Depressurization of CO₂ – a numerical benchmark study

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Abstract

A numerical benchmark study has been performed, comparing results from the OLGA pipeline simulator to data obtained using the multi-stage (MUSTA) centred scheme. The case considered is a depressurization of a pipeline. Care was taken to compare the same flow model and thermodynamic equation of state. The two methods appear to converge on fine grids, but on coarse grids, the MUSTA method is more accurate.

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1. Introduction

In CO₂ transport, the development of safe procedures for e.g. injection into reservoirs, first fill and depressurization of pipelines is an important issue. Pipeline integrity analyses are also gaining interest [1,3]. A depressurization will normally lead to phase transition, which could cause a strong cooling of the pipeline material. Due to the thermophysical properties, this effect is thought to be more pronounced for CO₂ than for e.g. natural gas. This motivates the study of single- and two-phase flow models for the flow of CO₂ in a pipeline. Furthermore, since the temperature is a function of pressure, there is a need for numerical methods that are able to capture pressure waves in a robust and accurate manner.

For two-phase flow, such numerical methods are not an off-the-shelf commodity. Munkejord et al. [7] discussed a drift-flux model for multi-component two-phase flows. The multi-stage (MUSTA) centred scheme by Toro and coworkers [9,10] was chosen as numerical method, based on its good robustness and accuracy properties, as well as its independence of the thermodynamic equation of state. The purpose of the present study is to compare the MUSTA method to the solution scheme of commercially available engineering tools.

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As a pipeline simulation tool we have chosen OLGA, version 5.3.2. OLGA is a multiphase thermo-hydraulic simulation tool originally developed by IFE and later improved and further developed by SPT Group. Our choice of OLGA was based upon availability, as well as the long track record within the industry as the chosen tool for simulating transient multiphase pipeline transport. The OLGA version used in this study is based upon a modified two-fluid model, i.e., separate continuity equations for the gas, liquid bulk and liquid droplets are applied [2]. These may be coupled through interfacial mass transfer.

We believe that the ability of a CO₂ pipeline simulation tool to predict pressure waves will be important for developing safe procedures for injection into reservoirs, first fill and depressurization of CO₂ pipelines. For applications requiring high resolution, such as the simulation of water-hammer effects and valve handling, it will be crucial that the chosen fluid model and numerical scheme is able to capture the essential dynamics.

The rest of this paper is organized as follows. The considered flow model and thermodynamic equation of state is briefly described in Section 2, while Section 3 presents our numerical simulations. Section 4 concludes the paper.

2. Model overview

When comparing different numerical models or tools, it is important to be able to distinguish between any differences arising from different mathematical models and those due to different numerical methods. Failing to do so will hamper the development of both the models and the numerical methods. Therefore, when the purpose is to compare different numerical schemes, the implemented models should ideally be identical. However, for the time being, we do not have an implementation of the MUSTA method for the two-fluid model found in OLGA. At the same time, there is no drift-flux model available in OLGA. On the other hand, we know that by limiting the pressure to the single-phase region, the drift-flux model will reduce to the Euler equations of single-phase flow. Without having access to the exact details of the OLGA model, we assume that a similar thing will happen there. Hence in this work, we will study the following model for single-phase one-dimensional compressible flow:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} &= 0, \\
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial p}{\partial x} &= \frac{4}{3} \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) - F_w, \\
\frac{\partial E}{\partial t} + \frac{\partial [(E+p)u]}{\partial x} &= \frac{4}{3} \frac{\partial}{\partial x} \left( \mu u \frac{\partial u}{\partial x} \right) - u F_w.
\end{align*}
\]

Herein, \(\rho\) is the density, \(u\) is the velocity, \(p\) is the pressure and \(\mu\) is the dynamic viscosity. \(E = \rho(e + 1/2u^2)\) is the total energy and \(e\) is the specific internal energy. \(F_w\) is the wall friction,

\[
F_w = \frac{f(Re,e)}{d} \frac{1}{2} \rho u^2,
\]

where \(f(Re,e)\) is the Darcy friction factor being a function of the Reynolds number, \(Re\), and the relative pipe roughness, \(e\). In the following calculations, the Colebrook-White formula will be used.

