised from Table S1 of Sanchez–Vicente13 [111]

7.1.5 Carbon Dioxide–Oxygen VLE Data

P (MPa)	v_{Bub} ($\text{m}^3\text{mol}^{-1}$)	v_{Dew} ($\text{m}^3\text{mol}^{-1}$)	T(K)	x_{CO_2}	x_{O_2}	y_{CO_2}	y_{O_2}	Usable Data Point?
12.4163655	—	—	259.99	—	—	0.5	0.5	No
12.4163655	—	—	259.83	—	—	0.5	0.5	No
12.4163655	—	—	259.19	—	—	0.5	0.5	No
10.501323	—	—	258.53	—	—	0.5	0.5	No
13.326264	—	—	253.71	—	—	0.5	0.5	No
13.39415175	—	—	253.68	—	—	0.5	0.5	No
15.32945925	—	—	248.04	—	—	0.5	0.5	No
15.60405	—	—	244.77	—	—	0.5	0.5	No
13.9321875	—	—	244.11	—	—	0.5	0.5	No
14.20677825	—	—	243.47	—	—	0.5	0.5	No
13.9321875	—	—	243.47	—	—	0.5	0.5	No
13.9321875	—	—	242.95	—	—	0.5	0.5	No
14.0699895	—	—	242.95	—	—	0.5	0.5	No
14.0699895	—	—	242.83	—	—	0.5	0.5	No
14.1388905	—	—	240.11	—	—	0.5	0.5	No
14.20677825	—	—	239.71	—	—	0.5	0.5	No
14.20677825	—	—	239.77	—	—	0.5	0.5	No
3.61020975	—	—	239.65	—	—	0.5	0.5	No
3.61020975	—	—	239.55	—	—	0.5	0.5	No
14.2523745	—	—	237.93	—	—	0.5	0.5	No
14.27770575	—	—	237.44	—	—	0.5	0.5	No
14.26757325	—	—	237.28	—	—	0.5	0.5	No
14.331408	—	—	235.06	—	—	0.5	0.5	No
14.6211975	—	—	235.52	—	—	0.5	0.5	No
14.27770575	—	—	235.57	—	—	0.5	0.5	No
10.9370205	—	—	252.92	—	—	0.4	0.6	No
10.9370205	—	—	252.89	—	—	0.4	0.6	No
11.0059215	—	—	252.49	—	—	0.4	0.6	No
11.0059215	—	—	252.26	—	—	0.4	0.6	No
11.0059215	—	—	252.03	—	—	0.4	0.6	No
11.0059215	—	—	251.85	—	—	0.4	0.6	No
11.0059215	—	—	252.09	—	—	0.4	0.6	No
9.074667	—	—	252.59	—	—	0.4	0.6	No
9.08378625	—	—	252.75	—	—	0.4	0.6	No
11.8813695	—	—	251.83	—	—	0.4	0.6	No
11.9502705	—	—	251.86	—	—	0.4	0.6	No
12.01410525	—	—	251.93	—	—	0.4	0.6	No
12.14988075	—	—	251.9	—	—	0.4	0.6	No
9.074667	—	—	251.41	—	—	0.4	0.6	No
12.01410525	—	—	251.48	—	—	0.4	0.6	No
11.952297	—	—	251.31	—	—	0.4	0.6	No
11.91278025	—	—	251.48	—	—	0.4	0.6	No
12.14988075	—	—	250.66	—	—	0.4	0.6	No
12.14988075	—	—	250.89	—	—	0.4	0.6	No
13.05167325	—	—	248.18	—	—	0.4	0.6	No
13.08207075	—	—	248.18	—	—	0.4	0.6	No
13.6444245	—	—	242.16	—	—	0.4	0.6	No
13.909896	—	—	242.16	—	—	0.4	0.6	No
13.909896	—	—	242.23	—	—	0.4	0.6	No
13.8713925	—	—	242.2	—	—	0.4	0.6	No
13.88659125	—	—	242.03	—	—	0.4	0.6	No
14.29189125	—	—	235.87	—	—	0.4	0.6	No
14.32228875	—	—	235.9	—	—	0.4	0.6	No
14.30709	—	—	235.9	—	—	0.4	0.6	No
14.30709	—	—	235.83	—	—	0.4	0.6	No
3.611223	—	—	233.97	—	—	0.4	0.6	No
3.611223	—	—	234.4	—	—	0.4	0.6	No
9.743412	—	—	240.18	—	—	0.3	0.7	No
9.743412	—	—	240.01	—	—	0.3	0.7	No
11.60272575	—	—	239.51	—	—	0.3	0.7	No
11.67162675	—	—	239.51	—	—	0.3	0.7	No
11.63312325	—	—	239.35	—	—	0.3	0.7	No
11.63312325	—	—	239.51	—	—	0.3	0.7	No
11.648322	—	—	239.51	—	—	0.3	0.7	No
11.66352075	—	—	239.51	—	—	0.3	0.7	No
10.77591375	—	—	241.01	—	—	0.3	0.7	No
10.77591375	—	—	240.84	—	—	0.3	0.7	No
11.05354425	—	—	240.61	—	—	0.3	0.7	No
11.05354425	—	—	240.71	—	—	0.3	0.7	No
10.432422	—	—	240.84	—	—	0.3	0.7	No
10.432422	—	—	240.94	—	—	0.3	0.7	No
9.123303	—	—	240.84	—	—	0.3	0.7	No
9.123303	—	—	241.18	—	—	0.3	0.7	No
12.91387125	—	—	235.22	—	—	0.3	0.7	No
13.05167325	—	—	235.22	—	—	0.3	0.7	No
13.7416965	—	—	233.08	—	—	0.3	0.7	No
13.8105975	—	—	233.74	—	—	0.3	0.7	No
5.333748	—	—	232.23	—	—	0.3	0.7	No
5.333748	—	—	232.07	—	—	0.3	0.7	No

Data summarised from TABLE I, II, III, IV, and V of Booth30 [76]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{O_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{O_2}}$	Usable Data Point?
10.5033495	—	—	228.29	—	—	0.2	0.8	No
10.5033495	—	—	228.22	—	—	0.2	0.8	No
11.1923595	—	—	223.25	—	—	0.2	0.8	No
11.2612605	—	—	223.31	—	—	0.2	0.8	No
11.1923595	—	—	223.21	—	—	0.2	0.8	No
11.2612605	—	—	223.25	—	—	0.2	0.8	No
10.19228175	—	—	224.39	—	—	0.2	0.8	No
10.19228175	—	—	224.92	—	—	0.2	0.8	No
10.19228175	—	—	224.42	—	—	0.2	0.8	No
10.19228175	—	—	223.28	—	—	0.2	0.8	No
10.8073245	—	—	223.38	—	—	0.2	0.8	No
5.333748	—	—	219.58	—	—	0.2	0.8	No
5.333748	—	—	219.65	—	—	0.2	0.8	No
11.7840975	—	—	221.09	—	—	0.2	0.8	No
11.7840975	—	—	220.99	—	—	0.2	0.8	No
12.8338245	—	—	215.27	—	—	0.2	0.8	No
12.8946195	—	—	215.27	—	—	0.2	0.8	No
3.509898	—	—	214.76	—	—	0.2	0.8	No
7.056273	—	—	213.25	—	—	0.2	0.8	No
13.14083925	—	—	212.89	—	—	0.2	0.8	No
13.103349	—	—	212.89	—	—	0.2	0.8	No
13.11854775	—	—	212.82	—	—	0.2	0.8	No
13.20974025	—	—	212.17	—	—	0.2	0.8	No
13.14083925	—	—	211.88	—	—	0.2	0.8	No
13.20974025	—	—	210.58	—	—	0.2	0.8	No
13.20974025	—	—	210.41	—	—	0.2	0.8	No
14.26554675	—	—	210.58	—	—	0.2	0.8	No
13.20974025	—	—	212.76	—	—	0.2	0.8	No
13.27053525	—	—	212.76	—	—	0.2	0.8	No
13.20974025	—	—	211.13	—	—	0.2	0.8	No
13.19960775	—	—	211.06	—	—	0.2	0.8	No
13.19960775	—	—	210.84	—	—	0.2	0.8	No
7.056273	—	—	212.88	—	—	0.2	0.8	No
7.056273	—	—	213.25	—	—	0.2	0.8	No
7.056273	—	—	213.08	—	—	0.2	0.8	No
7.056273	—	—	209.04	—	—	0.1	0.9	No
7.056273	—	—	208.07	—	—	0.1	0.9	No
8.778798	—	—	207.91	—	—	0.1	0.9	No
8.778798	—	—	207.84	—	—	0.1	0.9	No
8.778798	—	—	207.98	—	—	0.1	0.9	No
10.501323	—	—	205.92	—	—	0.1	0.9	No
10.501323	—	—	205.89	—	—	0.1	0.9	No
10.501323	—	—	205.79	—	—	0.1	0.9	No
13.946373	—	—	202.18	—	—	0.1	0.9	No
13.946373	—	—	202.15	—	—	0.1	0.9	No

