

Photo: Jostein Pettersen

Fundamental aspects of transport and injection of CO₂ with impurities

CO₂ Dynamics

<http://www.sintef.no/co2dynamics>

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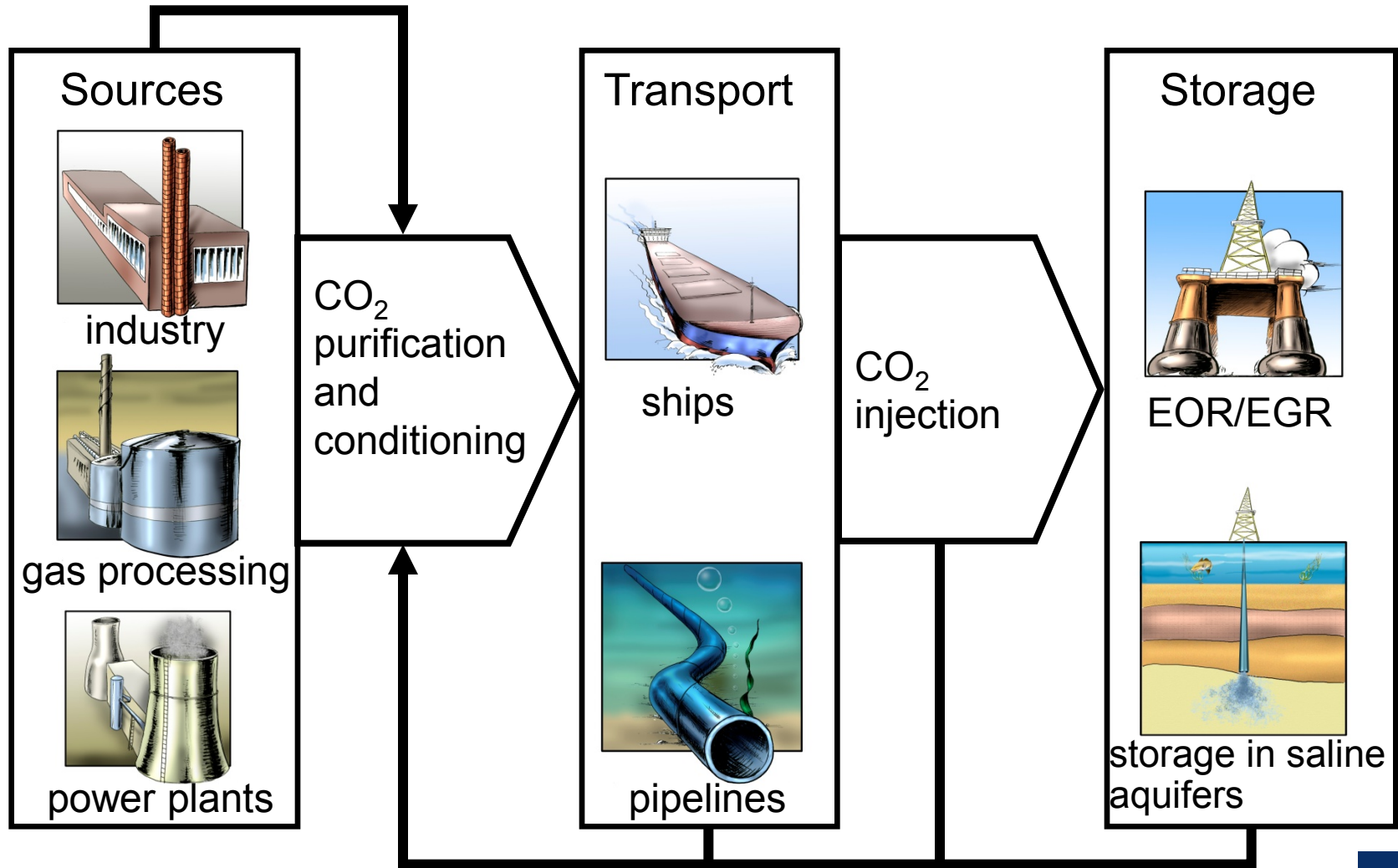
- Quick project overview
- Research challenges
- Examples:
 - Binary interaction parameters for a CO₂ mixture
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 - Effect of equilibrium assumptions on speed of sound
- Conclusions

