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A method for simulating two-phase pipe flow with real equations of state

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ABSTRACT

Common two-fluid models for pipe flow assume local non-equilibrium regarding phase transfer. To solve the two-fluid models together with accurate equations of state for real fluids will in most cases require mechanical, thermal and chemical equilibrium between the phases. The reason is that reference equations of state for real substances typically describe full thermodynamic equilibrium. In this paper, we present a method for numerically solving an equilibrium model analysed by Morin and Flåtten in the paper *A two-fluid four-equation model with instantaneous thermodynamical equilibrium*, 2013.

The four-equation two-fluid model with instantaneous thermodynamical equilibrium is derived from a five-equation two-fluid model with instantaneous thermal equilibrium. The four-equation model has one mass equation common for both phases, but allows for separate phasic velocities. For comparison, the five-equation two-fluid model is numerically solved, using source terms to impose thermodynamical equilibrium. These source terms are solved using a fractional-step method.

We employ the highly accurate Span–Wagner equation of state for CO_2, and use the simple and robust FORCE scheme with MUSCL slope limiting. We demonstrate that second-order accuracy may be achieved for smooth solutions, whereas the first-order version of the scheme even allows for a robust transition to single-phase flow, also in the presence of instantaneous phase equilibrium.

1. Introduction

In the frame of CO_2 capture and storage (CCS), large amounts of CO_2 have to be transported between the point of capture and the point of injection. In the two-degree scenario of the International Energy Agency [1], about seven gigatonnes of CO_2 emissions will be contained using CCS in 2050. This requires the development of an extensive CO_2 transport network. For large volumes of CO_2, pipeline transport is an option.

There are challenges related to the operation of a CO_2 pipeline, both in normal operation and during depressurisation events, either planned or accidental. The safety of operation has to be ensured, and it has to be demonstrated to the regulatory bodies. To facilitate this, and to reduce costly experimental procedures, reliable and accurate numerical simulation tools have to be developed.

In pipelines, the CO_2 will generally be transported in a dense phase, supercritical or liquid. However, during transient events, gas or solid phases may appear. In addition, impurities from the capture process will be present in the CO_2. These impurities may be for example water, residual chemicals or gases from combustion. They will impact the thermodynamic behaviour of the CO_2, for example the mixture density or the temperature of the mixture during phase change.

It is common to use the stiffened-gas equations of state, when modelling two-phase flow [2–5]. It has a simple analytical form, and can be used to describe meta-stable fluids. For long pipelines transporting CO_2 rich multi-component mixtures from a capture cite to an offshore injection well, these models might not predict the fluid properties accurately. In this case it is important to use real equations of state. The real equations of state are generally only valid for full thermodynamical equilibrium.

At least two types of transient events have to be studied, with very different characteristics. The first type covers the fast depressurisation events that occur when the pipe content is discharged to the atmosphere, either due to shutting down the pipeline, or due to a fracture [6]. The second type covers the load variations in the pipeline in normal operation, due to the capture processes delivering varying amounts of CO_2. These load variations will have time scales in the order of several hours.

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The kinetics of heat transfer between the phases, and of phase change can most probably not be neglected in fast transients related to fast depressurisation events. However, during slow transients related to load variation, one is interested in predicting the response of the mixture in the pipeline, to avoid too low temperatures or phase change through pumps for example. During these slow transients, the most important is to have a very accurate equation of state to describe CO_2-rich mixtures, rather than to describe the kinetics of internal heat transfer or phase change very accurately. The time scales of these processes are negligible compared to the time scale of the relatively slow load variation. Very accurate equations of state can be obtained for mixtures at equilibrium. Thus it seems to be reasonable to use a full-equilibrium fluid-dynamical model in this case, to be able to benefit from the equilibrium equations of state.

Therefore, in the present work, we study full equilibrium fluid-dynamical models where phase change and heat transfer between the phases are assumed to be instantaneous. The framework supports any equation of state, thus impurities may be added by using an equation of state for mixtures. Here we are using a very accurate equation of state for pure CO_2 [7]. We compare two approaches. The first one is based on a fluid-dynamical model out of chemical equilibrium, the two-fluid five-equation model with phase change [8]. Instantaneous phase change is achieved by performing flash calculations between each time step, such that the mixture returns to chemical equilibrium. The second one is based on a full-equilibrium two-fluid four-equation model presented in [9].

Numerical results are presented to show the performance of the methods, and to compare them to each other. The models have been solved using the finite-volume method with the FORCE flux [10, Sec. 14.5.1] and the second-order extension MUSCL [11]. They show that the four-equation based approach performs better in terms of computational time than the five-equation based approach. It also shows that we can achieve second-order convergence rate in smooth regions, and that the method satisfactorily handles the transition to single-phase flow.

In Section 2, the five-equation model is presented, as well as the procedure to ensure chemical equilibrium between the phases. Then, the four-equation model is presented in Section 3. In Section 4, the equation of state as well as the procedure to evaluate the new state of the fluid are explained. The characteristic wave-structure of the models are presented in Section 5. Subsequently, the numerical methods employed to solve the transport systems are described in Section 6. Finally, Section 7 shows the results of the numerical test cases, and Section 8 summarise this work.