Continued: Data summarised from TABLE I, II, III, IV, and V of Booth30 [76]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{O_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{O_2}}$	Usable Data Point?
0.93118	—	—	223.75	0.9960	0.0040	0.7778	0.2222	Vol. Est.
1.42666	—	—	223.75	0.9878	0.0122	0.5539	0.4461	Vol. Est.
2.59392	—	—	223.75	0.9694	0.0306	0.3547	0.6453	Vol. Est.
3.42479	—	—	223.75	0.9574	0.0426	0.2899	0.7101	Vol. Est.
5.04599	—	—	223.75	0.9244	0.0756	0.2229	0.7771	Vol. Est.
7.75136	—	—	223.75	0.8567	0.1433	0.1863	0.8137	Vol. Est.
8.71395	—	—	223.75	0.8192	0.1808	—	—	No
11.85503	—	—	223.75	0.6944	0.3056	0.2030	0.7970	Vol. Est.
12.72642	—	—	223.75	0.6587	0.3413	0.2192	0.7808	Vol. Est.
13.78020	—	—	223.75	0.6071	0.3929	0.2887	0.7113	Vol. Est.
14.23616	—	—	223.75	0.5538	0.4462	0.3760	0.6240	Vol. Est.

Data summarised from Table I of Fredenslund72 [123]

P (MPa)	v_{Bub} ($\mathrm{m^3 mol^{-1}}$)	v_{Dew} ($\mathrm{m^3 mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{O_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{O_2}}$	Usable Data Point?
1.01325	—	—	223.15	0.992	0.008	0.688	0.312	Vol. Est.
2.02650	—	—	223.15	0.975	0.025	0.383	0.617	Vol. Est.
3.03975	—	—	223.15	0.951	0.049	0.288	0.712	Vol. Est.
4.05300	—	—	223.15	0.929	0.071	0.239	0.761	Vol. Est.
5.06625	—	—	223.15	0.904	0.096	0.211	0.789	Vol. Est.
6.07950	—	—	223.15	0.883	0.117	0.191	0.809	Vol. Est.
7.09275	—	—	223.15	0.85	0.15	0.186	0.814	Vol. Est.
8.10600	—	—	223.15	0.811	0.189	0.182	0.818	Vol. Est.
9.11925	—	—	223.15	0.78	0.22	0.18	0.82	Vol. Est.
10.13250	—	—	223.15	0.733	0.267	0.181	0.819	Vol. Est.
11.14575	—	—	223.15	0.707	0.293	0.203	0.797	Vol. Est.
12.15900	—	—	223.15	0.666	0.334	0.22	0.78	Vol. Est.
13.17225	—	—	223.15	0.607	0.393	0.238	0.762	Vol. Est.
1.01325	—	—	233.15	—	—	0.882	0.118	No
2.02650	—	—	233.15	0.979	0.021	0.581	0.419	Vol. Est.
3.03975	—	—	233.15	0.959	0.041	0.411	0.589	Vol. Est.
4.05300	—	—	233.15	0.936	0.064	0.349	0.651	Vol. Est.
5.06625	—	—	233.15	0.913	0.087	0.305	0.695	Vol. Est.
6.07950	—	—	233.15	0.88	0.12	0.277	0.723	Vol. Est.
7.09275	—	—	233.15	0.859	0.141	0.259	0.741	Vol. Est.
8.10600	—	—	233.15	0.833	0.167	0.243	0.757	Vol. Est.
9.11925	—	—	233.15	0.795	0.205	0.234	0.766	Vol. Est.
10.13250	—	—	233.15	0.752	0.248	0.233	0.767	Vol. Est.
11.14575	—	—	233.15	0.726	0.274	0.24	0.76	Vol. Est.
12.15900	—	—	233.15	0.672	0.328	0.27	0.73	Vol. Est.
13.17225	—	—	233.15	0.62	0.38	0.298	0.702	Vol. Est.
2.02650	—	—	243.15	0.99	0.01	0.725	0.275	Vol. Est.
3.03975	—	—	243.15	0.969	0.031	0.537	0.463	Vol. Est.
4.05300	—	—	243.15	0.948	0.052	0.449	0.551	Vol. Est.
5.06625	—	—	243.15	0.92	0.08	0.391	0.609	Vol. Est.
6.07950	—	—	243.15	0.896	0.104	0.356	0.644	Vol. Est.
7.09275	—	—	243.15	0.86	0.14	0.329	0.671	Vol. Est.
8.10600	—	—	243.15	0.838	0.162	0.307	0.693	Vol. Est.
9.11925	—	—	243.15	0.809	0.191	0.311	0.689	Vol. Est.
10.13250	—	—	243.15	0.764	0.236	0.306	0.694	Vol. Est.
11.14575	—	—	243.15	0.734	0.266	0.318	0.682	Vol. Est.
12.15900	—	—	243.15	0.694	0.306	0.329	0.671	Vol. Est.
2.02650	—	—	253.15	0.994	0.006	0.939	0.061	Vol. Est.
3.03975	—	—	253.15	0.97	0.03	0.698	0.302	Vol. Est.
4.05300	—	—	253.15	0.958	0.042	0.6	0.4	Vol. Est.
5.06625	—	—	253.15	0.938	0.062	0.5	0.5	Vol. Est.
6.07950	—	—	253.15	0.908	0.092	0.46	0.54	Vol. Est.
7.09275	—	—	253.15	0.875	0.125	0.44	0.56	Vol. Est.
8.10600	—	—	253.15	0.859	0.141	0.426	0.574	Vol. Est.
9.11925	—	—	253.15	0.83	0.17	0.399	0.601	Vol. Est.
10.13250	—	—	253.15	0.78	0.22	0.401	0.599	Vol. Est.
11.14575	—	—	253.15	0.745	0.255	0.399	0.601	Vol. Est.
12.15900	—	—	253.15	0.7	0.3	0.43	0.57	Vol. Est.
3.03975	—	—	263.15	0.991	0.009	0.904	0.096	Vol. Est.
4.05300	—	—	263.15	0.965	0.035	0.737	0.263	Vol. Est.
5.06625	—	—	263.15	0.944	0.056	0.654	0.346	Vol. Est.
6.07950	—	—	263.15	0.921	0.079	0.583	0.417	Vol. Est.
7.09275	—	—	263.15	0.89	0.11	0.537	0.463	Vol. Est.
8.10600	—	—	263.15	0.866	0.134	0.507	0.493	Vol. Est.
9.11925	—	—	263.15	0.838	0.162	0.505	0.495	Vol. Est.
10.13250	—	—	263.15	0.805	0.195	0.5	0.5	Vol. Est.
11.14575	—	—	263.15	0.757	0.243	0.502	0.498	Vol. Est.
12.15900	—	—	263.15	0.701	0.299	0.554	0.446	Vol. Est.
4.05300	—	—	273.15	0.99	0.01	0.901	0.099	Vol. Est.
5.06625	—	—	273.15	0.958	0.042	0.786	0.214	Vol. Est.
6.07950	—	—	273.15	0.938	0.062	0.702	0.298	Vol. Est.
7.09275	—	—	273.15	0.91	0.09	0.664	0.336	Vol. Est.
8.10600	—	—	273.15	0.874	0.126	0.628	0.372	Vol. Est.
9.11925	—	—	273.15	0.853	0.147	0.602	0.398	Vol. Est.
10.13250	—	—	273.15	0.815	0.185	0.599	0.401	Vol. Est.
11.14575	—	—	273.15	0.753	0.247	0.638	0.362	Vol. Est.
5.06625	—	—	283.15	0.972	0.028	0.885	0.115	Vol. Est.
6.07950	—	—	283.15	0.96	0.04	0.839	0.161	Vol. Est.
7.09275	—	—	283.15	0.929	0.071	0.782	0.218	Vol. Est.
8.10600	—	—	283.15	0.913	0.087	0.737	0.263	Vol. Est.
9.11925	—	—	283.15	0.885	0.115	0.706	0.294	Vol. Est.
10.13250	—	—	283.15	0.813	0.187	0.737	0.263	Vol. Est.