CO₂ Dynamics – a research project

- Purpose: Given by the acronym KMB: Competence-building project with user involvement
- RCN funds 72% of the project
- Industry partners fund 9% each
- KMB project; an instrument for funding fundamental and pre-competitive research with higher risk than what the industry accepts to bear alone
- Industry participation to ensure an application-oriented direction and relevance
- Competence building for SINTEF and the consortium partners
- Duration: 2009-2013.
- Total budget: 26.5 MNOK (≈3.3 MEUR)

The CCS value chain

composition, T, P

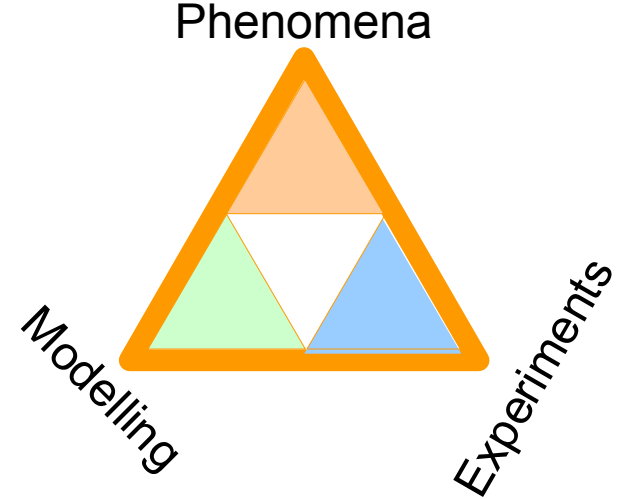


technical and legal CO₂ requirements

Research needs and objective

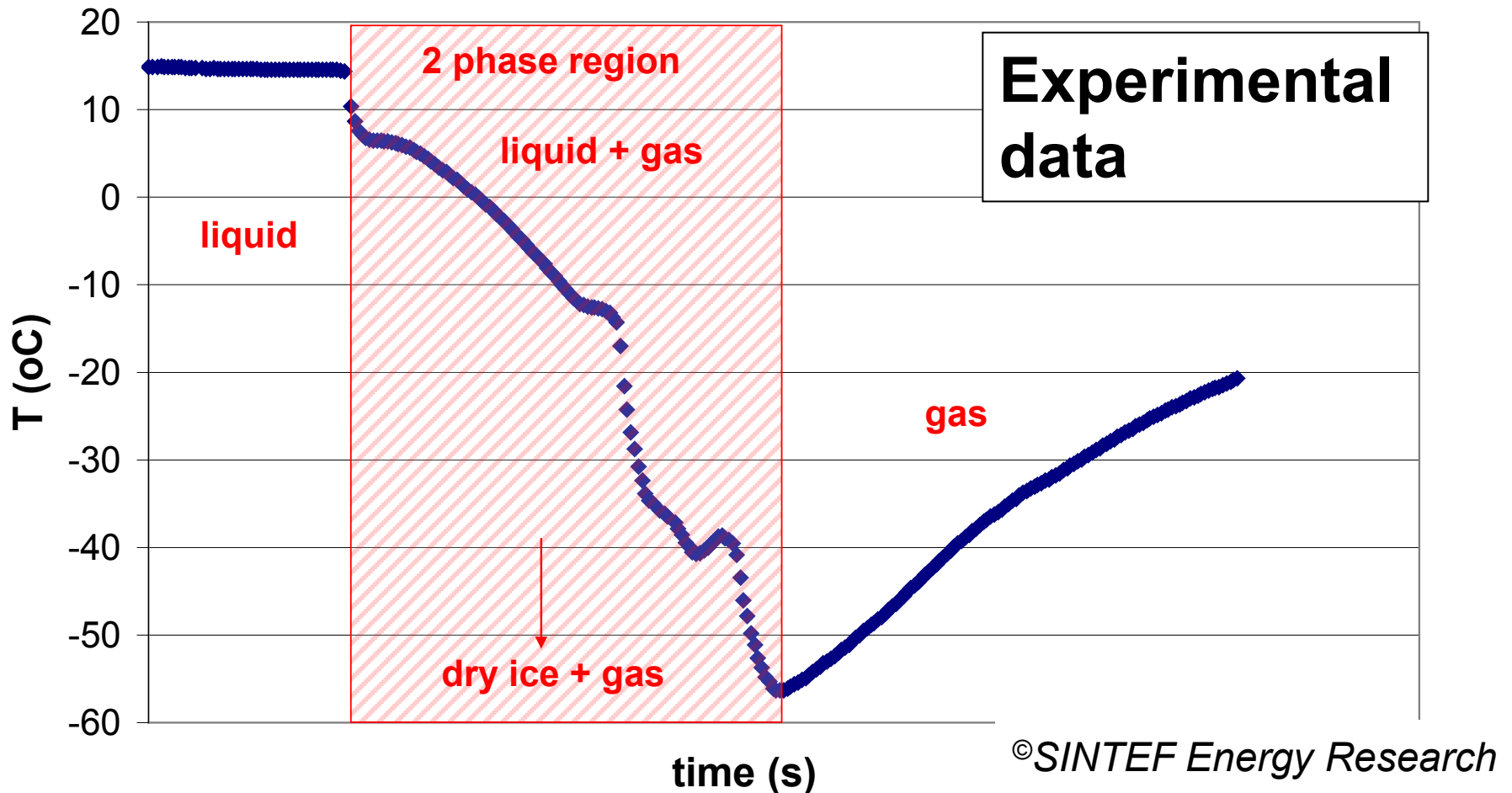
- **Objective:** Develop knowledge, methods and tools to enable safe design and operation of systems for CO₂ transport and injection
- **What is needed?**
 - **Thermodynamics:** Models and experimental data for phase equilibria, thermodynamic properties and transport properties.
 - **Fluid mechanics:** Models for multicomponent multiphase flow. In particular, models for flow regimes and phase interaction.
 - **Numerical methods:** The system of equations resulting from the thermodynamical and flow model must be solved in an accurate, robust and efficient way.
 - Each of the above areas contain many open research topics, and it is a challenging task even putting together a “simple” model which is able to some extent to account for the complex thermodynamical and fluid dynamical interplay that can occur in a CO₂ transport pipeline.

Research method



- In good research, we have a two-way coupling between modelling and experimental work:
 - Experiments are needed to develop and verify models.
 - Development and understanding of models will improve the understanding of the phenomena under study.
- There is no planned experimental activity in the present project, but available data will be employed.
- Since this is a competence-building project, the findings will be *published* in the open literature, mainly in peer-reviewed journals and at conferences (like here). See also the project home page.

CO₂ pipeline depressurization



Modified from: "Construction of a CO₂ pipeline test rig for R&D and operator training", Pettersen, J., de Koeijer, G. and Hafner, A., GHGT-8, Trondheim, June 2006

Research challenges

- Fluid dynamics
 - We need to consider multiphase flow models since phase transition can take place during decompression.
 - It is not clear which models should be employed in which situation.
 - Slip relation in the drift-flux model.
 - Interfacial friction, mass and heat transfer in the two-fluid model.
 - Etcetera.
 - The eigenstructure of the model determines the wave-propagation speed and hence the decompression and compression behaviour.
 - Analysis is needed for the models we are interested in.

