

# CERTIFICATION OF APPROVAL

DEVELOPMENT OF VOLUME TO MASS  
CONVERSION MODEL FOR  
NGV DISPENSING UNIT USING  
THERMODYNAMIC PROPERTIES

By

Nadiah Abu Hassan

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Approved by,



NorHayati Mellon

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1) Natural gas

## **CERTIFICATION OF ORIGINALITY**

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgement, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

  
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NADIYAH ABU HASSAN

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## 1.0 ABSTRACT

This research project is initiated as one of the sub studies in the implementation of natural gas vehicle usage in Malaysia. Developing a natural gas refueling station at lower cost is a challenge that needs to be handled by the university. One of the areas of interest is in the metering system. Regulatory requirement states that natural gas must be measured in mass flow rate. Coriolis meter is the only available mass flow meter in the market. But this meter is too costly. Thus a study to develop a cheaper metering system is required.

The best alternative is by measuring the flow rate of natural gas and then converts it to mass flow rate. This conversion can be done in various ways of calculations. Manual calculation using Equation of State, combination of several Equations of State and Activity Coefficient Method are the most commonly used method of calculation for natural gas component. The author used several equations of state in order to complete this research. But first, the properties of the natural gas such as its composition, vapor pressure and critical properties need to be determined first.

The calculation starts with the study to find the variation in mass as pressure of the natural gas is changed. For this calculation purpose, the tank is considered as an isothermal system with temperature maintained at 30<sup>0</sup>C. The system that been studied is the NGV's tank which volume is constant (55 liters). The calculation is done using Soave Redlich Kwong EOS and Peng Robinson EOS. To compare the data with the ideal condition, a plot using ideal gas equation is done as well. The calculation is repeated at different composition to see how the variations in composition affect the behavior of the graph.

Finally, the variation in mass as a function of temperature and pressure is done. At this stage, HYSIS is used to determine the data for the plot. The equations that been considered in the calculation are Soave Redlich Kwong EOS, Peng Robinson EOS and Lee Kesler Plocker EOS. The graphs are plotted to see the relationship.

## **2.0 INTRODUCTION**

### **2.1 Background of the Study**

Automotive industry is one of the fastest growing industries in the world. The car usage is increasing as the economic status is developing year by year. But unfortunately, these vehicles are major contributors to air pollution problem. Phenomenon such as photochemical smog, acid rain and increment in air pollution index is mainly contributed by emission from vehicles' exhaust. Thus, there are more alternatives been developed to create a more environmental friendly vehicle.

As the pollutant emitted from the vehicle come from its fuel, it is a good approach to change its fuel from diesel and gasoline to other type of fuel. Natural gas is one of the best options available. Natural gas is a product that been collected together with petroleum. It is colorless and odorless gas that can be easily combusted. It believed that natural gas is one of the cleanest, safest, and most useful of all energy sources.

Natural gas vehicle has become a more popular option of transportation worldwide. Natural gas contains less carbon than any other fossil fuel and thus produces lower carbon dioxide emission per vehicle traveled. NGV also emit very low level of carbon monoxide and volatile organic compound. Exhaust emission from a typical NGV are much lower than those from gasoline powered vehicles.

From safety point of view also, using natural gas offer a safer system. If a leak were to occur in an NGV fuel system, the natural gas would dissipate into the atmosphere because it is lighter than air. Natural gas has a high ignition temperature, about 1200<sup>0</sup>F and narrow range of flammability. Besides, natural gas is not toxic and will not contaminate ground water. Natural gas combustion produces no significant aldehydes or other air toxins, which are a concern in gasoline and other alternative fuels.

## 2.2 Problem Statement

UTP in corporation with other universities had conducted a study on the development of NGV usage in Malaysia. UTP's scope is to focus in designing the natural gas refueling system. The tasks are broken into smaller scope to be studied. The author scope is to concentrate in the natural gas metering system. Natural gas need to be measure in mass flow rate rather than the other fuel that been measured in volumetric flow rate.

There are several types of flow meter in the market that can measure natural gas flow from the natural gas dispensing unit to the vehicle. Coriolis meter, vortex flow meter, positive displacement flow meter and differential meter are among the most popular flow meter that been used to measure flow.

Among this four, only coriolis meter give the reading in mass per unit time while the other flow meter give the volumetric reading of volume per unit time. The high cost of this meter lead to the research of finding another alternative to measure mass flow. The best window that been considered is to have the volumetric flow rate measured, and then convert it to mass.

The conversion of volume to mass for natural gas is quite complicated as it involves changes in its properties. There are a lot of correlation been develop that can relate mass and volume by using thermodynamic properties such as temperature and pressure. The applicability of each correlation is different depending on its temperature range, pressure range and also composition of the fluid that been studied. The project to be conducted is to find several Equations of State that are suitable for natural gas and then use them for thermodynamic calculation.



## 2.3 Objectives

The objective of this research is to find the more economical method to measure the mass of natural gas. This is important in order to comply with SIRIM requirement in measuring natural gas in mass unit. Conversion from volumetric flow rate to mass flow rate is believed to be the best option. Using several thermodynamic Equations of State, the relation between thermodynamic properties such as pressure, temperature and density is studied. The calculation need to be repeated for several Equations of State.

The other objective is to find the composition effect in the mass of fuel being delivered. The study is conducted at two different compositions, namely the leanest and the richest composition. This result will be plotted in a graph and will be compared with the actual result from the real refueling procedure. Then only the best correlation can be selected.

## 2.4 Scopes of Study

The project is mainly concentrating in finding the variation mass of natural gas as the thermodynamic properties which is the temperature and pressure changed. The other studies such as finding the natural gas composition and volume of the system is considered done.

The scope of this research project can be summarized as follow;

1. Finding Equation of State that is applicable for natural gas calculation
2. calculate the variation of density for those EOS at different temperature and pressure
3. calculate the variation of density for different compositions
4. find the mass of the natural gas for constant volume tank

## 3.0 LITERATURE REVIEW AND THEORY

### 3.1 Theories

#### 3.1.1 Equation of State

##### 3.1.1.1 Ideal Gas Equation

The simplest equation that relates mass and volume for gas is the ideal gas equation.

$$PV = nRT$$

where  $n$  is the number of mole which can be converted to mass by multiplying with molecular weight. But unfortunately, the real condition is not as simple as ideal gas relationship. Assuming the gas behave ideally as there is no intermolecular interaction between the molecules might lead to major deviation from the real process. Ideal gas can be achieved if the density of the gas is too low. For ideal gas, the product of pressure and volume linearly increase with increasing temperature.

All substance behaves accordingly to this simple equation at sufficiently high specific volume (low density). This is because, at vanishing low density, the individual molecules are essentially point particle, occupying zero volume and never colliding with one another. Even in their ideal gas state, where no intermolecular interaction occurs, all substances still temperature dependent. The difference in heat capacity among species arise from their differing number of constituents atoms and the manner they are arrange in the molecules.

In engineering application, which are most often at atmospheric pressure or higher, no fluid is truly an ideal gas. However in many cases the assumption is within a few percent of being exact. In this study, ideal gas is used as a reference point. The result calculated using other EOS will be plotted in a same graph with ideal gas plot and the difference is noted.

### 3.1.1.2 Van der Waal Equation

The Van der Waals equation of state is derived from ideal gas by adding a term representative of intermolecular attraction,  $a/v^2$ , where  $a$  is an empirical constant specific for each substance. This force has some theoretical justification; the attractive London forces between molecules which exist because of mutually induced perturbations in their electron clouds, decay with the sixth order in intermolecular distance.

The square of volume is roughly proportional to this distance raised to the sixth power. Van der Waals was the first to use this force in a tractable equation of state; it is sometime referred to as van der Waals force.

The second modification is the addition of  $a$  term,  $b$ , specific to each substance, and the representative of the hard volume of the molecules themselves, that is the volume below which the system can never be compressed. The resulting equation is

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

Where

$$a = \frac{27R^2T_c^2}{64P_c}$$

$$b = \frac{1}{8} \frac{RT_c}{P_c}$$

$$v = \frac{\text{volume}}{\text{mole}} = \frac{MW}{\rho}$$

Because the Van der Waals equation is not a perfect representation of any substance, no perfect pair of constant will exactly match all the true isotherms. There are therefore many pairs,  $a$  and  $b$ , that can be found to fit best over some limited range.

### 3.1.1.3 Soave-Redlich-Kwong Equation

An empirical modification to the Van der Waals equation was made by Otto Redlich. He found that, whereas the first term in the equation was a reasonable assessment of the repulsive forces, the attractive force term needed temperature dependence to reproduce a large quantity of experimental data more accurately. He ended up with an equation known as Redlich Kwong equation written as;

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

where

$$a = 0.42748 \frac{R^2 T_c^{2.5}}{P_c}$$

$$b = 0.08664 \frac{RT_c}{P_c}$$

This Redlich-Kwong equation is reasonably good at describing liquid and vapor volumes, but when the process is inverted and vapor pressure is predicted, the results are severely in error. This led Soave to replace the constant  $a$  with the one that was dependent on temperature; he further put in a dependence on the acentric factor,  $\omega$ , which, in its development, was based on the vapor pressure behavior. The result is an equation that is not much better in predicting vapor pressures of pure components.

Soave-Redlich Kwong is written as;

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

$$\begin{aligned}
a(T_c) &= a_c = 0.42748(RT_c)^2 / P_c \\
b &= 0.08664 RT_c / P_c \\
a(T) &= a_c \cdot \alpha(T) \\
\alpha &= \left[1 + M(1 - \sqrt{T_r})\right]^2 \\
m &= 0.480 + 1.574\omega - 0.176\omega^2 \\
\omega &= -\log P_r - 1 \\
P_r &= P^* / P_c
\end{aligned}$$

Soave replaces a term in RK with a function that involve temperature and acentric factor. The  $\alpha$  function was devised to fit the vapor pressure data of hydrocarbons and the equation does fairly well for these material.

#### 3.1.1.4 Peng Robinson Equation

Peng Robinson equation is related to the the SRK and was developed to overcome the instability in the SRK equation near the critical point. Peng Robinson equation is put as below;

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

where

$$a(T) = 0.45724 \frac{(RT_c)^2}{P_c} \alpha(T)$$

$$b = 0.07780 \frac{RT_c}{P_c}$$

$$\sqrt{\alpha} = 1 + k \left[1 - \sqrt{\frac{T}{T_c}}\right]$$

$$k = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

This PR equation of state is developed 1976 to be applicable to all calculation of all fluid properties in natural gas properties. This correlation provides reasonable accuracy near critical point. As put in above, the parameter is expressed in term of critical properties. It is commonly used

to represent hydrocarbon and inorganic gases such as nitrogen, oxygen and hydrogen sulfide.

The generalized parameter of PR equation of state is function of critical pressure, critical temperature and acentric factor of the fluid. Thus this PR is said to be a three-parameter equation of state, where as the Van der Waals equation contain only two parameters which are critical pressure and critical temperature.

### 3.1.1.5 Lee Kesler Plocker Equation

Benedict Webb Rubin is an equation of state that has eight empirical constants and gives accurate predictions for vapor and liquid phase hydrocarbons. It can also be used for mixtures of light hydrocarbons with carbon dioxide and water.

Lee and Kesler extended the Benedict Webb Rubin equation to a wider variety for substance using the principle of corresponding state. The method was modified further by Plocker. The new method to calculate critical properties and other constants is introduced.

$$T_{c_{ij}} = (T_{c_i} T_{c_j})^{1/2}$$

$$T_{c_m} = T_{c_i} \quad T_{c_{ij}} = T_{c_j}$$

$$v_{c_m} = \sum_i \sum_j x_i x_j v_{c_{ij}}$$

$$v_{c_{ij}} = \frac{1}{8}(v_{c_i}^{1/3} + v_{c_j}^{1/3})^3$$

$$v_{c_i} = z_{c_i} \frac{RT_{c_i}}{p_{c_i}}$$

$$z_{c_i} = 0.2905 - 0.085\omega_i$$

$$p_{c_m} = z_{c_m} \frac{RT_{c_m}}{v_{c_m}}$$

$$z_{c_m} = 0.2905 - 0.085\omega_m$$

$$\omega_m = \sum_i x_i \omega_i$$

### 3.1.2 Variation of Composition in Natural Gas

Natural gas is a combustible mixture of hydrocarbon gases. While natural gas is formed primarily of methane, it can also include ethane, propane, butane and pentane. The composition of natural gas can vary widely, but below is a chart outlining the typical makeup of natural gas before it is refined.

Table 1 : Natural Gas Composition

Typical Composition of Natural Gas		
Methane	CH <sub>4</sub>	70-90%
Ethane	C <sub>2</sub> H <sub>6</sub>	0-20%
Propane	C <sub>3</sub> H <sub>8</sub>	
Butane	C <sub>4</sub> H <sub>10</sub>	
Carbon Dioxide	CO <sub>2</sub>	0-8%
Oxygen	O <sub>2</sub>	0-0.2%
Nitrogen	N <sub>2</sub>	0-5%
Hydrogen sulphide	H <sub>2</sub> S	0-5%
Rare gases	A, He, Ne, Xe	trace

In its purest form, such as the natural gas that is delivered to home, it is almost pure methane. Methane is a molecule made up of one carbon atom and four hydrogen atoms, and is referred to as CH<sub>4</sub>. Natural gas is considered 'dry' when it is almost pure methane, having had most of the other commonly associated hydrocarbons removed. When other hydrocarbons are present, the natural gas is 'wet'.

The variation in natural gas composition might affect the volume to mass conversion. This composition varies depend on several factor such as the location of the reservoir where the natural gas is collected

Presence of impurities is another concern in natural gas composition. In most occasions, hydrocarbons are produced with non-hydrocarbon impurities. The most common include water, carbon dioxide, hydrogen sulfide and nitrogen. Since water has a low vapor pressure and is virtually immiscible in the hydrocarbon liquid phase, it does not have a significant effect on the shape of the hydrocarbon phase envelope except at high temperature and low pressure.

The effect of  $\text{CO}_2$ ,  $\text{H}_2\text{S}$  and  $\text{N}_2$  is shown in figures below.

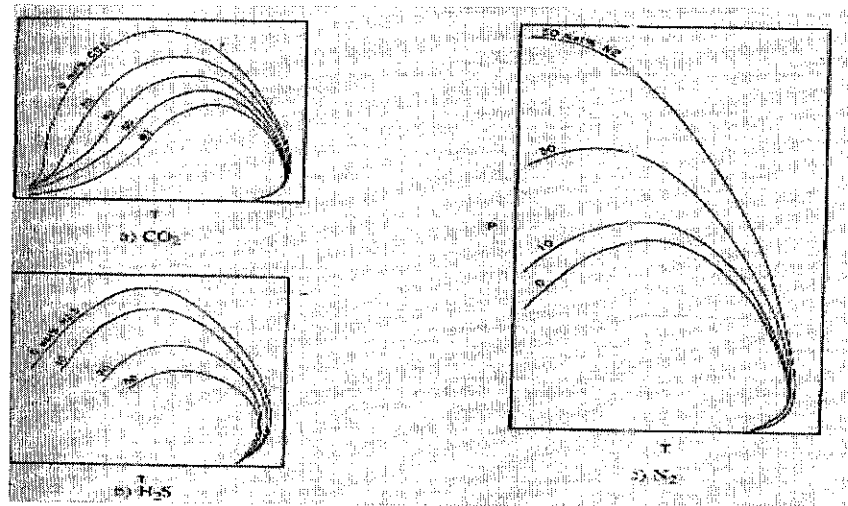


Figure 1: Effect of Impurities in Natural Gas

Cricondenbar is defined as the maximum pressure at which liquid and vapor might exist. Both  $\text{CO}_2$  and  $\text{H}_2\text{S}$  lower the cricondenbar of the mixture. If sufficient quantities of  $\text{CO}_2$  and  $\text{H}_2\text{S}$  component are added to the reservoir fluid and the reservoir pressure is kept above the phase enveloped, a single dense liquid phase exists.

Although the actual mechanism is more complex, it is this solubility that is the primary driving force behind miscible flood enhance oil recovery project. Natural gas components such as ethane, propane and butane have a similar effect. Nitrogen, on the other hand raises the criconcenbar and decrease miscibility. It is typically used for pressure maintenance.



### 3.2 Literature Review

Besides calculating the thermodynamic properties relationship with mass variation using the equations of state discussed before, there are also some studies that been conducted to find the best ways to relate all these properties. All these studies are to find the best solutions for each unique condition that the writer was working on.

Some of the studies are by incorporating several equation of state together. For example, the journal entitles efficient method for calculations of compressibility, density and viscosity of natural gas by N. Varotsis, G Steward and A.C Toddm Clancy. The writers use Whitson correlation to calculate boiling point, Lee Kesler Equation to calculate critical temperature and pressure, Edminster correlation to find acentric factor and Pitzer correlation is used to find critical compressibility factor.

The calculation involves the usage of a lot of equation and constant. The critical pressure and temperature is calculated by first finding a constant denoted by  $K_{inf}$  and  $J_{inf}$ .

$$J_{inf} = \alpha_0 + \left[ \alpha_1 \left( \frac{y_i T_C}{P_C} \right) \right]_{H_2S} + \left[ \alpha_2 \left( \frac{y_i T_C}{P_C} \right) \right]_{CO_2} + \left[ \alpha_3 \left( \frac{y_i T_C}{P_C} \right) \right]_{N_2} \\ + \left[ \alpha_4 \sum y_i \left( \frac{P_C}{T_C} \right) \right]_{C1-C6} + [\alpha_5 y_i MW]_{C7}$$

where

$$\alpha_0 = 0.036983$$

$$\alpha_1 = 1.043902$$

$$\alpha_2 = 0.894942$$

$$\alpha_3 = 0.792231$$

$$\alpha_4 = 0.882292$$

$$\alpha_5 = 0.018637$$

$$K_{inf} = \beta_0 \left[ \beta_1 \left( \frac{y_i T_C}{P_C^{0.5}} \right) \right]_{H_2S} + \left[ \beta_2 \left( \frac{y_i T_C}{P_C^{0.5}} \right) \right]_{CO_2} + \left[ \beta_3 \left( \frac{y_i T_C}{P_C^{0.5}} \right) \right]_{N_2}$$

$$+ \left[ \beta_4 \sum y_i \left( \frac{P_C}{T_C^{0.5}} \right) \right]_{C1-C6} + [\beta_5 y_i MW]_{C7}$$

where

$$\beta_0 = 0.7765003$$

$$\beta_1 = 1.0695317$$

$$\beta_2 = 0.9850308$$

$$\beta_3 = 0.8617653$$

$$\beta_4 = 1.0127054$$

$$\beta_5 = 0.4014645$$

Then the critical properties of the natural gas are calculated using the equation as below;

$$T_{PC} = \frac{K_{INF}^2}{J_{INF}}$$

$$P_{PC} = \frac{T_{PC}}{J_{INF}}$$

$$P_{PR} = \frac{P}{P_{PC}}$$

$$T_{PR} = \frac{T}{T_{PC}}$$

Finally, the compressibility factor is found using the equation below before inserting it in a normal relation to find the density of the natural gas.

$$z = \left[ C_1 + \frac{C_2}{T_{PR}} + \frac{C_3}{T_{PR}^3} + \frac{C_4}{T_{PR}^4} + \frac{C_5}{T_{PR}^5} \right] \rho_\tau + \left[ C_6 + \frac{C_7}{T_{PR}} + \frac{C_8}{T_{PR}^2} \right] \rho_\tau^2 - C_9 \left[ \frac{C_7}{T_{PR}} + \frac{C_8}{T_{PR}^2} \right] \rho_\tau^5$$

$$+ C_{10} \left( 1 + C_{11} \rho_\tau^2 \right) \frac{\rho_\tau^2}{T_{PR}^3} 3 \exp \left[ -C_{11} \rho_\tau^2 \right] + 1 (24)$$

This method of calculation is mainly concern with the presence of heptanes in the mixture. Thus might not be suitable for this study, but this research gives some idea on the correlation that normally been used and also prove that a combination of several equations of state is acceptable for calculation purpose in order to get the best fit data.

There is also a research that focused in a property method and calculation. Every equation of state is being studied further to find its suitable application. The research done shows the following result.