2. The five-equation model with phase change

The one-dimensional two-fluid models describe one-dimensional two-phase flows in pipes. In the six-equation model, the phases are at mechanical equilibrium [8]. This means that the two phases are at the same pressure at all times. The model is well known in the literature [12,13,4,14,15], and used in commercial simulation tools like CATHARE [16] or RELAP5 [17].

The five-equation model [8] is derived from the six-equation model by assuming instantaneous thermal equilibrium. This means that the phases are now at the same pressure and temperature at all times. This model contains one mass and one momentum equation for each phase, while only one mixture energy equation is present. This model is similar to the model used by the commercial flow simulation tool OLGA [18]. When viscous terms are neglected, and all external forces but gravity are ignored, the system of equations for the one-dimensional five-equation model becomes

$$\frac{\partial(\rho_g\alpha_g)}{\partial t}+\frac{\partial(\rho_g\alpha_g v_g)}{\partial x}=\Psi, \tag{1}$$

$$\frac{\partial(\rho_\ell\alpha_\ell)}{\partial t}+\frac{\partial(\rho_\ell\alpha_\ell v_\ell)}{\partial x}=-\Psi, \tag{2}$$

$$\frac{\partial(\rho_g\alpha_g v_g)}{\partial t}+\frac{\partial(\rho_g\alpha_g v_g^2)}{\partial x}+\alpha_g\frac{\partial p}{\partial x}+\tau_i=v_i\Psi+\rho_g\alpha_g g_x, \tag{3}$$

$$\frac{\partial(\rho_\ell\alpha_\ell v_\ell)}{\partial t}+\frac{\partial(\rho_\ell\alpha_\ell v_\ell^2)}{\partial x}+\alpha_\ell\frac{\partial p}{\partial x}-\tau_i=-v_i\Psi+\rho_\ell\alpha_\ell g_x, \tag{4}$$

$$\frac{\partial(E_g+E_\ell)}{\partial t}+\frac{\partial(E_g v_g+\alpha_g v_g p)}{\partial x}+\frac{\partial(E_\ell v_\ell+\alpha_\ell v_\ell p)}{\partial x} = g_x\alpha_g\rho_g v_g+g_x\alpha_\ell\rho_\ell v_\ell, \tag{5}$$

where the total energy E_k of phase $k \in \{g,\ell\}$ is the sum of kinetic and internal energy,

$$E_k=\rho_k\alpha_k\left(\frac{1}{2}v_k^2+e_k\right). \tag{6}$$

e is the specific internal energy.

Further, ρ is the mass density, v is the velocity, p is the pressure, α is the volume fraction, and g_x is the gravitational component along the x-axis. Ψ is the mass-transfer rate from the liquid to the gas phase, τ_i is the interfacial momentum exchange and v_i is the interfacial momentum velocity. The volume fractions must satisfy

$$\alpha_g+\alpha_\ell=1. \tag{7}$$

The interfacial momentum exchange is modelled with a differential term. In this term, the factor Δp represents the difference between the average bulk pressure and the pressure at the gas–liquid interface. In this work we use

$$\tau_i=-\Delta p\frac{\partial\alpha_\ell}{\partial x}. \tag{8}$$

For practical simulations, Δp should be physically modelled to account, for example, for the hydrostatic pressure in the liquid phase, or for the interfacial tension. However, for the purpose of the general model analysis performed in the present article, Δp is here chosen to be [19,8]

$$\Delta p=\delta\frac{\alpha_g\alpha_\ell\rho_g\rho_\ell}{\alpha_\ell\rho_g+\alpha_g\rho_\ell}(v_g-v_\ell)^2, \tag{9}$$

where $\delta=2$.

The unknowns of the system (1)–(5) are $\alpha_g, \alpha_\ell, v_g, v_\ell, p, \rho_g, \rho_\ell, e_g$ and e_ℓ. However, since we will be using the equation of state to solve the system, the temperature T must be included in the list. We have thus 10 unknowns. The 10 equations are (7), the transport Eqs. (1)–(5), plus two thermodynamic relations per phase given by the equation of state.

We may split the system (1)–(5) into two parts, which will prove useful in the course of the article. The first part is the flow model (1)–(5) where phase change is ignored ($\Psi=0$), while the second part only contains the contributions of phase change

$$\frac{\partial(\rho_g\alpha_g)}{\partial t}=\Psi, \tag{10}$$

$$\frac{\partial(\rho_\ell\alpha_\ell)}{\partial t}=-\Psi, \tag{11}$$

$$\frac{\partial(\rho_g\alpha_g v_g)}{\partial t}=v_i\Psi, \tag{12}$$

$$\frac{\partial(\rho_\ell\alpha_\ell v_\ell)}{\partial t}=-v_i\Psi. \tag{13}$$

The energy equation has disappeared in the second system, because mixture energy is not concerned by phase change, it is only an internal transfer.