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Entropy – stagnation enthalpy interpolation tables for calculation of the critical flow properties of compressible fluids

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Scope

- Motivation and objectives
- Methodology
- Results
- Conclusions and next steps

https://www.h2-view.com/story/in-focus-transitioning-the-uks-gas-networks-to-hydrogen/

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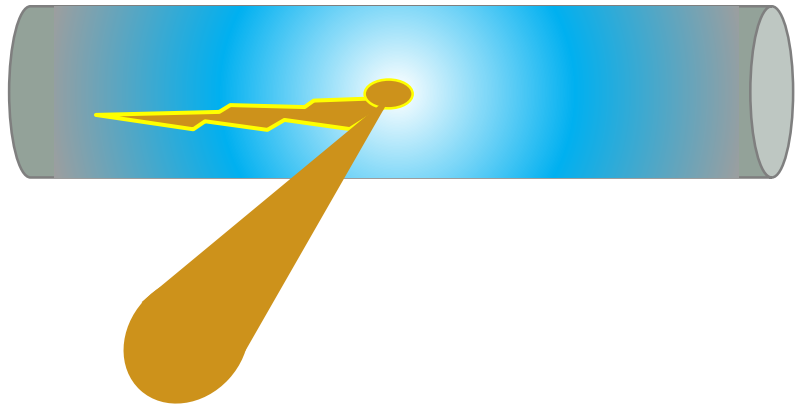
Motivation and objectives

- Pipeline transportation of industrial gases is mature technology.
- Due to hazardous nature of transported fluids and high operating pressures, safety of pipeline transportation is of serious concern.
- Mathematical models predicting pipeline decompression and the fluid discharge flow are in the heart of Qualitative Risk Assessment (QRA) predicting consequences of pipeline failure:
  - ✓ Significant cooling and dry ice formation during venting and accidental failure of CO_2 transport pipelines
  - ✓ Low-temperature induced brittle fracture upon accidental failure of ethylene and CO_2 transport pipeline
  - ✓ Safety assessment of hydrogen transport pipelines and facilities – with increasing demand for H_2 transport



Motivation and objectives

- Models have been developed in the past:
  - Homogeneous Equilibrium Mixture (HEM) and multi-fluid/ multiphase models for transient flow of compressible fluids in pipelines
  - Fluid properties calculation methods (EoS, interpolation tables) for single and multi-phase flows

- The accuracy and computational efficiency of the physical properties models is critical for the pipeline decompression flow simulations

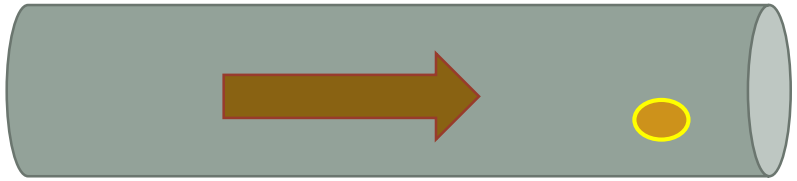
Physical properties involved

Governing equations for transient flow in a pipeline:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = -S_o$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} = -\frac{\partial p}{\partial x} - 2f_w \frac{\rho u^2}{D} - uS_o$$

$$\frac{\partial \rho e_{tot}}{\partial t} + \frac{\partial u(\rho e_{tot} + p)}{\partial x} = -2f_w \frac{\rho u^3}{D} + \frac{4q_w}{D} - h_{tot,o}S_o$$



where ρ, u, e_{tot} and p are respectively the mixture density, velocity, total energy and pressure, $u_o, h_{tot,o}$ and S_o are respectively the velocity, stagnation enthalpy and the mass flux source term associated with the local discharge flow.

Physical properties involved

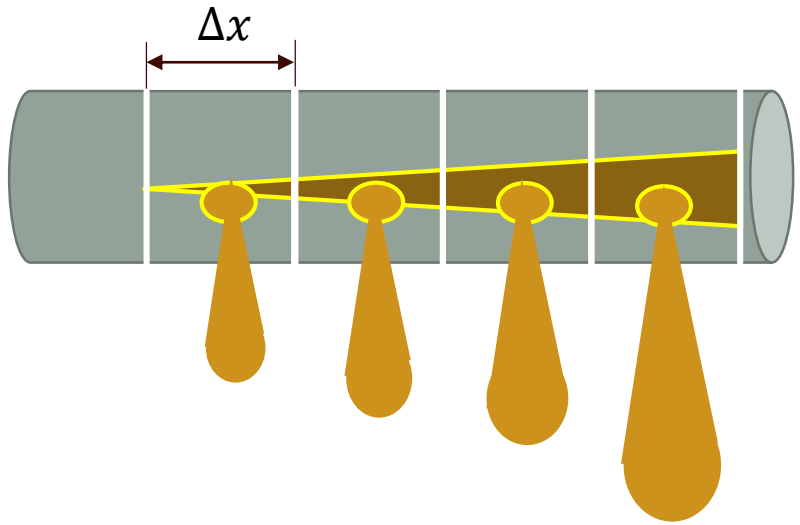
Discharge flow model – choked (critical) flow:

$$S_o = \frac{C_d\, \rho_o u_o A_o}{A \cdot \Delta x}$$

$$s_o = s_{up}$$

$$h_o + \frac{u_o^2}{2} = h_{tot,up}$$

$$u_o = c_{s,o}$$



where C_d is the local discharge coefficient for the rupture, Δx is the cell width, A is the pipe cross-sectional area, s is the entropy and the index "up" refers to stagnation conditions in the flow.

Physical properties involved

Density-energy flash calculations are performed as part of solution of the conservation equations describing the flow inside the pipe:

$$p, T, x = f(\rho, e)$$

Stagnation enthalpy – entropy flash calculations to obtain properties of choked (critical) flow:

$$c_s, \rho = f(s, H)$$

Physical Properties:

- Density
- Heat Capacity
- Speed of sound
- Joule-Thomson effect
- Phase equilibrium
- Viscosity
- Diffusivity
- Thermal conductivity

Mathematical model of pipeline flow:

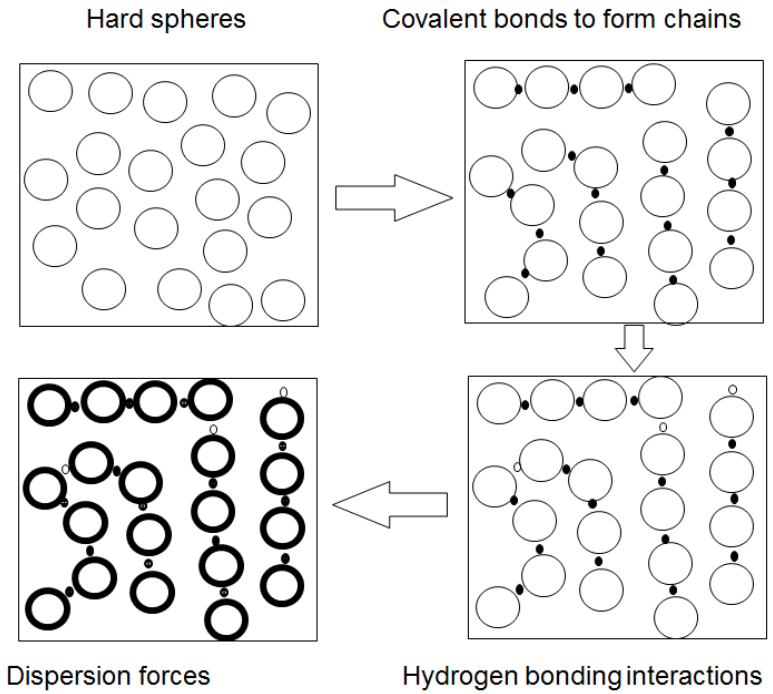
- Mass conservation
- Momentum conservation
- Energy conservation
- Viscous friction
- Heat transfer
- Interphase H&M transfer
- Fluid/structure interaction