Table 2 : Recommended Equation of State for Different System

Type of system	Recommended properties method
TEG Dehydrate	Peng robinson
Sour water	Peng robinson, sour PR
Cryogenic gas processing	PR, PRSV
Air separation	PR, PRSV
Atm crude tower	PR, PR option, GS
Vacuum tower	PR, PR option, GS, Braun K10, ESSO K
Ethylene tower	Lee Kesler Plocker
High H2 system	PR,ZJ, GS
Reservoir system	PR, PR option
Steam system	Steam package, CS, GS
Hydrate inhibition	PR
Chemical system	Activity model, PRSV
HF alkylation	PRSV, NRTL
TEG dehydration with aromatics	PR
Hydrocarbon system where H2O solubility in hydrocarbon is important	Kabadi Danner
System with selected gases and light hydrocarbon	PR, SRK, MBWR

The PR equation of state has been enhanced to yield accurate phase equilibrium calculations for systems ranging from low temperature cryogenic systems to high temperature, high pressure reservoir systems. The same equation of state satisfactorily predicts component distributions for heavy oil systems, aqueous glycol and CH<sub>3</sub>OH systems, and acid gas/sour water systems, although specific

sour water models (Sour PR and Sour SRK) are available for more specialized treatment.

High recommendation for the PR equation of state is largely due to the preferential attention that has been given to it by Hyprotech. Although the Soave-Redlich-Kwong (SRK) equation will also provide comparable results to the PR in many cases, it has been found that its range of application is significantly limited and it is not as reliable for non-ideal systems. For example, it should not be used for systems with  $\text{CH}_3\text{OH}$  or glycols.

The PR can also be used for crude systems, which have traditionally been modeled with dual model thermodynamic packages (an activity model representing the liquid phase behavior, and an equation of state or the ideal gas law for the vapor phase properties). These earlier models are suspect for systems with large amounts of light ends or when approaching critical regions. Also, the dual model system leads to internal inconsistencies.

The proprietary enhancements to the PR and SRK methods allow these EOSs to correctly represent vacuum conditions and heavy components (a problem with traditional EOS methods), as well as handle the light ends and high-pressure systems.

Although equation of state models have proven to be very reliable in predicting properties of most hydrocarbon based fluids over a large range of operating conditions, their application has been limited to primarily non-polar or slightly polar components. Thus there are some literature that had been conducted using other method of calculation such as using activity coefficient method.

Polar or non-ideal chemical systems have traditionally been handled using dual model approaches. In this approach, an equation of state is used for predicting the vapour fugacity coefficients (normally ideal gas assumption or the Redlich

Kwong, Peng-Robinson or SRK equations of state, although a Virial equation of state is available for specific applications) and an activity coefficient model is used for the liquid phase.

Although there is considerable research being conducted to extend equation of state applications into the chemical arena (e.g., the PRSV equation), the state of the art of property predictions for chemical systems is still governed mainly by Activity Models. Activity Models are much more empirical in nature when compared to the property predictions (equations of state) typically used in the hydrocarbon industry.

For example, they cannot be used as reliably as the equations of state for generalized application or extrapolating into untested operating conditions. Their tuning parameters should be fitted against a representative sample of experimental data and their application should be limited to moderate pressures. Consequently, more caution should be exercised when selecting these models for your simulation.

Although for ideal solutions the activity coefficient is unity, for most chemical (non-ideal) systems this approximation is incorrect. Dissimilar chemicals normally exhibit not only large deviations from an ideal solution, but the deviation is also found to be a strong function of the composition. To account for this non-ideality, activity models were developed to predict the activity coefficients of the components in the liquid phase. The derived correlations were based on the excess Gibbs energy function, which is defined as the observed Gibbs energy of a mixture in excess of what it would be if the solution behaved ideally, at the same temperature and pressure.

The individual activity coefficients for any system can be obtained from a derived expression for excess Gibbs energy function coupled with the Gibbs-Duhem equation. The early models (Margules, van Laar) provide an empirical

representation of the excess function that limits their application. The newer models such as Wilson, NRTL and UNIQUAC utilize the local composition concept and provide an improvement in their general application and reliability. All of these models involve the concept of binary interaction parameters and require that they be fitted to experimental data.

Since the Margules and van Laar models are less complex than the Wilson, NRTL and UNIQUAC models, they require less CPU time for solving flash calculations. However, these are older and more empirically based models and generally give poorer results for strongly non-ideal mixtures such as alcohol-hydrocarbon systems, particularly for dilute regions.

The Chien-Null model provides the ability to incorporate the different activity models within a consistent thermodynamic framework. Each binary can be represented by the model which best predicts its behavior. The following table briefly summarizes recommended models for different applications.

## 4.0 PROJECT OVERVIEW, METHODOLOGY AND PROJECT WORK

### 4.1 Project Work

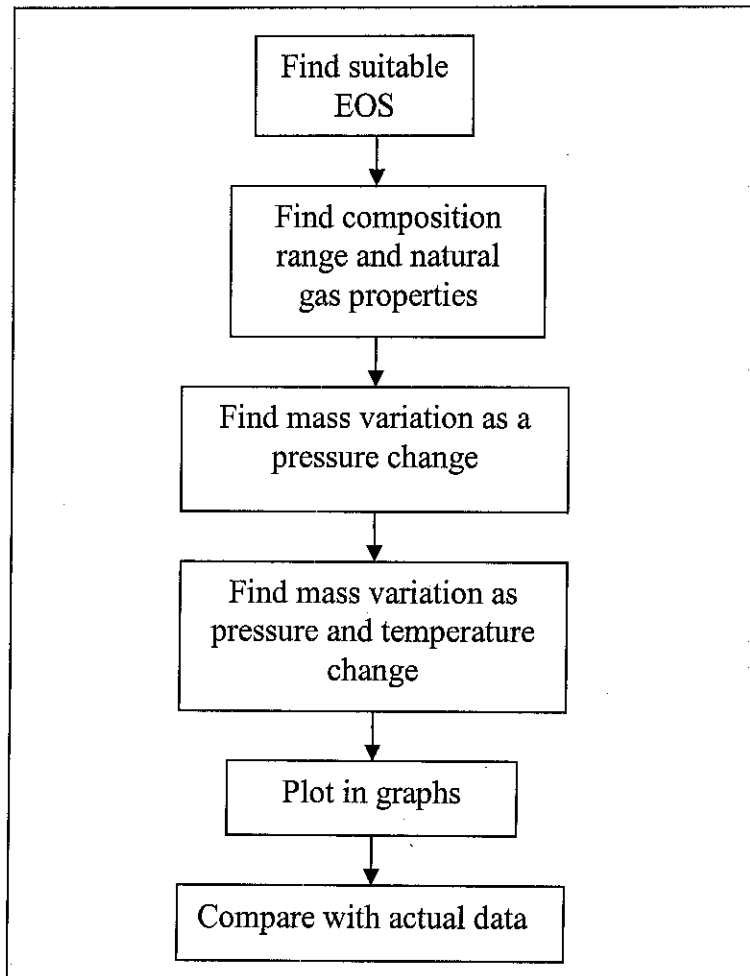


Figure 2 : Process Flow For This Research

#### 4.1.1 Finding Suitable Equation of State

The first step in this project is to find the most suitable Equation of State to be used. Not every equation of state can be used for natural gas calculation. The application of each equation of state is studied. Several equations of state are used and compared among each other.

Most equations of state have some empirical constant that should be used in the calculation. Thus these constants should be determined first before proceeding with the detail calculation. Books, journal and also internet search is the most useful tools to find this constant. HYSIS is also another option in getting the values to be used to plot graphs.

#### 4.1.2 Finding Composition and Natural Gas Properties

The second step is to find the range of composition variation for natural gas. The major concern is in the composition of methane, ethane and propane. The properties such as vapor pressure and critical properties of each natural gas component (critical temperature and critical pressure) should be determined as well.

Besides the properties for each component of natural gas, there are some other calculations that need to be completed first before start the calculation. The author has to determine the mass fraction, molecular weight of the natural gas mixture, vapor pressure for mixture, acentric factor for mixture and also critical properties of the mixture.

a) The calculation for mass fraction is as follow;

1. Assume 1 mole of natural gas mixture

2. Mass of component  $i$  = mole fraction x molecular weight of component  $i$

$$m_i = y_i \times MW$$

3. Find total mass of the natural gas

$$m_{total} = \sum_i m_i$$



This total mass is in gram. As the calculation is done by assuming 1 mole of natural gas, thus, the molecular weight of this natural gas is equal to this  $m_{total}$ .

4. Find mass fraction for each component

$$x_i = \frac{m_i}{m_{total}}$$

b) Vapor pressure prediction

if the normal boiling point (vapor pressure = 1 atm) and the critical temperature and pressure are known, then a straight line drawn through these two points on a plot of log pressure versus reciprocal absolute temperature can be used to make a rough estimation of the vapor pressure at intermediate temperature.

Several equations have been developed to express vapor pressure as a function of temperature. One of the most commonly used is the three term Antoine equation, which is given by;

$$\ln VP = A - \frac{B}{T + C}$$

where, VP = vapor pressure in mmHg

A,B,C = the Antoine coefficient

T= temperature, K

A more accurate equation that might be considered to calculate vapor pressure for pure component is as follow;

$$\ln VP = C_1 + \frac{C_2}{T} + C_3 \ln T + C_4 T^{C_5}$$

All the five constants are different for each component.

Once the vapor pressure of each composition is known, the vapor pressure for the mixture of natural gas could be determined.

$$VP_{mixture} = \sum_i x_i VP_i$$

Where  $x_i$  is the mass fraction of each component in the natural gas.

### c) Critical properties prediction

Critical properties that had become a concern here is the critical temperature and critical pressure. These critical properties can be determined for the individual component in the natural gas.

The critical values are found through a combination rule. They are not necessarily true value. Thus they are called pseudocriticals. The word pseudo means fake or not real. Thus a pseudocritical value is not a point on the phase curve. It is merely a correlating parameter that uses the concept of corresponding state format.

The value of critical properties of the mixture can be determined using Kay's Rule. This rule state that

$$P'_C = \sum x_i P_{Ci}$$

and

$$T'_C = \sum x_i T_{Ci}$$

where  $x_i$  is the mass fraction of each component in the mixture and  $T_{ci}$  and  $P_{ci}$  are the critical values for each component.

From these critical properties, the reduced properties can be determined. In corresponding state concept, physical and thermodynamic properties

are related to critical properties in universal ways. Mathematically, another way of stating this concept is to say that if an equation of state for any fluid is written in term of reduced properties, that equation is also valid for other fluid.

Reduced properties are defined as;

$$T_r = \frac{T}{T_c}$$
$$P_r = \frac{P}{P_c}$$

d) acentric factor estimation

Acentric factor was developed by Pitzer to describe the deviation of a fluid from simple fluid behavior, or its nonconformity with the corresponding state principle. For simple, noble gases like argon, zenon and the like,  $\omega$  is equal to zero.

The parameter  $\omega$  is defined by the equation

$$\omega = -\log P_r - 1$$

where  $P_r = P^*/P_c$ ;  $P^*$  is the vapor pressure at  $T^* = 0.7 T_c$

Once the acentric factor for each component is determined, the acentric factor of the mixture can be determined.

$$\omega_{mixture} = \sum x_i \omega_i$$

Using the raw data that had been determined before, the thermodynamic calculation can be done using the chosen equations of state. This calculation is done at constant volume condition. The volume that been referred to is the volume of the NGV's tank which is 55 liter. For this

purpose of calculation, the system is assumed to be exothermic. So, the calculation is only done at one temperature which is 30°C.

#### **4.1.3 Find Mass Variation as A Function of Pressure and Temperature.**

The next step is to calculate the variation of mass as pressure changes using the respective equation of state. This calculation is done by assuming an isothermal process. The result will be plotted in graph to have a clearer picture about the different in result given by each equation of state. Then the variation of temperature will be taken into account. The calculation will be done at some range of temperature. The result will be plotted in graph as well.

By right, the result that had been gained will be compared with the actual data gained from the refueling test. But this stage might not be possible if the equipment that been purchased cannot reach on time.

### **4.2 Tool Used**

For the completion of this project, the most useful packages that been used are:

#### **4.2.1 Microsoft Excel**

Microsoft excel is one of the most powerful that been wide use for engineering studies. It can be used to create a spread sheet, doing repetitive calculation at faster pace and also can be used to plot graphs. Microsoft Excel is a member of the spreadsheet family of software. Spreadsheet software is used to store information in columns and rows which can then be organized and or processed. Spreadsheets are designed to work well with numbers but often include text. Sometimes text in a spreadsheet is called a label, because it is labeling columns and rows of numbers. Numbers are called values sometimes, and can include numbers

for counts or measurements, dates, times, and calculations from numbers. Spreadsheets can help organize information, like alphabetizing a list of names or other text or reordering records according to a numeric field. However, spreadsheets are more often used for calculating, such as totaling a column of numbers or generating a more sophisticated formula to calculate some statistical measure on a list of numbers.

#### **4.2.2 HYSIS**

The property packages available in HYSYS help to predict properties of mixtures ranging from well defined light hydrocarbon systems to complex oil mixtures and highly non-ideal (non-electrolyte) chemical systems. HYSYS provides enhanced equations of state for rigorous treatment of hydrocarbon systems; semi empirical and vapor pressure models for the heavier hydrocarbon systems; steam correlations for accurate steam property predictions and activity coefficient models for chemical systems. All of these equations have their own inherent limitations.

HYSYS currently offers the enhanced Peng-Robinson (PR), and Soave-Redlich-Kwong (SRK) equations of state. In addition, HYSYS offers several methods which are modifications of these property packages, including PRSV, Zudkevitch Joffee (ZJ) and Kabadi Danner (KD). Lee Kesler Plocker (LKP) is an adaptation of the Lee Kesler equation for mixtures, which itself was modified from the BWR equation. Of these, the Peng-Robinson equation of state supports the widest range of operating conditions and the greatest variety of systems. The Peng-Robinson and Soave-Redlich-Kwong equations of state (EOS) generate all required equilibrium and thermodynamic properties directly. Although the forms of these EOS methods are common with other commercial simulators, they have been significantly enhanced by HYSIS to extend their range of applicability

## **5.0 RESULT AND DISCUSSION**

There are two approaches that been used to get the data for this research. The first attempt is by manual calculation and the second method is by using data from HYSIS. The result that been get is compared and the best one is then chosen.

### **5.1 Choosing Suitable Equations of State**

Equation of state is an algebraic expression which relates temperature, pressure and molar volume, for real fluid. Many equations o state had been developed of varying complexity. No one equation is sufficiently accurate to represent all real gases, under all condition.

The author has managed to study the application of each equation of state. Those equations of state that is suitable for natural gas application will be used.

#### **5.1.1 Ideal Gas**

Ideal gas equation is too simple to be considered in this process. The natural gas will be directed to the NGV's tank which originally at atmospheric pressure. During the refueling process, the pressure in the tank will be increasing up to 3500psi. At this condition, natural gas no longer shows an ideal behavior. The attractive and repulsive forces among the natural gas molecules become significant at higher pressure.

But natural gas plot might be helpful for comparison purpose. By using ideal gas equation the deviation of the real process from the ideal condition can be studied.

### **5.1.2 Van Der Waals Equation of State**

In some literature, Van der Waals equation of state is called the 'grandpa' of all equation of state. The development of this equation is done long time before with a lot of assumption and prediction of the behavior of the components. Although it had improved the ideal assumption in ideal gas equation by considering the forces exerted by the molecules, the applicability of this equation for natural gas is not satisfying.

The temperature dependent on the forces had been neglected. The forces are only assumed to be a function of volume and some empirical constant. But in this research, temperature is one of the main thermodynamic properties that need to be studied.

### **5.1.3 Soave-Redlich Kwong Equation of State**

SRK was found to be one of the best equations of state that can be used for natural gas calculation. This is because this equation of state is an upgraded version of Redlich Kwong equation by improving its usage toward hydrocarbon gases. Thus SRK can be considered as one of the suitable equation of state that can be used for the calculation of natural gas properties.

### **5.1.4 Peng Robinson Equation of State**

Peng Robinson is the improved version of Soave Redlich Kwong equation. The improvement was done to overcome the weaknesses of SRK equation near the critical point. But in this study, the range of properties changes that been studied is far away from the critical point. Thus, Peng Robinson and SRK can be considered as equally good for natural gas application.

### **5.1.5 Lee Kesler Plocker Equation of State**

Lee Kesler Plocker equation of state is the improved version of Benedict Webb Rubin equation of state that is developed mainly for the purpose of studying hydrocarbon properties both in liquid and vapor phase. So, this equation can be considered as very suitable to be used to study the thermodynamic properties of natural gas

### **5.2 Finding the Composition of Natural Gas**

Natural gas composition varies depending on the location where the natural gas is collected. For this research, natural gas will be supplied by Petronas. Thus, the composition range that needs to be taken into account should be according to Petronas's research.

This composition is the composition of natural gas after going through the treatment process. In the process, the impurities such as sulfur, carbon dioxide and nitrogen are extracted from the natural gas. This natural gas mainly contains methane. Other longer chain hydrocarbon such as ethane, propane, iso-butane and n-butane also present in small amount. There are two types of impurities in the natural gas composition that is nitrogen and carbon dioxide.

The data used for this variation in composition is collected by Petronas Research and Scientific Service (PRSS). The studied was conducted between June 1999 to January 2000 at various NGV dispensers and also at PGB Kapar. The result was summarized by having the range of gas composition being divided into two categories namely the leanest and the richest composition.



Table 3: Gas Composition as Analyzed by PRSS

Table 3: Gas Composition as Analyzed by PRSS  Gas composition		Typical Specification	
		Leanest	Richest
Methane	C1	96.42	89.04
Ethane	C2	2.29	5.85
Propane	C3	0.23	1.28
Iso-Butane	iC4	0.03	0.14
N-Butane	nC4	0.02	0.10
Iso-Pentane	iC5	n/a	n/a
N-Pentane	nC5	n/a	n/a
N-Hexane+	C6++	n/a	n/a
Condensate	C5+	0.00	0.02
Nitrogen	N2	0.44	0.47
Carbon dioxide	CO2	0.57	3.09
Gross Heating Value (GHV)		38.13	38.96

### 5.3 Finding Natural Gas Properties

The properties for each component in the natural gas are slightly different from each other. And after being mixed as natural gas, the properties also changes. Thus, appropriate calculation is used to get these parameters.

The calculation of mass fraction and molecular weigh was done using the method describes in the last section. Given in Table 3 is the composition of natural gas in term of mole fraction. This mole fraction needs to be converted to mass fraction because some calculation later requires the usage of mass fraction. The result can be summarized in the table as follow.

Table 4 : Mass Fraction For Natural Gas Component In Leanest Composition.

Component	Mol fraction	Molecular weight	Mass	Mass fraction
Methane	0.9642	16.04	15.466	0.928
Ethane	0.0229	30.09	0.689	0.0414
Propane	0.0023	44.09	0.101	0.061
Iso-butane	0.0003	58	0.0174	0.00104
n-butane	0.0002	58	0.0116	0.0007
Nitrogen	0.0044	28.02	0.123	0.0074
Carbon dioxide	0.0057	44.01	0.251	0.00151
Total	1	-	16.66	1

Table 5 : Mass Fraction For Natural Gas Component In Richest Composition.

