

# Simulation of CO<sub>2</sub> behavior in flow and depressurization: Treatment of formation of solid CO<sub>2</sub>

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## Background and motivation

Treatment of CO<sub>2</sub> in the oil & gas and process industry has become more focused over the last years. This concerns processing, transportation and storage. The combination of a rapid pressure drop and low temperatures in a CO<sub>2</sub> rich mixture can lead to formation of solid CO<sub>2</sub> (dry ice). There are several aspects within CCS where this subject arises, e.g.:

- **Blowdown of process equipment with high content of CO<sub>2</sub>.** During a blowdown process there is a risk of forming solid CO<sub>2</sub>. Solid particles might clog openings such as restriction orifices, reactor or column inventories and pipes. This may lead to a series of threats to the safety of installations.
- **Accidental depressurization during well-injection of CO<sub>2</sub>.** Knowledge and ability to predict behavior of CO<sub>2</sub> is crucial when modeling depressurization (or blow-out) of an injection well.
- **Long distance transport of CO<sub>2</sub>-rich mixtures in pipe lines.** As the pressure drops, there is a risk for solid CO<sub>2</sub> formation that can influence flow conditions.

Petrell is currently further developing the simulation system *Brilliant* (1), as part of the JIP SolidCO<sub>2</sub>Sim. *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<sub>2</sub> 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* 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 blow-down or blow-down 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<sub>2</sub> and CO<sub>2</sub>-rich mixtures, including formation of dry ice.

BRILLIANT  VESSFIRE

## Thermodynamic treatment of solid CO<sub>2</sub>

In collaboration with Tore Haug-Warberg (assoc. Prof at NTNU), a new thermodynamic module is being developed. The module consists of different models for specific equations of state (EOS), and a powerful and flexible equation solver part using Newton's method. The equation solving classes utilize the interface provided by the model system of Haug-Warberg. Different multiphase concepts can use different specialized equation setups, ensuring consistency throughout the solution of a control volume.

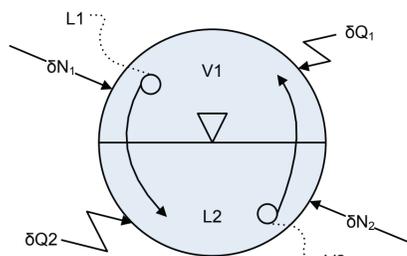


Figure 1: Schematic drawing of the thermodynamic control volume. Phases L1 and V2 are reference phases that handle condensation and evaporation, respectively.

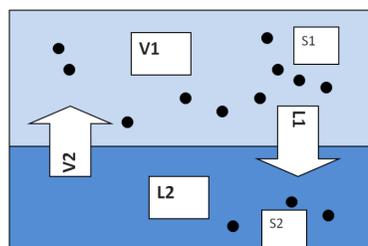
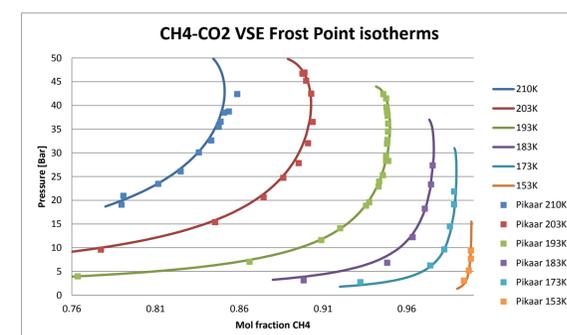
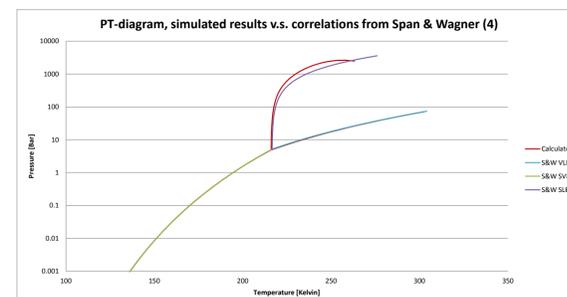


