Supporting Information for publication

Computational and experimental study of solid phase formation during the decompression of high pressure CO2 pipelines

by

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A1. The thermodynamic model

Assuming isentropic decompression from the initial state with entropy $s_o = s(p_o, T_o)$ to an equilibrium solid-vapour mixture at the triple point, the entropy can be expressed as:

$$s_o = s_v (1 - y_s) + s_s y_s \tag{A1}$$

This equation can be rearranged in terms of the mass fraction of the solid phase, y_s:

$$y_s = \frac{s_v - s_o}{s_v - s_s} \tag{A2}$$

Knowing y_s, the density of the vapour-solid mixture at the triple point, ρ, can be calculated using equation (6), and the corresponding volume fraction of solid phase can be determined:

$$\alpha_s = y_s \frac{\rho}{\rho_s} \tag{A3}$$

Then the mass of the solid-vapour mixture, M, and the mass of solid phase, M_s, within the pipe can be evaluated:

$$M = \rho V \tag{A4}$$

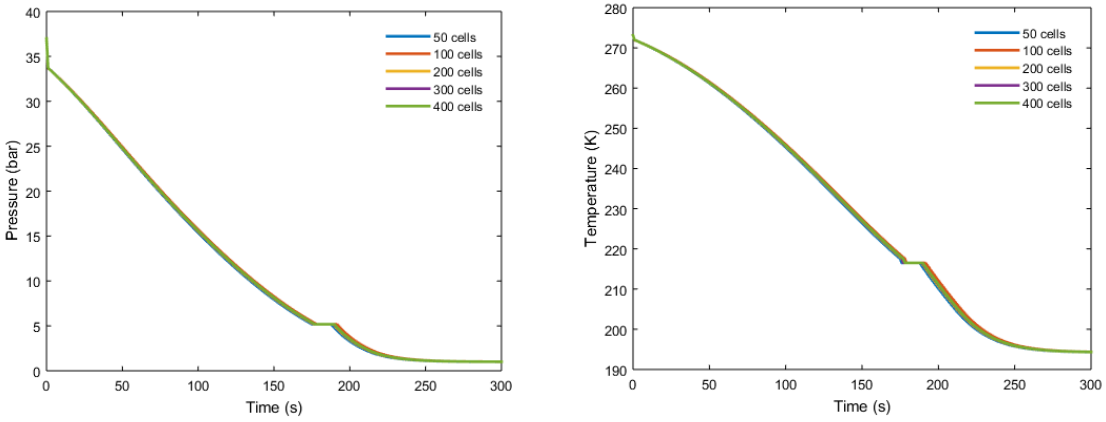
$$M_s = y_s M \tag{A5}$$

where V is the pipe volume.

A2. Convergence study

Figure A1 shows the results of calculation of pressure and temperature variation with time as predicted for conditions of Test 1 (Table 1) using 50, 100, 200, 300 and 400 computational cells. It can be seen that the results obtained using the 200, 300 and 400 cells are practically indistinguishable from each other, while using smaller number of cells result is marginal loss of accuracy at late stage of decompression after passing the triple point plateaux.

To illustrate the impact of discretisation level on the results, the pressure predicted at 50s in Test 1 (Table 1) is plotted as a function of the number of discretisation cells. The results in Figure A2 show that using more than 200 cells does not improve the accuracy of the results. On this basis the number of cells is set 200 cells in simulations of decompression tests in the present study.



(a) (b)

Figure A1. The histories of pressure (a) and temperature (b) variation at the second measurement point (Figure 2) in Test 1, predicted using 50, 100, 200, 300 and 400 computational cells.

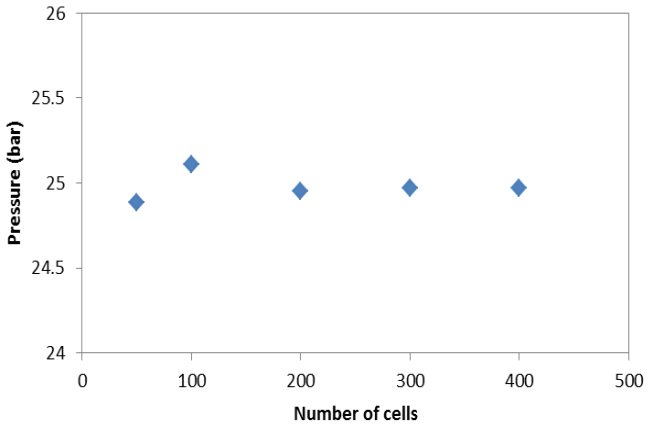


Figure A2. The impact of the number of cells on the pressure computed at the second measurement point (Figure 2) in Test 1 at 50 s.