Component	Mol fraction	Molecular weight	Mass	Mass fraction
Methane	0.8905	16.04	14.284	0.783
Ethane	0.0586	30.09	1.763	0.0967
Propane	0.0128	44.09	0.564	0.0309
Iso-butane	0.0014	58	0.0812	0.00445
n-butane	0.001	58	0.058	0.00318
Nitrogen	0.0047	28.02	0.1317	0.00722
Carbon dioxide	0.0309	44.01	1.3599	0.0745
Total	1	-	18.242	1

The second step is to calculate to critical properties of the natural gas. The raw data was given as follow;

Table 6 : Critical Properties of Natural Gas Component

Component	Pc(MPa)	Tc(K)
Methane	4.6	191
Ethane	4.88	305
Propane	4.25	370
Isobutane	3.65	408
N-Butane	3.8	425
Nitrogen	3.4	126
CO2	7.38	304

Thus, the critical properties of the mixture can then be calculated using Kay's Rule.

$$P_c^i = \sum x_i P_{Ci}$$

and

$$T_c^i = \sum x_i T_{Ci}$$

The result that been gained gives;

Table 7: Critical Properties for Different Concentration

Composition	Critical temperature	Critical pressure
Leanest	198.41 K	4.6409 MPa
richest	217.22 K	4.808MPa

Then, vapor pressure is calculated using the equation given

$$\ln VP = C_1 + \frac{C_2}{T} + C_3 \ln T + C_4 T^{C_5}$$

The values of the constants can be determined from Perry's Chemical Engineering Handbook. The constants are given as follow;

Table 8: Constants for Vapor Pressure Calculation

Component	C1	C2	C3	C4	C5
Methane	39.205	-1324.4	-3.4366	0.000031019	2
Ethane	51.857	-2598.7	-5.1283	0.000014913	2
Propane	59.078	-3492.6	-6.0669	0.000010919	2
Iso-Butane	100.18	-4841.9	-13.541	0.020063	1
N-Butane	66.343	-4363.2	-7.046	9.4509E-06	2
Nitrogen	58.282	-1084.1	-8.3144	0.044127	1
Co2	140.54	-4735	-21.268	0.040909	1

The temperature in the tank is assumed to be 30<sup>0</sup>C, which is equal to 303K. But, this temperature is not the temperature that been used for the calculation. This vapor pressure will be used to calculate the acentric factor, which been calculated at T\* = 0.7 T<sub>c</sub>.

Thus,

$$T_{\text{leanest}}^* = 0.7 \times 198.41$$

$$= 138.887K$$

$$T^*_{\text{richest}} = 0.7 \times 217.22$$

$$= 152.24K$$

The calculation will be done at these two temperature to find vapor pressure at  $T^*$  for the respective composition.

The calculation of vapor pressure for the mixture yields the result as below;

Table 9: Component Vapor Pressure at Different Composition

Component	Component vapor pressure for the leanest comp.(Pa)	Component vapor pressure for the richest comp (Pa)
Methane	6044717.2	1148556
Ethane	3403.227	11623.95
Propane	67.32525	365.2964
Isobutane	3.660636	29.37881
N-Butane	1.41519	12.09334
Nitrogen	5865583	9773952
Co2	1339.658	6531.119

The vapor pressure of the mixture can be determined by multiplying the mass fraction of each component with its vapor pressure.

The result is as below;

Vapor pressure at  $T^*$  for leanest composition = 604960 Pa

Vapor pressure at  $T^*$  for richest composition = 971508 Pa

#### 5.4 Variation in Mass as a Function of Pressure.

To relate mass with pressure variation, the author has tried the manual calculation which is a bit tedious and require sometime to be completed.

This manual calculation requires a lot of research and it is quite tedious. Before any calculation using the respective Equations of State can be done, there are a lot of parameters that need to be found first such as the mass fraction, vapor pressure, acentric factors and critical properties of each natural gas components. This manual calculation is

done to find mass variation as a function of temperature. The author managed to performed manual calculation for ideal gas, Peng Robinson and Soave Redlich Kwong Equation of State.

#### 5.4.1 Calculation Using Ideal Gas Equation

Ideal gas equation is given as below;

$$PV = nRT$$

where  $n$  is the number of mole that can be calculated by dividing the mass of the natural gas with its molecular weight. For the first part of the calculation, the temperature is assumed to be constant at 30<sup>0</sup>C.

Substitute  $n$  in term of mass and molecular weight, and then rearrange the equation will give;

$$m = \frac{PV(MW)}{RT}$$

where,  $V$  is the volume of NGV's tank, constant at 55 liter

$T$  is the temperature in the tank(assumed constant at 30<sup>0</sup>C)

$MW$  is the molecular weight of natural gas

$P$  is the pressure in Pascal

$R$  is the gas constant (8.314 J/molK)

$m$  is the mass of the natural gas transferred to tank, kg

The pressure is varies and the reading of mass is recorded. The calculation is done at both compositions. Then the result is plotted in the graph. The graph plotted is as below.

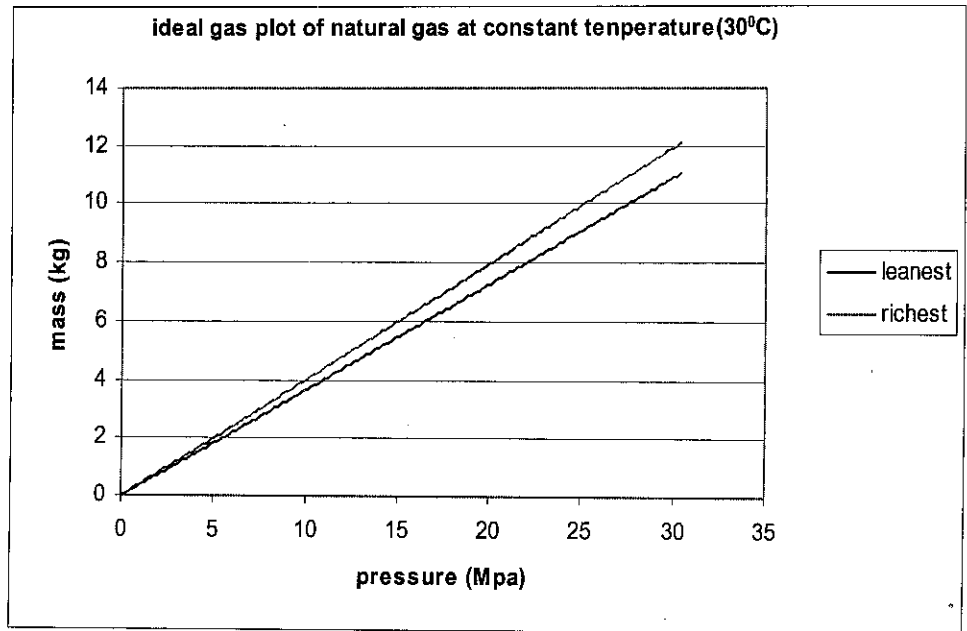


Figure 3: Ideal Gas Plot at 30°C

This graph shows the difference between the mass given by the leanest and the richest composition. As expected, the richest settle higher compared to the leanest composition. With higher molecular weight, the richest composition can be considered as denser than the leanest composition.

#### 5.4.2 Calculation Using Soave-Redlich-Kwong EOS

This SRK equation of state requires some additional calculation before can come out with the final equation.

Reduced pressure of the natural gas if found using

$$P_r = \frac{P}{P_c}$$

where P is the vapor pressure calculated at T\* (T\* = 0.7 T<sub>c</sub>)

From this reduced pressure, acentric factor is calculated using

$$\omega = -\log P_r - 1$$

since  $P_r$  is already the reduced pressure for the mixture, thus  $\omega$  is can straight away be considered as the acentric factor for the mixture.

reduced pressure and acentric for both compositions are as below;

Table 10: Properties of Natural Gas for Different Composition

	Leanest composition	Richest composition
Vapor pressure at T*	0.1330355	0.202059
Acentric factor	-0.115126	-0.305478

Then, the empirical parameter for SRK will be calculated using the formulas below.

$$a(T_c) = a_c = 0.42748 \frac{(RT_c)^2}{P_c}$$

$$b = 0.08664 \frac{RT}{P_c}$$

$$a(T) = a_c \cdot \alpha(T)$$

$$\alpha = \left[1 + M(1 - \sqrt{T_r})\right]^2$$

$$m = 0.480 + 1.574\omega - 0.176\omega^2$$

The calculated empirical constants are summarized in the table below;

Table 11 : Empirical Constant for SRK Calculation

Parameter	Leanest composition	Richest composition
$a(T_c)$	0.286923	0.289983
$b$	$3.08 \times 10^{-5}$	$3.25 \times 10^{-5}$
$a(T)$	0.250659	0.288175
$\alpha$	1.144671	0.993765
$m$	0.296459	-0.017246

these parameters will finally inserted in the SRK equation of state to get the final equation that will be used to plot the graph.

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

$v$  is the molar volume of the natural gas that can be expressed as

$$v = \frac{MW}{\left(\frac{m}{V}\right)}$$

Where MW and volume are known. Thus this equation can be inserted in SRK equation to have a relation between pressure and mass.



The graph that been plotted gives the result below;

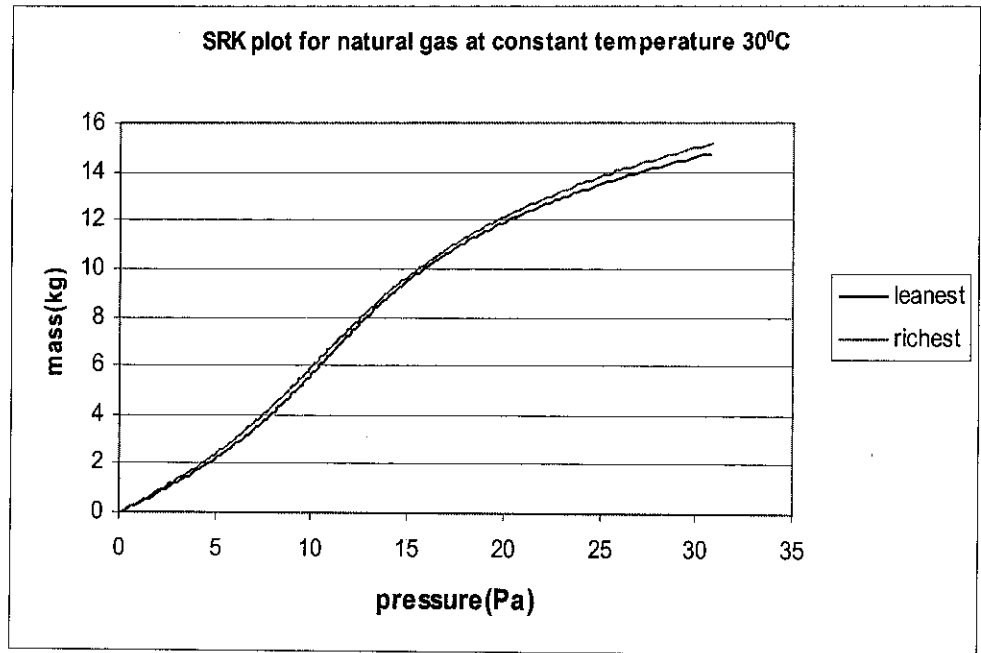


Figure 4: SRK Plot at 30°C

The result that had been determined shows a parabolic relationship between mass and pressure. The steepest slope occurs somewhere between 10 to 20 MPa. And as being observed in the ideal gas behavior, the richest composition gives slightly higher mass at a certain pressure.

#### 5.4.3 Calculation Using Peng Robinson EOS

The calculation for Peng Robinson is not much different from SRK's calculation. The only different is the formula used to get the empirical constants. The empirical constant is calculated using the formulas below;

$$a(T) = 0.45724 \frac{(RT_c)^2}{P_c} \alpha(T)$$

$$b = 0.07780 \frac{RT_c}{P_c}$$

$$\sqrt{\alpha} = 1 + k \left[ 1 - \sqrt{\frac{T}{T_c}} \right]$$

$$k = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

The data from this calculation is summarized below;

Table 12: Empirical Constants for Peng Robinson Calculation

Parameter	Leanest composition	Richest composition
$\omega$	-0.11513	-0.30497
$k$	0.19351	-0.12081
$\alpha$	0.910833	1.04423
$a(T)$	0.24419	0.3724
$b$	0.0000277	0.0000312

Then these values will be inserted in the Peng Robinson equation to get the final equation. The  $v$  term in the equation will be replaced in term of mass as done in SRK calculation.

Peng Robinson EOS is given as follow;

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

The result that been determined is plotted in the graph below;

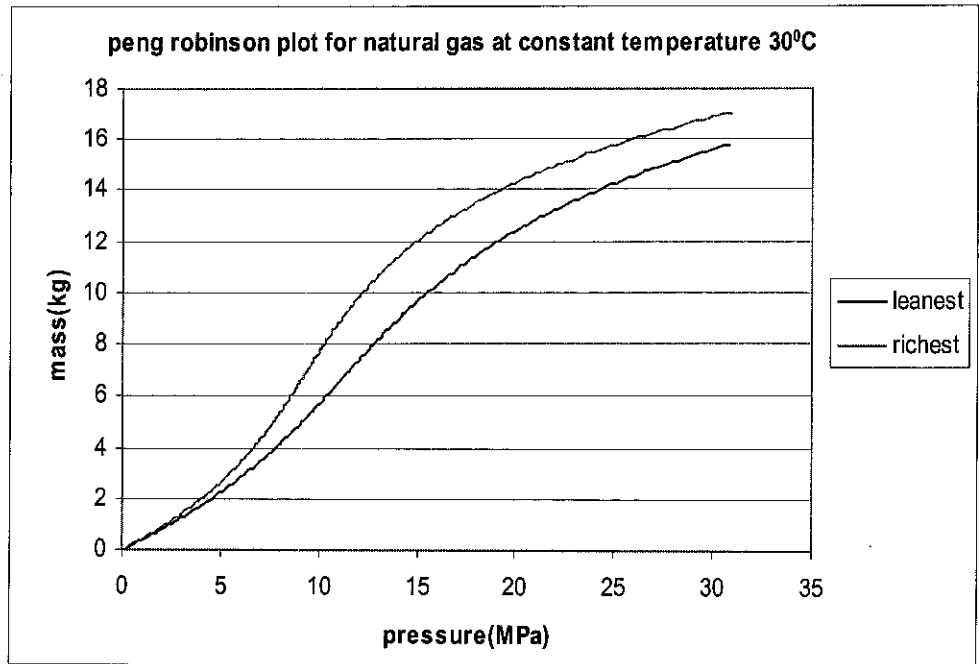


Figure 5: Peng Robinson Plot at 30<sup>0</sup>C

This plot show the same pattern as SRK plot. But the different in mass recorded between leanest and richest composition is more significant. Thus Peng Robinson is more sensitive to the changes in composition.

After the graph for each equation of state is determined, the comparison between these equations of state is studied. Graphs that combine all the equations of state are plotted.

The graphs that been plotted are as follow;

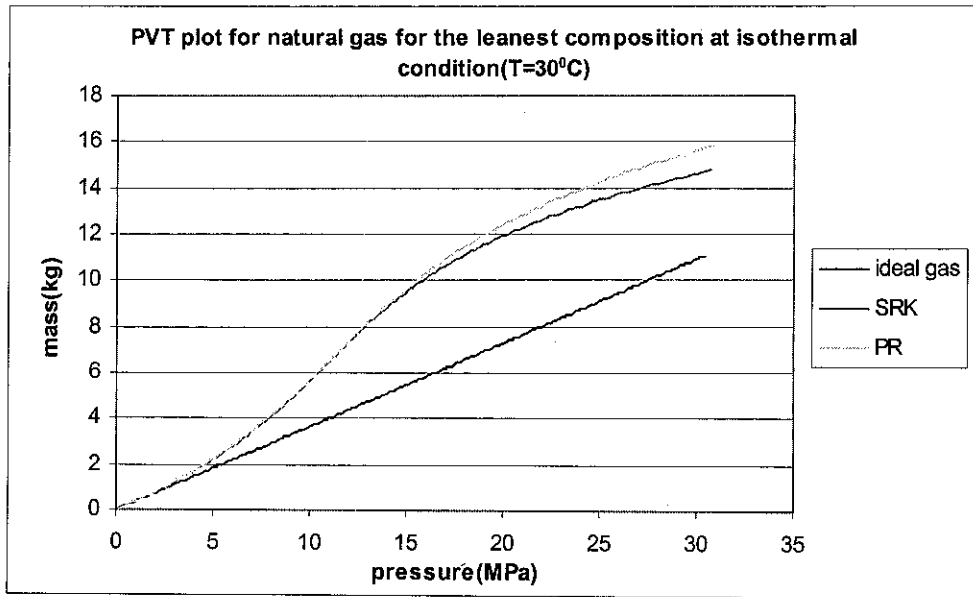


Figure 6 : PVT Plot for the Leanest Composition

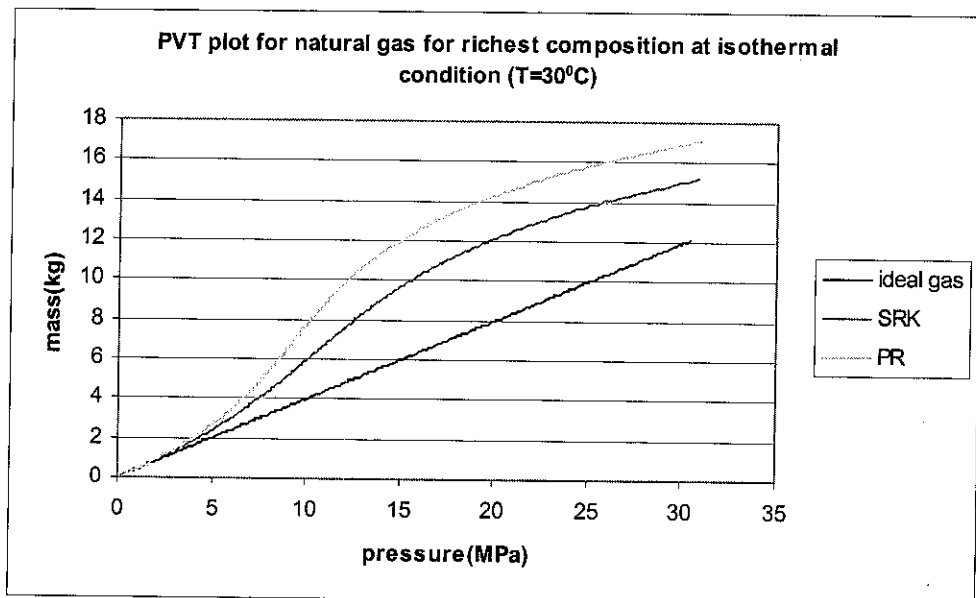


Figure 7 : PVT Plot for the Richest Composition

Basically, both graphs show the same pattern. Peng Robinson gives the highest mass at certain pressure, followed by Soave-Redlich-Kwong. The ideal gas equation settled much lower compared to the other equation of state. This is due

to its ideal assumption that there are no intermolecular forces between the molecules.

But in real condition, there are attractive and repulsive forces between the molecules. This attractive force between the hydrocarbon molecules makes the molecules get closer together occupying less volume. This will cause the density recorded become more than in ideal condition. Thus, this will lead to higher mass data.

From both of the graph, the three lines coincide at the beginning of the plot where the pressure is low. This is because, every equation of state manage to show an ideal behavior of the fluid at low density region. At thus point, the intermolecular forces can be neglected since the distances between each molecule are far from each other to introduce any interconnection between those molecules.

### **5.5 Variation of Mass as a Function of Pressure and Temperature**

Other thermodynamic property that becomes a concern is the temperature of the natural gas. During the refueling process, the tank will experience some reduction in temperature. This can be explained by Joule Thomson effect. The Joule Thomson coefficient is

$$\mu_{JT} = \frac{\partial T}{\partial P}$$

The value of this coefficient can be negative or positive depend on the reduced temperature and reduced temperature value. According to this principle, the cooling occurs when high pressure gas is expended. In this case, the gas from the dispensing unit is at high pressure going to a lower pressure tank in the natural gas vehicle.

The calculation to see the variation in temperature affect to mass is done at the range of 20<sup>0</sup>C to 32<sup>0</sup>C. Manual calculation might be too tedious to be repeated at

different temperature. If the temperature is changed, the other properties also change.

Thus a much simpler approach is considered to perform this calculation. HYSIS has become the best approach to study the relationship between mass, temperature and pressure. The method is rather simple. The author only has to choose which equation of state that want to be used and then enter the composition of the natural gas. Then, the parameters such as temperature and pressure are keyed in. The value of density will be displayed. This density will be easily converted to mass by multiplying with volume of the tank which is 55 liter.

Using this method enable the author to use more equation of state. Here, Lee Kesler Plocker is also been used as it was found to be suitable for natural gas application. The result is then plotted in graphs. Below are the results that been determined using the respective equation of state for the leanest composition.