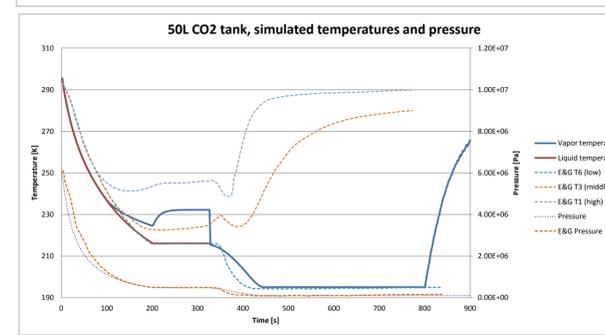
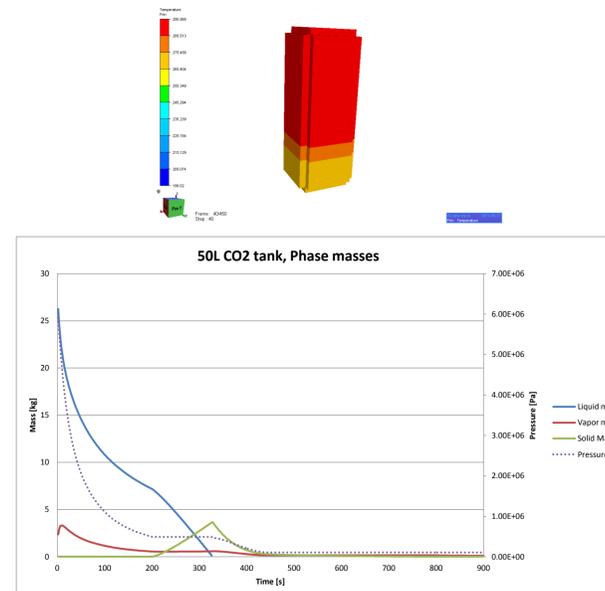
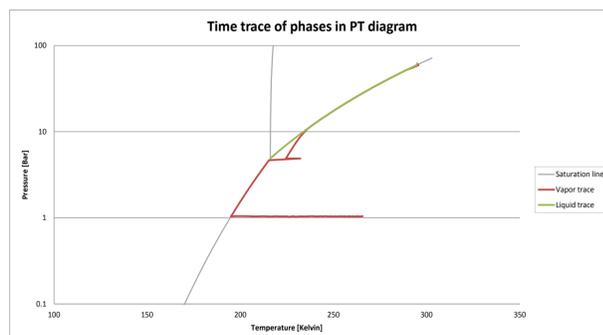
Figure 2: Solid is treated as particles dispersed into a bulk vapour or liquid phase



## Test case: Depressurization of a CO<sub>2</sub> tank

As a first test case, a depressurization simulation of a CO<sub>2</sub> filled tank has been performed. This has been done to demonstrate the current capabilities of treating formation and handling of dry-ice in a typical VessFire scenario. In order to validate against experimental data, the model was created similar to the CO<sub>2</sub> tank of Eggers & Green (3). The following conditions were used in the test case:

- Starting pressure: 60 bar
- Starting temperature: 295 K
- Initial level of liquid CO<sub>2</sub>: 86 vol%
- Volume of tank: 50L
- Time of depressurization: 400 s
- Steel wall thickness: 35 mm



## Perspectives

In the continuing work of the SolidCO<sub>2</sub>Sim project, important issues include: Multiphase flow with solids (i.e. particle flow), improved solution procedure for flow with large density variations, development and finalization of the thermodynamic module and GUI development.

## References

- (1) [www.brilliant-cfd.com](http://www.brilliant-cfd.com)
- (2) [www.vessfire.com](http://www.vessfire.com)
- (3) *Pressure discharge from a pressure vessel filled with CO<sub>2</sub>*. Eggers, E. og Green, V. 1990, J. Loss Prev. Process Ind.
- (4) *A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple-Point Temperature to 1100K at Pressures up to 800MPa*. Span, R. and Wagner, W.. 1996, J. Phys. Chem. Ref. Data, Vol 25

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