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Recommendations on models and modelling tools for CO_2 transport

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SUMMARY:

In order to predict the behaviour of CO_2 mixtures during pipeline transport, proper mathematical models and simulation tools are needed. This report gives an overview over existing models and tools, and their applicability to CO_2 pipeline transport. For each topic, a recommendation is given on what models and tools are best suited, or which further research is needed. A wide range of possible mathematical models for two-phase flow is presented, along with the relations necessary to close the model. This includes equations of state, and models for viscosity, friction, flow patterns, heat and mass transfer. Especially for equations of state, flow patterns and friction models, it is concluded that more experimental data for CO_2 mixtures is needed. Full-scale tests of running fractures are also recommended. Available simulation tools for pipeline flow are also presented, and their applicability to CO_2 pipeline flow is discussed. At the time of writing none of the commercially available tools seem fully capable of simulating flow of CO_2 with impurities.

KEYWORDS: Fluid dynamics, thermodynamics, CO_2 pipeline transport.

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1 Introduction

To properly predict the behaviour of CO_2 mixtures in pipeline flow, accurate and reliable mathematical models are necessary. Multiphase flow modelling has been an active field of research for the last five decades [19, 20, 30, 64]. This research has been driven particularly by two industry sectors: The nuclear industry, and the oil and gas industry. In the nuclear industry, two-phase flow of cooling fluid is a crucial part of a power plant. For this reason, the RELAP code was developed by the US Nuclear Regulatory Commission to simulate transients and accidents in water-cooled reactors [4]. In the oil and gas industry, three-phase flow of oil, gas and water in pipelines has been of particular interest. The development of models and simulation tools, such as the OLGA simulation tool [10], has played an important role in enabling such flows.

Carbon dioxide has a number of properties that makes it significantly different from oil, gas and water handled by the models mentioned above. Most notably, its critical point (73.8 bar at 31.1 °C) and triple point (5.18 bar at −56.6 °C) differ from those of gas and water. This means that CO_2 would be transported in a dense liquid state, whereas natural gas is transported in a dense gaseous state. Moreover, CO_2 captured from industry or power plants will not be pure, but will contain various impurities such as nitrogen, oxygen, water and methane. The presence of such impurities may significantly alter the thermodynamic and transport properties of the fluid. Developing good models for CO_2 with impurities is a challenging task and relies on good experimental data, and existing models still do not have adequate accuracy for all mixtures.

Under normal pipeline operation, the carbon dioxide mixture will be in a dense (single-phase) liquid-like state, which is the most energy-efficient transport mode. For such conditions, existing models for single-phase flow are expected to be adequate. However, if two-phase flow occurs, the flow behaviour is much more complex, and a number of modelling challenges arise. Two-phase flow may occur if the output from the CO_2 capture plant fluctuates over time, or during transient operations like the start-up and shutdown of a pipeline.

The distinction between a *model* and a *simulation tool* is an important one. The term *model* usually refers to a mathematical equation or expression for a certain phenomenon. A computer implementation that solves such models numerically is termed a *simulation tool*. An accurate model is not enough to describe the flow; its implementation must also be correct in order to give reliable results. In this report, we will present an overview over existing models and simulation tools for CO_2 pipeline flow. For each topic, we give a recommendation on which models or tools are best suited, based on our current experience and knowledge. For some topics, the recommendation is rather that more research is needed. The aim is not to include all models in their completeness, but rather to refer the reader to relevant literature.

The recommendations are to a large extent based on previous work in NORDICCS WP5, as well as our current experience with models and simulation tools for CO_2 pipeline flow in general. The main results of the work in NORDICCS WP5 are summed up in the next section.

1.1 NORDICCS Task 5.2

At the beginning of the NORDICCS project, a literature study [8] was performed, with focus on models and simulation tools for pipeline transport of CO_2 mixtures. This gave an updated knowledge of the current research and identified what further research was needed. The study

highlighted running ductile fractures as an important area of research, since such fractures present one of the main risks of CO_2 pipeline transport. These fractures propagate due to the high pressure inside the pipe, so accurate prediction of the speed of pressure waves, i.e. the speed of sound, is necessary. The speed of sound will depend on the flow topology and the model assumptions made on equilibrium in pressure, temperature, velocity and chemical potential. Experimental data for the speed of sound in CO_2 mixtures would therefore be useful to validate the modelling assumptions made.