Data summarised from Table I of Fredenslund70 [112]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{O_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{O_2}}$	
3.48530	0.00004735	0.0004505	273.15	1.0000	0.0000	1.0000	0.0000	Yes
3.79212	0.00004750	0.0004250	273.15	0.9934	0.0066	0.9520	0.0480	Yes
4.13685	0.00004700	0.0003980	273.15	0.9859	0.0141	0.9010	0.0990	Yes
4.48159	0.00004790	0.0003690	273.15	0.9782	0.0218	0.8550	0.1450	Yes
4.82633	0.00004810	0.0003410	273.15	0.9705	0.0295	0.8150	0.1850	Yes
5.17107	0.00004834	0.0003180	273.15	0.9625	0.0375	0.7782	0.2218	Yes
5.51581	0.00004858	0.0002960	273.15	0.9545	0.0455	0.7480	0.2520	Yes
5.86054	0.00004883	0.0002760	273.15	0.9461	0.0539	0.7225	0.2775	Yes
6.20528	0.00004911	0.0002570	273.15	0.9378	0.0622	0.7008	0.2992	Yes
6.55002	0.00004941	0.0002410	273.15	0.9290	0.0710	0.6820	0.3180	Yes
6.89476	0.00004974	0.0002260	273.15	0.9199	0.0801	0.6658	0.3342	Yes
7.23950	0.00005007	0.0002120	273.15	0.9101	0.0899	0.6512	0.3488	Yes
7.58423	0.00005045	0.0002010	273.15	0.9003	0.0997	0.6383	0.3617	Yes
7.92897	0.00005086	0.0001900	273.15	0.8901	0.1099	0.6268	0.3732	Yes
8.27371	0.00005131	0.0001800	273.15	0.8795	0.1205	0.6162	0.3838	Yes
8.61845	0.00005182	0.0001710	273.15	0.8680	0.1320	0.6070	0.3930	Yes
8.96318	0.00005239	0.0001620	273.15	0.8560	0.1440	0.5991	0.4009	Yes
9.30792	0.00005300	0.0001530	273.15	0.8435	0.1565	0.5940	0.4060	Yes
9.65266	0.00005368	0.0001440	273.15	0.8300	0.1700	0.5915	0.4085	Yes
9.99740	0.00005445	0.0001350	273.15	0.8165	0.1835	0.5915	0.4085	Yes
10.34214	0.00005540	0.0001260	273.15	0.8020	0.1980	0.5935	0.4065	Yes
10.68687	0.00005650	0.0001170	273.15	0.7861	0.2139	0.5980	0.4020	Yes
11.03161	0.00005795	0.0001080	273.15	0.7685	0.2315	0.6080	0.3920	Yes
11.37635	0.00006040	0.0000998	273.15	0.7485	0.2515	0.6250	0.3750	Yes
11.54872	0.00006230	0.0000938	273.15	0.7340	0.2660	0.6405	0.3595	Yes
11.74177	0.00007600	0.0000760	273.15	0.6880	0.3120	0.6880	0.3120	Yes

Data summarised from Table IV of Muirbrook64 [54]

P (MPa)	v_{Bub} ($\mathrm{m^3mol^{-1}}$)	v_{Dew} ($\mathrm{m^3mol^{-1}}$)	T(K)	$x_{\mathrm{CO_2}}$	$x_{\mathrm{O_2}}$	$y_{\mathrm{CO_2}}$	$y_{\mathrm{O_2}}$	Usable Data Point?
6.028838095	—	—	273.15	0.9199	0.0801	0.6980	0.3020	Vol. Est.
6.099765602	—	—	273.15	0.9370	0.0630	0.6980	0.3020	Vol. Est.
6.018705594	—	—	273.15	0.9397	0.0603	0.7020	0.2980	Vol. Est.
5.319563025	—	—	273.15	0.9568	0.0432	0.7460	0.2540	Vol. Est.
6.971160688	—	—	273.15	0.9157	0.0843	0.6470	0.3530	Vol. Est.
8.491035838	—	—	273.15	0.8707	0.1293	0.5930	0.4070	Vol. Est.
9.42322593	—	—	273.15	0.8400	0.1600	0.5795	0.4205	Vol. Est.
10.40607853	—	—	273.15	0.8015	0.1985	0.5780	0.4220	Vol. Est.
11.1052211	—	—	273.15	0.7630	0.2370	0.6010	0.3990	Vol. Est.
13.87139387	—	—	232.85	0.5980	0.4020	0.2370	0.7630	Vol. Est.
12.39204872	—	—	232.85	0.6690	0.3310	—	—	No
12.53390374	—	—	232.85	0.6600	0.3400	0.2800	0.7200	Vol. Est.
11.1457511	—	—	232.85	0.7240	0.2760	0.2470	0.7530	Vol. Est.
9.463755934	—	—	232.85	0.7830	0.2170	0.2320	0.7680	Vol. Est.
7.771628267	—	—	232.85	0.8355	0.1645	0.2300	0.7700	Vol. Est.
13.48635883	—	—	232.85	0.5970	0.4030	0.2930	0.7070	Vol. Est.
14.77318646	—	—	232.85	0.4690	0.5310	—	—	No
14.87451147	—	—	232.85	—	—	0.4560	0.5440	No
14.29695891	—	—	232.85	0.5030	0.4970	0.3830	0.6170	Vol. Est.
5.917380584	—	—	232.85	0.8870	0.1130	0.2260	0.7740	Vol. Est.
7.275135718	—	—	232.85	—	—	0.2300	0.7700	No
4.924395486	—	—	232.85	—	—	0.2510	0.7490	No
3.789555374	—	—	232.85	—	—	0.2840	0.7160	No
2.664847763	—	—	232.85	—	—	0.4470	0.5530	No
3.85035038	—	—	232.85	—	—	0.3290	0.6710	No
2.188620216	—	—	218.15	0.9670	0.0330	0.2960	0.7040	Vol. Est.
3.941542889	—	—	218.15	0.9280	0.0720	0.1880	0.8120	Vol. Est.
5.907248083	—	—	218.15	0.8810	0.1190	0.1530	0.8470	Vol. Est.
7.883085778	—	—	218.15	0.8260	0.1740	0.1470	0.8530	Vol. Est.
9.717068459	—	—	218.15	0.7660	0.2340	0.1490	0.8510	Vol. Est.
11.82462867	—	—	218.15	0.6880	0.3120	0.1780	0.8220	Vol. Est.
13.01013128	—	—	218.15	0.6180	0.3820	0.2110	0.7890	Vol. Est.
14.02338138	—	—	218.15	0.5320	0.4680	0.2640	0.7360	Vol. Est.

Data summarised from TABLE 1 of Zenner63 [103]

