Computationally efficient simulation of two-phase flows of CO_2 mixtures

Solomon Brown, Sergey Martynov, Haroun Mahgerefteh

UCL

Loukas Peristeras, Ilias Nikolaidis, Georgios C. Boulougouris, Dimitrios M. Tsangaris and Ioannis Economou

NCSR

2nd International Forum on Recent Developments of CCS Implementation

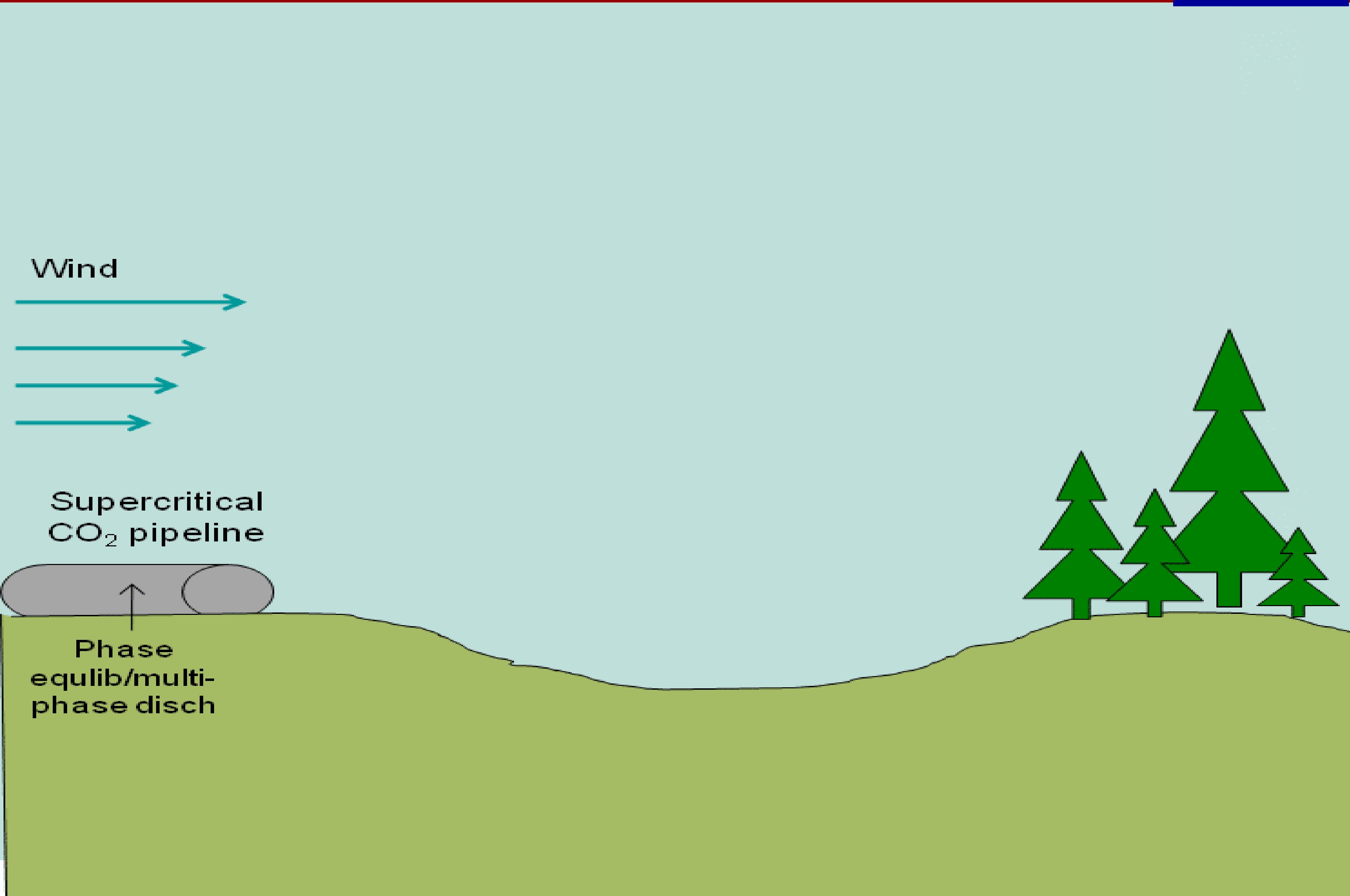
16th – 17th December 2015, Athens, Greece

Background

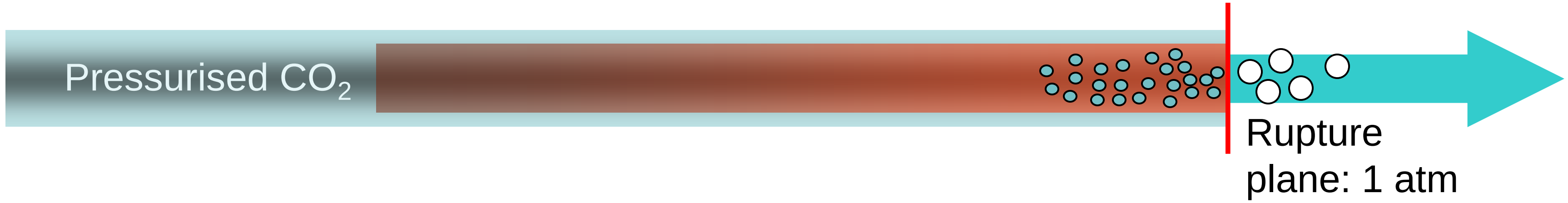
By 2050 200,000-360,000 km of pipeline will be required for transportation of CO_2 captured from fossil fuel power plant for subsequent sequestration (IEA, 2009).

IEA, Energy technology perspectives 2012: Pathways to a clean energy system.

CO_2 pipeline transportation – hazards cont.



