Simulation of CO_2 behavior in flow and depressurization

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Background and motivation

Accurate modeling of CO_2 behavior in flow and depressurization is important for handling CO_2 safely and optimally. By coupling a compressible flow solver with rigorous thermodynamic models we can assess several issues within carbon capture and storage (CCS):

- **Blowdown of process equipment with high content of CO_2.** Blowdown of initially supercritical CO_2 will typically form liquid, vapor and solid. Accurate modeling of this process enables better design of the depressurization system.

- **Accidental depressurization during well-injection of CO_2.** Knowledge and ability to predict behavior of CO_2 is crucial when modeling depressurization (or blow-out) of an injection well.

- **Identification of formation of solid CO_2.** Identifying risks associated with formation of solid CO_2 is important. Using a multiphase flow modeling approach, we can help address these risks.

Petrell is currently further developing the simulation system *Brilliant* (1) , as part of the JIP *Simulation of CO_2 behavior in flow and depressurization*. *Brilliant* is a general finite volume based CFD-system (Computational Fluid Dynamics) with integrated FEM abilities (Finite Element Method) for stress analysis. Brilliant is designed to fully support multiphysics applications. With the introduction of thermodynamic models capable of treating solid CO_2 in *Brilliant*, complex scenarios involving possible dry ice formation may be simulated in a fully 3-dimensional and transient framework.

VessFire (2) is a *Brilliant*-based simulation system, tailor made for analysis of depressurization of process equipment. *VessFire* is already in widespread use, and the multiphysics simulation approach enables safer design of process equipment. *VessFire* will utilize the knowledge and technology developed during this project. Addressing the thermo-mechanical response of vessels and pipes subject to extreme temperatures, e.g. in relation to cold blowdown or blowdown when the process system is exposed to fire, is important when designing and dimensioning process equipment. With the aid of this project, *VessFire* will be able to accurately handle CO_2 and CO_2-rich mixtures, including formation of dry ice.

BRILLIANT VESSFIRE

Thermodynamic treatment of CO_2

A new thermodynamic module, ThermoProp, has been developed for *Brilliant*. The module is based on the thermodynamic software solution from HAUG Technology (5). By utilizing a generic programming interface the equation solver layer in ThermoProp has been written entirely independent of which equation of state (EOS) is being used. Currently we use a special purpose dry ice model for the solid, Peng Robinson EOS for mixtures and Span Wagner EOS for pure CO_2. Figure 1 shows pressure and temperatures of a pure CO_2 depressurization, where the simulation dynamically starts from a vapor-liquid entering into a vapor-liquid-solid state and finally entering a vapor-solid state. Comparison with the experimental results of Eggers & Green (3) shows excellent agreement. Figure 2 shows pressure transients starting from three different supercritical states.

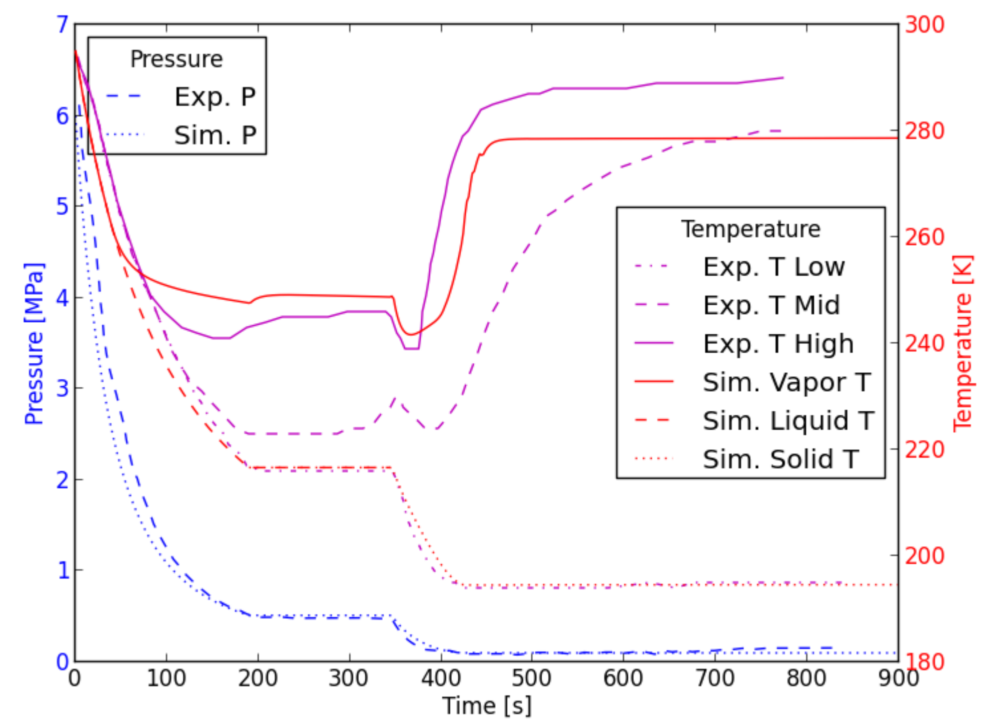

Figure 1: Simulated results of depressurization of a pure CO_2 vessel compared with the experimental results of Eggers & Green (3). The initial conditions is in the two phase region with pressure 60 bar, temperature 300 K and a liquid volume fraction of 80%. At approximately 200s the liquid reaches the triple point and starts forming dry ice. At approx. 350s the liquid vanishes and only solid and vapor remains in the vessel. The experimental temperature curves are from three different vertical levels in the vessel. Excellent agreement is seen on the pressure and temperature transients.