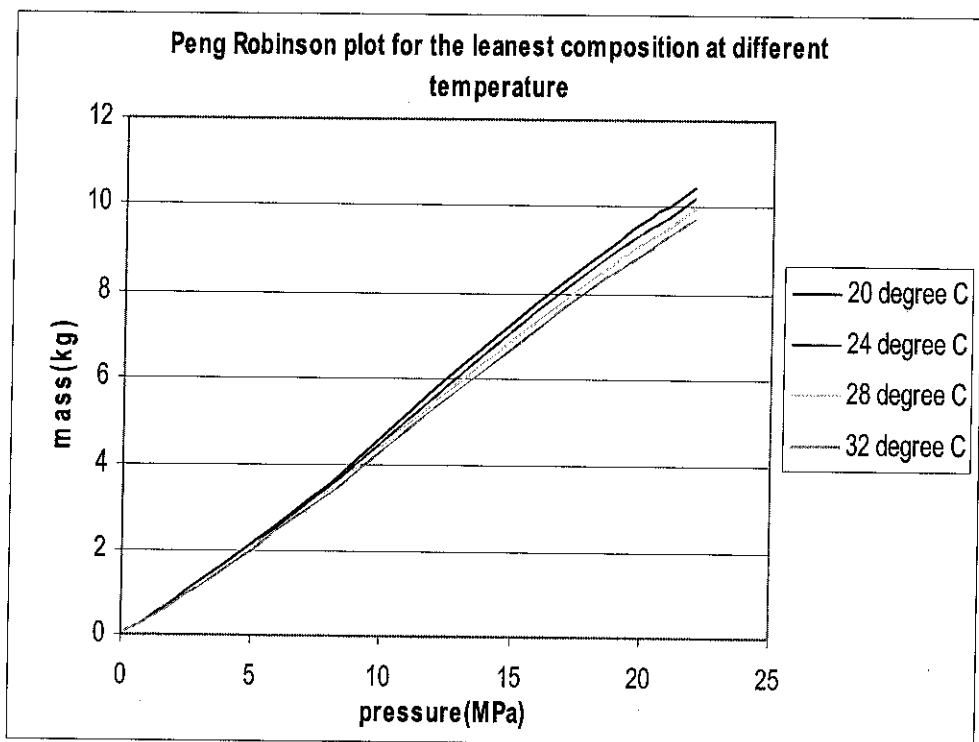


Figure 8: Peng Robinson Plot at Different Temperature

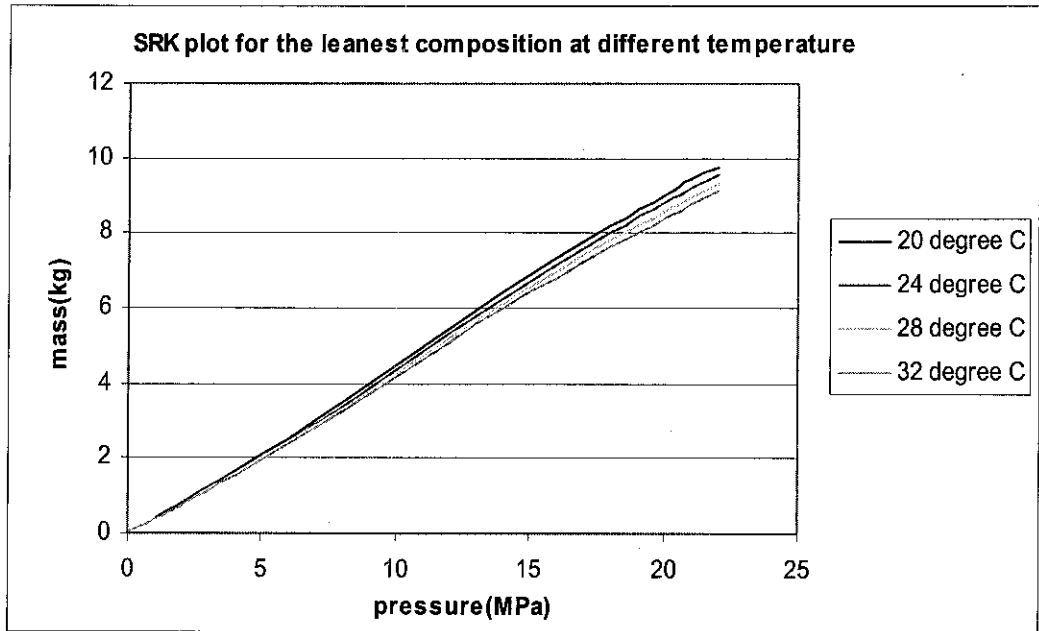


Figure 9: SRK Plot at Different Temperature

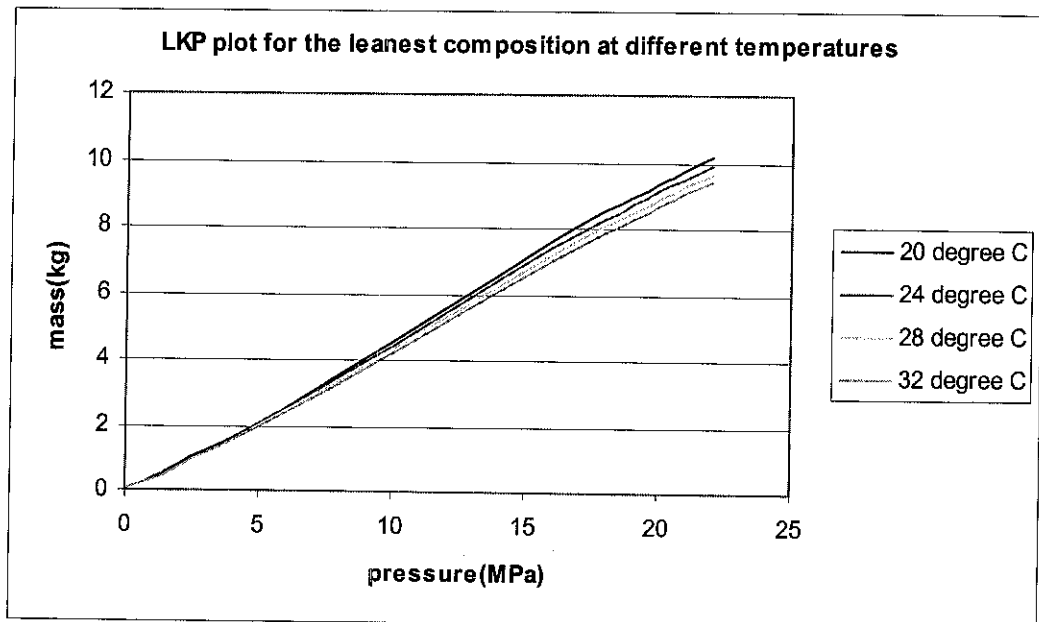


Figure 10: LKP Plot at Different Temperature

Basically, the three equations of state give almost a similar relationship. At certain pressure, higher temperature gives lower volume. This phenomenon is theoretically correct. At higher temperature, there is more thermal energy being transferred to the molecules that lead to increment in their kinetic energy.

The molecules moves faster and occupy larger volume. Thus the density of the component decreased causing a reduction in mass in a constant volume container. But the reduction in the mass is not too significant as the temperature changes. Gas is more sensitive to pressure changes as it is easily compressible.

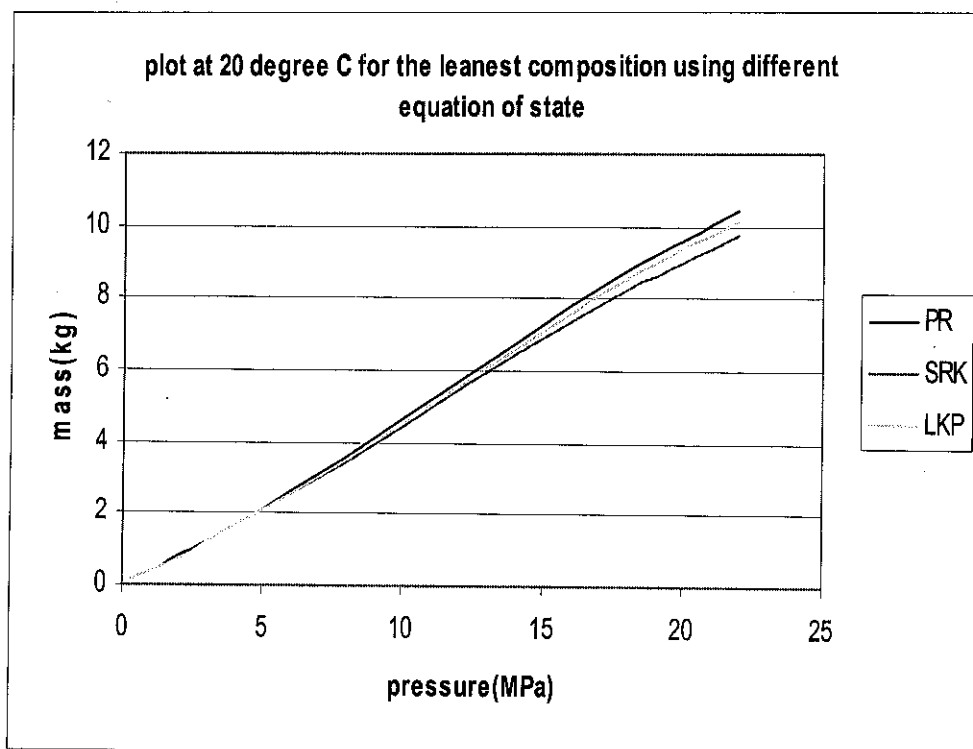


Figure 11: Plot at 20<sup>0</sup>C Using Different Equation of State

Take for example the graph that been plot above. At a certain temperature and composition, Peng Robinson gives the highest mass while SRK gives the lowest. Lee Kesler plot settled somewhere in between these two equation of state.



In most literature, Peng Robinson is always the best equation of state for hydrocarbon. Data gained from calculation is compared with the actual data in those literatures. The same should have been done in this project. But unfortunately, the equipment can need to be used for the test cannot reach within this research period. The only comparison that managed to be done is between the data determined from this research with data from literature. But this comparison might not be too accurate as the composition of natural gas used in the literature is not the same with the one in this research.

Note : for more graph at different composition and temperature, please refer appendix.

## 6.0 CONCLUSION AND RECOMMENDATION

The objective of the research to convert natural gas volume to its mass using its thermodynamic properties has been achieved. The relationship between natural gas properties and its variation in density and mass can be observed as well.

The density and mass is directly proportional with pressure. If pressure in the system increased, the density will also increase. This is because, at higher pressure, there will be more force been exerted on the molecules causing them to get closer to each other. This cause an increase in density and at constant volume, the mass of the system also increases.

Temperature on the other hand cause reduction in mass as temperature is increased. At higher temperature, the molecules get more power in form of heat causing them to move more frequently and occupy larger volume. The distance between the molecules is increasing causing a reduction in density. And for an isochoric system, the mass of the natural gas will decrease if the temperature is increase and the pressure is kept constant.

From the literature, Peng Robinson is the best equation of state that can be applied for natural gas system. Peng Robinson is developed as an improvement of Soave Redlich Kwong thus offering a more accurate reading compared to SRK. Besides, many literatures had been done and conclude that Peng Robinson is best suited for light hydrocarbon calculation. In this research, Peng Robinson gives higher reading of mass at a certain pressure and temperature compared to Soave Redlich Kwong and Lee Kesler Plocker.

The effect of composition is been determined in this research. The richest composition which has higher molecular weight gives a higher reading of mass at certain pressure and temperature. The same pattern is observed for every Equations of State.

Peng Robinson is considered as the best by referring to the theoretical research. There is a necessity to have the data been compared and justified by real test. Since there is no facilities that can be used to test the data, the procedure could not be performed. Thus, in

future, when the equipment is purchased and ready for used, the test to confirm this data should be conducted. This test is important to determine which Equation of State gives the best data that can fit the actual process.

Calculation using combination of several equation of state and activity coefficient method could be test as well. The result might give a better data that can fit the real process much better compared to the single Equation of State. At some range of temperature and pressure, one Equation of State might be used and then at another range, the other Equation of State could be implemented.

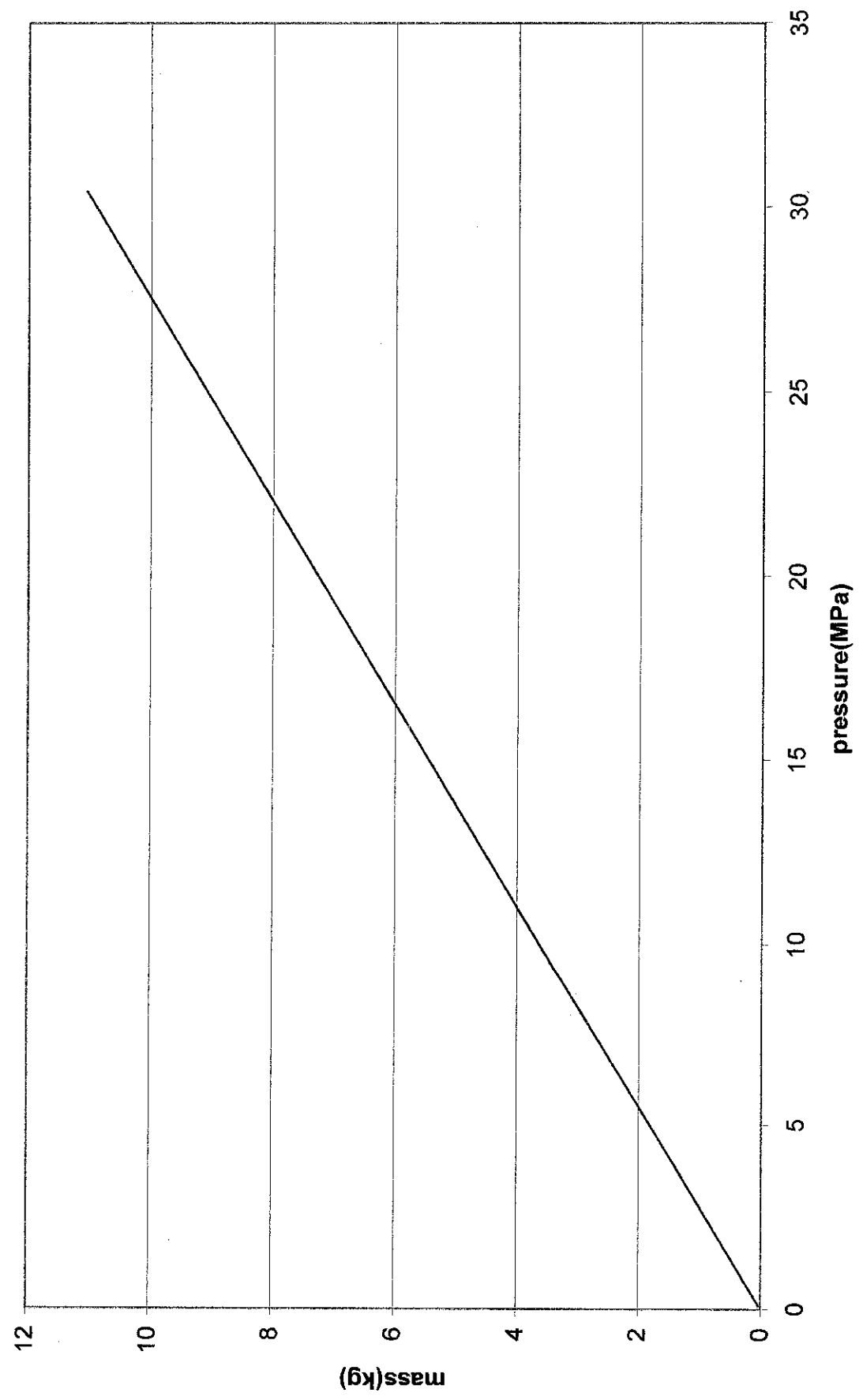
A wider range of composition might also be studied. More data from PRSS is required in order to perform this calculation. Calculation might be done by creating own composition, but this might not be practical. It would be much better if the compositions that been used are the one available in market.

Basically, the objectives of the project to convert volume of natural gas to its density had been achieved. Hopefully, this research can help to build a natural gas refueling station at lower cost.

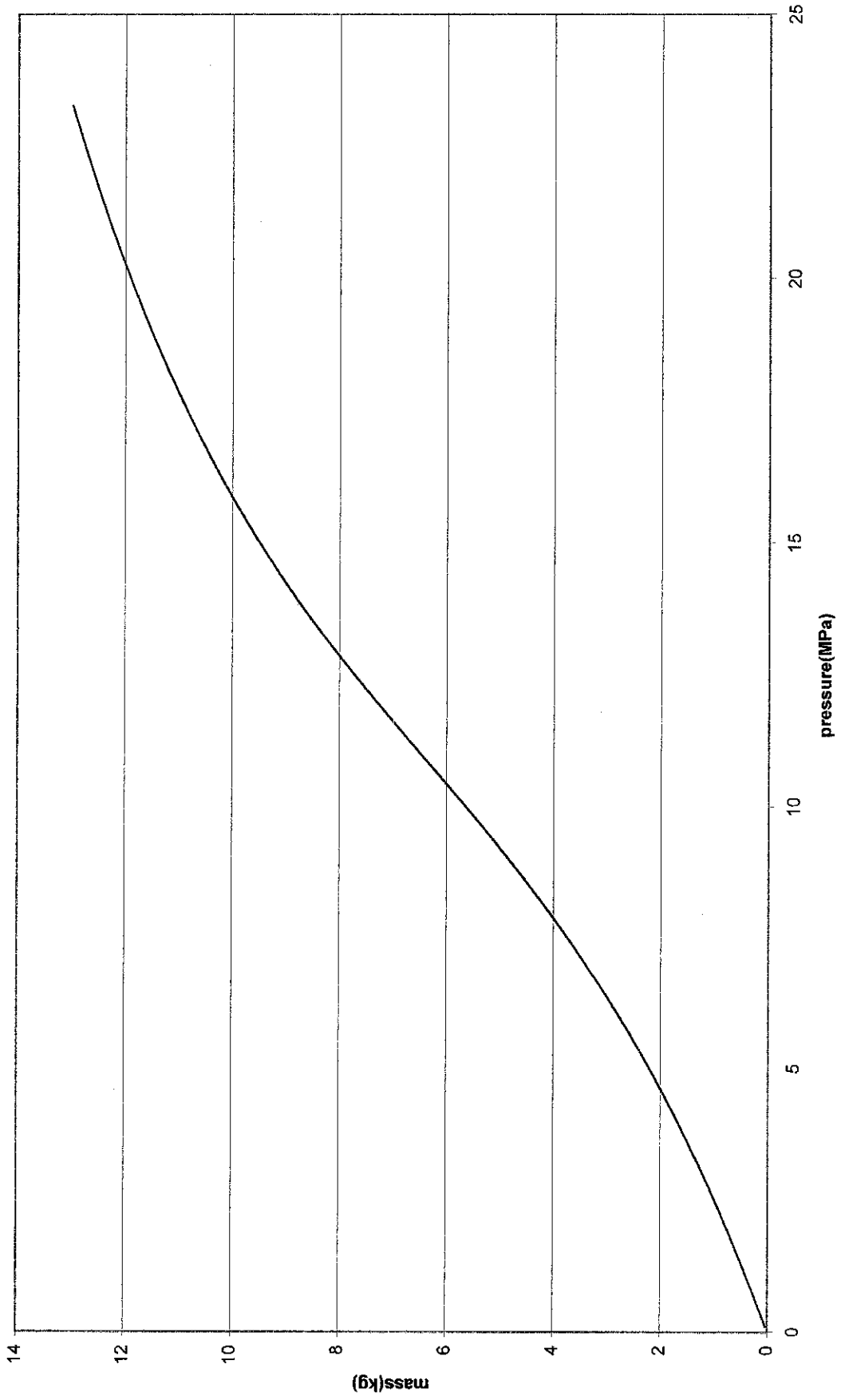
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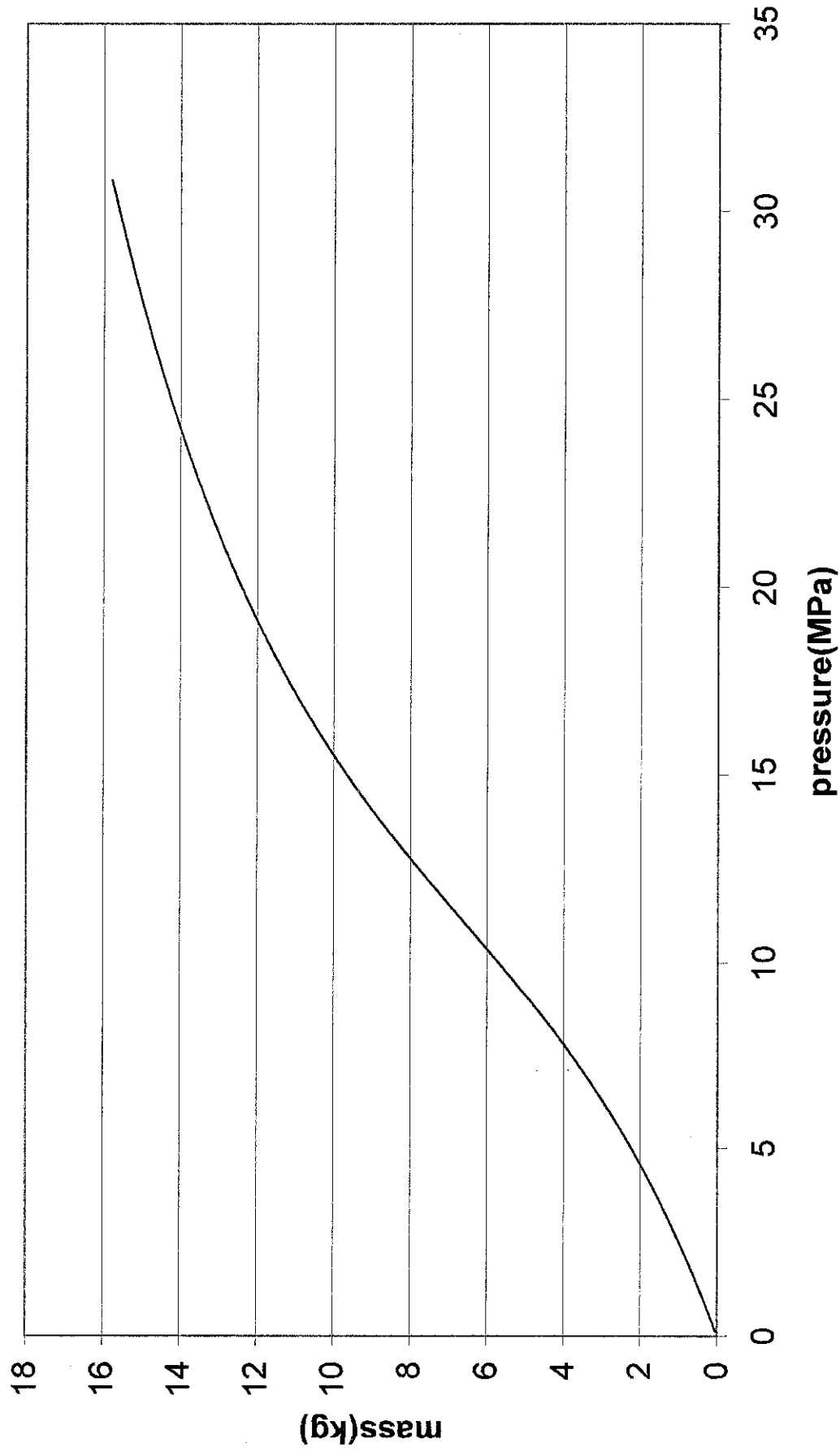
ideal gas plot for the leanest composition at constant temperature 30°C