In the equation system (1), a thermodynamic equation of state (EOS) is required. Since this work is a benchmark study, we have opted at using an EOS as simple as possible. Hence the stiffened-gas equation of state [4,5] was employed. Herein, the pressure law is

\[
p(\rho, e) = (\gamma - 1) \rho e - \gamma p_w.
\]

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \\
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial p}{\partial x} = \frac{4}{3} \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) - F_w, \\
\frac{\partial E}{\partial t} + \frac{\partial [(E+p)u]}{\partial x} = \frac{4}{3} \frac{\partial}{\partial x} \left( \mu u \frac{\partial u}{\partial x} \right) - u F_w.
\]

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\[
p(\rho, e) = (\gamma - 1) \rho e - \gamma p_w.
\]
and the temperature law is
\[ T(\rho, e) = \frac{1}{c_v} \left( e - \frac{p_\infty}{\rho} \right), \]
where the specific-heat ratio \( \gamma = \frac{c_p}{c_v} \), the specific heat at constant pressure, \( c_p \), and the reference pressure, \( p_\infty \), are model constants. The stiffened-gas model can be seen as a linearization about a given state. With \( p_\infty = 0 \), the ideal-gas law is recovered.

3. Numerical simulations

We consider the following benchmark case: A pipe of length 1000 m and inner diameter \( d = 0.3 \) m is filled with initially motionless \( \text{CO}_2 \), with a pressure of \( p = 20 \) MPa and a temperature of \( T = 300 \) K. The pipe is closed at the left-hand side. At time \( t = 0 \) s, the pressure at the right-hand side is decreased to 10 MPa, and then set back to 20 MPa at \( t = 1 \) s. A rarefaction wave followed by a shock wave will propagate to the left.

The EOS parameters are given in Table 1. They have been set using data from [8] at \( p = 15 \) MPa and \( T = 300 \) K. The stiffened-gas equation of state is not implemented in OLGA. We have therefore supplied the thermodynamic variables in the form of a fluid table. Further, a constant dynamic viscosity of \( \mu = 8.4 \times 10^{-5} \) Pa s has been employed, and the relative pipe roughness was \( \varepsilon = 1.67 \times 10^{-4} \).

Table 1. Equation-of-state parameters

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol (unit)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific-heat ratio</td>
<td>( \gamma ) (–) 1.4</td>
</tr>
<tr>
<td>Spec. heat at const. pres.</td>
<td>( c_p ) (J/(kg K)) 2400</td>
</tr>
<tr>
<td>Reference pressure</td>
<td>( p_\infty ) (Pa) 1.5 \times 10^8</td>
</tr>
</tbody>
</table>

The MUSTA method is a first-order multi-stage centred scheme aimed at approaching the accuracy of upwind schemes while retaining the simplicity of centred schemes [10]. The calculations performed using the MUSTA method have been run with a Courant–Friedrichs–Lewy (CFL) number of 0.9, employing the two-stage MUSTA scheme with two local cells. Increased resolution can be obtained by increasing the number of stages and cells, and by employing the MUSCL method to obtain second-order accuracy for smooth solutions. These issues are described and discussed by Munkejord et al. [6]. In particular, for two-phase flow models, a high number of stages is required before the accuracy of MUSTA can be compared to that of e.g. the Roe scheme.

In the following, where noted, some reference solutions have been obtained using the MUSCL-MUSTA scheme using a CFL number of 0.5.

We do not have access to the details of the OLGA model and the numerical implementation of the model. However, OLGA is known to utilize a semi-implicit integration scheme. This allows for taking long time steps suitable for simulating rather slow mass transients and providing efficient run times for long transport lines. However, limiting the time integration step based upon the mass transport will not allow us to capture the essential dynamics of the pressure waves investigated in the present study. Therefore, we have enabled a CFL criterion including the speed of sound, similar to that of the MUSTA method, using a CFL number of 0.9.
3.1. Effect of sub-models

We will start by investigating the effect of the terms on the right-hand side of the governing equations (1). The first term on the right-hand side of the second and third equations represents the \( x \) component of the viscous stress tensor. The rest of the viscous stress tensor is modelled by the wall-friction term. Since we are interested in the model in itself, the high-resolution MUSCL-MUSTA scheme was employed with a fine grid of 5000 cells. Pressure profiles calculated at time \( t = 1.51 \) s are displayed in Figure 1.

