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

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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 CO₂ transport pipelines
✓ Low-temperature induced brittle fracture upon accidental failure of ethylene and CO₂ transport pipeline
✓ Safety assessment of hydrogen transport pipelines and facilities – with increasing demand for H₂ 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:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} &= -S_o \\
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} &= -\frac{\partial p}{\partial x} - 2f_w \frac{\rho u^2}{D} - uS_o \\
\frac{\partial \rho e_{tot}}{\partial t} + \frac{\partial u(\rho e_{tot} + p)}{\partial x} &= -2f_w \frac{\rho u^3}{D} + \frac{4q_w}{D} - h_{tot,o}S_o
\end{align*}
\]

where \( \rho \), \( u \), \( e_{tot} \) 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:

\[ S_0 = \frac{C_d \rho_0 u_0 A_0}{A \cdot \Delta x} \]

\[ s_o = s_{up} \]

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

\[ u_o = c_{s,o} \]

where \( C_d \) is the local discharge coefficient for the rupture, \( \Delta x \) 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.
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:**

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

*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
• Motivation and objectives
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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:

\[ s_o = s_{up} \]
\[ h_o + \frac{c_{s,o}^2}{2} = h_{tot,up} \]

\[ h_{tot,o} \]

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

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

Step 2: Interpolation (inverse mapping)

\[ p, T, \rho, x, ... = f(s, h_{tot}) \]
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, \( \alpha \) is the vapour volume fraction.

The speed of sound in saturated VLE mixture of ethylene, predicted using the homogeneous frozen mixture model.
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 \( (\rho) \),
- 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 \( T(\rho, e) \).
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Density-energy ($\rho - e$) interpolant data – Ethylene
\[(h_{\text{tot}} - s)\] interpolant data – Ethylene

![Graph showing the interpolation of \(h_{\text{tot}} - s\) data for Ethylene.]
Density-energy ($\rho-e$) phase diagram – CO$_2$

![Graph showing the phase diagram of CO$_2$ with different states and phases: solid, liquid, and gaseous.](image)
(h_{tot} - s) phase diagram – CO_2
The accuracy of the inverse interpolation method is assessed by comparing the original input data \((\rho^o, e^o)\) used for the inverse mapping with the \((\rho, e)\) data returned by EoS based on the interpolation results \((T, p)\):

\[
\Delta \rho = |\rho^o - \rho_{EoS}[T_{interp}(\rho^o, e^o); \ p_{interp}(\rho^o, e^o)]|
\]
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 \(\phi_i^o\) and \(\phi_i\) 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 \( \tau_i \) 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 (\( \tau_{CPU} \)) 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
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https://c4u-project.eu/
https://twitter.com/C4Uproject
https://www.linkedin.com/company/c4u-project/

Successful demonstration of CO₂ capture from industrial sources
Economic & safe demonstration of integrated CCUS value chain
Viable pathways to rollout CCUS in areas with high concentrations of CO₂ emitting industries

WP1: DISPLACE process for reheating ovens
WP2: CASOH process for blast furnace gas
WP3: Integration of CO₂ capture technologies in steel plant
WP4: Integration of CO₂ capture in industrial clusters
WP5: Societal readiness and public policy
WP6: Long term business models
WP7: Dissemination, communication and public engagement
WP8: Project management

WP1

WP2

WP3

WP4

WP5

WP6

WP7

WP8

Testing and demonstration of capture technologies at TRL7

Integrating CO₂ capture in industrial installations and clusters

Societal readiness, public policy and the business case

WP8: Project management

Impacts

https://c4u-project.eu/
References


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