7.1.6 Carbon Dioxide–Oxygen Density Data

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{O_2}	Usable Data Point?
1.003	0.002413887	303.22	0.9393	0.0607	Yes
2.004	0.001157555	303.22	0.9393	0.0607	Yes
3.000	0.000725096	303.22	0.9393	0.0607	Yes
4.000	0.000510389	303.22	0.9393	0.0607	Yes
5.002	0.000377868	303.22	0.9393	0.0607	Yes
6.003	0.000284668	303.22	0.9393	0.0607	Yes
7.000	0.000212568	303.22	0.9393	0.0607	Yes
8.001	0.000149399	303.22	0.9393	0.0607	Yes
9.002	9.38565E-05	303.22	0.9393	0.0607	Yes
10.001	7.35358E-05	303.22	0.9393	0.0607	Yes
11.002	6.63849E-05	303.22	0.9393	0.0607	Yes
12.004	6.25647E-05	303.22	0.9393	0.0607	Yes
13.000	5.99933E-05	303.22	0.9393	0.0607	Yes
14.000	5.82109E-05	303.22	0.9393	0.0607	Yes
15.002	5.68231E-05	303.22	0.9393	0.0607	Yes
16.001	5.56647E-05	303.22	0.9393	0.0607	Yes
17.001	5.46871E-05	303.22	0.9393	0.0607	Yes
18.001	5.37799E-05	303.22	0.9393	0.0607	Yes
19.006	5.30034E-05	303.22	0.9393	0.0607	Yes
20.003	5.23691E-05	303.22	0.9393	0.0607	Yes
1.000	0.002577784	323.18	0.9393	0.0607	Yes
2.003	0.001243349	323.18	0.9393	0.0607	Yes
3.003	0.000797365	323.18	0.9393	0.0607	Yes
4.002	0.000572122	323.18	0.9393	0.0607	Yes
5.001	0.000435729	323.18	0.9393	0.0607	Yes
6.001	0.000343092	323.18	0.9393	0.0607	Yes
7.003	0.000275693	323.18	0.9393	0.0607	Yes
8.001	0.000223883	323.18	0.9393	0.0607	Yes
9.001	0.000182289	323.18	0.9393	0.0607	Yes
10.001	0.000148421	323.18	0.9393	0.0607	Yes
11.000	0.000121552	323.18	0.9393	0.0607	Yes
12.001	0.000101589	323.18	0.9393	0.0607	Yes
13.000	8.80984E-05	323.18	0.9393	0.0607	Yes
14.000	7.96031E-05	323.18	0.9393	0.0607	Yes
15.001	7.37514E-05	323.18	0.9393	0.0607	Yes
16.001	6.97203E-05	323.18	0.9393	0.0607	Yes
17.001	6.67886E-05	323.18	0.9393	0.0607	Yes
18.000	6.4459E-05	323.18	0.9393	0.0607	Yes
19.001	6.25936E-05	323.18	0.9393	0.0607	Yes
20.003	6.10073E-05	323.18	0.9393	0.0607	Yes
1.020	0.002834381	343.15	0.9393	0.0607	Yes
2.006	0.0013649	343.15	0.9393	0.0607	Yes
3.001	0.000886542	343.15	0.9393	0.0607	Yes
4.010	0.000643871	343.15	0.9393	0.0607	Yes
5.002	0.000489051	343.15	0.9393	0.0607	Yes
6.001	0.000391082	343.15	0.9393	0.0607	Yes
7.001	0.000320933	343.15	0.9393	0.0607	Yes
8.003	0.000268726	343.15	0.9393	0.0607	Yes
9.001	0.000227939	343.15	0.9393	0.0607	Yes
10.003	0.000194951	343.15	0.9393	0.0607	Yes
11.000	0.000168225	343.15	0.9393	0.0607	Yes
12.001	0.000146601	343.15	0.9393	0.0607	Yes
13.001	0.000128816	343.15	0.9393	0.0607	Yes
14.002	0.000114536	343.15	0.9393	0.0607	Yes
15.003	0.000103397	343.15	0.9393	0.0607	Yes
16.001	9.45847E-05	343.15	0.9393	0.0607	Yes
17.001	8.76435E-05	343.15	0.9393	0.0607	Yes
18.002	8.236E-05	343.15	0.9393	0.0607	Yes
19.002	7.81584E-05	343.15	0.9393	0.0607	Yes
20.002	7.47358E-05	343.15	0.9393	0.0607	Yes
1.004	0.003147709	363.15	0.9393	0.0607	Yes
2.010	0.001457763	363.15	0.9393	0.0607	Yes
3.011	0.000960732	363.15	0.9393	0.0607	Yes
4.006	0.000690617	363.15	0.9393	0.0607	Yes
5.000	0.000531185	363.15	0.9393	0.0607	Yes
6.000	0.000429588	363.15	0.9393	0.0607	Yes
7.003	0.000358881	363.15	0.9393	0.0607	Yes
8.002	0.000304431	363.15	0.9393	0.0607	Yes
9.004	0.000262627	363.15	0.9393	0.0607	Yes
10.002	0.000229012	363.15	0.9393	0.0607	Yes
11.001	0.000201795	363.15	0.9393	0.0607	Yes
12.000	0.000179306	363.15	0.9393	0.0607	Yes
13.001	0.00016046	363.15	0.9393	0.0607	Yes
14.000	0.00014469	363.15	0.9393	0.0607	Yes
15.003	0.000131461	363.15	0.9393	0.0607	Yes
16.001	0.000120483	363.15	0.9393	0.0607	Yes
17.001	0.000111317	363.15	0.9393	0.0607	Yes
18.001	0.000103687	363.15	0.9393	0.0607	Yes
19.001	9.73328E-05	363.15	0.9393	0.0607	Yes
20.003	9.18585E-05	363.15	0.9393	0.0607	Yes

Data summarised from Table 6 and 7 of Mantovani12 [109]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{O_2}	Usable Data Point?
1.009	0.003376052	383.14	0.9393	0.0607	Yes
2.002	0.001594143	383.14	0.9393	0.0607	Yes
3.001	0.001022225	383.14	0.9393	0.0607	Yes
4.001	0.000744683	383.14	0.9393	0.0607	Yes
5.002	0.000581265	383.14	0.9393	0.0607	Yes
6.001	0.000472758	383.14	0.9393	0.0607	Yes
7.000	0.00039631	383.14	0.9393	0.0607	Yes
8.001	0.000339193	383.14	0.9393	0.0607	Yes
9.000	0.000294669	383.14	0.9393	0.0607	Yes
10.000	0.000259121	383.14	0.9393	0.0607	Yes
11.000	0.000230341	383.14	0.9393	0.0607	Yes
12.002	0.000206523	383.14	0.9393	0.0607	Yes
13.002	0.000186693	383.14	0.9393	0.0607	Yes
14.002	0.000169956	383.14	0.9393	0.0607	Yes
15.001	0.000155597	383.14	0.9393	0.0607	Yes
16.000	0.000143448	383.14	0.9393	0.0607	Yes
1.001	0.002503509	303.22	0.8709	0.1291	Yes
2.001	0.001180414	303.22	0.8709	0.1291	Yes
3.000	0.000746082	303.22	0.8709	0.1291	Yes
4.001	0.000530545	303.22	0.8709	0.1291	Yes
5.002	0.000398756	303.22	0.8709	0.1291	Yes
6.001	0.000309359	303.22	0.8709	0.1291	Yes
7.001	0.000242529	303.22	0.8709	0.1291	Yes
8.002	0.000190666	303.22	0.8709	0.1291	Yes
9.003	0.000148408	303.22	0.8709	0.1291	Yes
10.000	0.000114954	303.22	0.8709	0.1291	Yes
11.003	9.35623E-05	303.22	0.8709	0.1291	Yes
12.003	8.09863E-05	303.22	0.8709	0.1291	Yes
13.002	7.35001E-05	303.22	0.8709	0.1291	Yes
14.004	6.86525E-05	303.22	0.8709	0.1291	Yes
15.001	6.51449E-05	303.22	0.8709	0.1291	Yes
16.003	6.26099E-05	303.22	0.8709	0.1291	Yes
17.003	6.06296E-05	303.22	0.8709	0.1291	Yes
18.005	5.89879E-05	303.22	0.8709	0.1291	Yes
19.001	5.76081E-05	303.22	0.8709	0.1291	Yes
20.001	5.64756E-05	303.22	0.8709	0.1291	Yes
1.004	0.002709605	323.18	0.8709	0.1291	Yes
2.002	0.001277746	323.18	0.8709	0.1291	Yes
3.004	0.000818891	323.18	0.8709	0.1291	Yes
4.006	0.000590453	323.18	0.8709	0.1291	Yes
5.001	0.000454064	323.18	0.8709	0.1291	Yes
6.001	0.000360989	323.18	0.8709	0.1291	Yes
7.002	0.000294265	323.18	0.8709	0.1291	Yes
8.002	0.000243712	323.18	0.8709	0.1291	Yes
9.002	0.000203887	323.18	0.8709	0.1291	Yes
10.001	0.000172089	323.18	0.8709	0.1291	Yes
11.000	0.000146463	323.18	0.8709	0.1291	Yes
12.001	0.000126071	323.18	0.8709	0.1291	Yes
13.000	0.000110259	323.18	0.8709	0.1291	Yes
14.001	9.82086E-05	323.18	0.8709	0.1291	Yes
15.001	8.92738E-05	323.18	0.8709	0.1291	Yes
16.002	8.25996E-05	323.18	0.8709	0.1291	Yes
17.001	7.75544E-05	323.18	0.8709	0.1291	Yes
18.001	7.35497E-05	323.18	0.8709	0.1291	Yes
19.003	7.04477E-05	323.18	0.8709	0.1291	Yes
20.001	6.78809E-05	323.18	0.8709	0.1291	Yes
1.000	0.002975439	343.15	0.8709	0.1291	Yes
2.003	0.001386207	343.15	0.8709	0.1291	Yes
3.001	0.000890136	343.15	0.8709	0.1291	Yes
4.001	0.000653424	343.15	0.8709	0.1291	Yes
5.001	0.000504569	343.15	0.8709	0.1291	Yes
6.006	0.000405032	343.15	0.8709	0.1291	Yes
7.003	0.00033541	343.15	0.8709	0.1291	Yes
8.005	0.00028312	343.15	0.8709	0.1291	Yes
9.000	0.000242778	343.15	0.8709	0.1291	Yes
10.001	0.000210446	343.15	0.8709	0.1291	Yes
11.001	0.000184158	343.15	0.8709	0.1291	Yes
12.002	0.000162636	343.15	0.8709	0.1291	Yes
13.002	0.000144814	343.15	0.8709	0.1291	Yes
14.003	0.00013012	343.15	0.8709	0.1291	Yes
15.001	0.000118028	343.15	0.8709	0.1291	Yes
16.003	0.000108119	343.15	0.8709	0.1291	Yes
17.001	0.000100065	343.15	0.8709	0.1291	Yes
18.001	9.35314E-05	343.15	0.8709	0.1291	Yes
19.001	8.81762E-05	343.15	0.8709	0.1291	Yes
20.001	8.37317E-05	343.15	0.8709	0.1291	Yes