The literature study also points out the need for accurate, robust and efficient thermodynamic models for CO_2 mixtures. Small amounts of impurities can be challenging to handle due to small phase envelopes, and needs special care. Since CO_2 has a high triple point (5.18 bar), the models also need to include dry ice. Finally, it is concluded that existing commercial simulation tools are mainly suited for oil–gas–water flow, and are not directly applicable to flow of CO_2 with impurities.

In normal operation of a pipeline, single-phase flow will be the most energy efficient transport mode. However, the flow may intermittently enter the two-phase region due to varying flow rate and temperature. This could cause unstable flow regimes (such as slug flow) and be detrimental to compressors and pumps. In NORDICCS report D5.2.1301 [49], it was investigated how the presence of certain impurities influences the occurrence of two-phase flow. It was found that some impurities indeed have an effect on whether two-phase flow occurs or not. Moreover, whether the pipe is buried or not also has a significant effect.

NORDICCS report D5.2.1302 [7] investigated the impact of certain volatile impurities (N_2, CH_4, O_2) on the lowest temperature reached during depressurization through a valve. These impurities did not have any negative effect on the temperature reached. However, it was demonstrated that the valve area has a very significant effect: Larger area leads to a larger temperature drop. This temperature drop is important to predict to allow pipeline operators to stay within the temperature tolerance limits of the pipeline, valves and other equipment.

In 2013, a researcher from SINTEF Energy Research visited Gassco to run the commercial simulator OLGA for some test cases relevant for CO_2 transport. The results were then compared with an in-house code at SINTEF Energy Research and presented in D5.2.1304 [51]. Good agreement was found for depressurization of a horizontal pipe, but for a pipeline with a basin profile, the results differed. One of the main causes for this discrepancy was the low-order numerical method used by the SINTEF code. For this reason, a higher-order numerical method was implemented [52]. This improved the accuracy of the results significantly, and better correspondence between the results from the two codes was found.

2 Averaged 1D models for pipeline flow

The complexity of multiphase pipeline flow makes it computationally intractable to describe it using three-dimensional models for most cases. For this reason, the majority of models and simulation tools for multiphase pipeline flow are one-dimensional. These models may be obtained by *averaging* a three-dimensional formulation over space and time (see e.g. Drew and Passman [19]). To represent the complex interaction between the two phases in a one-dimensional model,

closure relations are necessary. These relations can represent friction, heat transfer and mass transfer between the phases, and will be described in more detail in section 3.

In this section, we present the averaged one-dimensional models most relevant for multiphase pipeline flow. In general, they can be divided in two groups: two-fluid models and drift-flux models. They differ in the way they handle velocity differences between phases. We will consider models for two-phase (liquid–gas) flow, but the principles behind them can also be extended to flow with three phases (or more).

2.1 Two-fluid models

Two-fluid models allow the two phases to have independent velocities. The velocities are nevertheless coupled through friction between the phases described by a friction correlation. The Baer–Nunziato model [9] serves as a basis for many other two-fluid models. It consist of seven equations describing conservation of mass, momentum and energy for each phase, and advection of the volume fraction. The volume fraction, α_k, is defined as the fraction of the total volume that is occupied by phase k.

The seven equations of the model can be expressed as follows [9, 42, 62]:

- Volume advection:

$$\frac{\partial \alpha_\mathrm{g}}{\partial t} + v_\mathrm{i}\frac{\partial \alpha_\mathrm{g}}{\partial x} = \mathscr{P}(p_\mathrm{g} - p_\ell). \tag{1}$$

- Conservation of mass:

$$\frac{\partial \alpha_\mathrm{g}\rho_\mathrm{g}}{\partial t} + \frac{\partial \alpha_\mathrm{g}\rho_\mathrm{g}v_\mathrm{g}}{\partial x} = \mathscr{M}(\mu_\ell - \mu_\mathrm{g}), \tag{2}$$

$$\frac{\partial \alpha_\ell\rho_\ell}{\partial t} + \frac{\partial \alpha_\ell\rho_\ell v_\ell}{\partial x} = \mathscr{M}(\mu_\mathrm{g} - \mu_\ell). \tag{3}$$