Equation of state models

- Peng – Robinson (PR) EoS: $$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)}$$

Easy to implement, computationally efficient

- Perturbed Chain – Statistical Association Fluid Theory (PC-SAFT) EoS:



$$a(T,\rho) = a^{ideal}(T,\rho) + a^{hard-sphere}(T,\rho) + a^{dispersion}(T,\rho) + a^{chain}(T,\rho) + a^{association}(T,\rho)$$

Highly-accurate, but can be computationally demanding

Equation of state models

- To speed-up the properties calculations, **interpolation tables** can be used instead of EoS, provided that the interpolation method is:
  - accurate and robust, and
  - suits the *pipe flow* and *discharge flow models*

Objectives

- To develop the physical properties interpolation method for use in the pipeline decompression flow simulations
- To apply the method for calculation of physical properties of real fluids
- To evaluate the accuracy and computational efficiency of the interpolation method

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Physical properties inverse interpolation

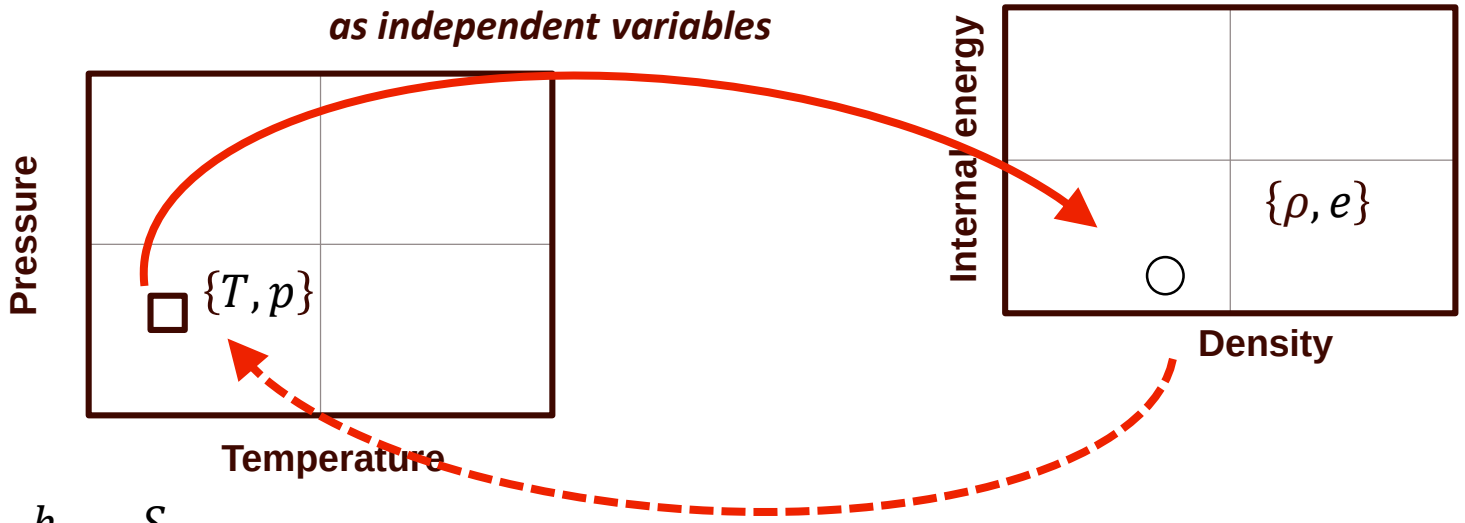
Pipe flow model equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = -S_o$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} = -\frac{\partial p}{\partial x} - 2f_w \frac{\rho u^2}{D} - uS_o$$

$$\frac{\partial \rho e_{tot}}{\partial t} + \frac{\partial u(\rho e_{tot} + p)}{\partial x} = -2f_w \frac{\rho u^3}{D} + \frac{4q_w}{D} - h_{tot,o} S_o$$

Step 1: Construct the interpolant data using EoS (direct mapping) with $\{T, p\}$ as independent variables



Step 2: Interpolation (inverse mapping)

$$p, T, x, \ldots = f(\rho, e)$$

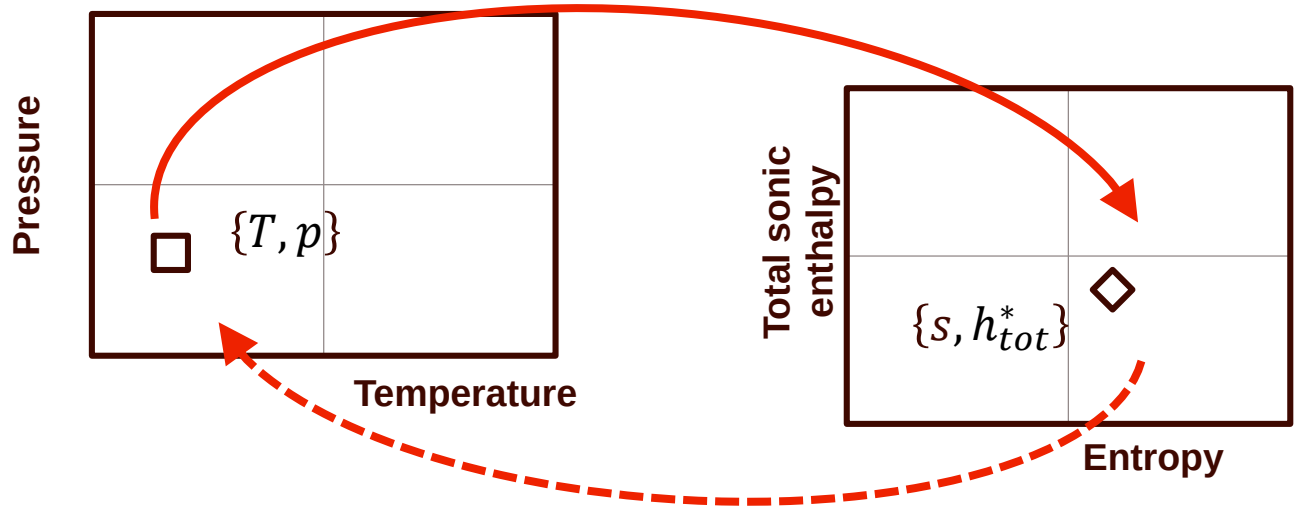
Physical properties inverse interpolation

Critical discharge flow model:

$$s_o = s_{up}$$

$$\underbrace{h_o + \frac{c_{s,o}^2}{2}}_{h_{tot,o}^*} = h_{tot,up}$$

Step 1: Construct the interpolant data using EoS (direct mapping) with $\{T, p\}$ as independent variables