Physics of decompression



- At the rupture plane the fluid is exposed to ambient air
- Following the rupture, the rarefaction wave starts propagating along the pipe
- The vapour phase emerges in the expansion wave
- Due to rapid cooling of the fluid in the decompression wave, the solid phase may also be released from the pipe

Mathematical model -Pipeline discharge

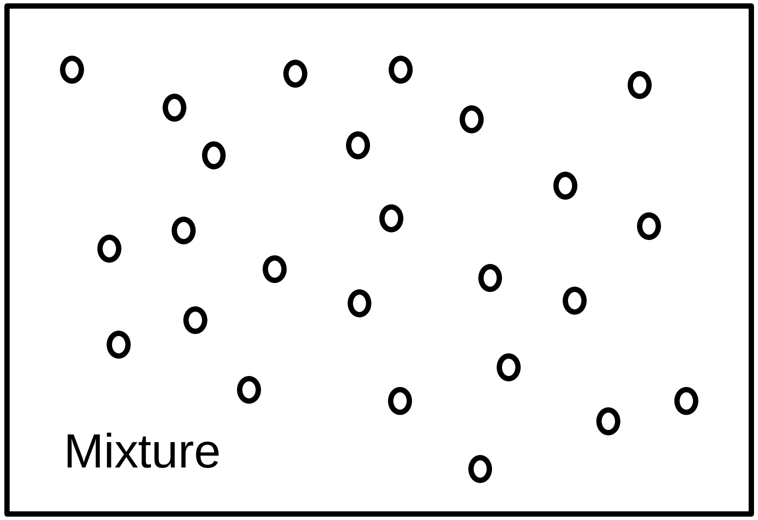
Homogeneous Equilibrium Model

Balance equations:

$$\frac{\partial \rho_{mix}}{\partial t} + \frac{\partial \rho_{mix} u_{mix}}{\partial x} = S_\rho$$

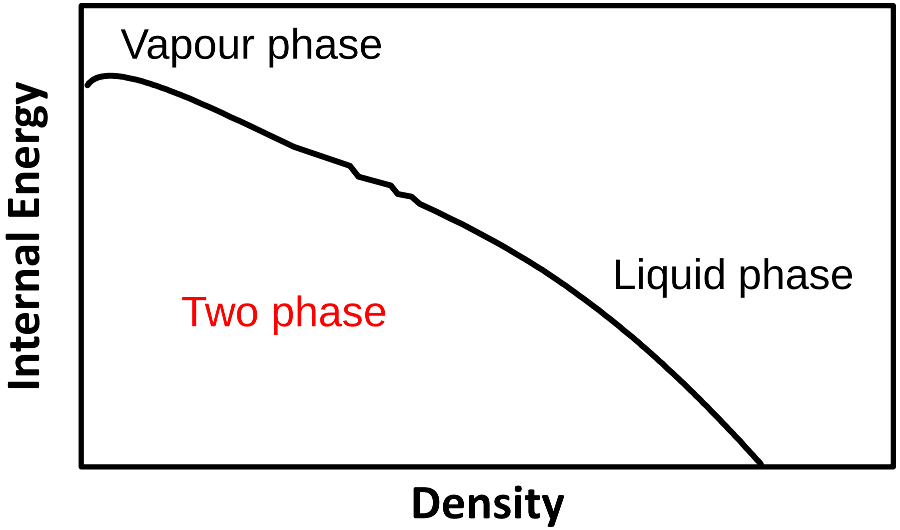
$$\frac{\partial \rho_{mix} u_{mix}}{\partial t} + \frac{\partial \rho_{mix} u_{mix}^2 + P}{\partial x} = S_u$$

$$\frac{\partial \rho_{mix} E_{mix}}{\partial t} + \frac{\partial \rho_{mix} H_{mix}}{\partial x} = S_e$$