Continued: Data summarised from Table 6 and 7 of Mantovani12 [109]

P (MPa)	v (m^3mol^{-1})	T(K)	x_{CO_2}	x_{O_2}	Usable Data Point?
1.000	0.003185259	363.15	0.8709	0.1291	Yes
2.002	0.001473777	363.15	0.8709	0.1291	Yes
3.002	0.00095608	363.15	0.8709	0.1291	Yes
4.000	0.000701231	363.15	0.8709	0.1291	Yes
5.002	0.000547794	363.15	0.8709	0.1291	Yes
6.003	0.000444788	363.15	0.8709	0.1291	Yes
7.002	0.0003718	363.15	0.8709	0.1291	Yes
8.003	0.000317692	363.15	0.8709	0.1291	Yes
9.000	0.00027555	363.15	0.8709	0.1291	Yes
10.003	0.000241714	363.15	0.8709	0.1291	Yes
11.000	0.000214464	363.15	0.8709	0.1291	Yes
12.000	0.000191907	363.15	0.8709	0.1291	Yes
13.000	0.000173149	363.15	0.8709	0.1291	Yes
14.000	0.000157257	363.15	0.8709	0.1291	Yes
15.002	0.000143833	363.15	0.8709	0.1291	Yes
16.001	0.000132475	363.15	0.8709	0.1291	Yes
17.001	0.000122904	363.15	0.8709	0.1291	Yes
18.000	0.000114765	363.15	0.8709	0.1291	Yes
19.001	0.000107724	363.15	0.8709	0.1291	Yes
20.003	0.000101639	363.15	0.8709	0.1291	Yes
1.002	0.003586107	383.14	0.8709	0.1291	Yes
2.003	0.001638731	383.14	0.8709	0.1291	Yes
3.003	0.001046574	383.14	0.8709	0.1291	Yes
4.004	0.0007627	383.14	0.8709	0.1291	Yes
5.005	0.000596174	383.14	0.8709	0.1291	Yes
6.001	0.000486754	383.14	0.8709	0.1291	Yes
7.003	0.000408933	383.14	0.8709	0.1291	Yes
8.003	0.000351021	383.14	0.8709	0.1291	Yes
9.000	0.000306213	383.14	0.8709	0.1291	Yes
10.002	0.000270271	383.14	0.8709	0.1291	Yes
11.000	0.000241179	383.14	0.8709	0.1291	Yes
12.001	0.000217173	383.14	0.8709	0.1291	Yes
13.000	0.000197165	383.14	0.8709	0.1291	Yes
14.003	0.000180226	383.14	0.8709	0.1291	Yes
15.001	0.000165734	383.14	0.8709	0.1291	Yes
16.002	0.000153322	383.14	0.8709	0.1291	Yes
17.001	0.000142635	383.14	0.8709	0.1291	Yes
18.000	0.000133215	383.14	0.8709	0.1291	Yes
19.001	0.000125113	383.14	0.8709	0.1291	Yes
20.001	0.000118137	383.14	0.8709	0.1291	Yes

Continued: Data summarised from Table 6 and 7 of Mantovani12 [109]

7.2 Published Paper

Presented over the following eight pages our paper [40] published in May 2013 as part of the work done for this EngD. Its contents are broadly aligned with those which are presented in Chapter 4.

Bibliography

[1] Nicholas Stern. *The Economics of Climate Change: The Stern Review*. Cambridge University Press, January 2007.

[2] Bert Metz, Ogunlade Davidson, Heleen de Coninck, Manuela Loos, and Leo Meyer (Eds.). IPCC Special Report on Carbon Dioxide Capture and Storage, 2005.

[3] Lauren Elmegreen Rafelski, Stephen C. Piper, and Ralph F. Keeling. Climate Effects on Atmospheric Carbon Dioxide over the Last Century. *Tellus Series B–Chemical and Physical Meterology*, 61(5):pp. 718—731, November 2009.

[4] Ralph Keeling. http://www.theguardian.com/environment/2013/may/14/record-400ppm-co2-carbon-emissions. (Online), Tuesday 14th May 2013.

[5] Department of Trade and Industry. *Energy White Paper: Our Energy Future — Creating a Low Carbon Economy*. The Stationary Office, 2003.

[6] Department of Trade and Industry. *Energy White Paper: Meeting the Energy Challenge*. The Stationary Office, 2007.

[7] Jorge Leis and Kurt Zenz House. The Green Edge: Why Carbon Competitiveness Matters. Bain and Company, 2010.

[8] Sarah M. Forbes, Preeti Verma, Thomas E. Curry, S. Julio Friedmann, and Sarah M. Wade. *CCS Guidelines: Guidelines for Carbon Dioxide Capture, Transport, and Storage*. World Resources Institute, 2008.

[9] John Davison. CO_2 Capture Ready Plants. (Presentation Slides), March 2008. Presentation at 3rd Oxy–Combustion Network Meeting, Yokohama, Japan.

[10] Stephen Tindale and Simon Tilford. Carbon Capture and Storage: What the EU Needs to do. Centre for European Reform, 2010.

[11] Bp energy outlook 2030. Technical report, BP, 2013.

[12] The Guardian. Carbon Targets Pledged at Copenhagen 'Fail to Keep Temperature Rise to 2C'. (Newspaper Article), Friday 12th February 2010.

[13] Department of Energy and Climate Change. UK Renewable Energy Roadmap, July 2011.

[14] Charles Perrow. *Normal Accidents: Living with High–Risk Technologies*. Princeton University Press, 1999.

[15] Danielle Demetriou. http://www.telegraph.co.uk/news/worldnews/asia/japan/8953574/japan-earthquake-tsunami-and-fukushima-nuclear-disaster-2011-review.html. (Online), Monday 19th December 2011.

[16] Sara Vaughan. Energy Efficiency — Is It Ever Going to Happen? (Presentation Slides), Thursday 7th October 2010.

[17] Brendan Beck. CCS Technology: Capture, Transport and Storage of CO_2. (Presentation Slides), September 2007.

[18] A. Rao. An Assessment of CO_2 Compression Options for Near Zero Emission Power Plants. (Presentation Slides), May 2007. Presentation at ASME Turbo Expo, May 2007.

[19] R. Dennis and M. Klein. CO_2 Compression Opportunities in Fossil Fuelled Power Plants. (Presentation Slides), May 2007. Presentation at ASME Turbo Expo, May 2007.

[20] P. N. Seevam, J. M. Race, and M. J. Downie. Theme A6: CO_2 Transport Infrastructure. (Presentation Slides), 2008.

[21] DG Environment News Alert Service. Transport Challenges for CCS (Special Issue 3). Science for Environmental Policy, April 2008.

[22] J. Barrie, K. Brown, P. R. Hatcher, and H. U. Schellhase. Carbon Dioxide Pipelines: A Preliminary Review of Design and Risks. 2003.

[23] Recommended Practice: DNV—RP–J202: Design and Operation of CO_2 Pipelines. Det Norske Veritas, April 2010.