- Conservation of momentum:

$$\frac{\partial \alpha_\mathrm{g}\rho_\mathrm{g}v_\mathrm{g}}{\partial t} + \frac{\partial (\alpha_\mathrm{g}\rho_\mathrm{g}v_\mathrm{g}^2 + \alpha_\mathrm{g}p_\mathrm{g})}{\partial x} - p_\mathrm{i}\frac{\partial \alpha_\mathrm{g}}{\partial x} = v_\mathrm{i}\mathscr{M}(\mu_\ell - \mu_\mathrm{g}) + \mathscr{V}(v_\ell - v_\mathrm{g}) + f_{b,\mathrm{g}} + f_{f,\mathrm{g}}, \tag{4}$$

$$\frac{\partial \alpha_\ell\rho_\ell v_\ell}{\partial t} + \frac{\partial (\alpha_\ell\rho_\ell v_\ell^2 + \alpha_\ell p_\ell)}{\partial x} - p_\mathrm{i}\frac{\partial \alpha_\ell}{\partial x} = v_\mathrm{i}\mathscr{M}(\mu_\mathrm{g} - \mu_\ell) + \mathscr{V}(v_\mathrm{g} - v_\ell) + f_{b,\ell} + f_{f,\ell}. \tag{5}$$

- Conservation of energy:

$$\begin{aligned}\frac{\partial E_\mathrm{g}}{\partial t} + \frac{\partial \left(E_\mathrm{g}v_\mathrm{g} + \alpha_\mathrm{g}v_\mathrm{g}p_\mathrm{g}\right)}{\partial x} - p_\mathrm{i}v_\mathrm{i}\frac{\partial \alpha_\mathrm{g}}{\partial x} &= -p_\mathrm{i}\mathscr{P}(p_\mathrm{g} - p_\ell) \\ &\quad + \left(\mu_\mathrm{i} + \frac{1}{2}v_\mathrm{i}^2\right)\mathscr{M}(\mu_\ell - \mu_\mathrm{g}) \\ &\quad + v_\mathrm{i}\mathscr{V}(v_\ell - v_\mathrm{g}) + \mathscr{T}(T_\ell - T_\mathrm{g}) + f_{b,\mathrm{g}}v_\mathrm{g} + Q_{\mathrm{w,g}},\end{aligned} \tag{6}$$

$$\frac{\partial E_\ell}{\partial t} + \frac{\partial \left(E_\ell v_\ell + \alpha_\ell v_\ell p_\ell\right)}{\partial x} - p_\mathrm{i} v_\mathrm{i} \frac{\partial \alpha_\ell}{\partial x} = -p_\mathrm{i} \mathscr{P}(p_\ell - p_\mathrm{g}) + \left(\mu_\mathrm{i} + \frac{1}{2} v_\mathrm{i}^2\right) \mathscr{M}(\mu_\mathrm{g} - \mu_\ell) + v_\mathrm{i} \mathscr{V}(v_\mathrm{g} - v_\ell) + \mathscr{T}(T_\mathrm{g} - T_\ell) + f_{b,\ell} v_\ell + Q_{\mathrm{w},\ell}. \tag{7}$$

Here subscripts g and ℓ denote gas and liquid, respectively. The pressure, temperature, density, velocity, chemical potential of phase k are denoted p_k, T_k, ρ_k, v_k and μ_k, respectively. The total energy density is $E_k = \alpha_k \rho_k (e_k + \frac{1}{2} v_k^2)$, where e_k is the internal energy. Body forces (such as gravity) and friction from the pipe wall are denoted $f_{b,k}$ and $f_{f,k}$, respectively, whereas heat transferred from the wall to the fluid is denoted $Q_{\mathrm{w},k}$. The interfacial velocity v_i, pressure p_i and chemical potential μ_i need to be modelled in such a way that the model is well-posed, i.e. that is has a well-defined solution. Similar equations for a solid phase could also be added to the model if necessary.

The right-hand sides of eqs. (1)–(7) contain a number of terms that describe transfer of volume, mass, heat and momentum between the two phases, formulated as relaxation processes. These processes drive the system towards equilibrium where the pressures, temperatures, velocities and chemical potentials of the two phases are equal. The factors $\mathscr{P}$, $\mathscr{M}$, $\mathscr{V}$ and $\mathscr{T}$ determine the rates of these processes. By assuming that one or more of these relaxation processes are instantaneous, i.e. that $\mathscr{P}$,$\mathscr{M}$,$\mathscr{V}$, and/or $\mathscr{T} \to \infty$, one can derive new models in which one or more of p, T, μ and v are always equal (i.e. in equilibrium) in the two phases.