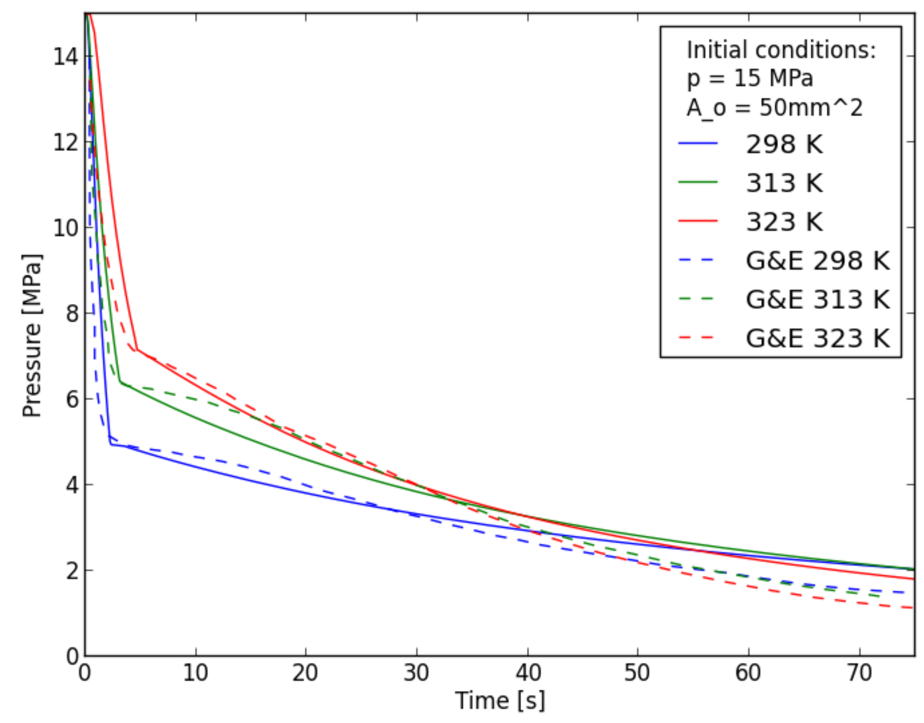

Figure 2: Pressure transients starting from three different temperatures in the supercritical region. The dashed lines are the experimental results of Gebbeken & Eggers (4). The characteristic bend in the pressure transient occurs when the two phase region is entered and flash evaporation occurs. The rapid vapor formation opposes the effect of depressurization.

Flow simulations with CO_2

Brilliant offers a general CFD framework, and couples different physical models into one simulation. A compressible flow solver coupled with thermodynamic models of CO_2 (pure or in mixtures) enables detailed analysis of CO_2 rich processes. In addition to solving full 3D flow problems with a fine grid, simplified 1D flow solution methods that are suitable for simulating flow between process components is being developed. Offering simulation software that is sufficiently fast and stable for practical applications is the main focus. Multiphase flow is also part of our activity, where dispersed flows (particles, bubbles or droplets) and stratified flows have been the main focus so far. Figure 3 shows simulation results from a buoyancy driven bubble flow. The simulation involve flow field solution of both the continuous liquid phase and the dispersed vapor bubble phase. Also, the thermodynamic module updates the state of each phase in each control volume per time step (including mass transfer, although there is no mass transfer in this particular case). Figure 4 shows the temperature on a 3D grid of a steel vessel wall.