Step 2: Interpolation (inverse mapping)

In this work the inverse interpolation method is applied for the entropy - stagnation enthalpy flash calculations

$$p, T, \rho, x, \ldots = f(s, h_{tot})$$

Physical properties of homogeneous vapour-liquid mixture

$$e = e_v x + e_l(1-x)$$

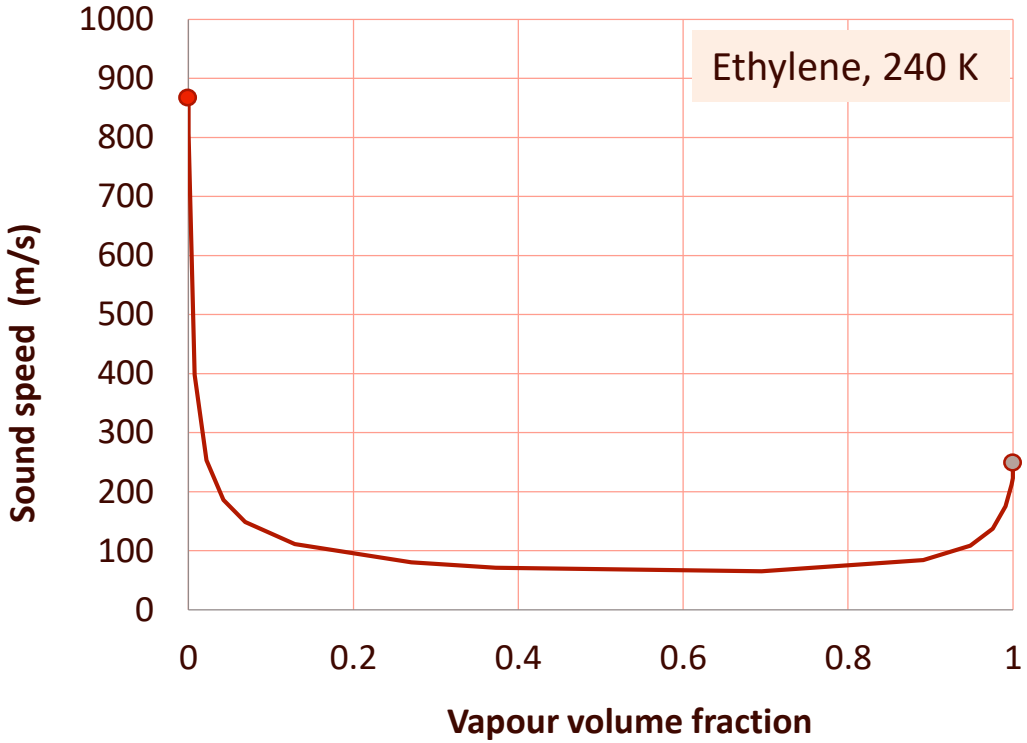
$$s = s_v x + s_l(1-x)$$

$$\rho = \rho_v \alpha + \rho_l(1-\alpha)$$

The speed of sound in a two-phase homogeneous frozen mixture (Wood, 1930):

$$c_s = \left[\frac{\rho\alpha}{\rho_v c_{s,v}^2} + \frac{\rho(1-\alpha)}{\rho_l c_{s,l}^2}\right]^{-1/2}$$

Where x is the vapour mass fraction,
α is the vapour volume fraction.



The speed of sound in saturated VLE mixture of ethylene, predicted using the homogeneous frozen mixture model.

Physical properties inverse interpolation method

Step 0: Construct the $\{T, p\}$ grid by seeding non-uniformly points along isotherms in the $T - p$ domain.

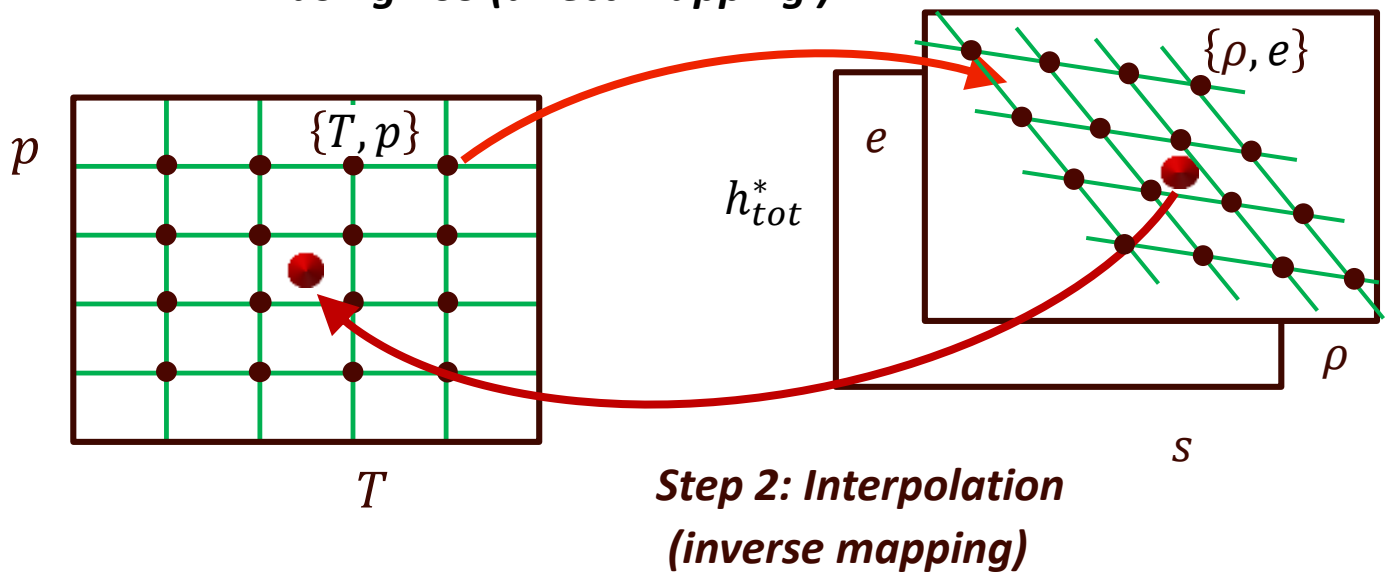
Step 1: *Direct* mapping: Use EoS to obtain the interpolant data on $\{T, p\}$:

- internal energy (e),
- density (ρ),
- mass fraction (x),
- entropy (s), and
- the total sonic enthalpy h^*_{tot}:

$$h^*_{tot} = h + \frac{c_s^2}{2}$$

Step 2: Use the interpolant data to fit Akima splines for the *inverse* interpolation, e.g.: $p(\rho, e)$ and $T(\rho, e)$.