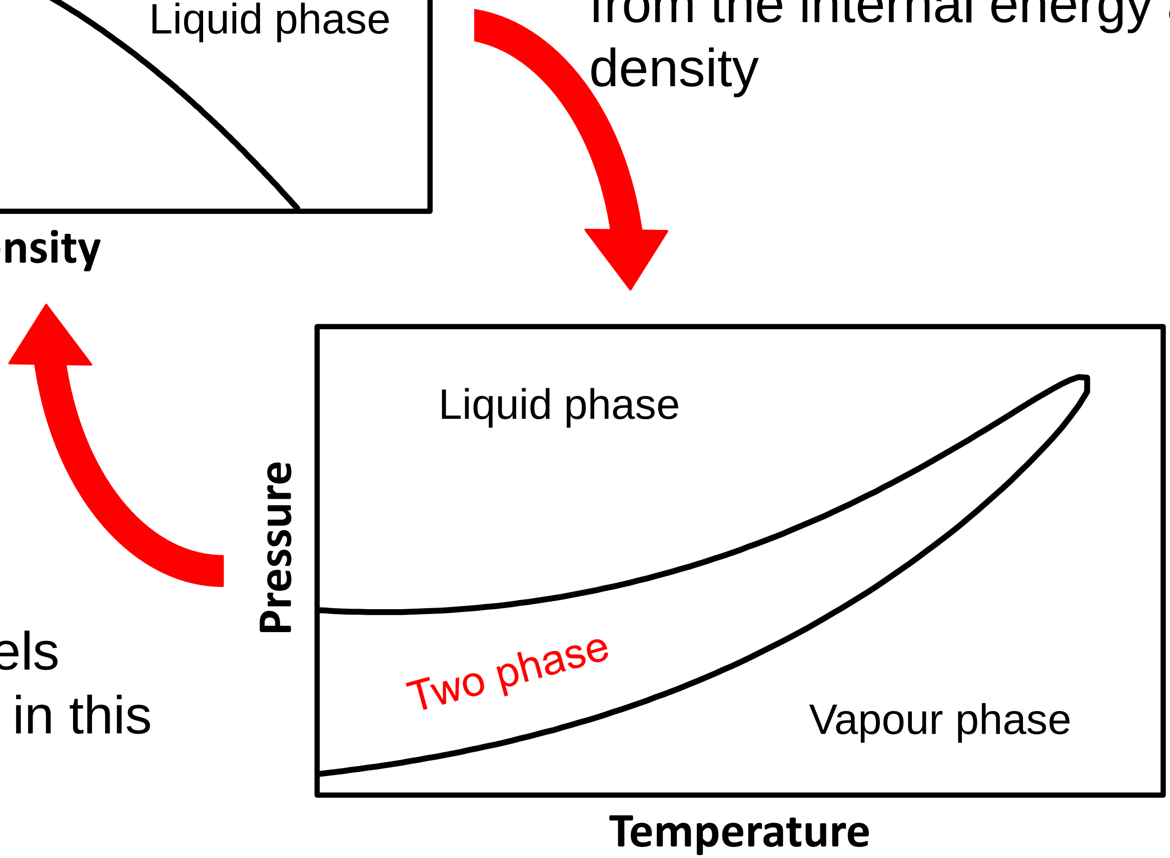


where ρ, u, P, H and E are the density, velocity, pressure, total enthalpy and total energy of a two-phase fluid mixture as function of time t and space x.

Thermodynamic evaluation

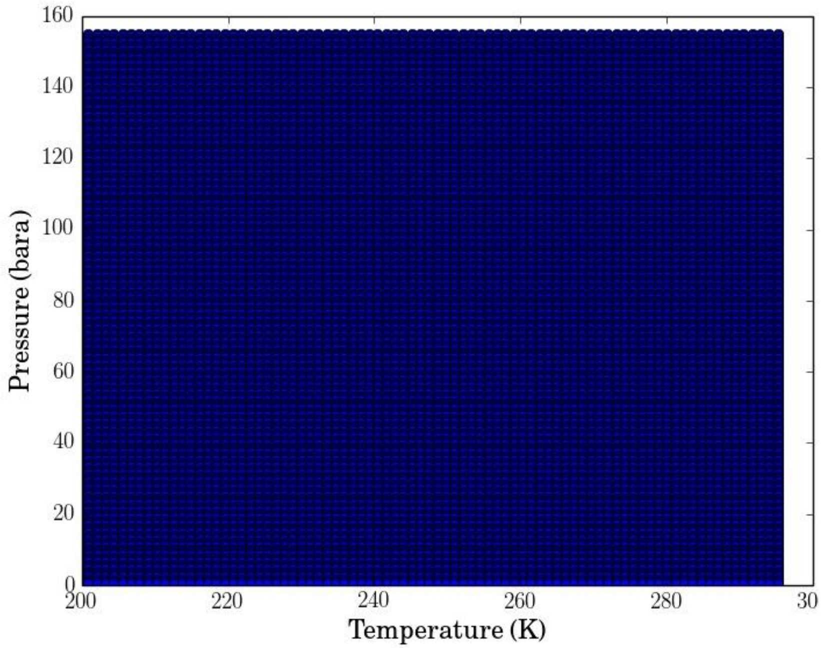


We would like to calculate the pressure and temperatures for our fluid from the internal energy and density



Robust evaluation of thermodynamic models usually only possible in this direction