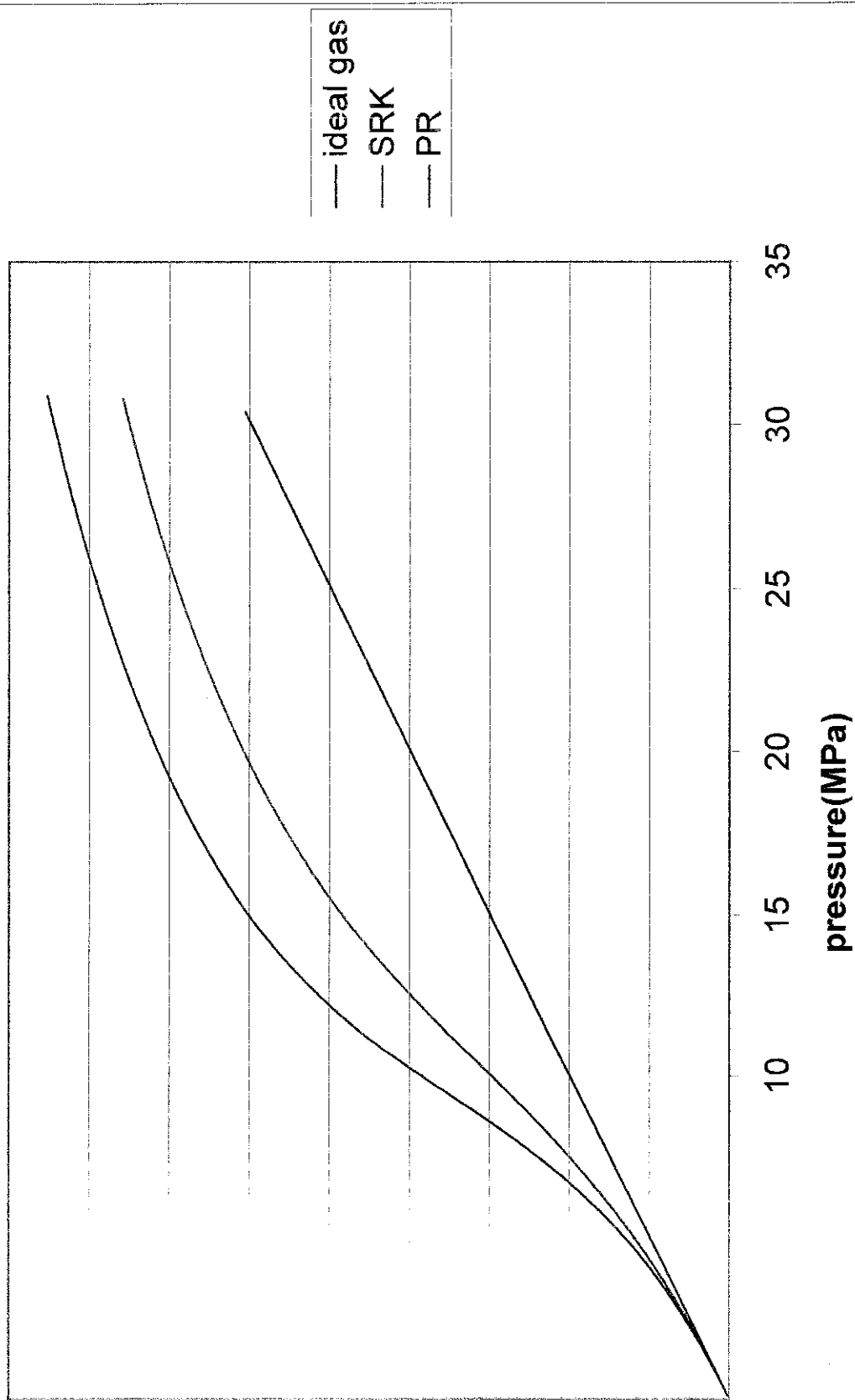
SRK plot for the leanest composition at constant temperature 30°C



**peng robinson plot for the leanest composition at 30°C**

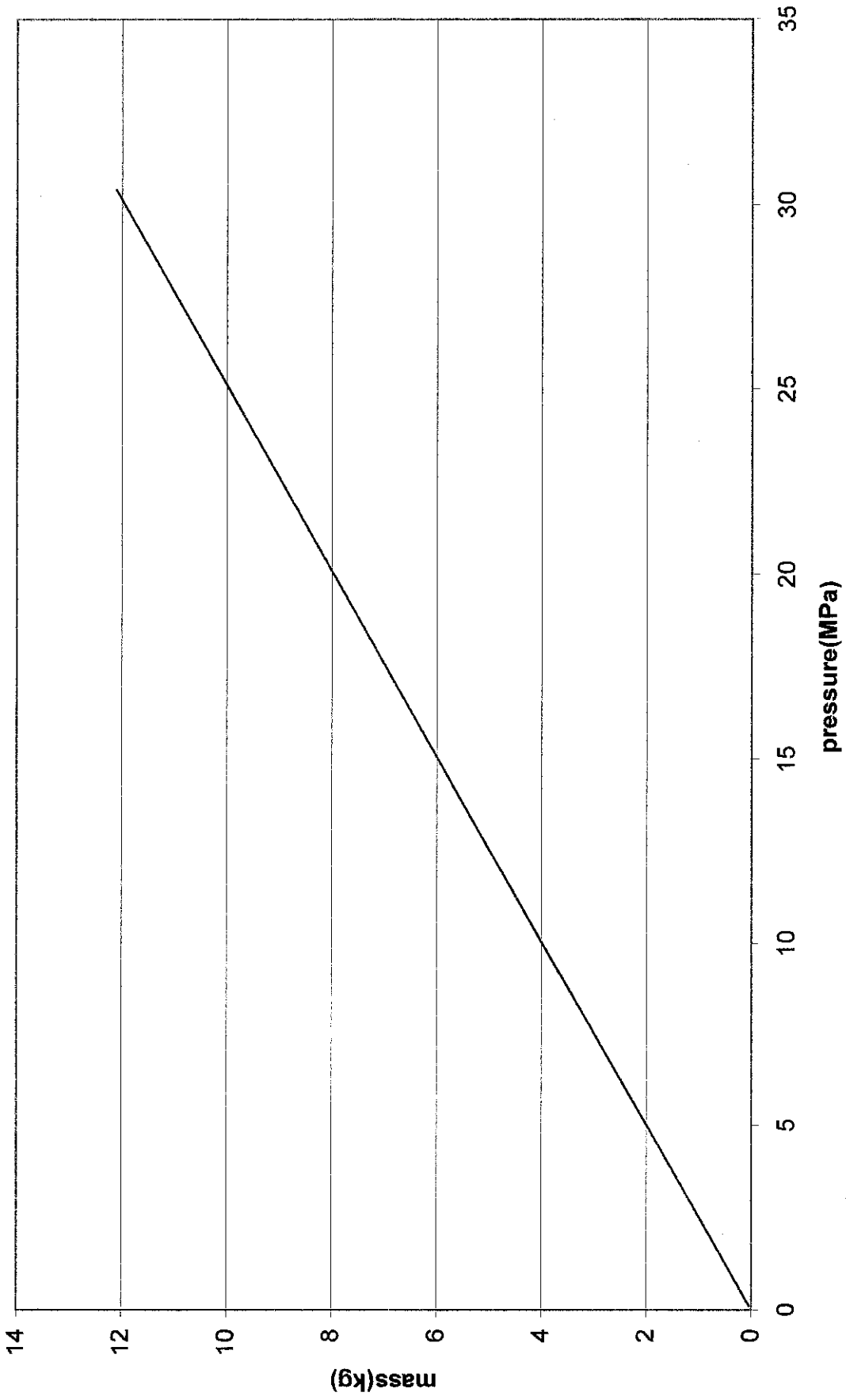


# Pressure for richest gas for richest composition at isothermal condition ( $T=30^{\circ}\text{C}$ )

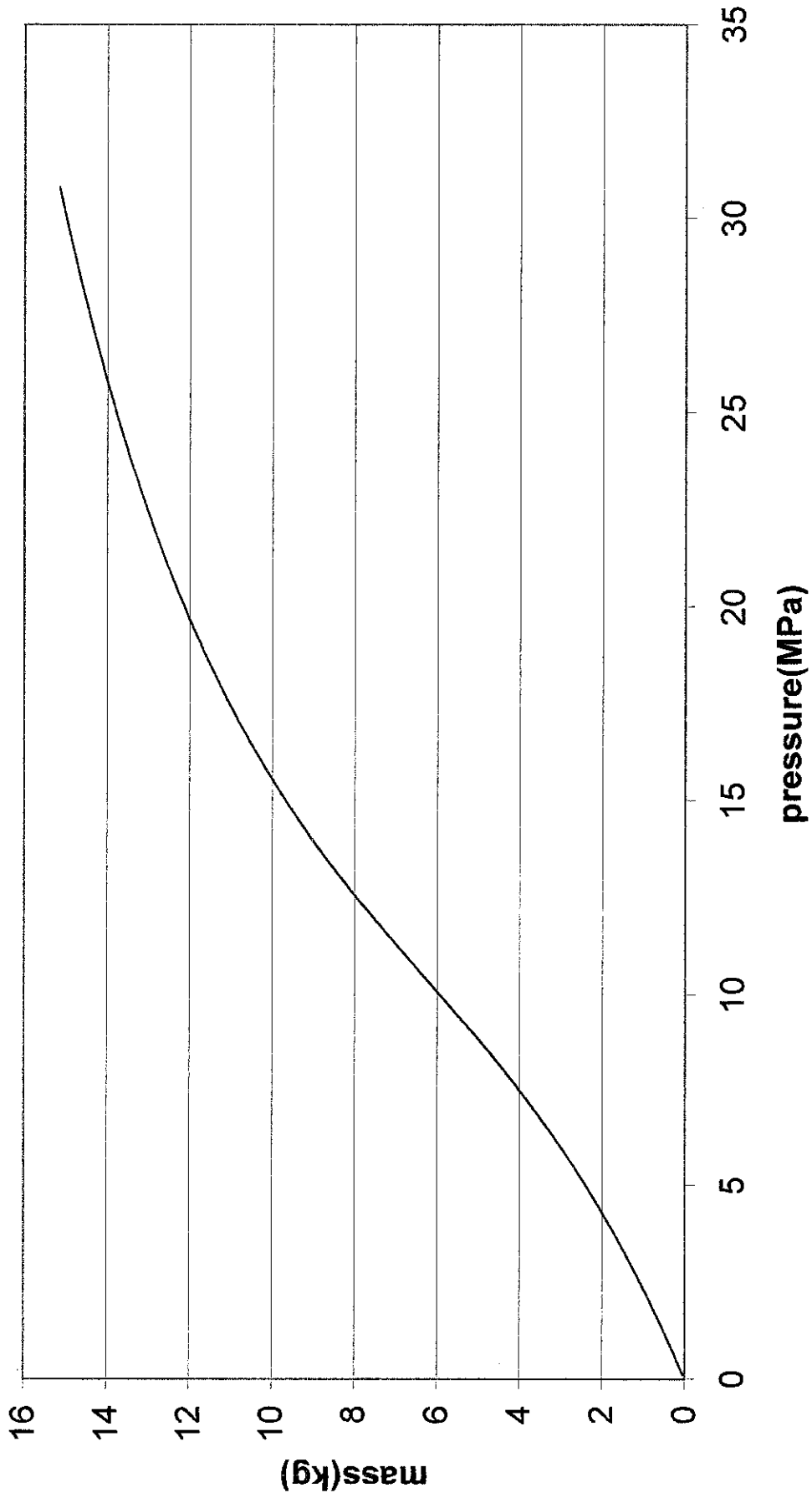




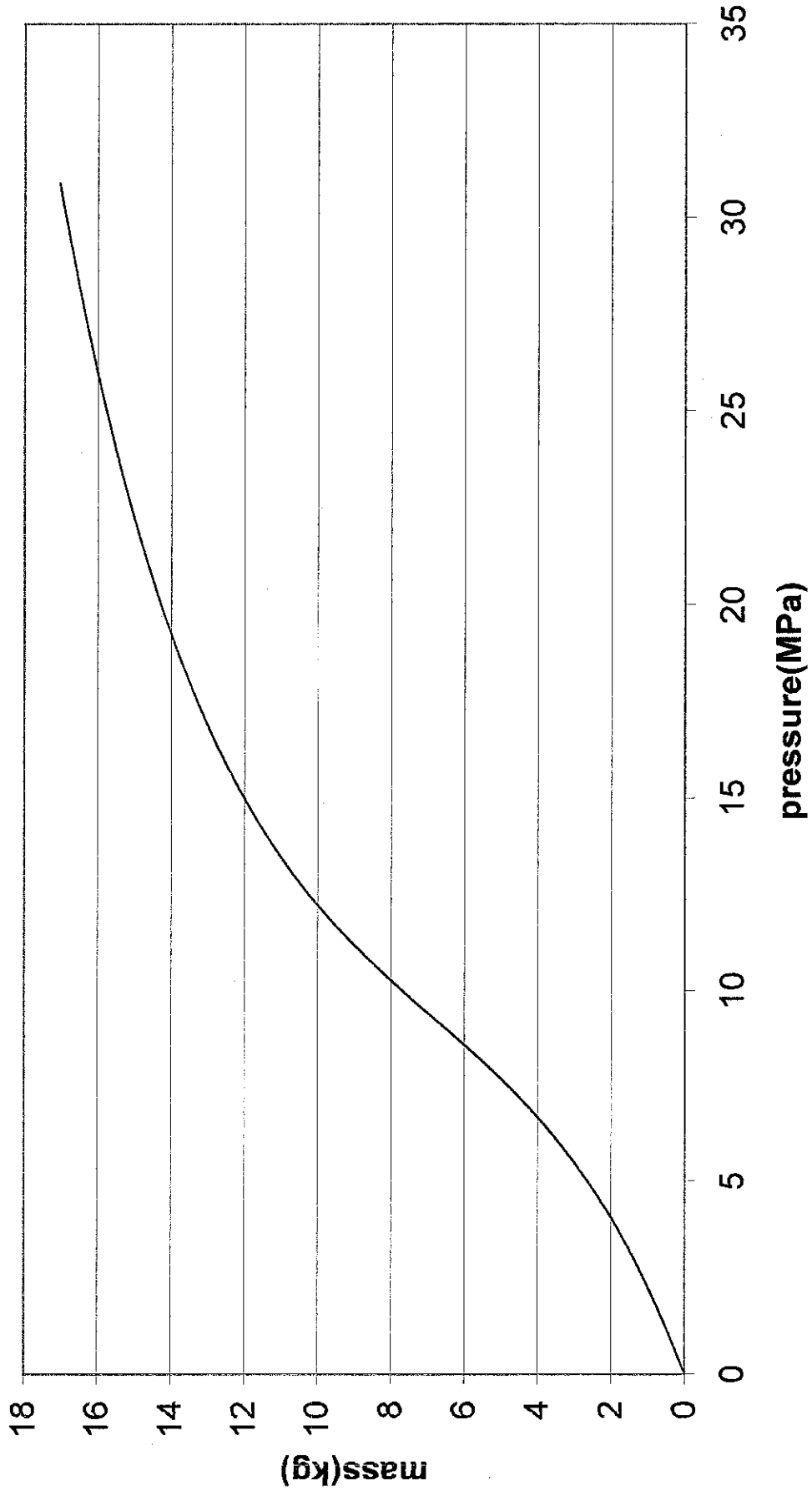
**ideal gas plot for the richest composition at constant temperature 30°C**