Step 1: Constructing interpolant data using EoS (direct mapping)



Step 2: Interpolation (inverse mapping)

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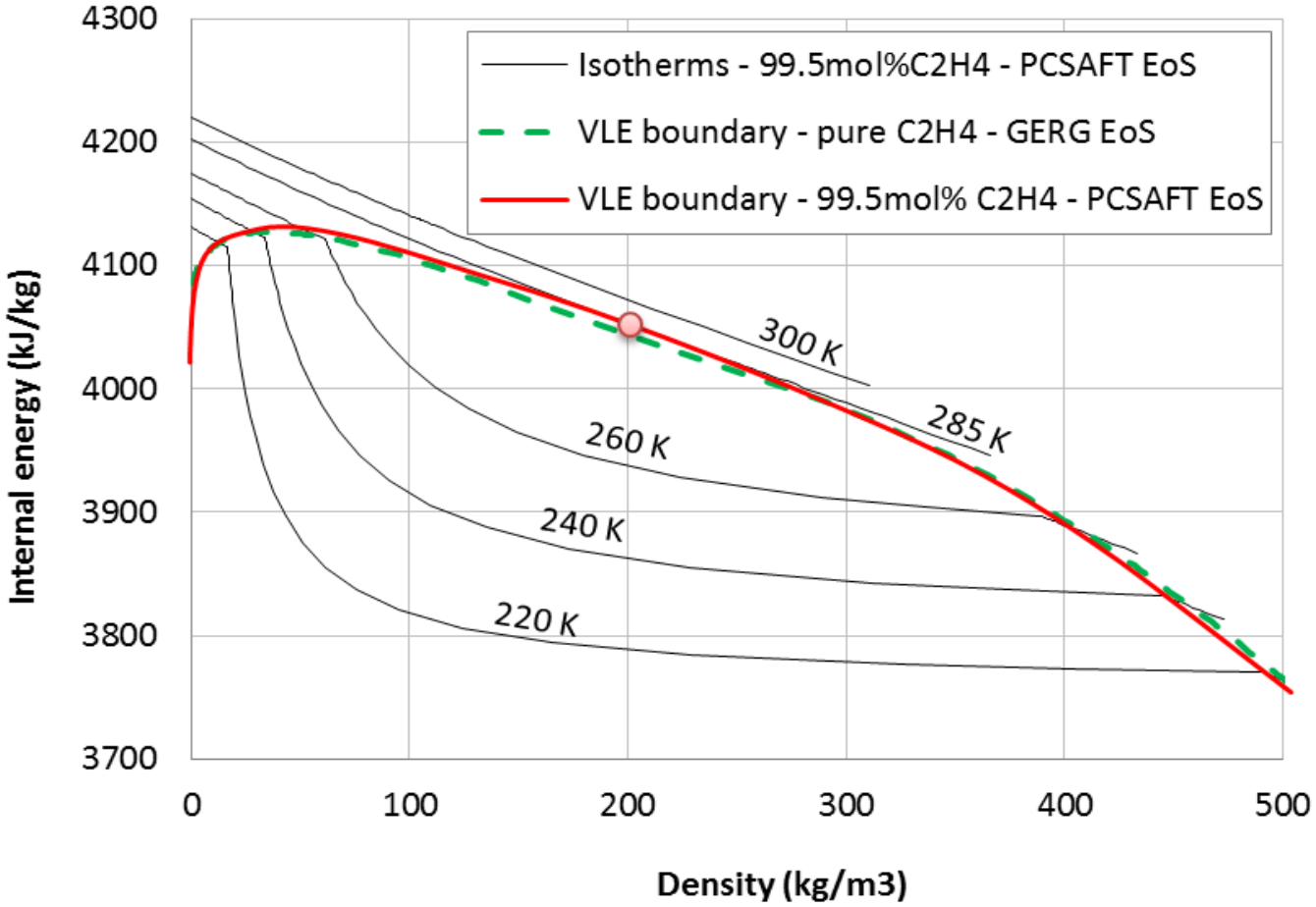
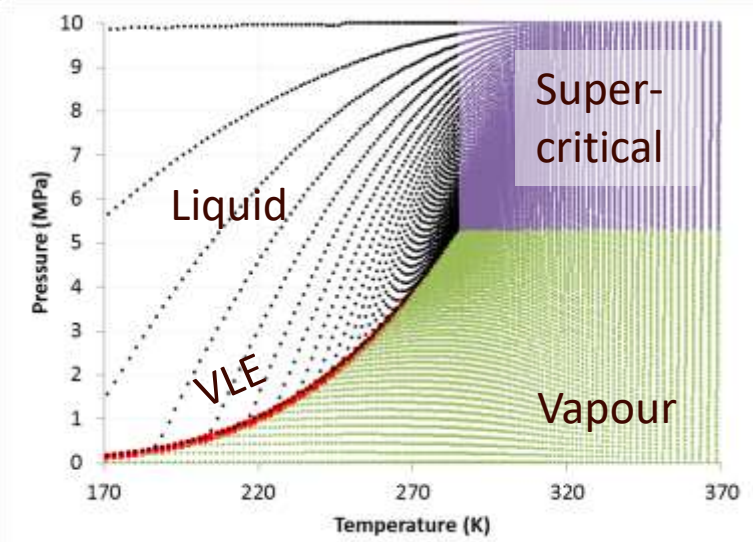
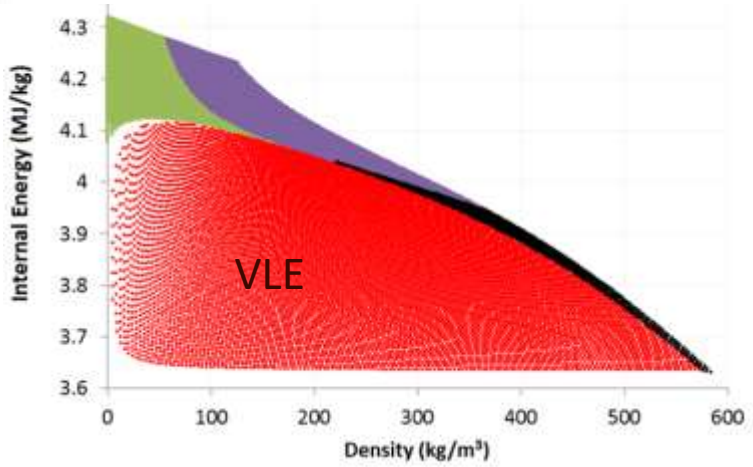
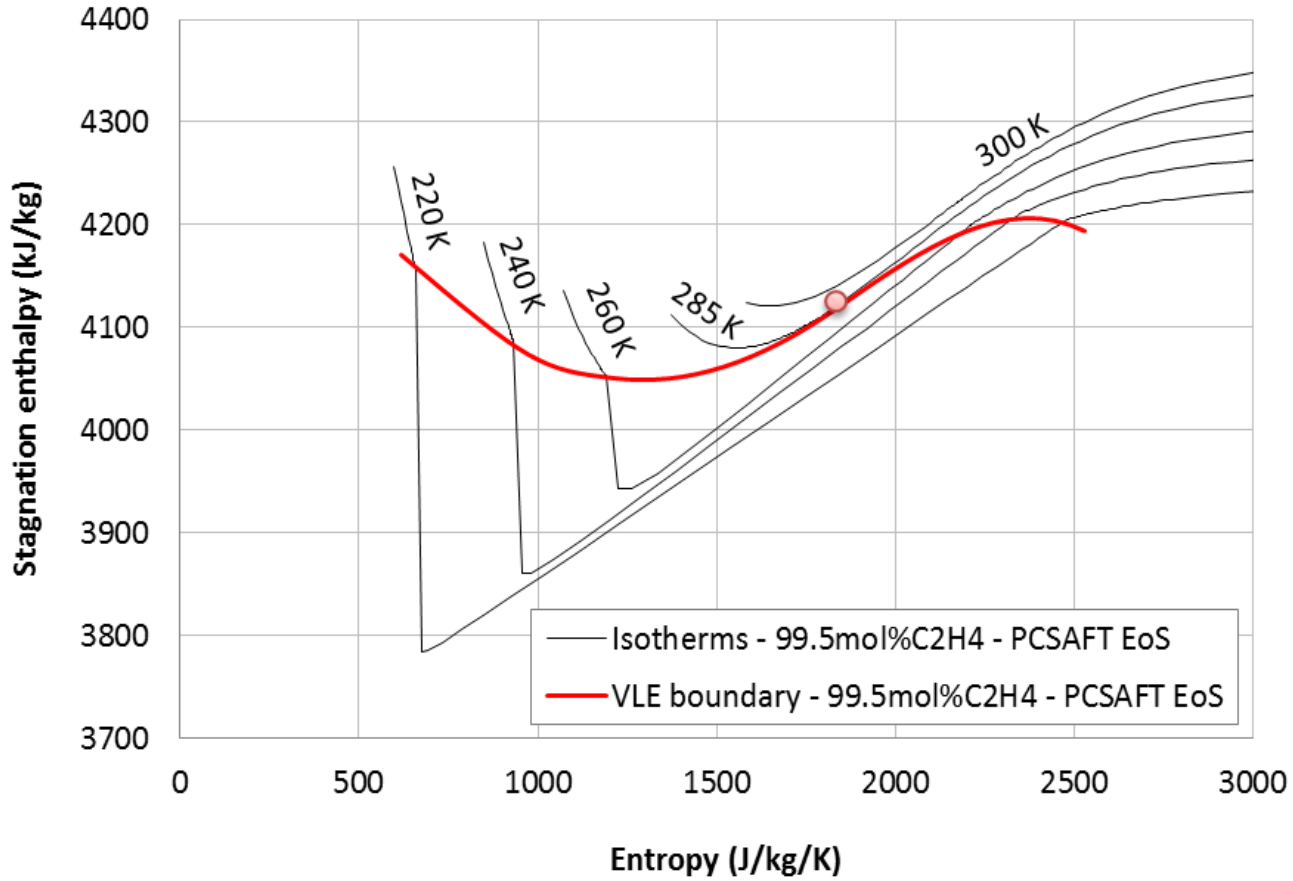
Density-energy (ρ- e) interpolant data – Ethylene