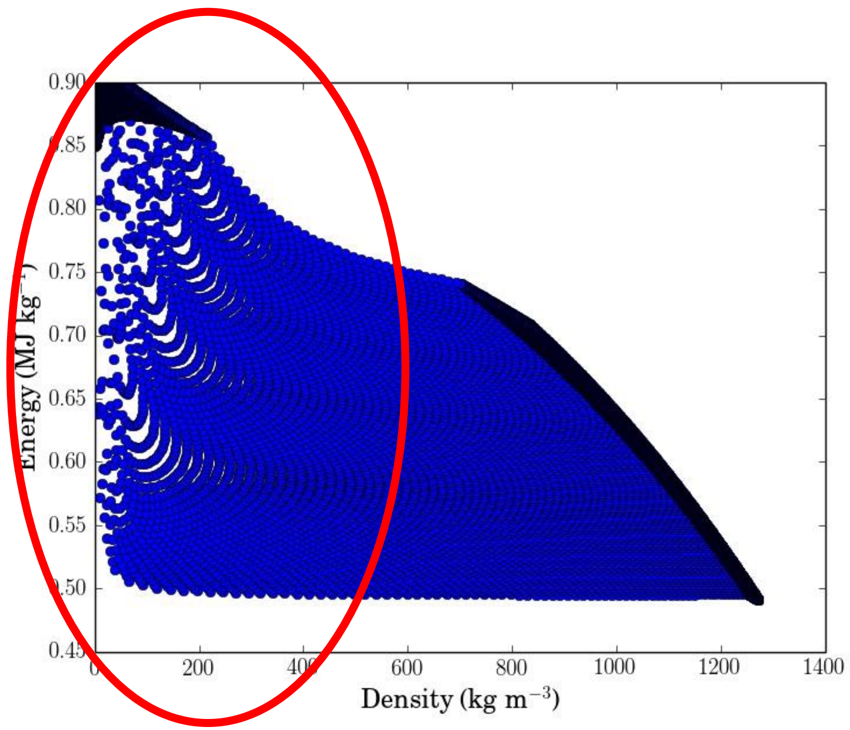
Inverse interpolation grids



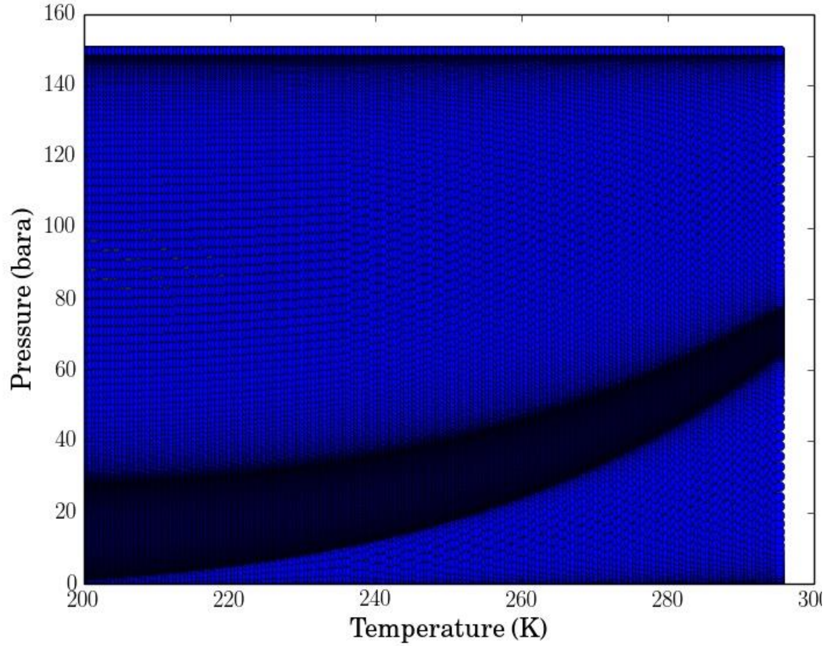
Naïve uniform sampling throughout the P-T space of interest using isothermal flash algorithms.

This produces an ill distributed grid of points in e-ρ points

…this region is so badly covered that simulations are impossible

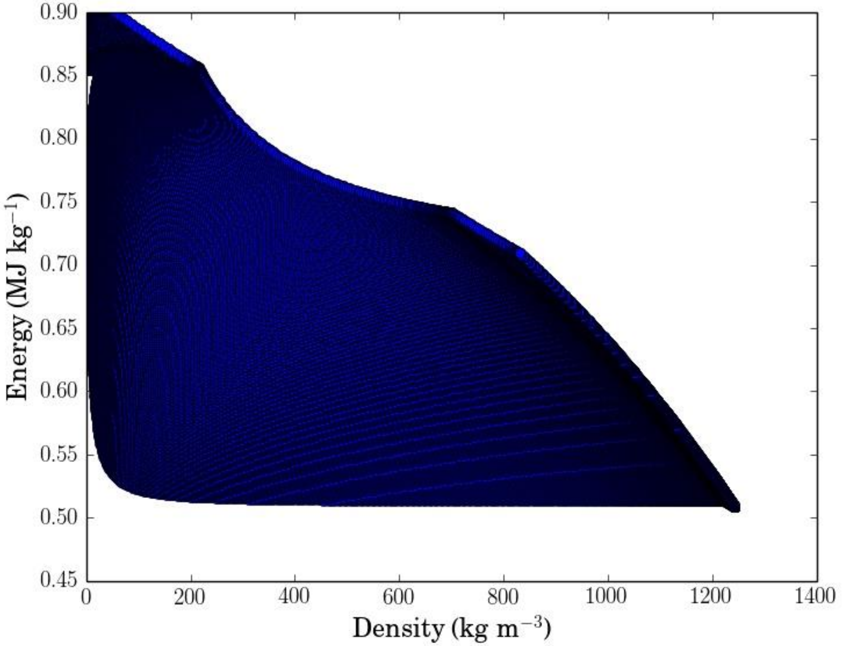


Interpolation grids



Instead we use a sampling which is heavier within the phase envelope and weighted towards phase boundaries…

…together with a re-distribution of points along isotherms gives an accurate interpolation grid



Mixture compositions of interest

Input Parameter	Binary mixture	Quinternary mixture
Fluid Composition (% vol./vol.)	N_2 – 4.04 CO_2 – 95.96	H_2 – 1.15 N_2 – 4 O_2 – 1.87 CH_4 – 1.95 CO_2 – 91.03

Cosham, A. et al.. "The Decompression Behaviour of Carbon Dioxide in the Dense Phase." In *Proceedings of the 2012 9th International Pipeline Conference*, 447. Asme, 2012. doi:10.1115/IPC2012-90461.

Equation of State and accuracy

We apply the PC-SAFT (Perturbed Chain Statistical Associating Fluid Theory) Equation of State.

Written as a summation of residual Helmholtz free energy terms that occur due to different types of molecular interactions in the system under study.

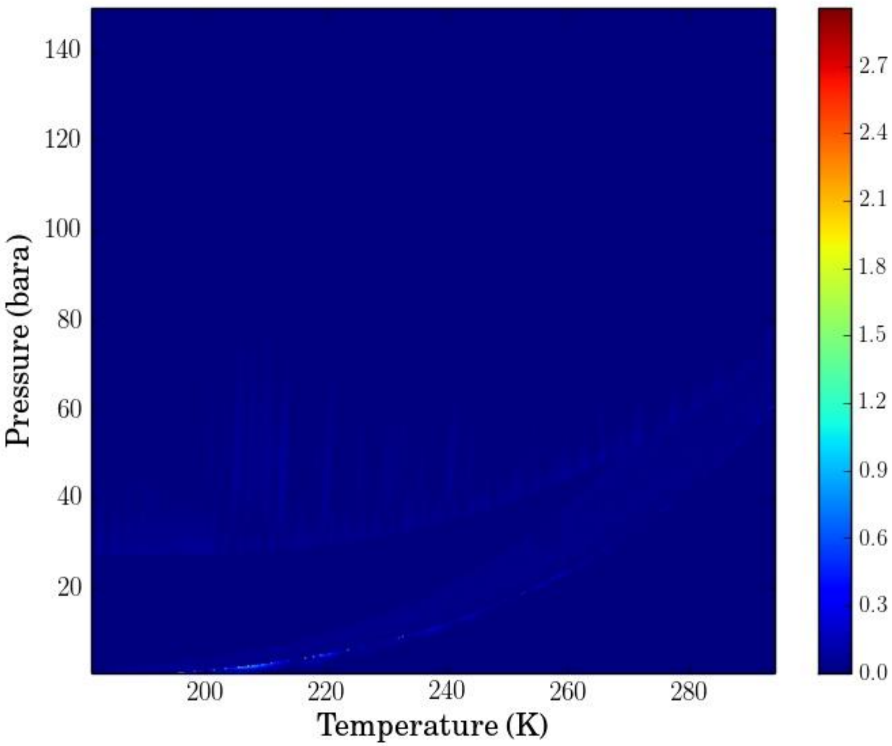
$$\frac{A^{res}(\rho, T)}{NRT} = \frac{a^{hs}}{RT} + \frac{a^{chain}}{RT} + \frac{a^{disp}}{RT} + \frac{a^{assoc}}{RT}$$