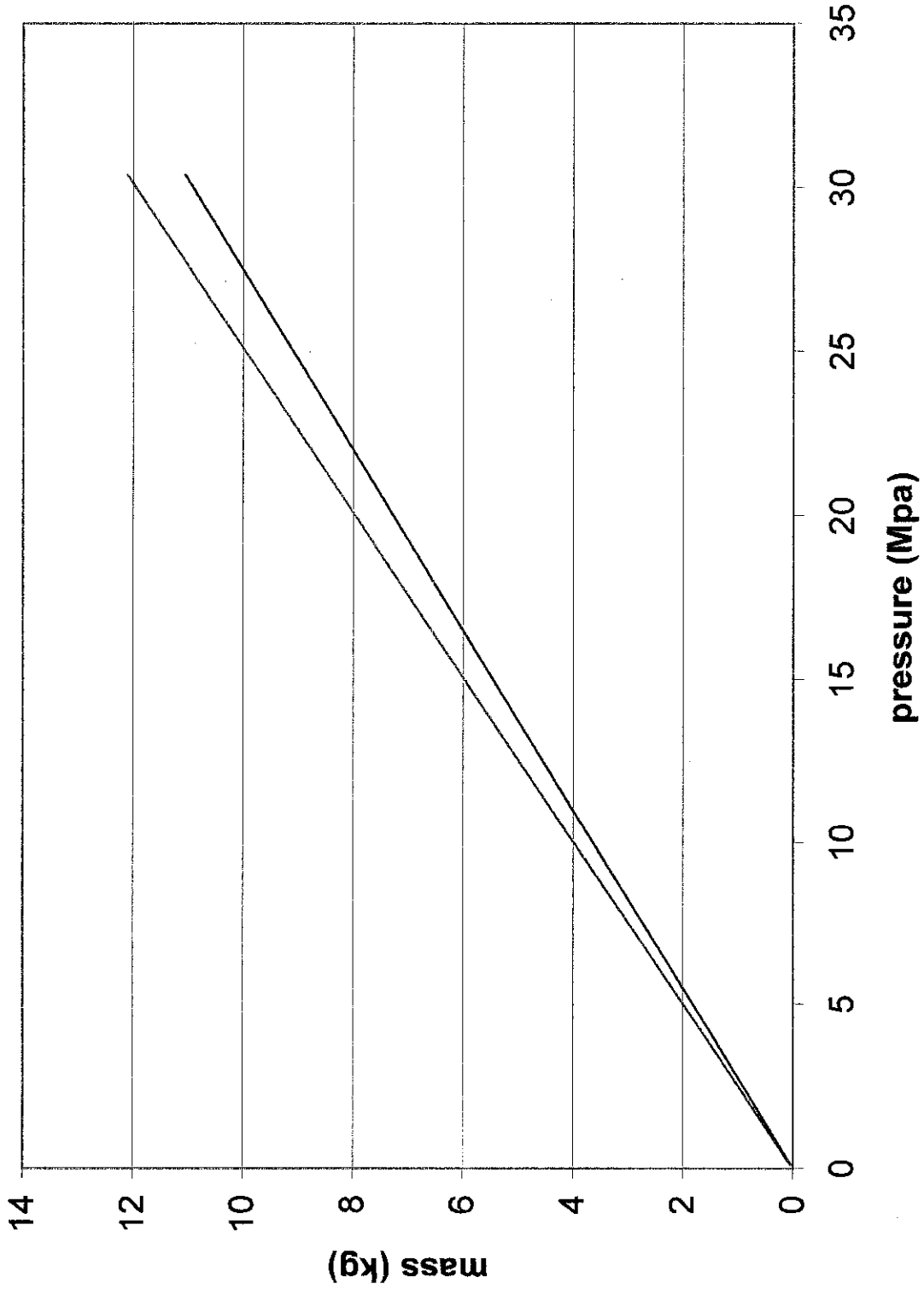
# SRK plot for the richest composition at constant temperature 30°C



**peng robinson plot for the richest composition at constant  
temperature 30°C**

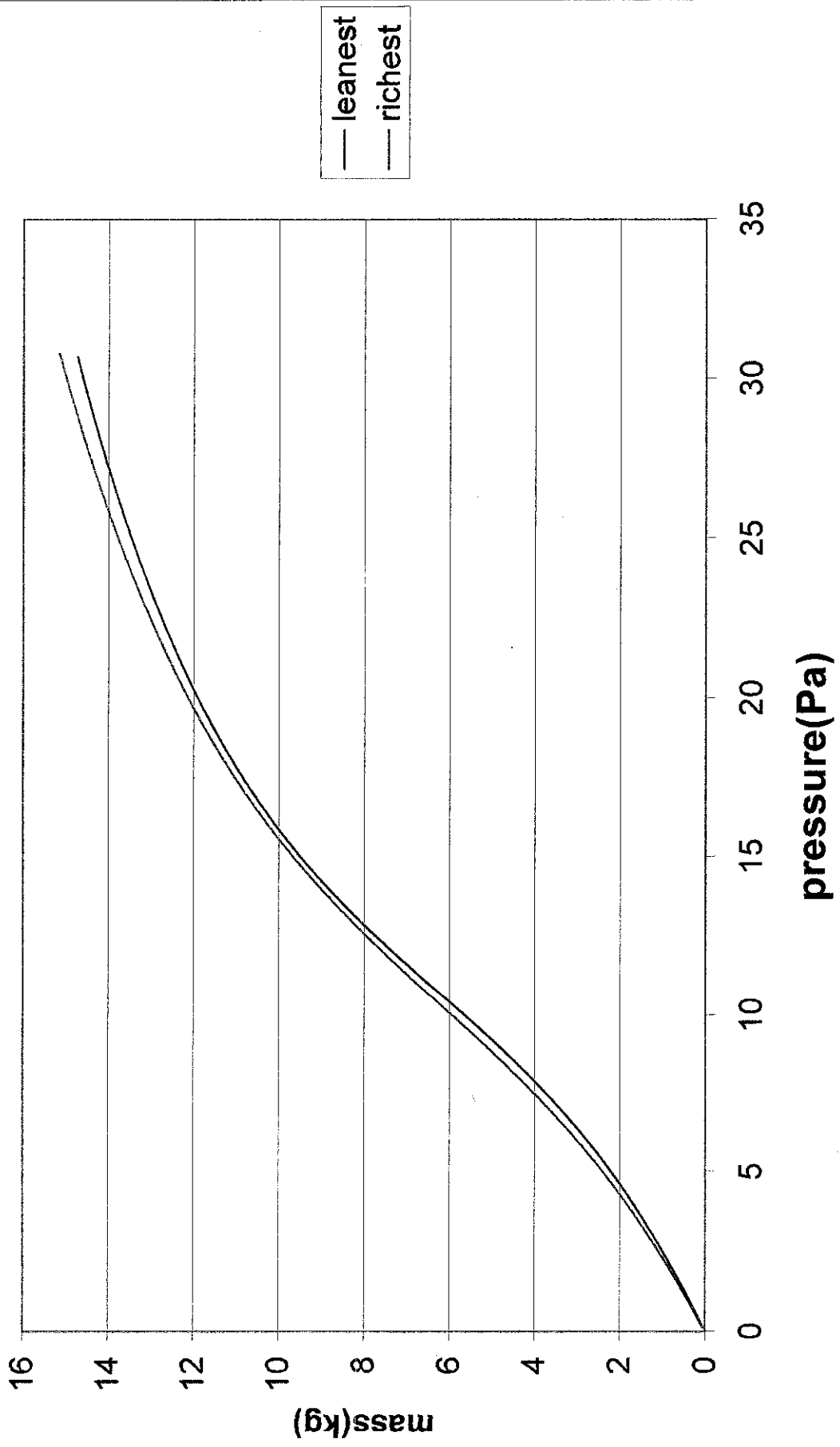


ideal gas plot of natural gas at constant temperature(30°C)

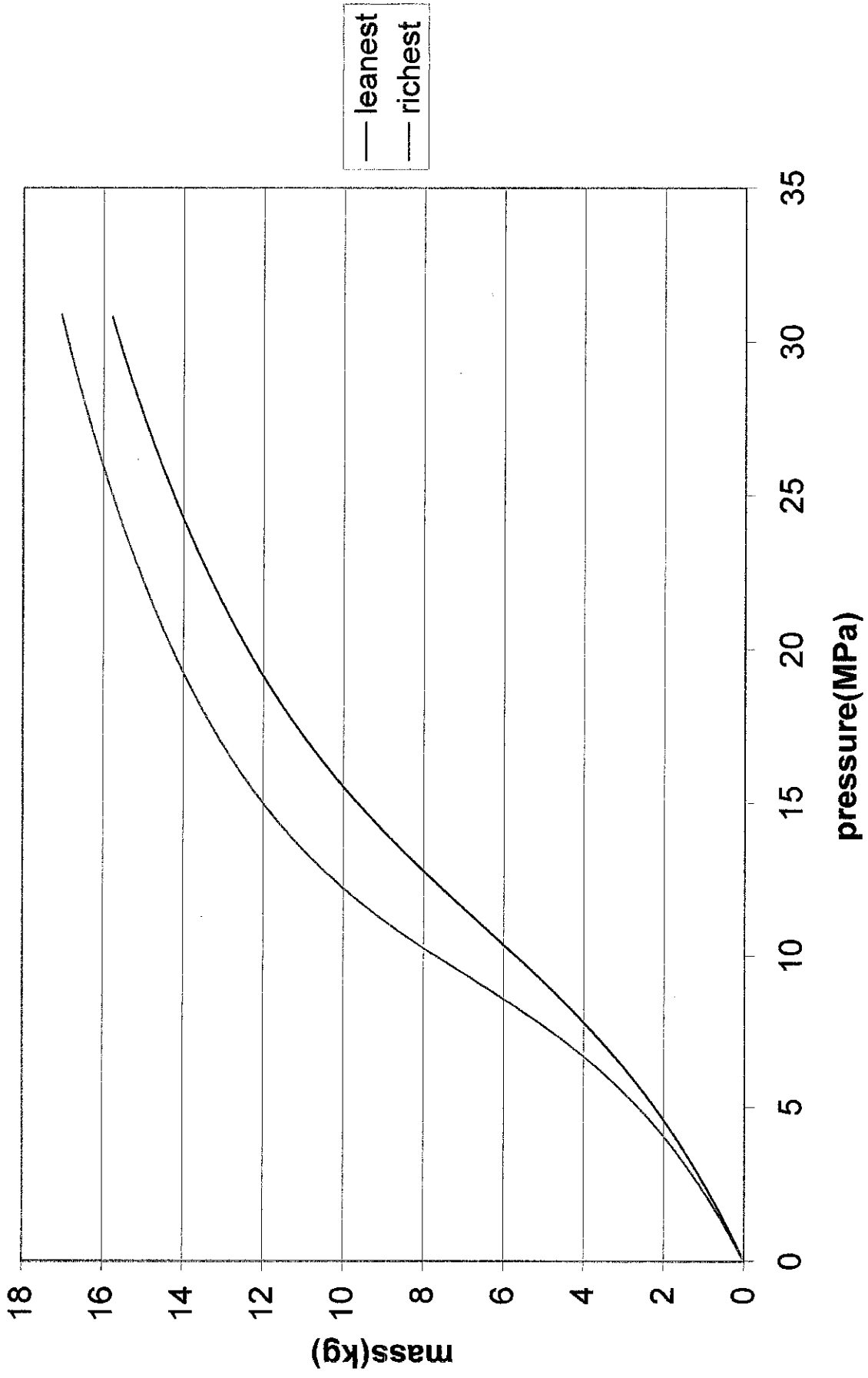


— leanest  
- - richest

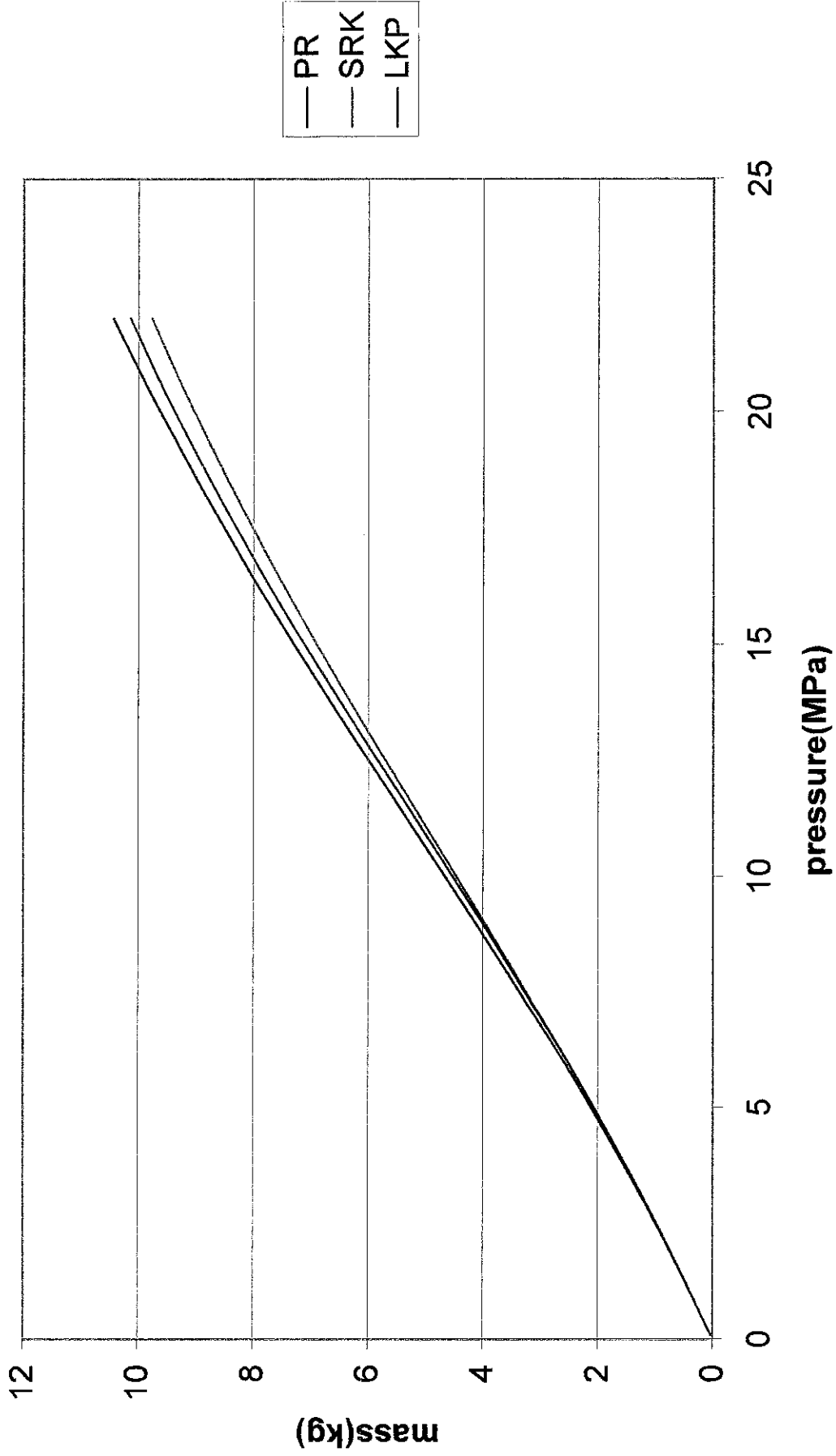
SRK plot for natural gas at constant temperature 30°C



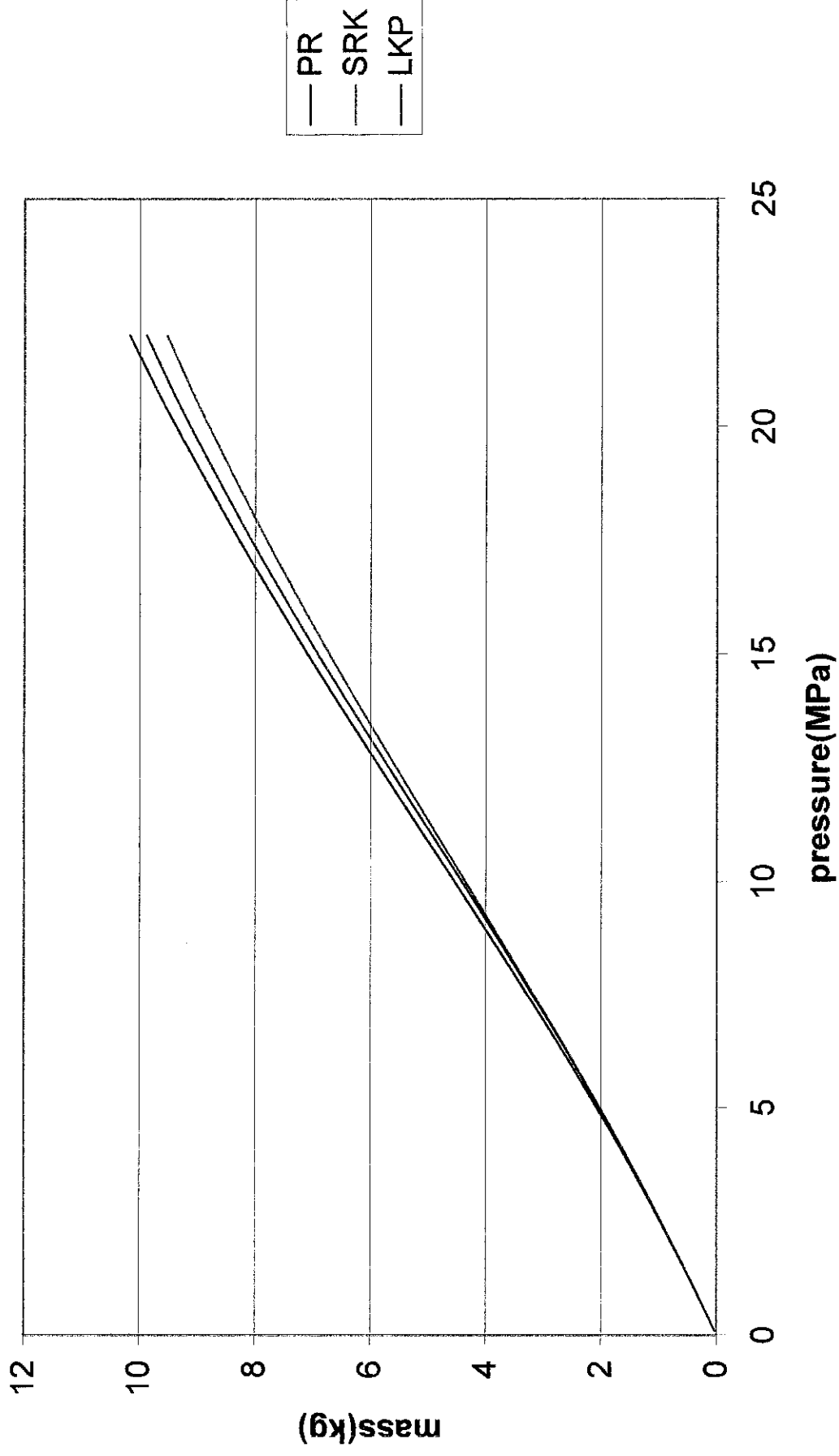
peng robinson plot for natural gas at constant temperature 30°C



plot at 20 degree C for the leanest composition using different equation of state