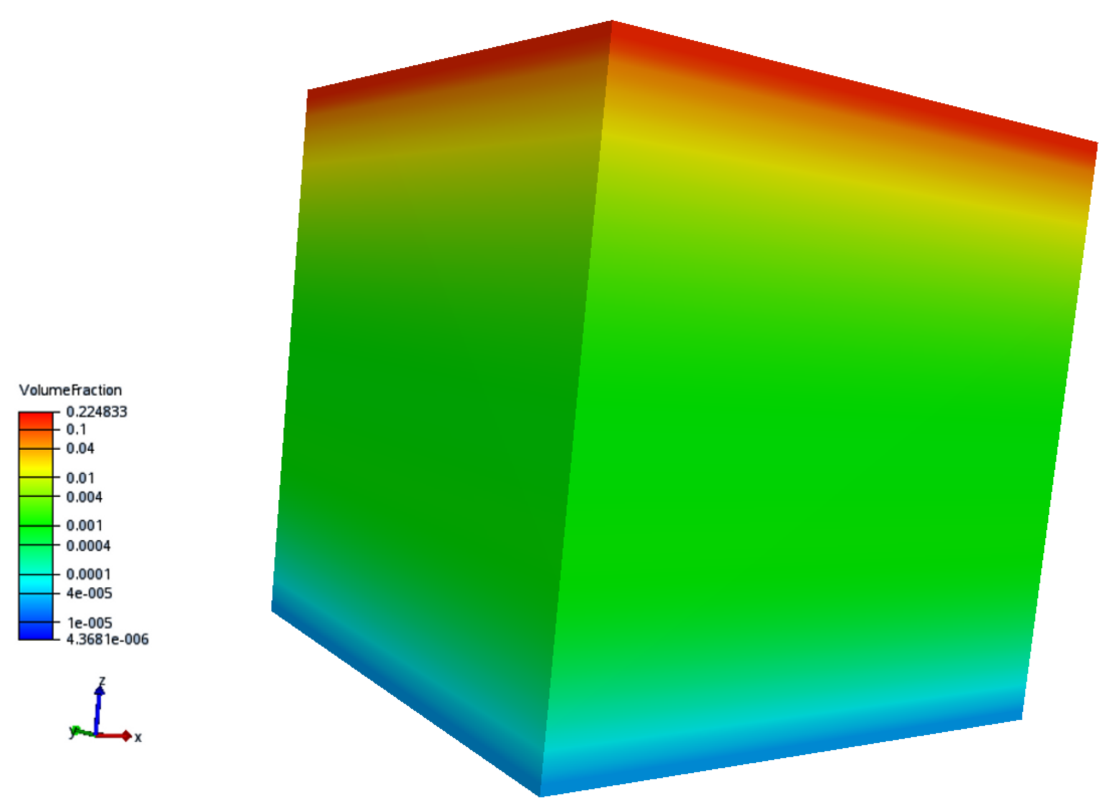

Figure 3: Simulation of a column with CO_2 bubbles in liquid water, where the buoyancy transports the bubbles upwards. Initially the entire domain starts with a uniform distribution of bubbles. During the simulation bubbles start accumulating in the top part of the column. This is shown by the bubble density (volume fraction) in the figure.

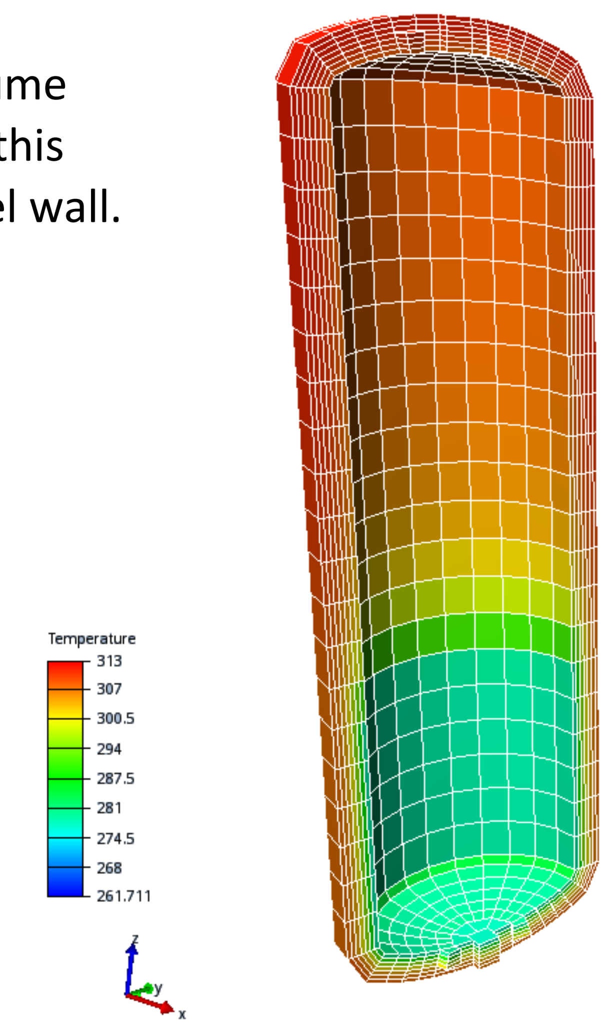

Figure 4: A 3D model of a steel vessel showing temperature during a depressurization simulation. The temperature is lower in the bottom part of the vessel due to a lower temperature in the liquid phase, which occupies approximately one third of the vessel volume.

Perspectives

In the third and last phase of the *Simulation of CO2 behavior in flow and depressurization* JIP, Petrell will utilize *Brilliant* and *VessFire* for various case studies presented by the JIP partners. Other activities include a continued effort on multiphase flow and finalization of a new release of VessFire that supports formation of dry ice and flow between process components.

References

(1) Theory and descriptions of structure for the multi physic simulation system Brilliant, Geir Berge. (www.brilliant-cfd.com)

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(3) Pressure discharge from a pressure vessel filled with CO2. Eggers, E. and Green, V. 1990, J. Loss Prev. Process Ind.

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(5) HAUG Technology. Contact: Tore Haug-Warberg, Assoc. Prof. NTNU.

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