Zein et al. [77] indicate that the pressure relaxation process is much faster than that of temperature, which in turn is much faster than that of chemical potential. This can justify a model where one assumes that pressure relaxation is instantaneous, i.e. $\mathscr{P} \to \infty$, and possibly also for temperature relaxation ($\mathscr{T} \to \infty$).

The hierarchy of models created by different combinations of equilibrium assumptions is illustrated as a four-dimensional hypercube in fig. 1 [42]. The basic seven-equation model is shown in red and forms the base of the hierarchy. The models shown in yellow have been analysed by Flåtten and Lund [22] and Lund [43]. The models described by Martínez Ferrer et al. [46] are shown in green, and the model presented by Morin and Flåtten [53] is shown in blue. The rightmost model is essentially the Euler equations (see e.g. White [75]) with an equilibrium two-phase equation of state. This model is also often referred to as the homogeneous equilibrium model (HEM).

The models with equal phase velocities (yellow nodes in fig. 1) are usually not referred to as two-fluid models, but can rather be seen as special cases of drift-flux models. Other similar combinations of conservation equations are used by commercial simulation tools, which will be discussed in more detail in section 5.

2.2 Drift-flux models

Drift-flux models are suitable for modelling flow patterns where the velocities of the two phases are tightly coupled, such as in bubbly flow. These models use an explicit relation between the two velocities known as a slip relation,

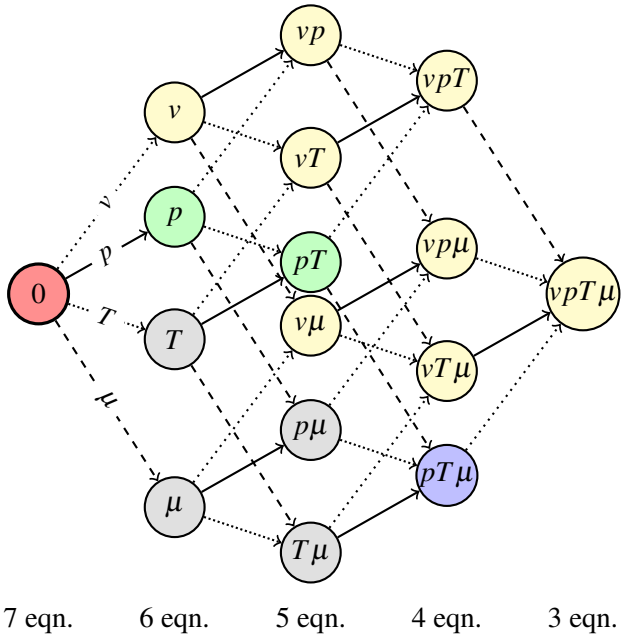

Figure 1: A hierarchy of models illustrated as a 4-dimensional hypercube. Each node represents a model, identified by the variables that are in equilibrium in that model. Each arrow represents a relaxation process. The coloured models have previously been studied by various authors, while the gray models are currently uninspected. From Linga [42].

$$v_g - v_\ell = \Phi(\alpha_g, p, T, v_g), \tag{8}$$

see e.g. Hibiki and Ishii [29], Ishii [31], Zuber and Findlay [78]. Such an explicit relation allows us to reduce the complexity of the model by having only one conservation equation for momentum instead of two. In other words, the two momentum equations (4) and (5) can be added to yield

$$\frac{\partial(\alpha_g\rho_g v_g + \alpha_\ell\rho_\ell v_\ell)}{\partial t} + \frac{\partial(\alpha_g\rho_g v_g^2 + \alpha_\ell\rho_\ell v_\ell^2 + \alpha_g p_g + \alpha_\ell p_\ell)}{\partial x} = f_{b,g} + f_{b,\ell}. \tag{9}$$

This equation, together with eqs. (1)–(3) and (6)–(7), can be seen as a basic model from which other drift-flux models can be derived.

As previously mentioned, the drift-flux model is intended to represent well-mixed flow patterns, such as bubbly flow. Hence it is only expected to give accurate results for such flow patterns. The RELAP code [59] is one of the industry standard codes for simulation of two-phase flow in the cooling system of nuclear reactors. It uses a drift-flux formulation only for bubbly flow and slug flow. Drift-flux models are also employed in the petroleum industry, such as TACITE [57] and RK-Kick [73].