% AAD between interpolation and EOS

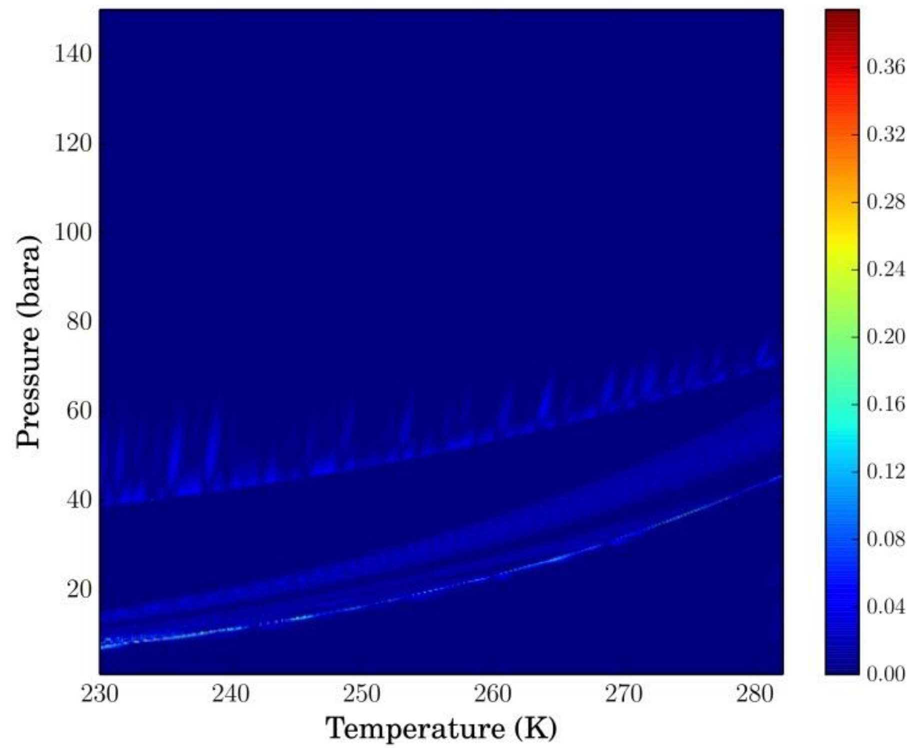
Input Parameter	Binary	Quinternary
Temperature	0.005	0.002
Pressure	0.44	0.07

Diamantonis, N. et al. “Evaluation of Cubic, SAFT, and PC-SAFT Equations of State for the Vapor–Liquid Equilibrium Modeling of CO2 Mixtures with Other Gases.” *Industrial & Engineering Chemistry Research* 52, 10: 3933–3942. doi:10.1021/ie303248q.