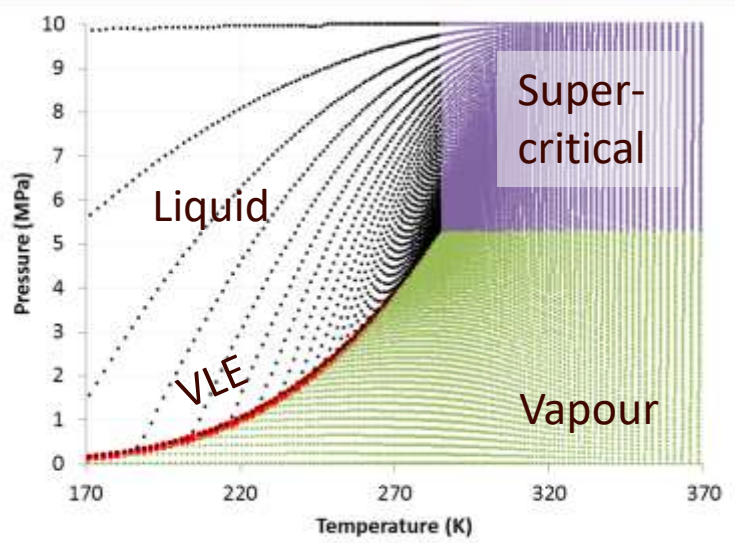


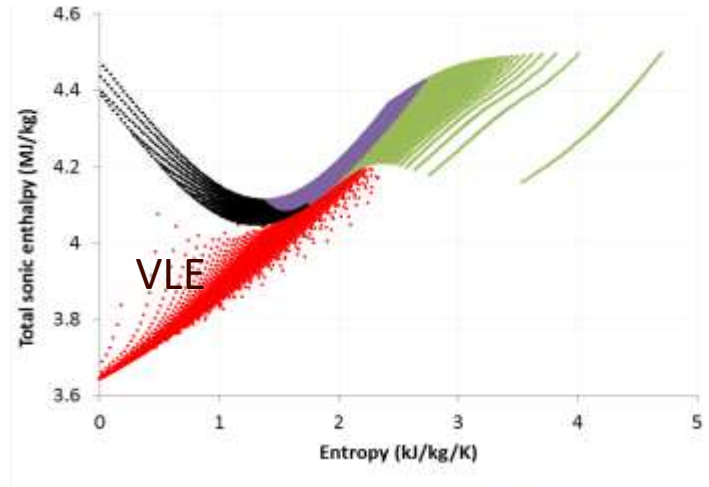




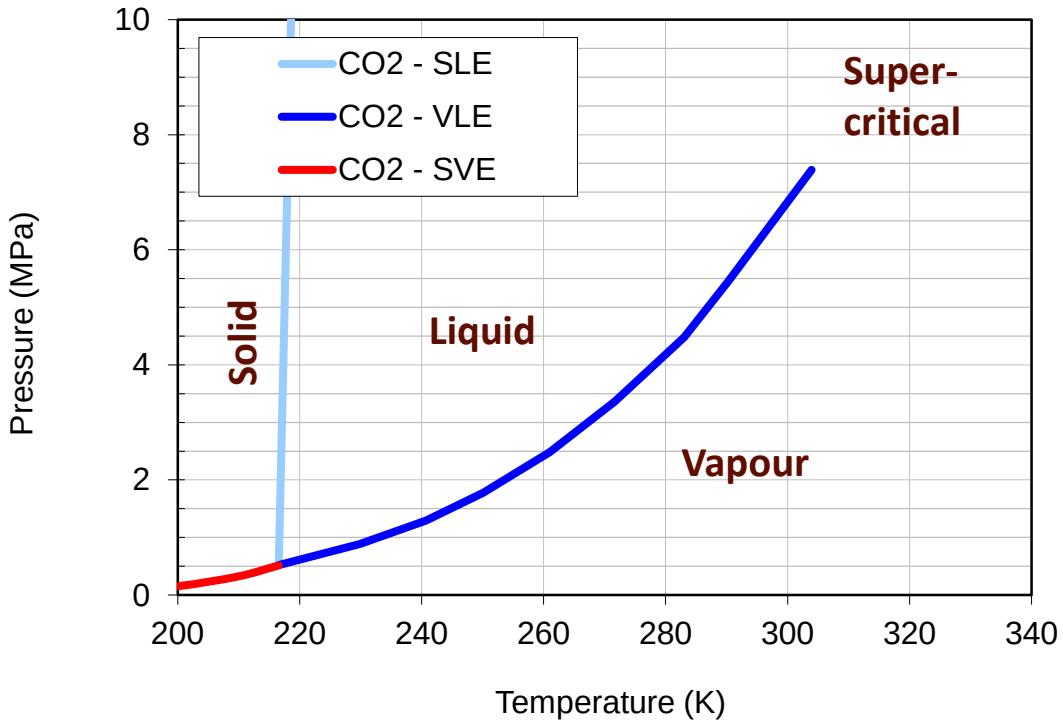
(h_{tot}- s) interpolant data – Ethylene

