D 1.3.2 The influence of CO₂ mixture composition and equations of state on simulations of transient pipeline decompression

In a carbon capture and storage (CCS) infrastructure, CO₂ transport is an essential component. For transport of large volumes of CO₂, pipelines are often the most cost-efficient solution. For efficient transport, the CO₂ is compressed to a high pressure, equivalent to around 100 atmospheres, so that it is in a liquid-like form. Pipelines may need to be emptied (or decompressed) due to maintenance or be accidentally emptied due to a rupture.

It is of interest to predict the temperature and pressure in the pipeline during a decompression for (at least) two specific reasons. First, as the pressure drops, the liquid will expand and eventually start to boil, which cools the pipe down. Low temperatures can be damaging to the pipe or to other equipment such as valves and pumps. Second, the pressure when the liquid starts to boil is relevant for running fractures. Running fractures occur when the pressure in the pipe is high enough to keep a fracture running along the length of the pipe. It is therefore of interest to predict the pressure at which the CO2 liquid starts to boil, since this in practice will be the pressure at the tip of the fracture in many cases. For these reasons, we need accurate mathematical models to predict the temperature and pressure during a decompression. When CO₂ is captured from industry, it will rarely be pure, but will be mixed with other gases such as e.g. nitrogen, oxygen, methane and ethane. Such CO2 mixtures can have significantly different properties from pure CO₂, which must be taken into account when predicting the temperature and pressure. A key component necessary to describe flow of CO₂ mixtures is the thermodynamic model, which relates properties like pressure, temperature and density to each other. In this work, we examine whether it is beneficial to use highly accurate thermodynamic models (EOS-CG and GERG) instead of a much simpler model (Peng-Robinson) when predicting temperature and pressure during a decompression. We also investigate whether the amount of other gases has any significant effect on temperature and pressure.

Our results show that for decompression, the choice of thermodynamic model matters much less than the amount of other gases. When the amount of other gases is increased, the boiling pressure can increase significantly, which can increase the risk of running fractures. It was found that the lowest temperature depends neither significantly on the amount of other gases nor on the choice of thermodynamic model. For other CO₂ pipeline considerations, however, the choice of thermodynamic model have larger impacts.



Figure: A comparison of the region where gas and liquid coexist as a function of temperature and pressure for pure CO₂ (solid line), CO₂ with 2% nitrogen (dotted fill), and CO₂ with 2% hydrogen (hatched fill). Also shown is the temperature–pressure evolution of a decompression event from an initial liquid state of 100 bar and 20 _C. An important parameter when designing pipelines to avoid running ductile fractures is the saturation pressure (red dots), which is the pressure where the liquid starts to boil. As seen, these impurities significantly increase the saturation pressure, and thus they increase the risk of running ductile fracture.