Temperature errors



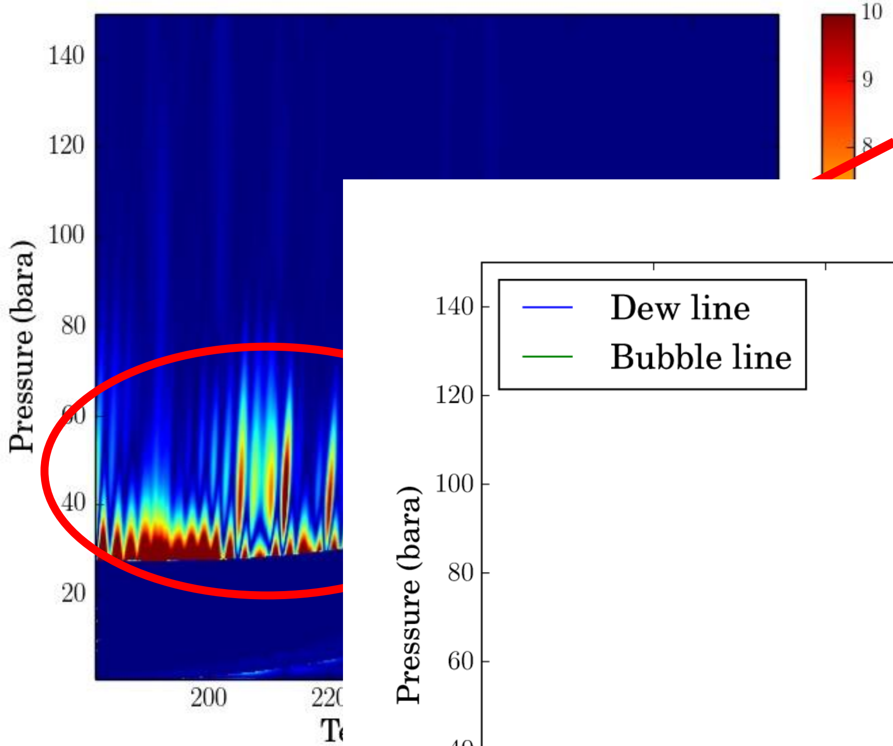
Binary

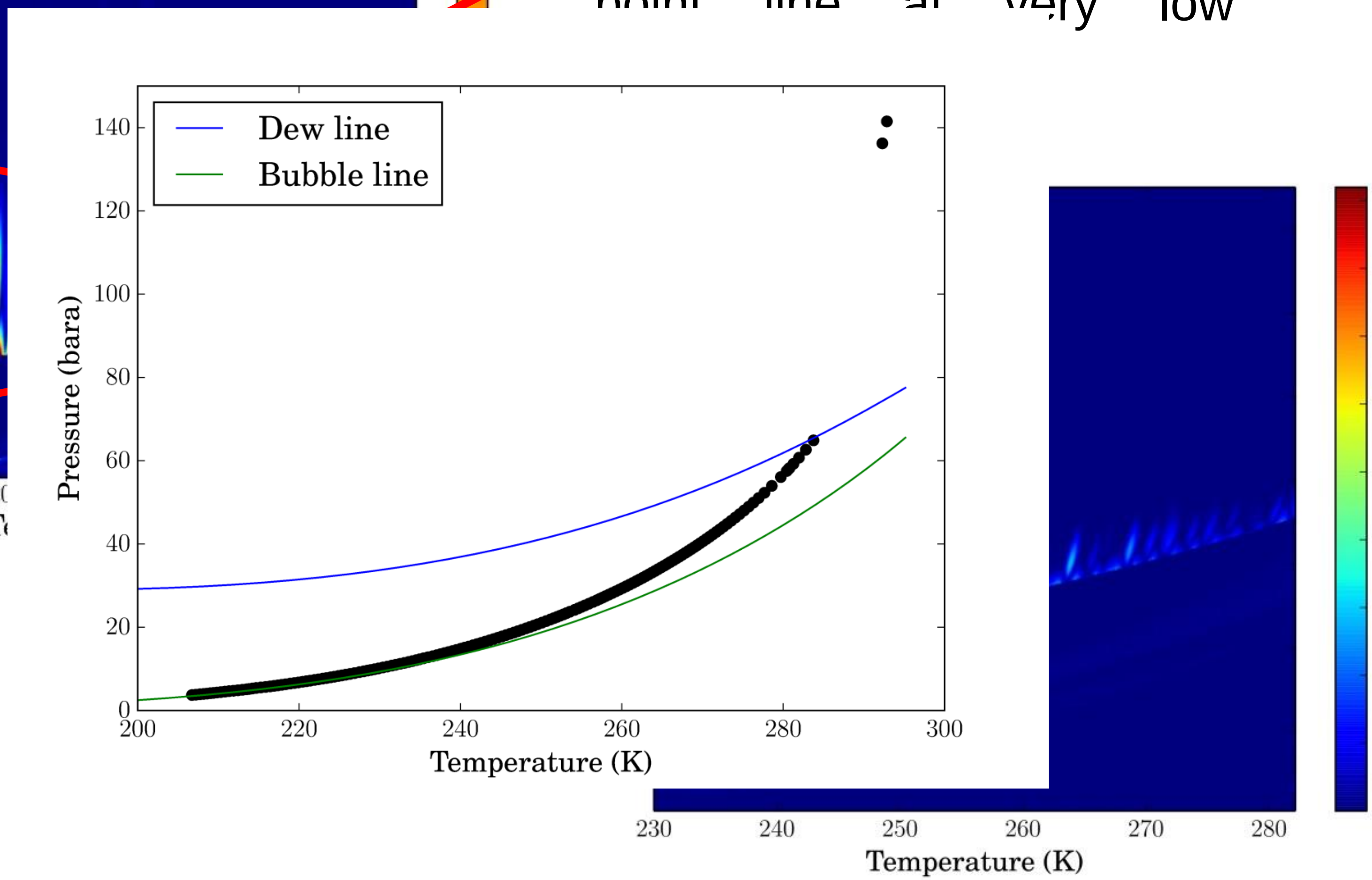


Quinternary

Pressure errors

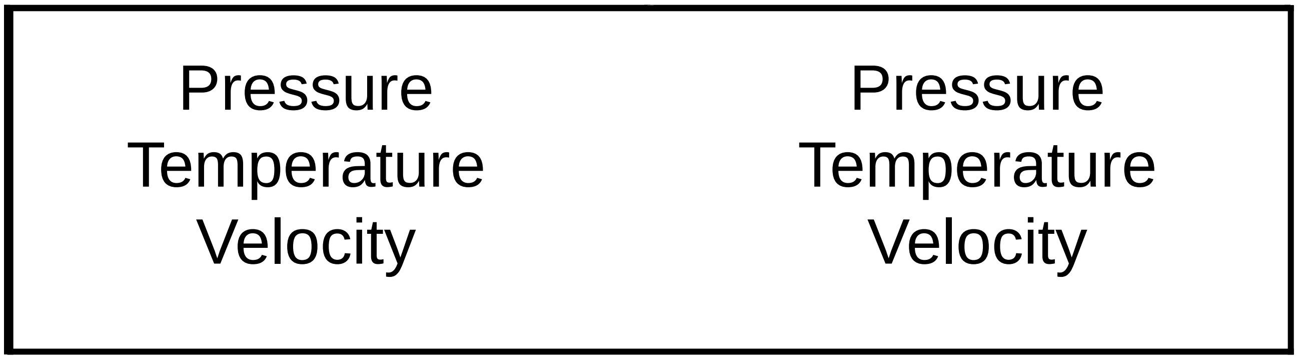
The greatest error is observed above the bubble point line at very low