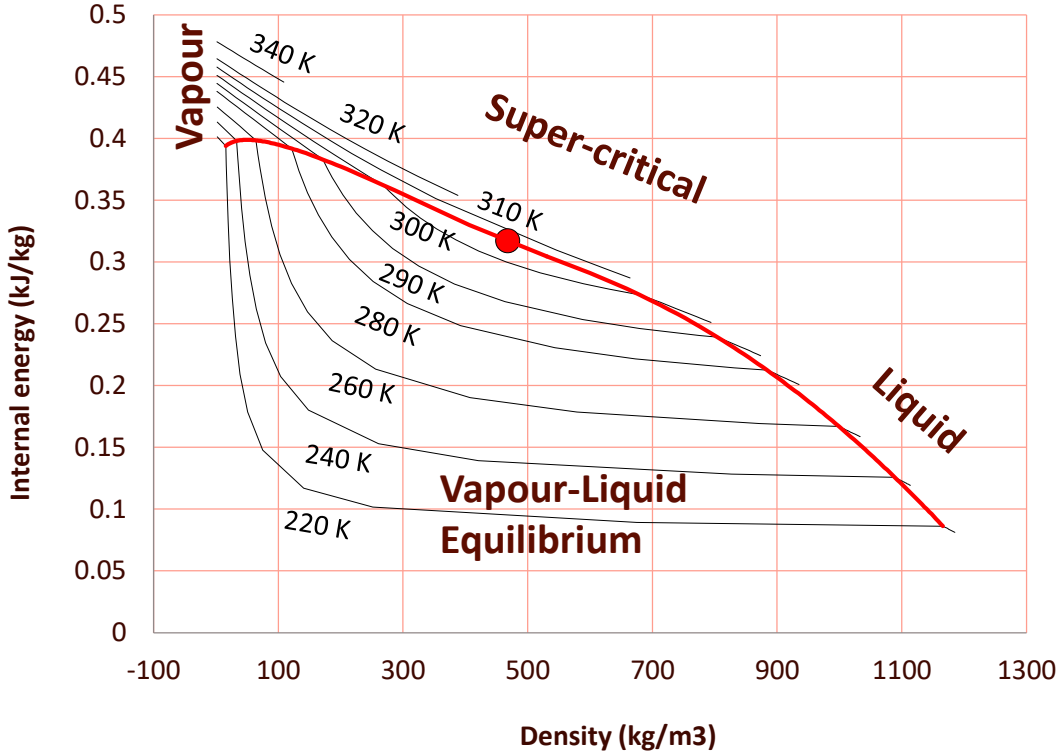




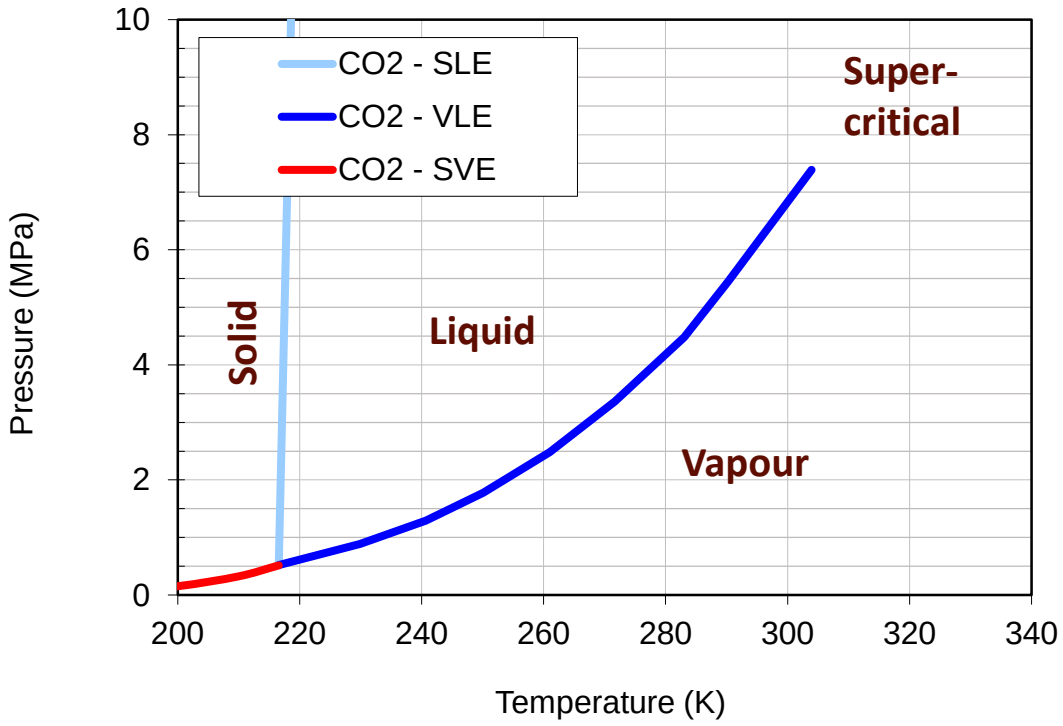


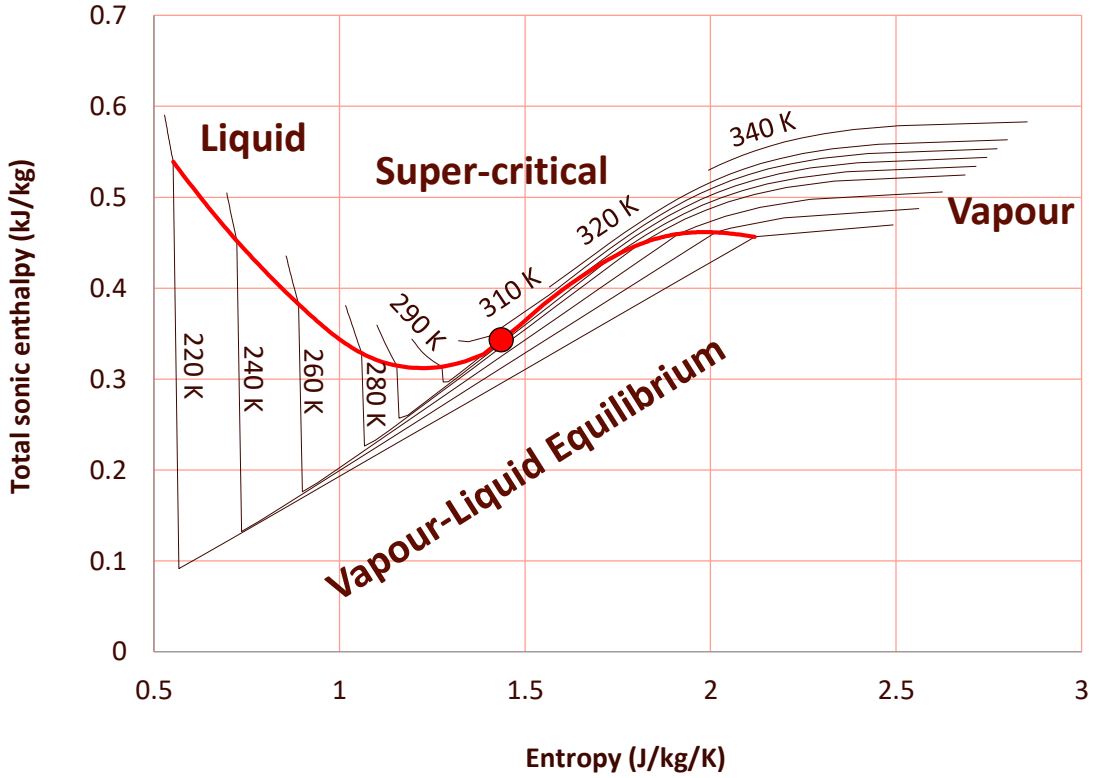
Density-energy (ρ- e) phase diagram – CO_2