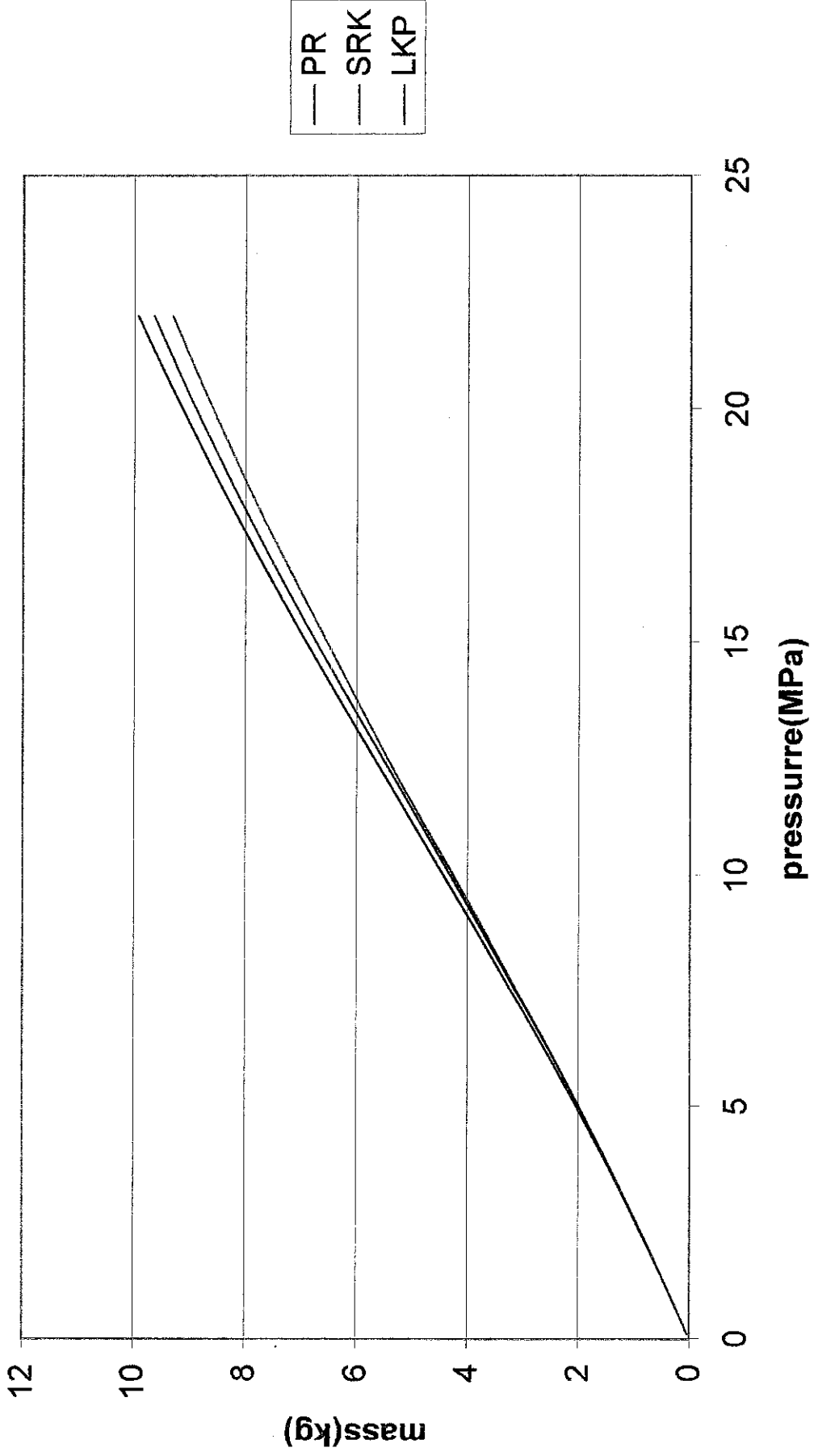


plot at 24 degree C for the leanest composition using different equation of state

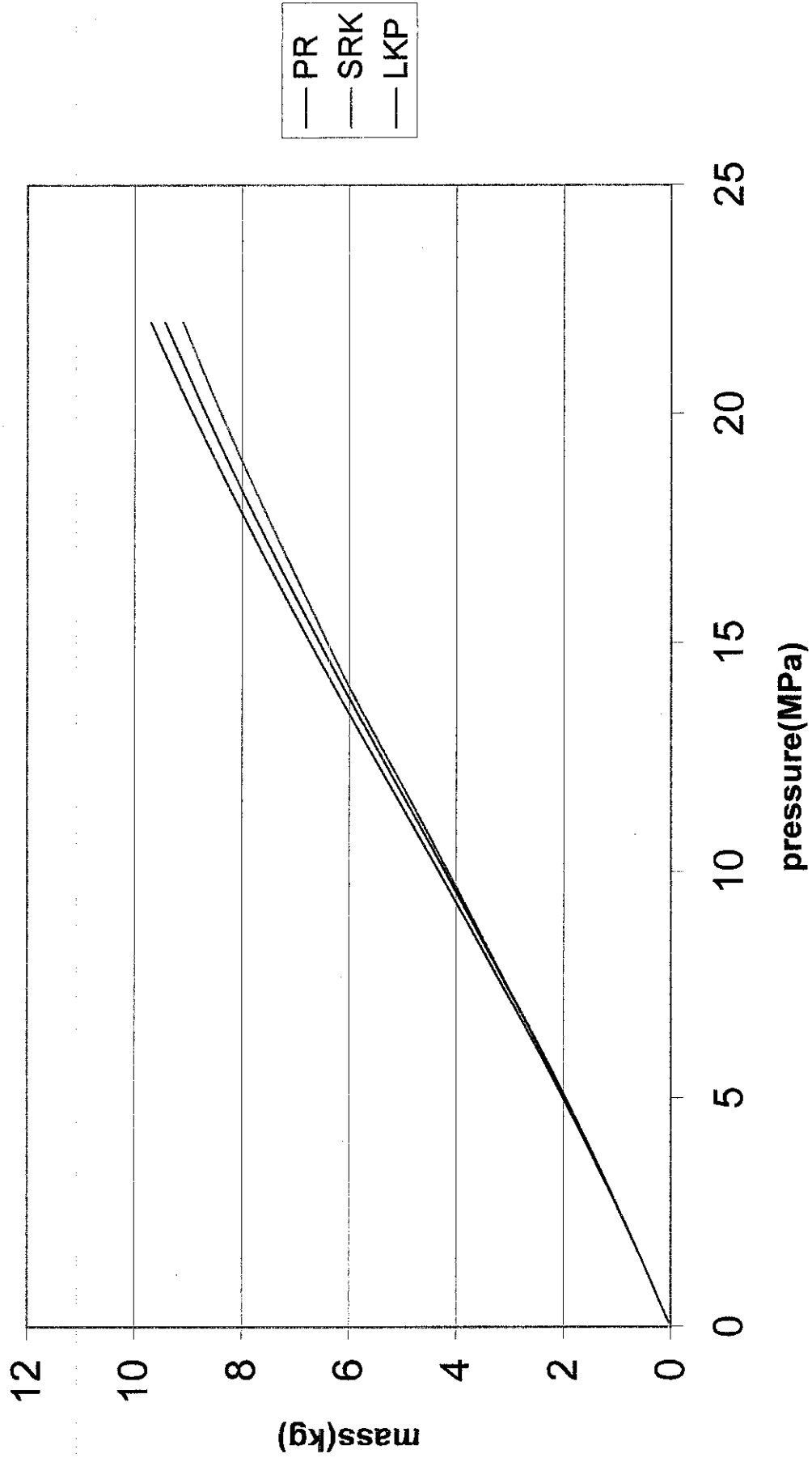




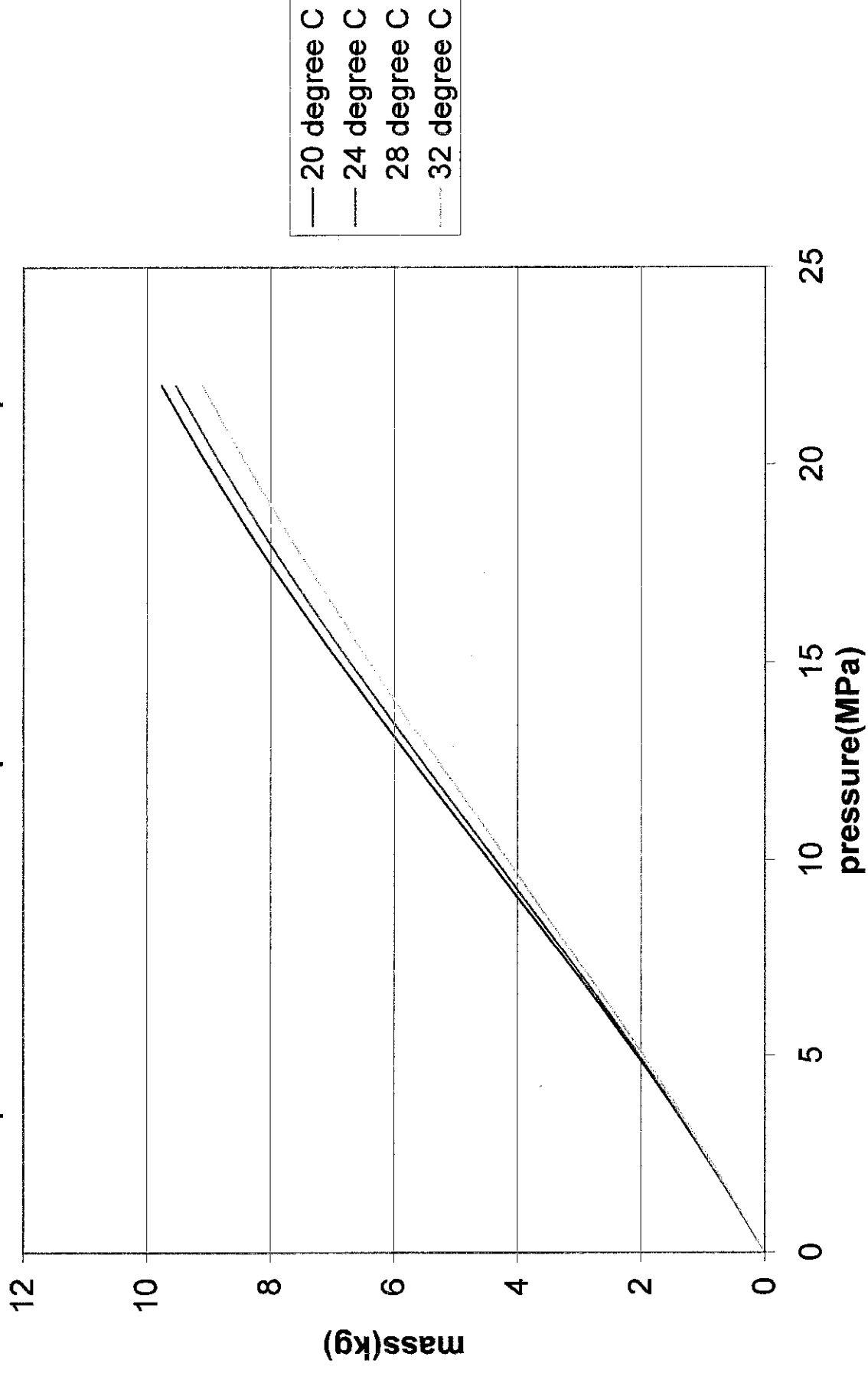
plot at 28 degree C for the leanest composition using different equations of state



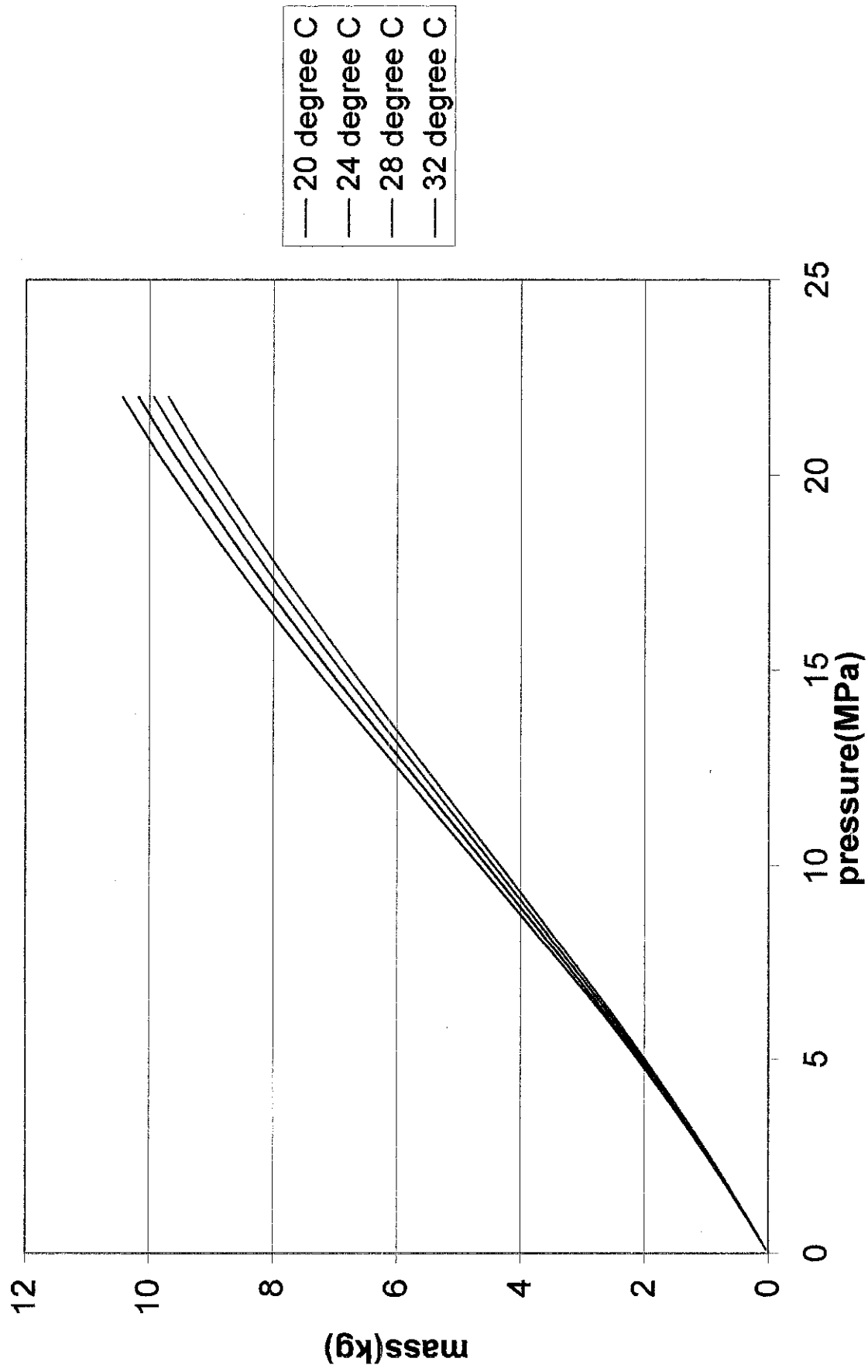
plot at 32 degree C for the leanest composition using different equation of state



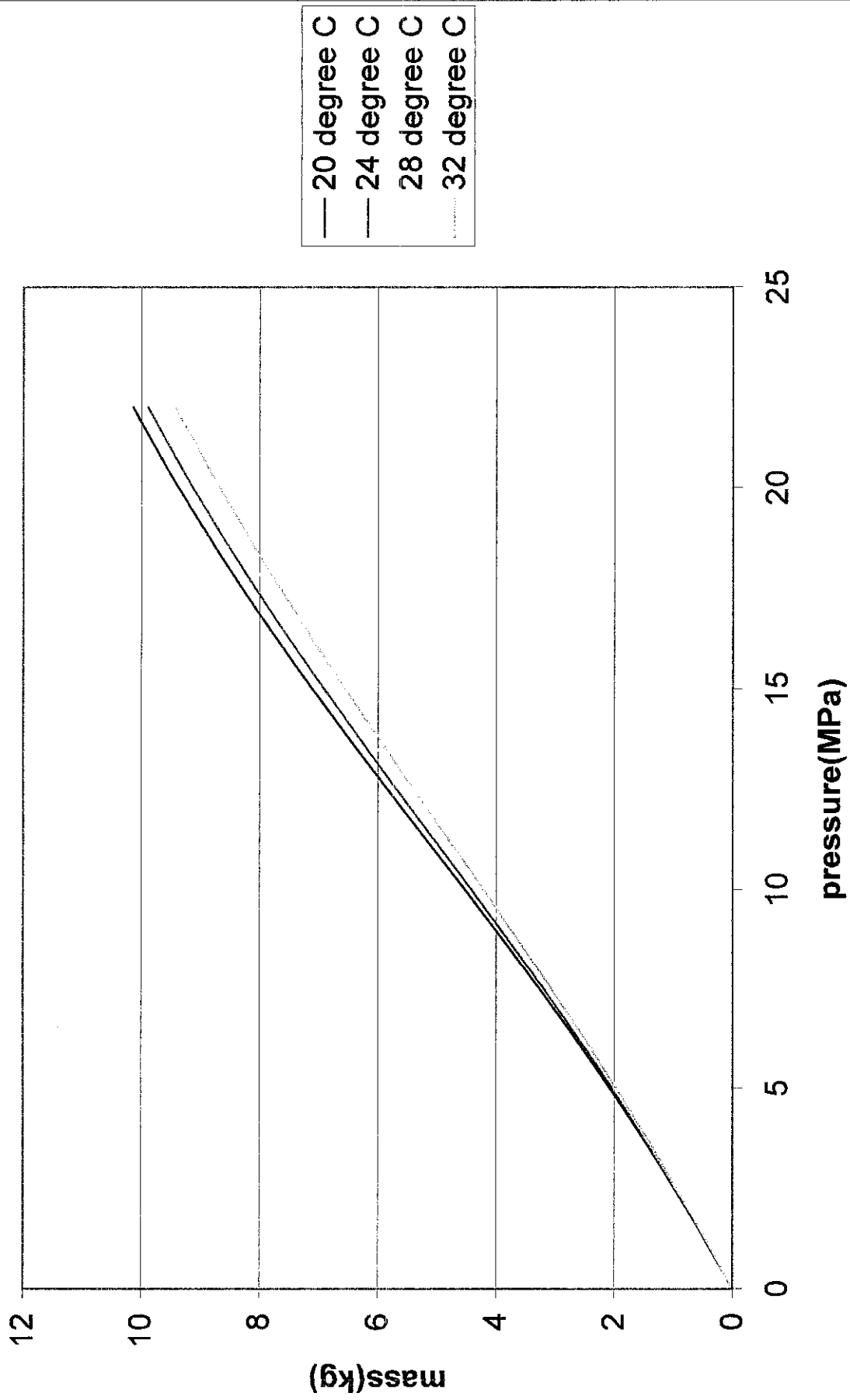
SRK plot for the leanest composition at different temperature



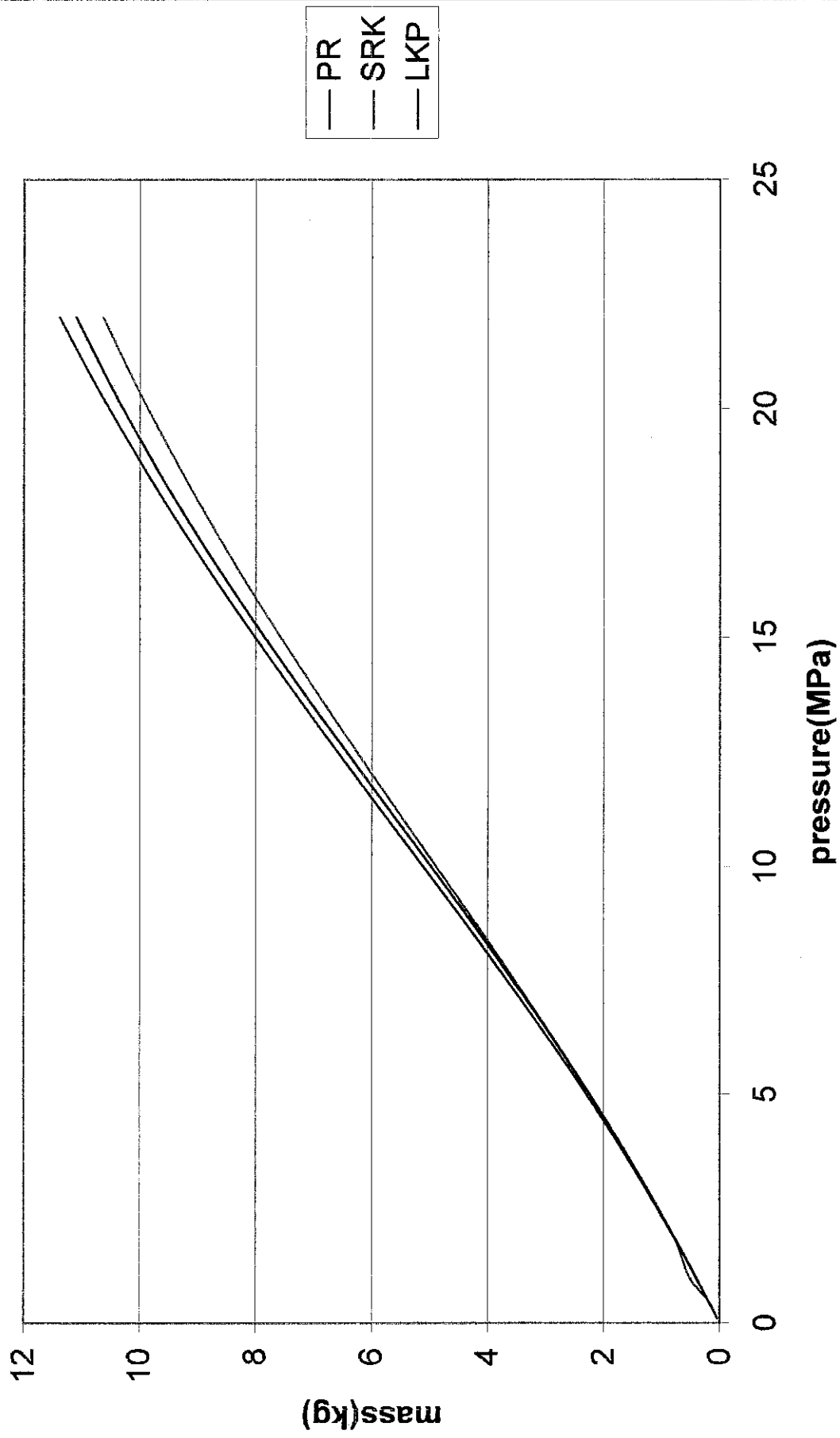
Peng Robinson plot for the leanest composition at different temperature