An advantage of a drift-flux model in contrast to a two-fluid model is that there are fewer closure relations that need modelling. On the other hand, the assumption that the phase velocities can be expressed explicitly using a slip relation (8) will not always be reasonable. A further

advantage of the drift-flux model is the absence of non-conservative terms in the momentum equation, something which eases the development of consistent and robust numerical methods.

2.3 Recommendation

If one is to simulate two-phase flow in flow patterns other than bubbly flow and slug flow, a two-fluid model with independent phase velocities is expected to give the most accurate results. Two-fluid models can have many different formulations, depending on which assumptions are made regarding equilibrium in pressure, temperature and/or chemical potential. The fewer equilibrium assumptions are made, the more terms (for heat and mass transfer between the phases) need to be modelled explicitly, and the accuracy of the two-fluid model stands or falls by the accuracy of these closure relations. As mentioned earlier, an assumption of equal phase pressure can be reasonable [77]. Modelling of heat and mass transfer terms is discussed in section 3.

3 Closure relations

3.1 Equation of state

In order to relate thermodynamic variables such as pressure, temperature, density, energy and heat capacity to each other, an equation of state (EOS) is needed. For single-component CO_2, the Span-Wagner EOS [65] is considered the reference. This EOS is valid for temperatures from 200 K to 1100 K and for pressures up to 800 MPa, which is more than sufficient to describe CO_2 pipeline flow.

For mixtures of CO_2 and other components relevant for CCS, available experimental data is more scarce. Li et al. [40] argue that no equation of state shows any clear advantage over any other when it comes to suitability for CCS applications. Cubic equations of state have a simple structure and give reasonable results, but are inaccurate at pressures above the critical point [8, 76]. There exists many other equations of state, often with a trade-off between accuracy and computational cost. Simple equations of state often have large errors in density and speed of sound (20% or more) due to few adjustable parameters.

To account for the interaction between different components in a mixture, interaction parameters are needed [76]. Such parameters are available for cubic equations of state and several CO_2 mixtures [39], while they are lacking for many other equations [76]. Ruhr-Universität Bochum is developing an equation of state for combustion gases and combustion-gas-like mixtures (EOS-CG [24]) that aims for improved accuracy for CCS applications. EOS-CG is derived from the GERG-2008 [36] formulation, introducing new Helmholtz energy mixing rules for some of the impurities in CO_2 mixtures. EOS-CG is primarily tuned for CO_2 mixtures, while GERG-2008 primarily is developed and tuned for natural gas mixtures. Even still, GERG-2008, available through REFPROP [38] developed by the US National Institute of Standards and Technology (NIST), is also applicable to CO_2 mixtures.

EOS-CG and GERG-2008 are known to give good predictions for density and speed of sound, but are very expensive to evaluate compared to the simple cubic equations of state. As an intermediate solution, corresponding state models [76] can be used at a computational cost similar to

the cubic models, but with improved density and speed-of-sound predictions. For CO_2 mixtures containing H_2O, the Cubic Plus Association (CPA) [35] show promise.

As shown in NORDICCS reports by Morin [50, 51], the presence of impurities can significantly affect the temperature at which two-phase flow occurs in a pipeline. Two-phase flow should generally be avoided in pipelines if possible, so it is important to model the effect of impurities properly.

Most equations of state require a separate model for the solid phase of CO_2 (dry ice). The models by Jäger and Span [32] and Trusler [71, 72] can calculate these properties accurately. Other solid phases may occur as well at low temperatures. Hydrates, solid phases consisting of CO_2 and water, can be described using a model by Jäger et al. [33].

3.1.1 Recommendation

For pure CO_2, the Span-Wagner EOS is highly accurate and suitable for simulations, although with a higher computational cost than a cubic EOS. For CO_2 mixtures, one often has to make a compromise between accuracy and speed, since the most accurate equations of state are also computationally expensive. If only limited accuracy is needed, cubic equations of state are a reasonable option with low computational cost. For better accuracy, more advanced equations of state such as EOS-CG [24] can be used. For simulations, a slightly less accurate but significantly less expensive EOS like CPA may be a better choice. Interpolation (look-up) tables can also be used to drastically improve computational speed, if necessary. To limit the amount of memory necessary, interpolation tables often assume constant mixture composition, which is a reasonable assumption in many cases.