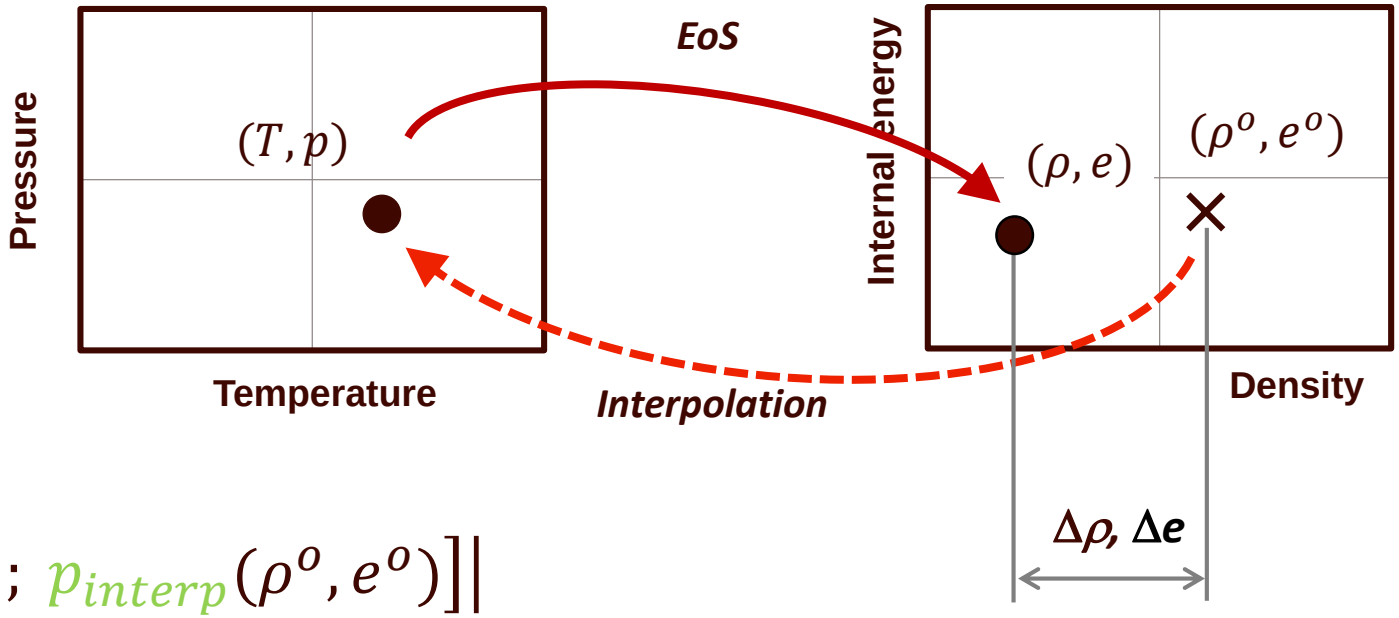
(h_{tot}- s) phase diagram – CO_2





The accuracy of the interpolation method

The accuracy of the inverse interpolation method is assessed by comparing the original input data (ρ^o, e^o) used for the inverse mapping with the (ρ, e) data returned by EoS based on the interpolation results (T, p):

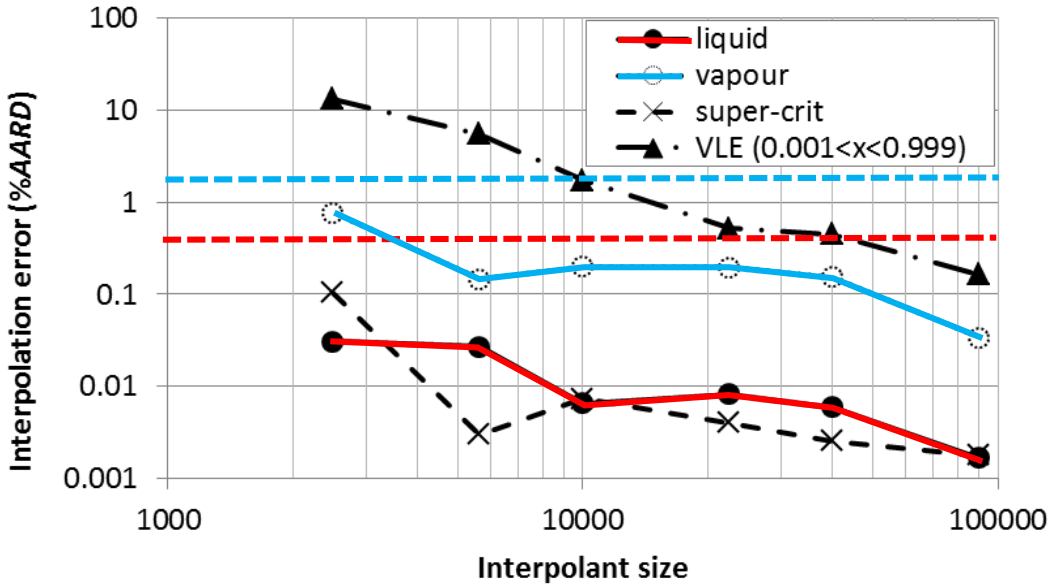


$$\Delta\rho = \left|\rho^o - \rho_{EOS}\left[T_{interp}(\rho^o, e^o);\ p_{interp}(\rho^o, e^o)\right]\right|$$

The accuracy of the interpolation method (ethylene)

$$\%AARD = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{\phi_i - \phi_i^o}{\phi_i^o}\right|$$

where ϕ_i^o and ϕ_i are respectively the reference value and the interpolated property at a point i, and n is the number of points in the thermodynamic phase region.



The accuracy of the PC-SAFT EoS (Nikolaidis, et al 2018):

- the saturated vapour : 2.37%,
- the saturated liquid: 0.42%,
- the supercritical fluid: 1.24%.

The interpolation method' errors are the order of magnitude smaller than the accuracy of EoS.