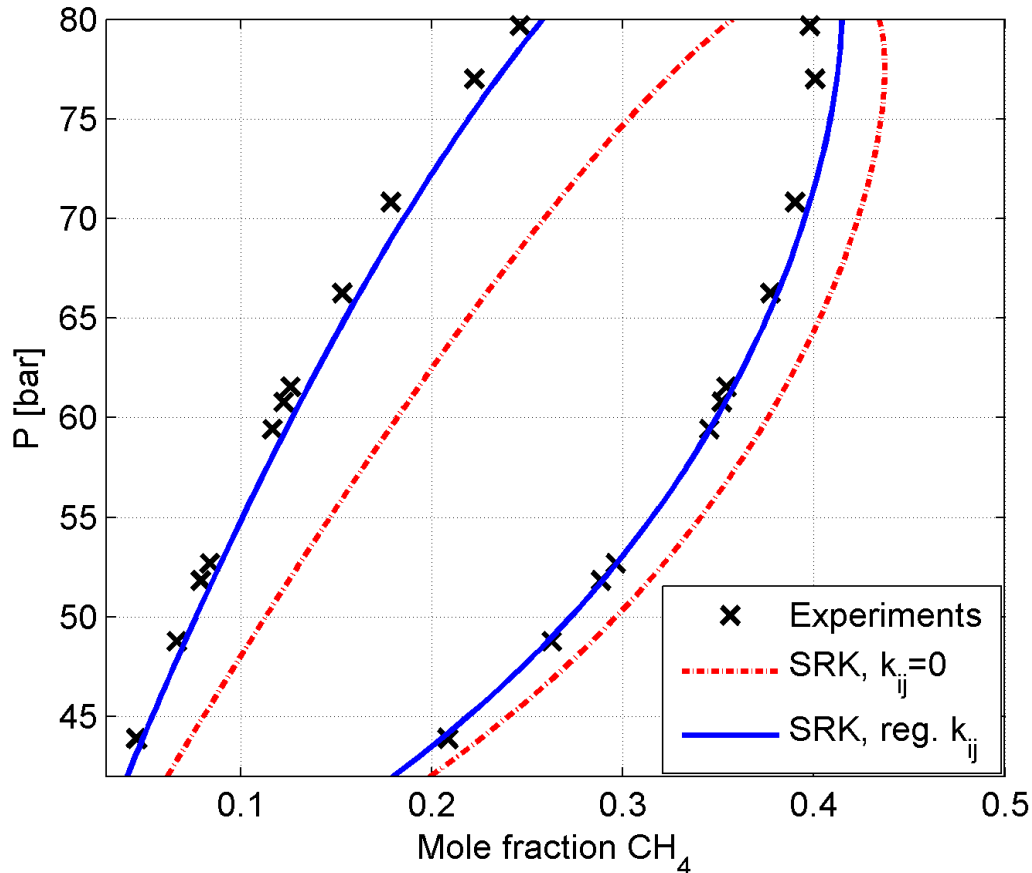
Research challenges

- Numerical methods
 - Numerical methods are not an off-the-shelf commodity for multiphase-flow models.
 - We need to be ascertained that we can obtain an accurate solution of the mathematical model. Only then can we infer that any discrepancy with experimental observations is due to wrong or simplified models (and experimental uncertainties).
- Thermodynamics
 - Fluid dynamics and thermodynamics are tightly coupled.
 - We need robust and accurate algorithms for cases when pressure and temperature are unknowns.
 - Further development of equations of state regarding consistency, accuracy, and, if possible, efficiency, for the relevant mixtures.

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Prediction of vapour-liquid equilibrium



- $\text{CO}_2\text{-CH}_4$ mixture at 270 K
- SRK equation of state
- Red: No binary interaction parameters, k_{ij}
- Blue: With regressed k_{ij}
- Thermodynamic models should not be used in a “black box” approach