3.2 Viscosity model

For pure CO_2, viscosity models have been presented by Vesovic et al. [74] and Fenghour and Wakeman [21]. For CO_2 with impurities, there are accurate models for the viscosity of the gas phase [60]. For the liquid phase, however, very little experimental data is available [41], hence few models exist. Some experimental work to fill these gaps is ongoing [61, 67]. Viscosity can also be calculated using molecular simulations, see e.g. Lachet et al. [37].

3.2.1 Recommendation

The available data for viscosity in the liquid phase of CO_2 mixtures is scarce, so more experiments are necessary to develop better viscosity models [58]. Funds were allocated to construct a CO_2-mixture viscosity apparatus by the Norwegian Government in 2013 as part of the European Carbon Dioxide Capture and Storage Laboratory Infrastructure (ECCSEL) Phase 1. Work is underway at SINTEF Energy Research to establish a project to realize this apparatus and collect experimental data.

3.3 Flow pattern prediction

Friction and heat transfer is often very dependent on which flow pattern is present in the flow, i.e. whether the flow is bubbly, stratified, annular or slug flow. There exist very little experimental data for flow patterns in CO_2 flow, especially in vertical or large diameter pipes [69]. Most of the available data on flow patterns seem to be focused on flow in small channels for air conditioning and heat pump applications. However, there is an abundance of data on flow patterns in e.g. water-steam and water-oil-gas flow, although many of these data are not publicly available. Correlations based on these data can potentially be used for carbon dioxide flow if they are based on dimensionless parameters. This would typically require values for surface tension, for which experimental data for CO_2 mixtures are scarce. Kolev [34] gives a thorough description of flow patterns for horizontal and vertical flow with and without boiling, which might also be relevant for CO_2 pipeline flow.

3.3.1 Recommendation

Current flow pattern maps are to a large extent based on experimental data for fluids like water and hydrocarbons, since experimental data for flow patterns in CO_2 flow is scarce, especially for large diameter pipes. It is therefore not guaranteed that these flow pattern maps are applicable for CO_2, which has a much lower surface tension than water. Existing flow pattern maps could be used with caution, but more experimental data for CO_2 flow patterns would be beneficial.

3.4 Friction

For both two-fluid models and drift-flux models, a model for friction between the fluid and the wall is needed. In eqs. (4)–(5) wall friction is represented by $f_{f,\mathrm{g}}$ and $f_{f,\ell}$. Aakenes [1], Aakenes et al. [2] compared experimental data for frictional pressure drop of CO_2 flow to friction models by Friedel [23] and Cheng et al. [14]. She found that the Friedel model gave significantly better predictions of pressure drop, even though the model by Cheng et al. was developed especially for CO_2.

The two-fluid model also requires a model for friction between the two phases, denoted as $\mathscr{V}$ in eqs. (4) to (5). Kolev [34] and Ransom et al. [59] describe a wide range of friction correlations for all flow patterns which may also be applicable to CO_2 flow. For horizontal flow with small differences between the gas and liquid velocities, the flow will be stratified, and the Spedding–Hand correlation [66] can be used.

3.4.1 Recommendation

For single-phase flow, reliable friction models exist, as long as correct viscosity values are available. For two-phase flow, more experimental data would be beneficial to validate the existing friction correlations.

3.5 Heat transfer

Heat transfer between the pipe wall and the fluid is typically modelled using a correlation for the Nusselt number Nu, which is related to the heat transfer rate as

$$Q_{\mathrm{w}} = \frac{k \cdot \mathrm{Nu}}{D}(T_{\mathrm{wall}} - T_{\mathrm{fluid}}), \tag{10}$$

where k is the thermal conductivity of the fluid and D is the pipe diameter. For turbulent single-phase pipeline flow, both the Dittus–Boelter [18] and the Gnielinski [25] correlations are well established.

For boiling two-phase flow, the Gungor–Winterton [26] correlation is commonly used. For condensing flow, the correlation by Boyko and Kruzhilin [13] can be used. These correlations do not necessarily give good predictions for all flow patterns. Collier and Thome [16] and Kolev [34] give comprehensive overviews of heat transfer correlations that apply to different flow patterns. For flow models where the two phases have individual temperatures, correlations are also needed for the heat transfer between the two phases, written as $\mathscr{T}$ in eqs. (6) to (7).