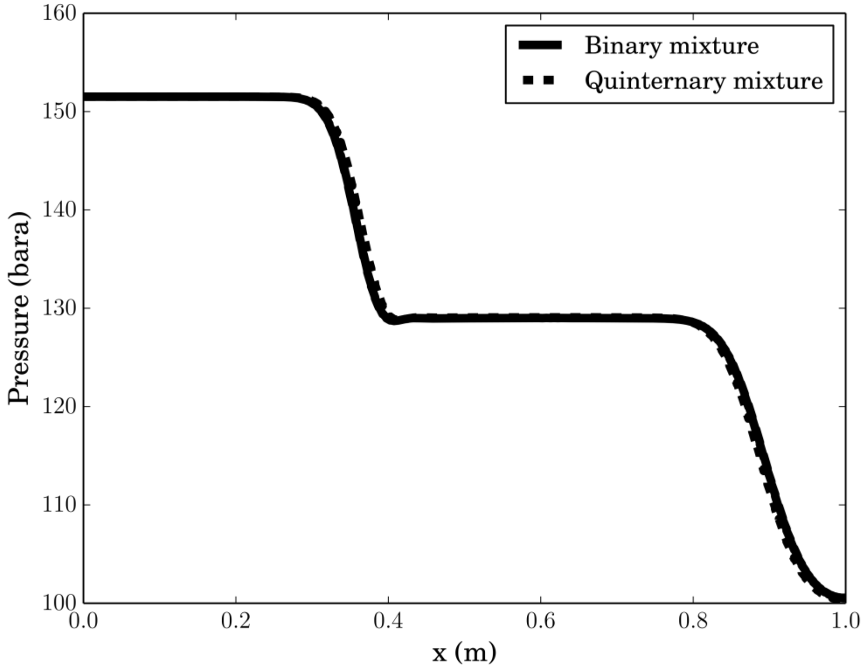
Quinternary

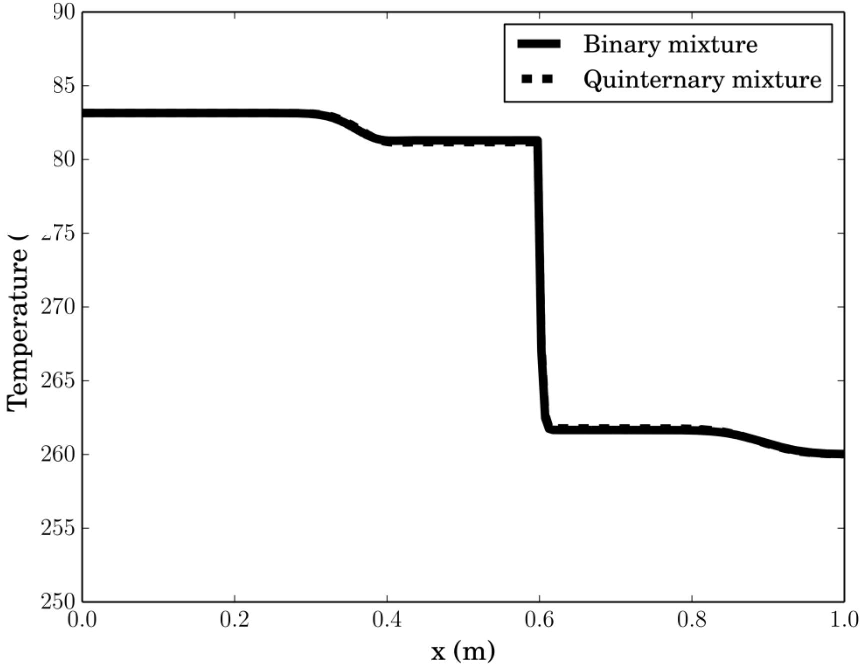
Fluid tests for stability – shock tubes



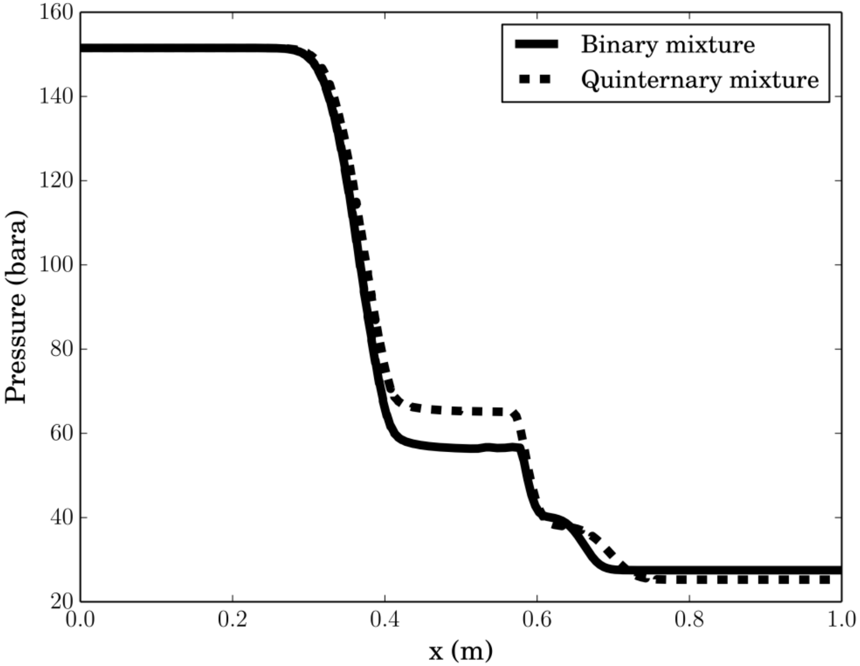
Input Parameter	P (bara)	Temperature (K)	Velocity (m s^{-1})
	Single-phase test		
Left state	151	283.15	0
Right state	100	260.00	0
	Two-phase test		
Left state	151	283.15	0
Right state	P_{dew}+2	260.00	0