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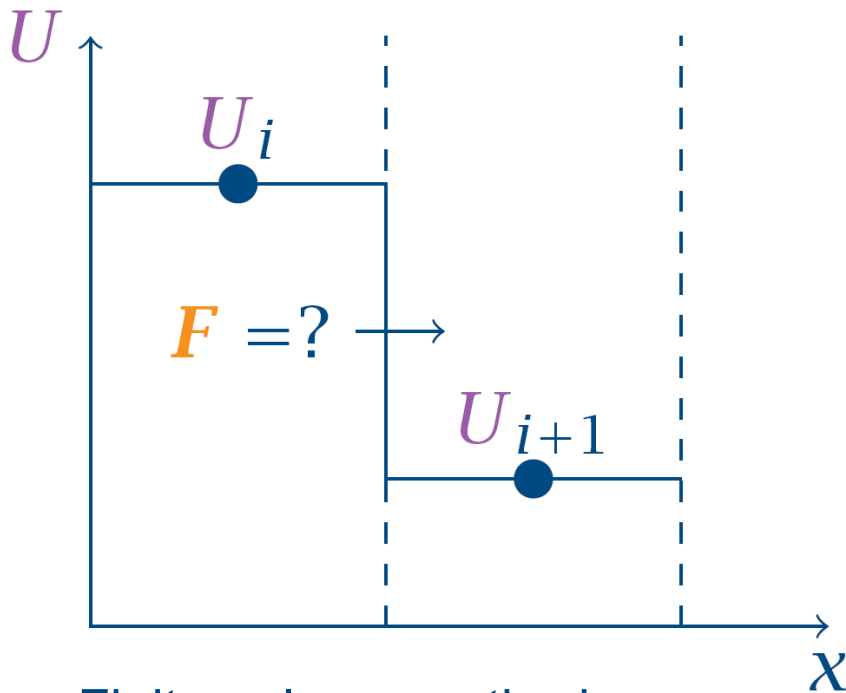
The numerical flux

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = Q(U)$$

Conservation law

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + \frac{F_{j+1/2} - F_{j-1/2}}{\Delta x} = Q_j^n,$$

Discretization



Finite-volume method

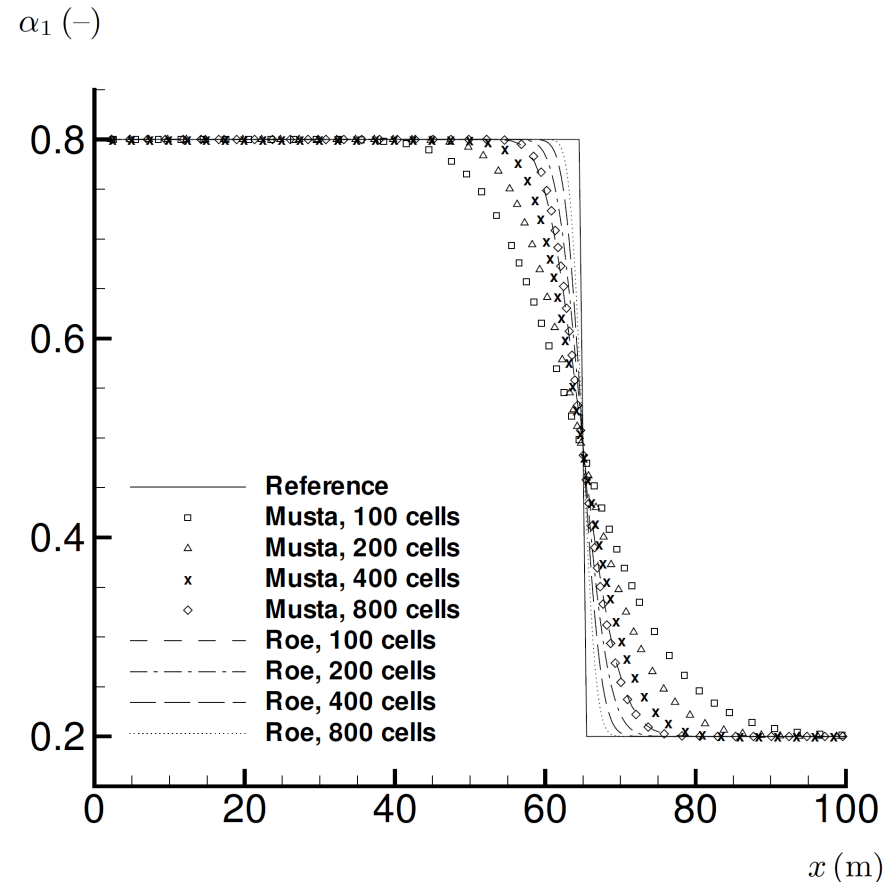
- The core of the finite-volume method
- Finding the numerical flux F is (still) a research task for multiphase flow models
- One way is via the quasi-conservative form