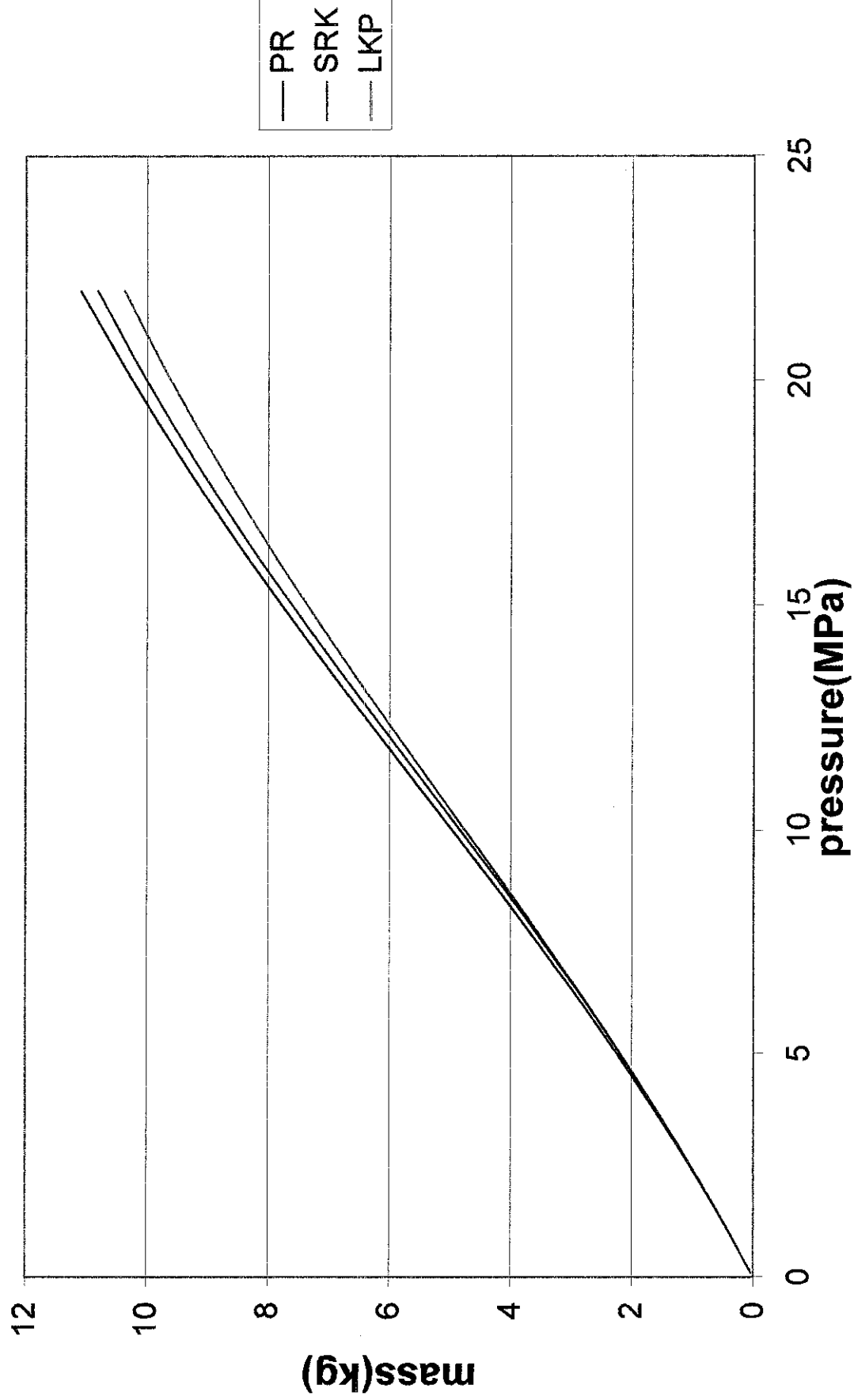
LKP plot for the leanest composition at different temperatures



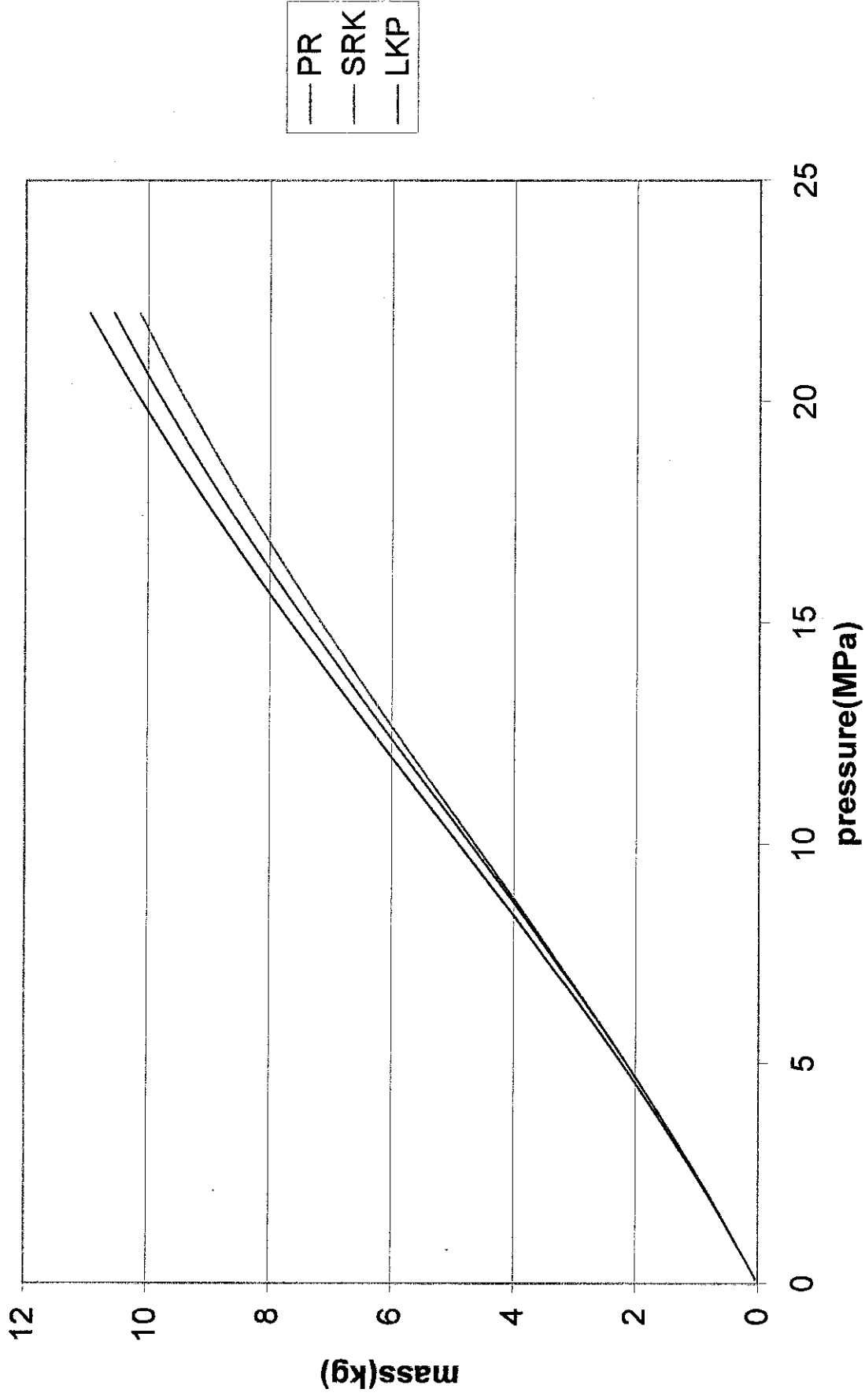
plot at 20 degree c for the richest composition using different EOS



plot at 24 degree C for the richest composition using different EOS

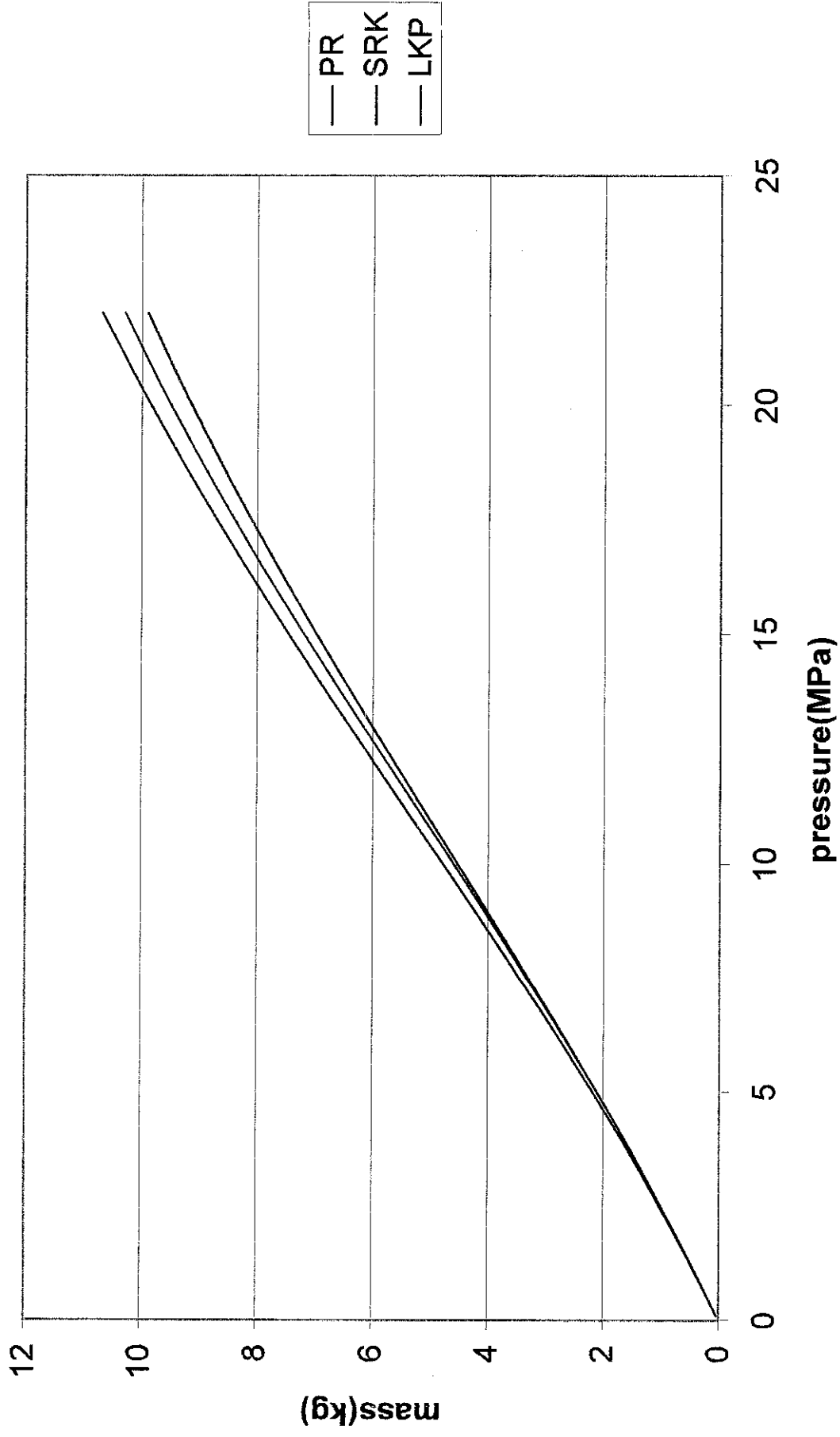


plot at 28 degree C for the richest composition using different EOS

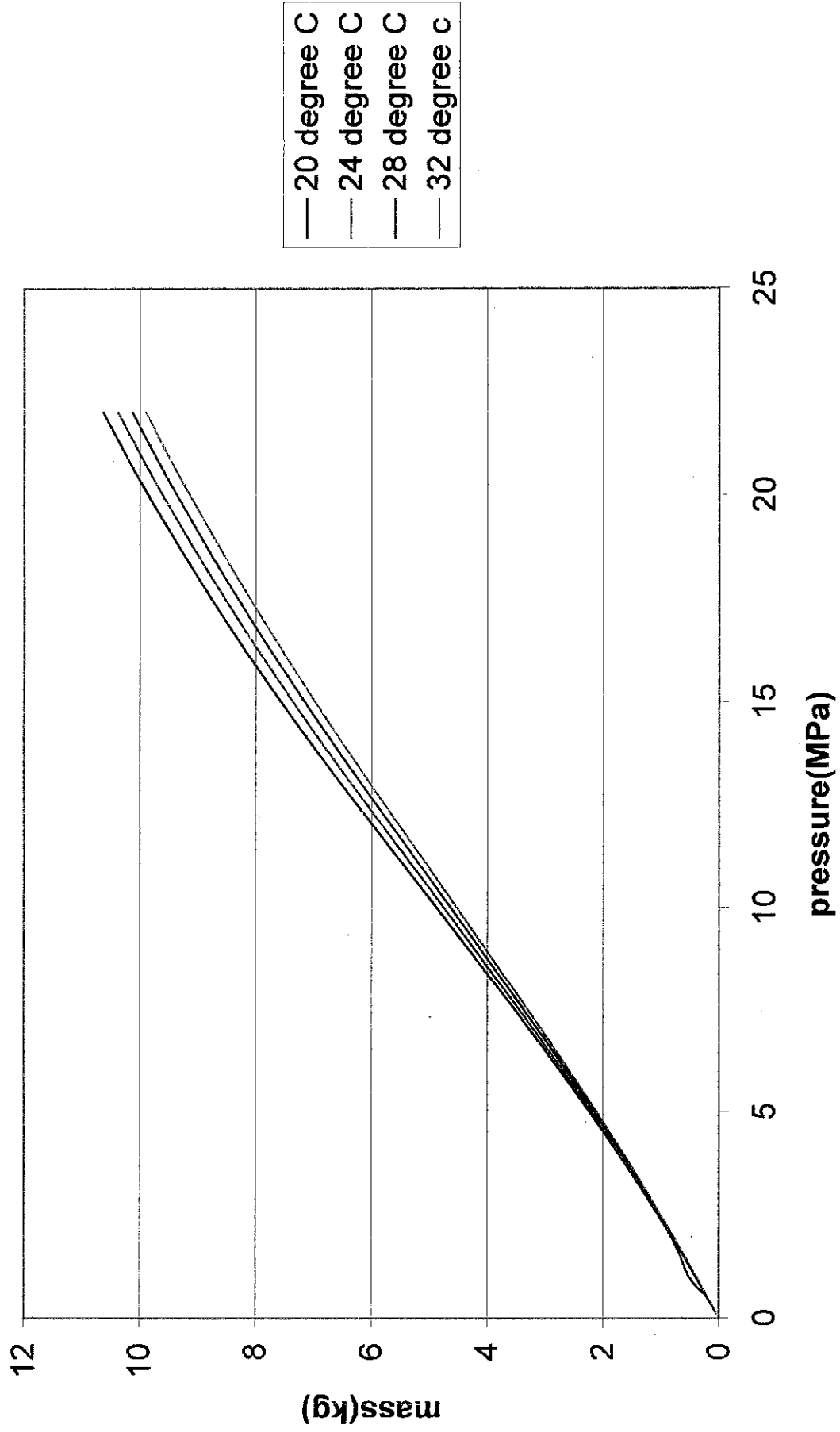




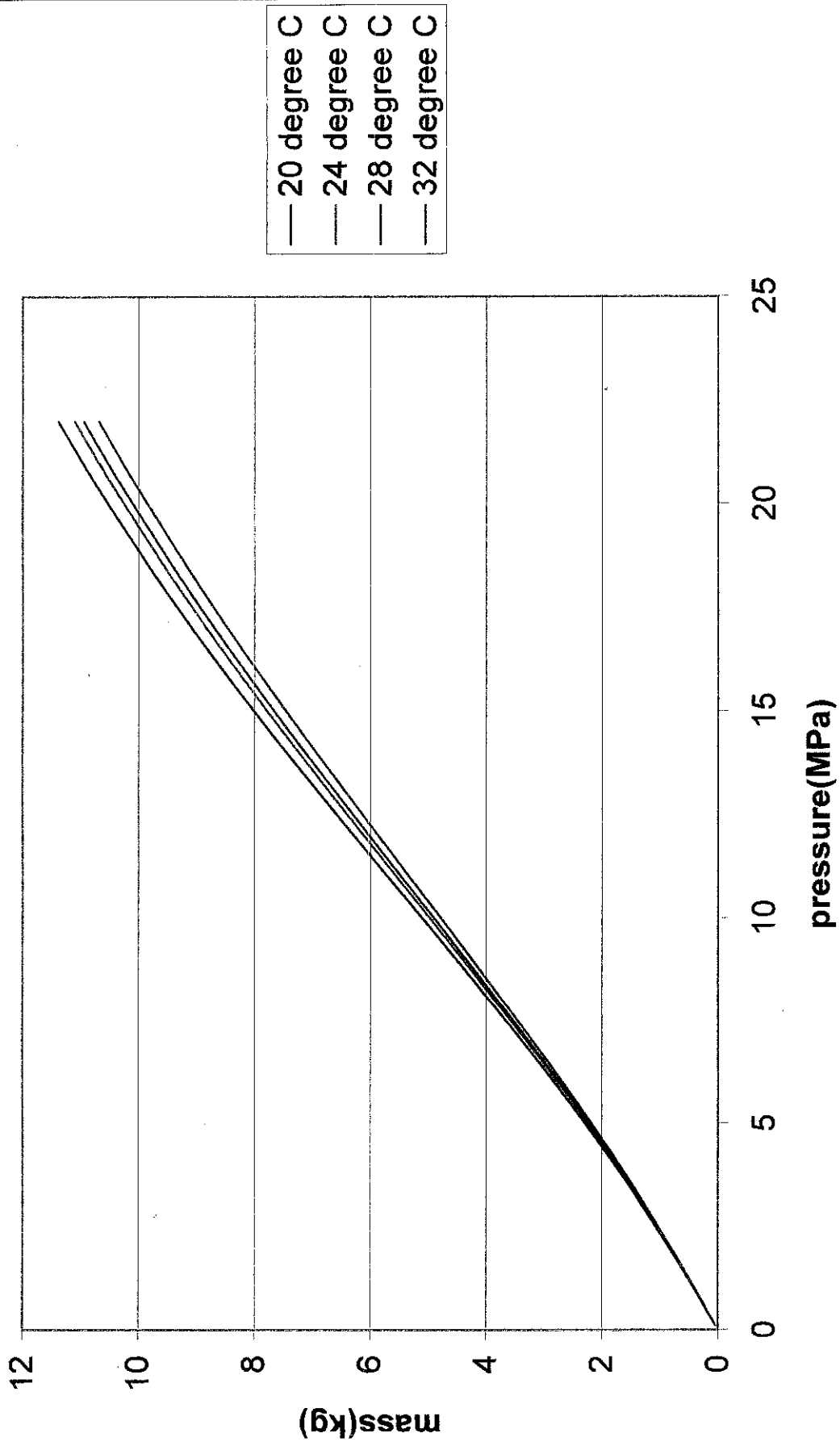
plot at 32 degree C for the richest composition using different EOS



SRK plot for the richest composition at different temperatures



Peng robinson plot for the richest composition at different temperature



LKP plot for the richest composition at different temperatures