[24] Audun Aspelund and Truls Gundersen. A Liquefied Energy Chain for Transport and Utilization of Natural Gas for Power Production with CO_2 Capture and Storage — Part 4: Sensitivity Analysis of Transport Pressures and Benchmarking with Conventional Technology for Gas Transport. *Applied Energy*, 86:pp. 815—825, 2009.

[25] Sandrine Decarre, Julien Berthiaud, Nicolas Butin, and Jean-Louis Guillaume-Combecave. CO_2 Maritime Transportation. *International Journal of Greenhouse Gas Control*, 4(5):pp. 857—864, 2010.

[26] Georg Hegerland, Terje Jørgensen, and John O. Pande. Liquefaction and Handling of Large Amounts of CO_2 for EOR. 2004.

[27] NWT. http://groen.blog.nl/files/2009/03/co2-opslag-cover-nwt.jpg. (Online).

[28] Mitsubishi Heavy Industries Ltd. Ship transport of CO_2: Report Number PH4/30. Technical report, IEA Greenhouse Gas R & D Programme, July 2004.

[29] Audun Aspelund and Kristin Jordal. A Study of the Interface Between CO_2 Capture and Transport. 2006.

[30] Audun Aspelund and Kristin Jordal. Gas Conditioning — The Interface Between CO_2 Capture and Transport.

[31] Erika de Visser, Chris Hendriks, Maria Barrio, Mona J. Mølnvik, Gelein de Koeijer, Stefan Liljemark, and Yann Le Gallo. Dynamis CO_2 Quality Recommendations. *International Journal of Greenhouse Gas Control*, 2:pp. 478—484, 2008. 4th Trondheim Conference on CO2 Capture, Transport and Storage, Trondheim, Norway, OCT 16-17, 2007.

[32] Sam Holloway, Anhar Karimjee, Makoto Akai, Riitta Pipatti, and Kristin Rypdal. *2006 IPCC Guidelines for National Greenhouse Gas Inventories. Chapter 5: Carbon Dioxide Transport, Injection and Geological Storage*, chapter 5. Volume 2: Energy, 2006.

[33] Otto Redlich and J. N. S. Kwong. On the Thermodynamics of Solutions. V. An Equation of State. Fugacities of Gasseous Solutions. In *Proceedings of the Symposium on Thermoynamics and Molecular Structure of Solution, Portland, Oregon*, pages pp. 233—244. Shell Development Company, September 1948.

[34] Ding-Yu Peng and Donald B. Robinson. A New Two–Constant Equation of State. *Ind. Eng. Chem. Fundam.*, 15(1):pp. 59—64, 1976.

[35] R. Span and W. Wagner. A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple–Point Temperature to 1100 K at Pressures up to 800 MPa. *J. Phys. Chem. Ref. Data*, 25(6):pp. 1509—1596, 2996.

[36] Equation of State Prediction of Carbon Dioxide Properties (Document Number KCP–GNS–FAS–DRP–0001). Technical report, E.On UK, 2012.

[37] Haroun Mahgerefteh, Solomon Brown, and Garfield Denton. Modelling the Impact of Stream Impurities on Ductile Fractures in CO_2 Pipelines. *Chemical Engineering Science*, 2012.

[38] H. Mahgerefteh, S. Brown, and S. Martynov. A Study of the Effects of Friction, Heat Transfer, and Stream Impurities on the Decompression Behavior in CO_2 Pipelines. *Greenhoue Gases Science and Technology*, 2012.

[39] Sean T. McCoy and Edward S. Rubin. An Engineering–Economic Model of Pipeline Transport of CO_2 with Application to Carbon Capture and Storage. *International Journal of Greenhouse Gas Control*, 2:pp. 219—229, 2008.

[40] Thomas A. Demetriades, Trevor C. Drage, and Richard S. Graham. Developing a New Equation of State for Carbon Capture and Storage Pipeline Transport. *Proc IMechE Part E: J. Process Mechanical Engineering*, 227(2):pp. 117—124, 2013.

[41] Trevor Drage, Jie Ke, Yolanda Sanchez-Vicente, Andrew Parrott, Richard Graham, Thomas Demetriades, Mike George, and Martyn Poliakoff. Measuring the Physical Properties of CO_2 Mixtures for CCS: An Update on Experimental Results and Comparison with Equations of State. 2012. (In preparation).

[42] M. Downie, J. Race, and P. Seevam. Some Technical Aspects of CO_2 Transport for Large Scale CCS. (Presentation Slides), January 2008. Presentation at International Workshop on Power Generation with CCS in India.

[43] Carbon Capture Journal. AMEC — Developing CCS Clusters. *Carbon Capture Journal*, 15:pp. 12—13, May/June 2010.

[44] V. Vandeginste and K. Piessens. Pipeline Design for a Least–Cost Router Application for CO_2 Transport in the CO_2 Sequestration Cycle. *International Journal of Greenhouse Gas Control*, 2:pp. 571—581, 2008. 4th Trondheim Conference on CO2 Capture, Transport and Storage, Trondheim, Norway, OCT 16-17, 2007.

[45] A. N. Sabirzyanov, A. P. Il'in, A. R. Akhunov, and F. M. Gumerov. Solubility of Water in Supercritical Carbon Dioxide. *High Temperature*, 40(2):pp. 203—206, 2002.

[46] W. Alan Propp, Tom E. Carleson, Chen M. Wai, Pat R. Taylor, Kirk W. Daehling, Shaoping Huang, and Masud Abdel-Latif. Corrosion in Supercritical Fluids. Technical report, Idaho National Engineering Laboratory, 1996.

[47] Alberto Mazzoldi, Tim Hill, and Jeremy Colls. A Consideration of the Jet–Mixing Effect when Modelling CO_2 Emissions from High Pressure CO_2. *Energy Procedia*, 1:pp. 1571—1578, 2009.

[48] Martin Downie, Julia Race, and Patricia Seevam. Transport of CO_2 for Carbon Capture and Storage in the UK (Report Number SPE 109060). September 2007. Presented at Offshore Europe 2007.

[49] Andreas Fredenhagen and Rudolf Eggers. The Effect of Hydrate Formation on the Pressure Release of Wet Carbon Dioxide. *Chem. Eng. Technol.*, 24(8):pp. 785—789, 2001.

[50] Torleif Holt, Erik Lindeberg, and Dag Wessel-Berg. EOR and CO_2 Disposal — Economic and Capacity Potential in the North Sea. *Energy Procedia*, 1:pp. 4159—4166, 2009.

[51] Y. Savidis and M. Bilio. Proposed Changes to the Pipeline Safety Regulations and the Broader Expectations of the Regulator for CO_2 Pipeline Design and Risk Assessment. Health and Safety Executive, July 2010. Presentation at the First International Forum on the Transportation of CO_2 by Pipeline, Newcastle, UK.

[52] http://www.chemistry-blog.com/wp-content/uploads/2009/02/phasediagramco2.png. (Online).

[53] Yashuhiko Arai, Gen-Ichi Kaminishi, and Shozaburo Saito. The Experiemntal Determination of the P–V–T–X Relations for the Carbon Dioxide–Nitrogen and the Carbon Dioxide–Methane Systems. *Journal of Chemical Engineering of Japan*, 4(2):pp. 113—122, 1971.

[54] Newell Knight Muribrook. *Experimental and Thermodynamic Study of the High–Pressure Vapor–Liquid Equilibria for the Nitrogen–Oxygen–Carbon Dioxide System.* PhD thesis, University of California, 1964.

[55] Hailong Li, Jana P. Jakobsen, Ø ivind Wilhelmsen, and Jinyue Yan. $PVTxy$ Properties of CO_2 Mixtures Relevant for CO_2 Capture, Transport and Storage: Review of Available Experimental Data and Theoretical Models. *Applied Energy*, 88:pp. 3567—3579, 2011.

[56] Antonie Oosterkamp and Joakim Ramsen. State–of–the–Art Overview of CO_2 Pipeline Transport with Relevance to Offshore Pipelines (Report Number POL–O–2007–138–A). Polytec, 2008.

[57] S. C. Page, A. G. Williamson, and I. G. Mason. Carbon Capture and Storage: Fundamental Thermodynamics and Current Technology. *Energy Policy*, 37:pp. 3314—3324, 2009.

[58] Universidade Salvador and Petroleo Brasileiro S. A. *Optimum Design of CO_2 Compression and Pipeway Transport System*, 2003.

[59] A. Aspelund, M. J. Mølnvik, and G. de Koeijer. Ship Transport of CO_2: Technical Solutions and Analysis of Costs, Energy Utilization, Exergy Efficiency and CO_2 Emissions. *Chemical Engineering Research and Design*, 84(A9, SI):pp. 847—855, 2006.