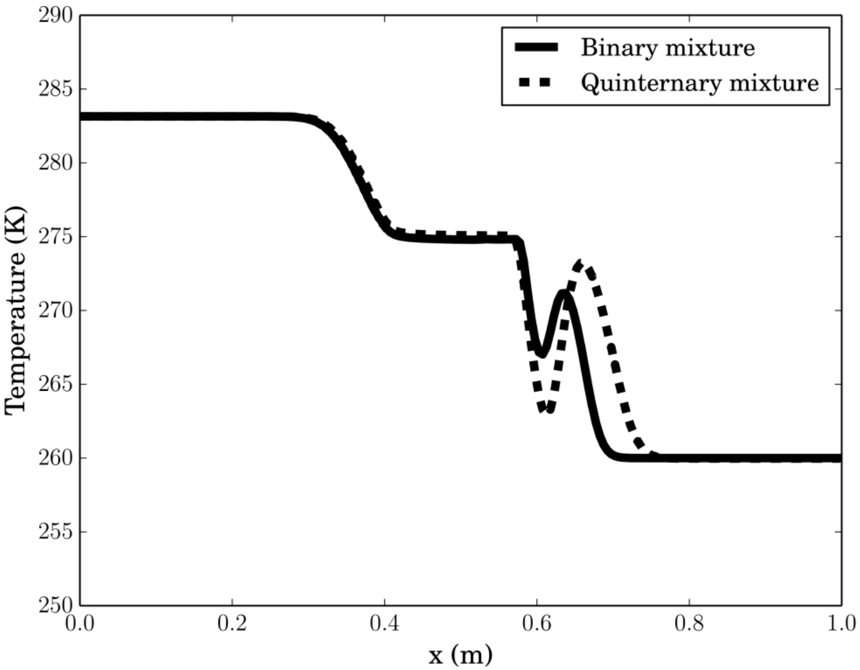
Single-phase shock tube test





Two-phase shock tube test





Decompression in CO_2 pipelines

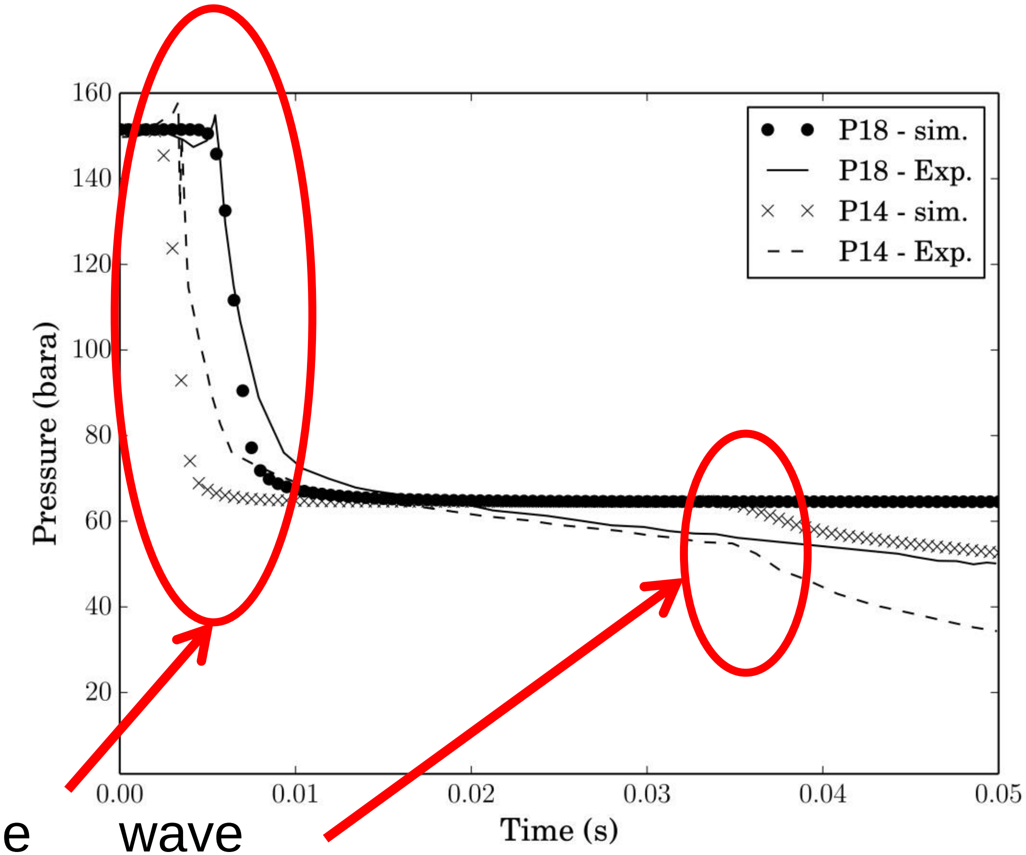
Pipeline characteristics and fluid conditions

Parameter	Value
Pipe internal diameter (m)	0.150
Pipe length (m)	144
Pipe wall roughness (mm)	0.005
Feed pressure (bara)	141
Feed temperature (K)	278.35

Cosham, A. et al.. “The Decompression Behaviour of Carbon Dioxide in the Dense Phase.” In *Proceedings of the 2012 9th International Pipeline Conference*, 447. Asme, 2012. doi:10.1115/IPC2012-90461.

Quinternary mixture decompression

Pressure profiles at two points within 4 m of release end



Capturing the wave speeds during decompression

Cosham, A. et al.. "The Decompression Behaviour of Carbon Dioxide in the Dense Phase." In *Proceedings of the 2012 9th International Pipeline Conference*, 447. Asme, 2012. doi:10.1115/IPC2012-90461.

Conclusions

- I showed the development and application of a robust interpolation method for the prediction of thermodynamic properties and phase equilibria of complex mixtures.

- Assessment of the method’s ability to reproduce the results of the EoS showed, for the most part, an error no greater than 0.5 %.

- Large errors were observed only for the liquid phase at low temperatures, where the physical model represented by the EoS is not applicable.

- Method was used in the simulation of flows containing CO_2 rich mixtures and was found to be robust.

- Comparison of the predictions against experimental decompression data, showed that the interpolation method produced robust and highly reliable results for simple and complex mixtures.

Acknowledgements and Disclaimer

The research leading to the results described in this presentation has received funding from the European Union 7th Framework Programme FP7-ENERGY-2012-1-2STAGE under grant agreement number 309102.

The presentation reflects only the authors' views and the European Union is not liable for any use that may be made of the information contained therein.