$$\frac{\partial U}{\partial t} + A(U) \frac{\partial U}{\partial x} = Q(U)$$

where $A(U) = \frac{\partial F(U)}{\partial U}$

Moving discontinuity

- Contact discontinuity
 - All variables uniform except a jump in volume fraction, α .
 - Riemann problem containing waves at flow velocity only.
- Features
 - Slow-moving wave
 - Difficult to resolve sharply
 - The diffusion increases with decreasing time-step length
- Roe (upwind) with 100 cells performs as well as Musta (centred) with 800 cells.
 - (Musta is a good scheme)

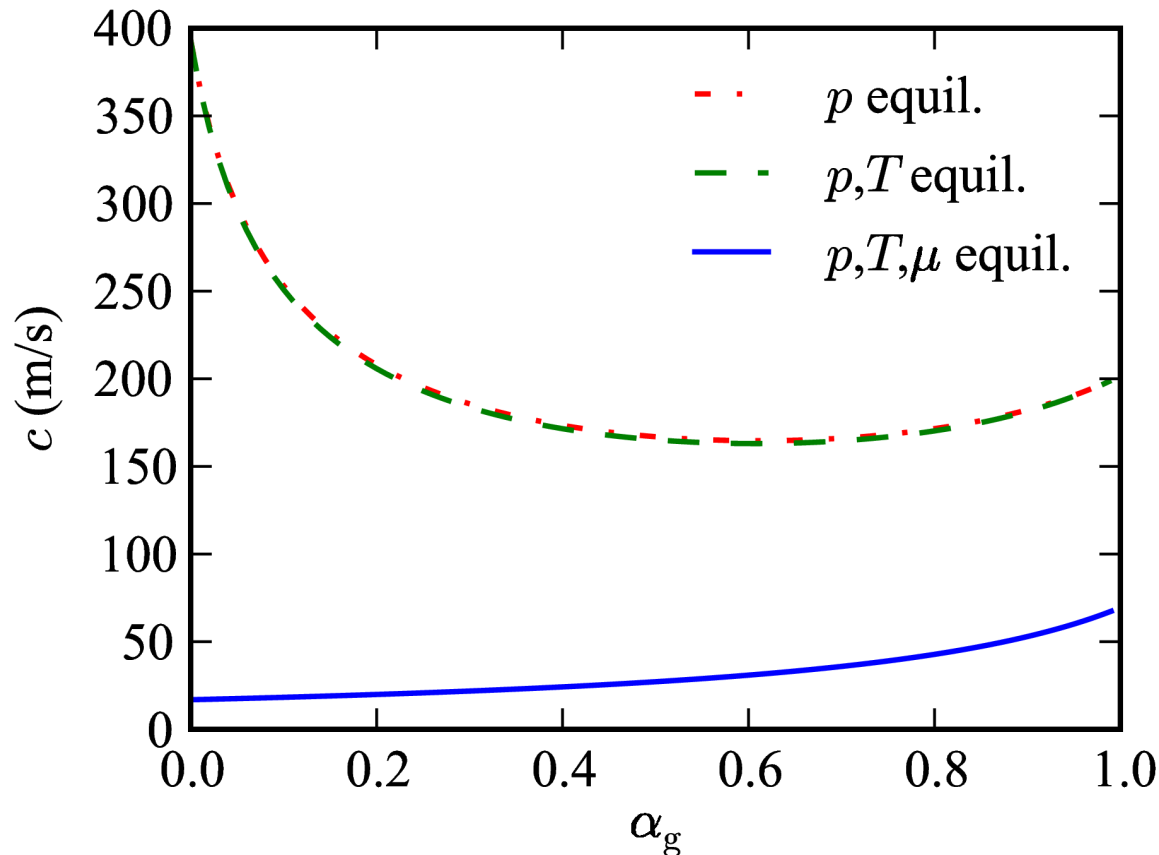


CO₂ volume fraction for the MUSTA and Roe schemes. CFL=0.9

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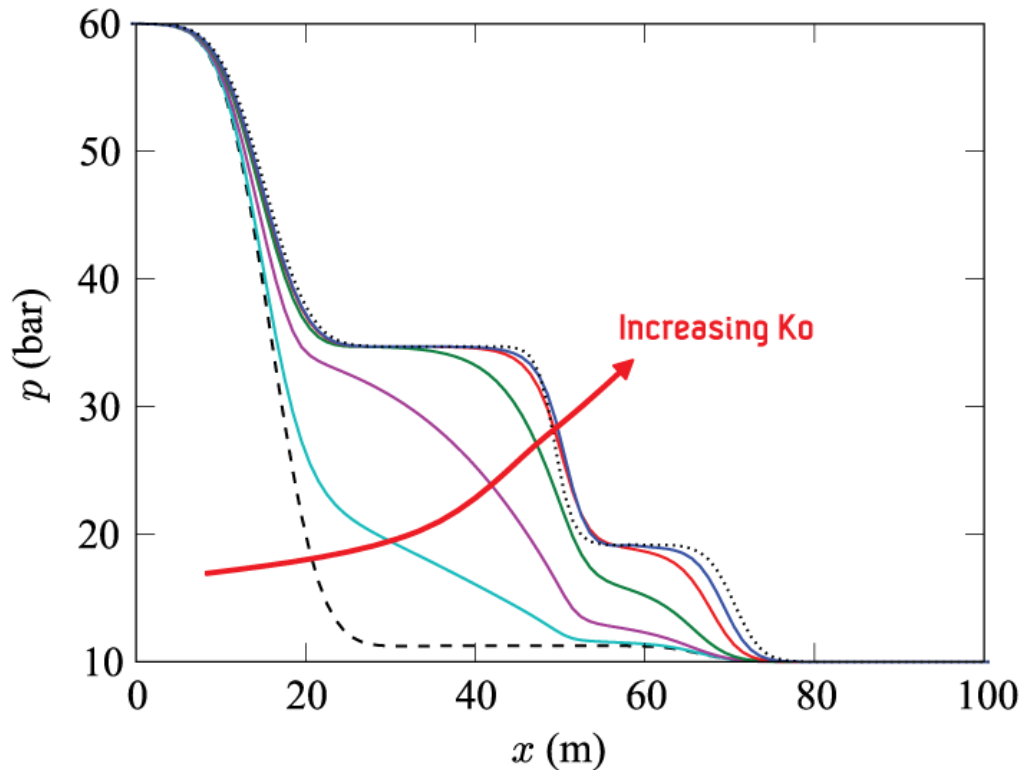
Speed of sound and different equilibria



- Equal pressure, temperature and chemical potential in gas and liquid gives
 - Very low speed of sound
 - Discontinuous speed of sound at single-phase limit

- Speed of sound as a function of gas volume fraction

Wave speed and phase equilibrium



- Model including phase transition
- High K_0 : Always phase equilibrium
- $K_0=0$: No phase transfer
- Equilibrium gives slower pressure waves

- Depressurization with slow \rightarrow fast phase equilibrium

Conclusions

- In CO₂ Dynamics, models and numerical methods for thermodynamics and fluid dynamics are analysed and developed.
- Accurate and consistent thermodynamic models for CO₂ mixtures are needed.
- Fluid problems involving pressure waves are of interest in safety analyses and otherwise.
- Therefore, we need to be able to calculate both pressure and volume-fraction waves in multicomponent multiphase flow.
 - Robust and accurate numerical methods are not an off-the-shelf commodity.
- The model assumptions regarding equilibrium (pressure, temperature, chemical potential) strongly influence the pressure wave propagation velocity (speed of sound).

Thank you for your attention

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This work was financed through the CO₂ Dynamics project.

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