[60] Shawn P. Lawlor and Peter Baldwin. Conceptual Design of a Supersonic CO_2 Compressor (Report Number GT2005–68349). (Presentation Slides), June 2005. Presentation at ASME Turbo Expo, June 2005.

[61] Jeffrey Moore, Klaus Brun, Marybeth Nored, and Ryan Gernentz. Novel Concepts for the Compression of Large Volumes of CO_2. (Presentation Slides), May 2007. Presentation at ASME Turbo Expo, May 2007.

[62] P. Chiesa. Impact of Gas Phase Impurities on CO_2 Compression. (Presentation Slides), May 2007. Presentation at ASME Turbo Expo.

[63] H. Miller. Carbon Dioxide Compression. In *ASME Turbo Expo, May 2007*. Dresser Rand Co., July 2007.

[64] P. L. Bovon and R. Habel. CO_2 Compression Challenges. (Presentation Slides), May 2007. Presentation at ASME Turbo Expo, May 2007.

[65] Nils Markusson and Stuart Haszeldine. 'Capture Readiness' — Lock–in Problems for CCS Governance. In *Greenhouse Gas Control Technologies*, volume 1 of *Energy Procedia*, pages pp. 4625—4632, 2009. 9th International Conference on Greenhouse Gas Control Technologies, Washington, DC, NOV 16-20, 2008.

[66] Implementation of Directive 2009/31/EC on the Geological Storage of Carbon Dioxide. Technical report, CO_2 Storage Life Cycle Risk Management Framework, 2011.

[67] Wordpress. http://barendrecht.groenlinks.nl/files/imageupload/sticky. (Online).

[68] R. Steeneveldt, B. Berger, and T. A. Torp. CO_2 Capture and Storage: Closing the Knowing–Doing Gap.

[69] Clair Gough. State of the Art in Carbon Dioxide Capture and Storage in the UK: An Experts' Review. *International Journal of Greenhouse Gas Control*, 2:pp. 155—168, 2008.

[70] Zero Emissions Platform. The Costs of CO_2 Transport. Technical report, European Technology Platform for Zero Emission Fossil Fuel Power Plants, 2012.

[71] *Perry's Chemical Engineering Handbook, Eighth Edition.* McGraw–Hill, 2007.

[72] Hasan Orbey and Stanley I. Sandler. *Modeling Vapor–Liquid Equilibira: Cubic Equations of State and Their Mixing Rules.* Cambridge University Press, 1998.

[73] P. M. Chaikin and T. C. Lubensky. *Principles of Condensed Matter Physics.* Cambridge University Press, 1995.

[74] The National Institute of Standards and Technology (NIST) Database.

[75] James F. Ely, J. W. Magee, and W. M. Haynes. Research Report RR–110: Thermophysical Properties for Special High CO_2 Content Mixtures. Technical report, National Bureau of Standards, Boulder, Colorado, May 1987.

[76] Harold Simmons Booth and James Maurice Carter. The Critical Constants of Carbon Dioxide–Oxygen Mixtures. *J. Phys. Chem.*, 34(12):pp. 2801—2825, 1930.

[77] Horacio A. Duarte-Garza, James C. Holste, Kenneth R. Hall, Kenneth N. Marsh, and Bruce E. Gammon. Isochoric pVT and Phase Equilibrium Measurements for Carbon Dioxide + Nitrogen. *J. Chem. Eng. Data*, 40:pp. 704—711, 1995.

[78] G. J. Esper, O. M. Bailey, J. C. Holste, and K. R. Hall. Volumetric Behaviour of Near–Equimolar Mixtures for CO_2 + CH_4 and CO_2 + N_2. *Fluid Phase Equilibria*, 49:pp. 35—47, 1989.

[79] N. K. Muirbrook and J. M. Prausnitz. Multicomponent Vapor–Liquid Equilibria at High Pressures: Part 1. Experimental Study of the Nitrogen–Oxygen–Carbon Dioxide System at 0°C. *A. I. Ch. E. Journal*, 11(6):pp. 1092—1096, November 1965.

[80] Ho-Mu Lin, Herbert M. Sebastian, and Kwang-Chu Chao. Vapor–Liquid Equilibrium in Ternary Mixtures of Hydrogen + Carbon Dioxide + l–Methylnaphthalene. *Fluid Phase Equilibria*, 7:pp. 87—91, 1981.

[81] Jeffery C. Seitz and James G. Blencoe. Volumetric Properties for $\{ (1-x)\ CO_2 + x CH_4 \}$, $\{ (1-x) CO_2 + x N_4 \}$, and $\{ (1-x) CH_4 + x N_2 \}$, at the Pressures (19.94, 29.94, 39.94, 59.93, 79.93, and 99.93) MPa and the Temperature 673.15 k. *J. Chem. Thermodynamics*, 28:pp. 1207—1213, 1996.

[82] Donnld M. Bailey, Gunter J. Esper, James C. Holste, Kenneth R. Hall, Philip T. Eubank, Kenneth M. Marsh, and William J. Rogers. Research Report RR–122: Properties of CO_2 Mixtures with N_2 and with CH_4. Technical report, A Joint Research Report by the Gas Processors Association and the Gas Research Institute, July 1989.

[83] H. Duarte-Garza, H. B. Brugge, C.-A. Hwang, P. T. Eubank, J. C. Holste, and K. R. Hall. Research Report RR–140: Thermodynamic Properties of CO_2 + N_2 Mixtures. Technical report, A Joint Research Report by the Gas Processors Association and the Gas Research Institute, June 1995.

[84] Masahiro Yorizane, Shô shin Yoshimura, and Hirokatsu Masuoka. Das Dampf–Flü ssigkeits–Gleichgewicht bei hohem Druck Das N_2–CO_2 und das H_2–CO_2–System. *Chemical Engineering of Japan*, 34:pp. 1—14, 1970. (In German and Japanese).

[85] H. B. Brugge, C.-A. Hwang, W. J. Rogers, J. C. Holste, and K. R. Hall. Experimental Cross Virial Coefficients for Binary Mixtures of Carbon Dioxide with Nitrogen, Methane and Ethane at 300 and 320 K. *Physica A*, 156:pp. 382—416, 1989.

[86] Hunter B. Brugge, James C. Holste, Kenneth R. Hall, Bruce E. Gammon, and Kenneth N. Marsh. Densities of Carbon Dioxide + Nitrogen from 225 K to 450 K at Pressures up to 70 MPa. *J. Chem. Eng. Data*, 42:pp. 903—907, 1997.

[87] Ivan D. Mantilla, Diego E. Cristancho, Saquib Ejaz, Kenneth R. Hall, Mert Atilhan, and Gustavo A. Iglesias-Silva. P–ρ–t Data for Carbon Dioxide from (310 to 450) K up to 160 MPa. *J. Chem. Eng. Data*, 55(11):pp. 4611—4613, 2010.

[88] J. F. Ely, W. M. Haynes, and B. C. Bain. Isochoric (p, V_m, T) Measurements on CO_2 and on ($0.982CO_2$ + $0.018N_2$) from 250 to 330 K at Pressures to 35 MPa. *J. Chem. Thermodynamics*, 21:pp. 879—894, May 1989.

[89] Ivan D. Mantilla, Diego E. Cristancho, Saquib Ejaz, Kenneth R. Hall, Mert Atilhan, and Gustavo A. Iglesias-Silva. New P–ρ–t Data for Nitrogen at Temperatures from (265 to 400) K at Pressures up to 150 MPa. *J. Chem. Eng. Data*, 55(10):pp. 4227—4230, 2010.

[90] K. Bezanehtak, G. B. Combes, F. Dehghani, N. R. Foster, and D. L. Tomasko. Vapor–Liquid Equilibrium for Binary Systems of Carbon Dioxide + Methanol, Hydrogen + Methanol, and Hydrogen + Carbon Dioxide at High Pressures. *J. Chem. Eng. Data*, 47:pp. 161—168, 2002.

[91] Baigui Bian, Yanru Wang, Jun Shi, Ensheng Zhao, and Benjamin C.-Y. Lu. Simultaneous Determination of Vapor–Liquid Equilibrium and Molar Volumes for Coexisting Phases up to the Critical Temperature with a Static Method. *Fluid Phase Equilibria*, 90:pp. 177—187, 1993.