![Figure 1: Depressurization case, effect of sub-models. MUSCL-MUSTA method on a 5000-cell grid. Pressure versus position at \( t = 1.51 \) s.](image)

In the figure, “no source” denotes a right-hand side of 0 in the governing equations (1). The data labelled “viscous” are calculated with the viscous term, but with zero wall friction. “Friction” means that the wall-friction term has been included. It can be seen from the figure that in this case, the \( x \) component of the viscous stress tensor has nothing to say. Wall friction, on the other hand, has a clear effect on the pressure drop, as expected. It can be noted, though, that wall friction causes practically no smearing of the rarefaction and the shock wave. The results presented in the following are obtained using the wall-friction model.
3.2. Effect of second-order extension

The first-order MUSTA method and the high-resolution MUSCL-MUSTA method are compared in Figure 2 using a grid of 100 cells. Data obtained using the first-order MUSTA method with a fine grid of 10000 cells are plotted as reference. The figure indicates a clear improvement in resolution by employing the MUSCL-MUSTA method compared to the first-order MUSTA method.

![Graph showing the effect of second-order extension](image)

Figure 2: Depressurization case, effect of second-order extension (MUSCL). First-order MUSTA method and MUSCL-MUSTA are compared using a grid of 100 cells, whereas data from the first-order MUSTA on a 10000-cell grid is used as reference. Pressure versus position at $t = 1.51$ s.
3.3. Comparison between OLGA and MUSTA

Figure 3 and Figure 4 display pressure profiles as a function of position and of time, respectively, comparing results obtained using the MUSTA method and with OLGA. As can be seen, the two methods give similar results, and the calculated wave-propagation speed agrees well. However, compared to the OLGA results, the MUSTA method produces a sharper wave resolution. Indeed, the results of the two methods appear to converge, but even for a fine grid of 10000 cells, there is a visible difference. This is also an indication of what would happen in the two-phase region. If pressure waves are smeared out, an underestimation of both the water hammer effect and the pipe cooling could be a result.

The wave-propagation speeds can be read off Figure 3. Both the ‘centre’ of the rarefaction wave and the shock wave have a speed of about 530 m/s. This agrees well with the speed of sound of 533 m/s at $T = 300$ K and $p = 16$ MPa [8].

Figure 3: Comparison of OLGA and the MUSTA method, depressurization case. Pressure versus position at $t = 1.51$ s.
Since, in the above calculations, the results have been obtained using the same kind of “compressible” time-step restriction, and a first-order time-integration scheme, the differences are thought to be mainly a function of the spatial discretization. There is possibly also a connection with the way the semi-implicit time-integration method is implemented in OLGA, and it is expected that this will influence the results providing less accurate prediction of the pressure waves, especially for low resolution grids. This means that to obtain a given accuracy, a finer grid, and hence longer CPU times, would be required.

4. Conclusions

A benchmark case for depressurization of a CO$_2$ pipeline in the single-phase region has been proposed. Numerical results from the OLGA code have been compared to calculations using the multi-stage (MUSTA) centred scheme. In particular, the stiffened-gas equation of state was employed in both cases. The two methods appear to converge on fine grids, but on coarse grids, the method in OLGA produced more smeared-out results.

We believe that the ability of a CO$_2$ pipeline simulation tool to predict pressure waves will be important for developing safe procedures for injection into reservoirs, first fill and depressurization of CO$_2$ pipelines. For applications requiring high resolution, such as the simulation of water-hammer effects and valve handling, it will be crucial that the chosen fluid model and numerical scheme is able to capture the essential dynamics.

Future work will include a benchmark case accounting for phase transition.
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