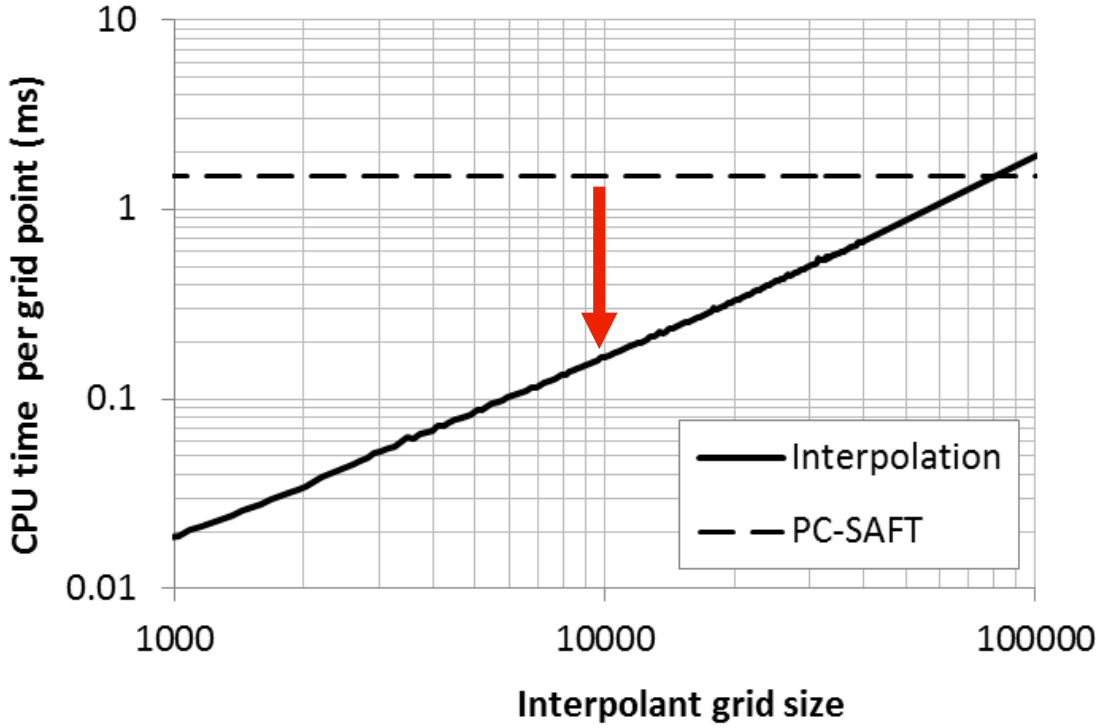
Relative errors of density predictions by the PC-SAFT based on the interpolated *p-T* data, and with the accuracy of PC-SAFT EoS [Nikolaidis et al, 2018).

The computational runtime (ethylene)

$$\tau_{CPU} = \frac{1}{N_{ref}} \sum_{i=1}^{N_{ref}} \tau_i$$

where τ_i is the CPU time spent on interpolation at a point i

The proposed interpolation method can speed up the property calculations, compared to using directly the PC-SAFT EoS, when using less than 80,000 interpolant points



Average computational runtimes (τ_{CPU}) spent on the interpolation of density and using directly the PC-SAFT EoS.

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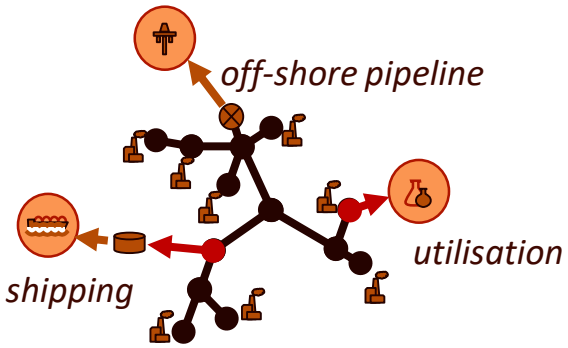
Conclusions and next steps

- ✓ Constructed $h^*_{tot} - s$ phase diagrams for the inverse interpolation flash calculations of critical (choked) flow
- ✓ Developed methodology for assessment of accuracy & computational efficiency of interpolation tables
- ✓ Demonstrated the methods for ethylene

- ✓ Ongoing work: validation against pipeline decompression data for ethylene and applying the method to carbon dioxide

H2020 project:

C⁴U - Advanced Carbon Capture for Steel Industries Integrated in CCUS Clusters



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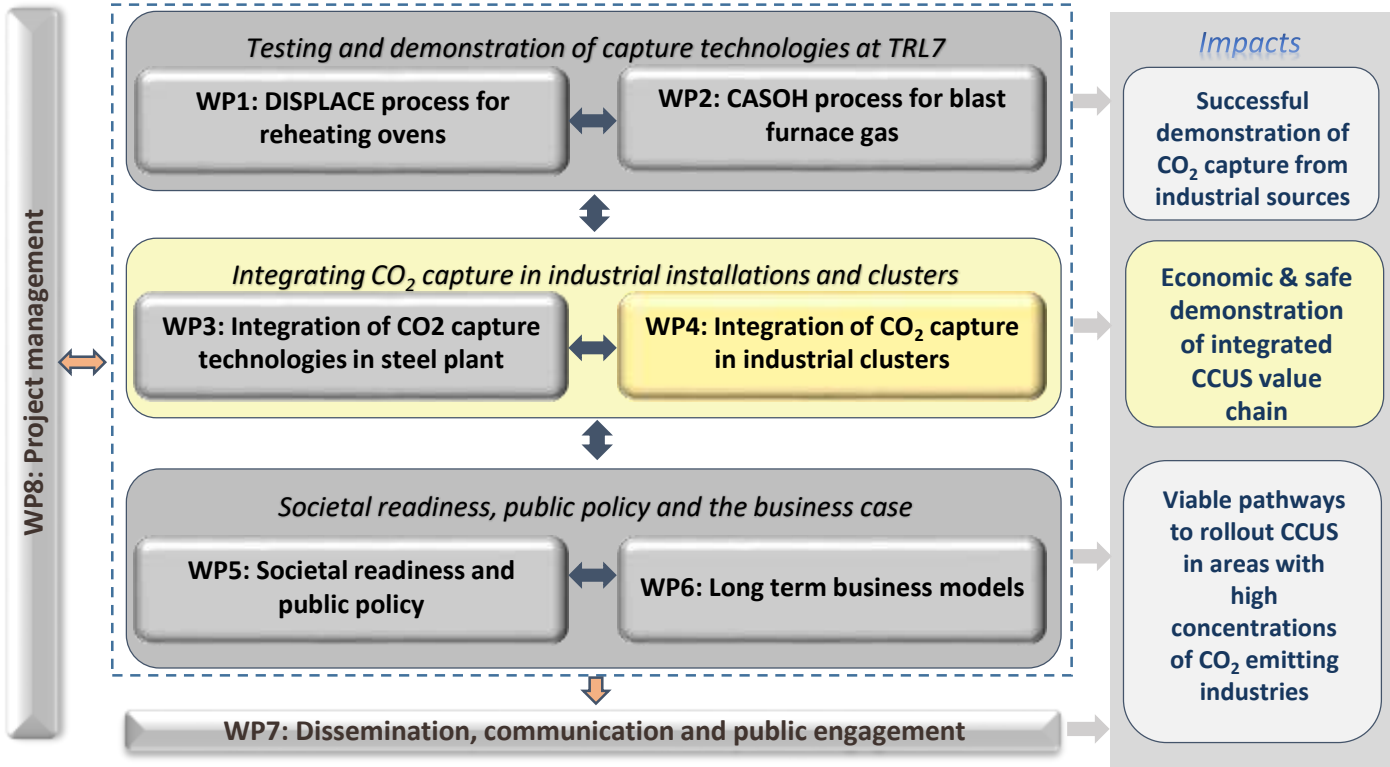

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- The statements made herein are solely the responsibility of the authors.