[92] Norman P. Freitag and Donald B. Robinson. Equilibrium Phase Properties of the Hydrogen–Methans–Carbon Dioxide, Hydrogen–Carbon Dioxide–*n*–Pentane and Hydrogen–*n*–Pentane Systems. *Fluid Phase Equilibria*, 31:pp. 183—201, 1986.

[93] Dimitris Bertsimas and John Tsitsiklis. Simulated Annealing. *Statistical Science*, 8(1):pp. 10—15, February 1993.

[94] William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. *Numerical Recipes in C: The Art of Scientific Computing (Second Edition)*. Cambridge University Press, 2 edition, 1992.

[95] T. S. Brown, V. G. Niesen, E. D. Sloan, and A. J. Kidnay. Vapor–Liquid Equilibria for the Binary Systems of Nitrogen, Carbon Dioxide, and *n*–Butane at Temperatures from 220 to 344 K. *Flurd Phase Equilibria*, 53:pp. 7—14, 1989.

[96] T. S. Brown, E. D. Sloan, and A. J. Kidnay. Vapor–Liquid Equilibria in the Nitrogen + Carbon Dioxide + Ethane System. *Fluid Phase Equilibria*, 51:pp. 299—313, 1989.

[97] Fahad A. Somait and Arthur J. Kidnay. Liquid–Vapor Equilibria at 270.00 K for Systems Containing Nitrogen, Methane, and Carbon Dioxide. *Journal of Chemical and Engineering Data*, 23(4):pp. 301—305, 1978.

[98] Belgin Yucelen and Arthur J. Kidnay. Vapor–Liquid Equilibria in the Nitrogen + Carbon Dioxide + Propane System from 240 to 330 K at Pressures to 15 MPa. *J. Chem. Eng. Data*, 44:pp. 926—931, 1999.

[99] I. R. Kritschewsky and V. P. Markov. The Compressibility of Gas Mixtures. *Acta Pysicochimica U. R. S. S.*, XII(1):pp. 59—66, 1940.

[100] G. Kaminishi and T. Toriumi. Vapour–Liquid Phase Equilibria in the CO_2–H_2, CO_2–N_2, and CO_2–O_2 Systems. *Kogyo Kagaku Zasshi*, 69:pp. 175—178, 1966. (In Japanese).

[101] D. S. Tsiklis. Heterogeneous Equilibria in Binary Systems. *Russian Journal of Physical Chemistry*, 20(2):pp. 181—188, 1946.

[102] Wolfram Weber, Sebastian Zeck, and Helmut Knapp. Gas Solubilities in Liquid Solvents at High Pressures: Apparatus and Results for Binary and Ternary Systems of N_2, CO_2, and CH_3OH. *Fluid Phase Equilibria*, 18:pp. 253—278, 1984.

[103] G. H. Zenner and L. I. Dana. Liquid–Vapor Equilibrium Compositions of Carbon Dioxide–Oxygen–Nitrogen Mixtures. *Chemical Engineering Progress Symposium Series*, 59(44):pp. 36—41, 1963.

[104] Masahiro Yorizane, Shoshin Yoshimura, Hirokatsu Masuoka, Yoshimori Miyano, and Yukihiko Kakimoto. New Procedure for Vapor–Liquid Equilibria. Nitrogen + Carbon Dioxide, Methane + Freon 22, and Methane + Freon 12. *J. Chem. Eng. Data*, 30(2):pp. 174—176, 1985.

[105] María Engracia Mondéjar Montagud. *Contribution to the Development and Introduction of Renewable Gaseous Fuels Through the Thermodynamic Characterization of Mixtures of their Components by using an Optimized Single Sinker Densimeter with Magnetic Suspension Coupling.* PhD thesis, University of Valladolid, 2012.

[106] Nanping Xu, Junhang Dong, Yanru Wang, and Jun Shi. High Pressure Vapor Liquid Equilibria at 293 K for Systems Containing Nitrogen, Methane and Carbon Dioxide. *Fluid Phase Equilibria*, 81:pp. 175—186, 1992.

[107] Shaoyi Jiang, Yanru Wang, and Jun Shi. Determination of Compressibility Factors and Virial Coefficients for the Systems Containing N_2, CO_2 and $CHClF_2$ by the Modified Burnett Method. *Fluid Phase Equrilibria*, 57:pp. 105—117, February 1990.

[108] Roy E. D. Haney and Harding Bliss. Compressibilities of Nitrogen–Carbon Dioxide Mixtures. *Industrial and Engineering Chemistry*, 36(11):pp. 985—989, November 1944.

[109] Mario Mantovani, Paolo Chiesa, Gianluca Valenti, Manuele Gatti, and Stefano Consonni. Supercritical Pressure–Density–Temperature Measurements

on CO_2–N_2, CO_2–O_2 and CO_2–Ar Binary Mixtures. *J. of Supercritical Fluids*, 61:pp. 34—43, 2012.

[110] C. Y. Tsang and W. B. Strett. Phase Equilibria in the H_2 / CO_2 System at Temperatures from 220 to 290 K and Pressures to 172 MPa. *Chemical Engineering Science*, 36:pp. 993—1000, 1981.

[111] Yolanda Sanchez-Vicente, Trevor C. Drage, Martyn Poliakoff, Jie Ke, and Michael W. George. Densities of the Carbon Dioxide Plus Hydrogen, A System of Relevance to Carbon Capture and Storage. *International Journal of Greenhouse Gas Control*, 13:pp. 78—86, March 2013.

[112] Aage Fredenslund and G. A. Sather. Gas–Liquid Equilibrium of the Oxygen–Carbon Dioxide System. *Journal of Chemical and Engineering Data*, 15(1):pp. 17—22, 1970.

[113] Jü rgen Stoll, Jadran Vrabec, and Hans Hasse. Vapor–liquid equilibria of mixtures containing nitrogen, oxygen, carbon dioxide, and ethane. *AIChE Journal*, 2003.

[114] Wikipedia. (Online).

[115] Taher A. Al-Sahhaf, Arthur J. Kidnay, and E. Dendy Sloan. Liquid + Vapor Equilibria in the N_2 + CO_2 + CH_4 System. *Ind. Eng. Chem. Fundam.*, 22:pp. 372—380, 1983.

[116] Taher A. Al-Sahhaf. Vapor–Liquid Equilibria for the Ternary System N_2 + CO_2 + CH_4 at 230 and 250 K. *Fluid Phase Equilibria*, 55:pp. 159—172, 1990.

[117] Gü nter Trappehl. *Experimentelle Untersuchung der Damff–Flussigkeits–Phasengleichgewichte und Kalorischen Eigenschaften bei Tiefen Temperaturen und hohen Drü cken an Stoffgemischen Bestehend aus N_2, CH_4, C_2H_6, C_3H_8 und CO_2*. PhD thesis, Technischen Uriversitt Berlin, 1987. (In German).

[118] V. V. Altunin and D. H. Chin. Thermal Properties of a CO_2–N_2 Gas Mixture at Elevated Temperature. *Unknown Journal*, pages pp. 64—70, 1972. (In Russian).

[119] Andrzej Hacura, Jong-Ho Yoon, and Frank G. Baglin. Density Values of Carbon Dioxide and Nitrogen Mixtures from 500 to 2500 bar at 323 and 348 K. *J. Chem. Eng. Data*, 33:pp. 152—154, 1988.

[120] N. D. Kosov and I. S. Brovanov. The Compressibility of Binary Mixtures of Helium, Nitrogen and Argon with Carbon Dioxide from 59 $\times$ 10^5 to 590 $\times$ 10^5 Pa. *Teploenergetika*, 22(11):pp. 87—89, 1975.

[121] Andrew J. Parrott, James Calladine, Maria-Jose Tenorio, Jie Ke, Trevor Drage, Michael W. George, and Martyn Poliakoff. COOLTRANS 3% H_2 + 97% CO_2 Binary Mixture VLE study. February 2013.

[122] B. V. Mallu and D. S. Viswanth. Compression Factors and Second Virial Coefficients of H_2, CH_4, { $x CO_2 + (1-x) H_2$ }, and { $x CO_2 + (1-x) CH_4$ }. *J. Chem. Thermodynamics*, 22:pp. 997—1006, 1990.

[123] Aage Fredenslund, Jørgen Mollerup, and Ole Persson. Gas–Liquid Equilibrium of Oxygen–Carbon Dioxide System. *Journal of Chemical and Engineering Data*, 17(4):pp. 440—443, 1972.