There are large uncertainties in heat transfer correlations, especially for two-phase flow, and the heat transfer may depend heavily on which flow pattern is present. Another disadvantage with many of the existing correlations is that few of them (if any) are based on experimental data for CO_2, which adds to the uncertainty.

3.5.1 Recommendation

For single-phase flow, it is expected that existing models for heat transfer are sufficient for CO_2 pipeline flow. For two-phase flow, heat transfer is highly dependent on flow pattern. If the flow pattern is predicted correctly, it is expected that also heat transfer can be estimated using existing correlations [16, 34, 59]. It should be noted that for most pipeline operations, heat transfer is much faster between the pipe and the inside fluid than between the pipe and the surroundings. This will reduce the impact of any uncertainties in the inner heat transfer model, since the pipe steel nevertheless will have the same temperature as the fluid.

3.6 Mass transfer

If our two-phase flow model includes two mass equations, we need to model the mass transfer that occurs between the two phases due to condensation and evaporation, represented as $\mathscr{V}$ in eqs. (2) to (3). A number of models in the literature include mass transfer terms [12, 63, 68, 70], but common for many of them is that they contain unknown rate constants that need to be tuned. Lund and Aursand [44] gives an explicit expression with few tunable parameters, but this has not yet been validated experimentally.

Two-phase flow models with individual chemical potentials in the two phases seem to be rather uncommon in the literature. If the chemical potentials are equal, mass transfer is explicitly coupled to heat and volume transfer ($\mathscr{T}$ and $\mathscr{P}$ in eqs. (1) to (7)) between the phases, as shown by e.g. Flåtten and Lund [22].

3.6.1 Recommendation

There does not seem to exist many experimentally based mass transfer models, hence such models should be used with care. An alternative might be to use a model with equal chemical potentials and pressures, but independent temperatures.

4 Depressurization

Depressurization of a pipeline may be caused by planned operations or accidents, and can involve complex interplay between mechanical, fluid-mechanical and thermodynamic phenomena. In this section, we focus on two relevant causes: Running ductile fractures and emptying of a pipe through a valve.

4.1 Running ductile fractures

One of the possible issues with CO_2 pipeline transport is the potential for running ductile fractures [48]. Running fractures occur when the pressure inside the pipe is large enough to keep a crack running along the length of the pipe. Such fractures may arise if the pipe steel is weakened due to an accident or a material defect. Both Aursand et al. [5] and Mahgerefteh et al. [45] found that CO_2 pipelines may be more susceptible to running fractures than natural gas pipelines.

The risk of running ductile fractures is often assessed using semi-empirical methods like the Battelle method [47]. This method assumes that the fracture propagation and the fluid flow out of the crack are uncoupled. Since it is a semi-empirical method, it cannot be readily applied to new pipeline materials and fluids, as it would need recalibration [55].

According to O'Donoghue et al. [56], the three most important phenomena for running ductile fractures are the large-scale elasto-plastic deformation of pipe walls, the three-dimensional transient fluid dynamics and the inelastic dynamic crack-extension process. These three phenomena are all rather complex, hence only a few coupled models exist. In a collaboration between SINTEF Energy Research and SINTEF Materials and Chemistry, a coupled material-fluid methodology has been developed for predicting crack arrest for natural gas and hydrogen pipelines [11, 55], which has shown good agreement with full-scale tests [3]. Applied to CO_2 pipelines, this coupled model predicts a larger necessary pipe thickness than semi-empirical methods [6], which may indicate that the latter are not conservative enough. To our knowledge, only very limited experimental data for running fractures in CO_2 pipelines have been published so far. Cosham et al. [17] conducted West–Jefferson tests with pipes of limited length for pure CO_2 and CO_2+N_2. They found that the shape of the fracture depends on the size of the initial defect and the steel toughness, but also that more tests are needed.

4.1.1 Recommendation

Models for prediction of running ductile fractures are currently under development and steadily improving. Experimental data from full-scale tests with CO_2 pipelines would help validate these models. Their output could be essential for determining the pipe steel thickness necessary to prevent running ductile fractures.

4.2 Valves

In a controlled shutdown of a CO_2 pipeline, which might be necessary for some maintenance operations, the pipe will be vented through one or more valves. Depending on the rate of depressurization, very low temperatures may occur, which causes the pipe steel to become brittle and more susceptible to damage. For this reason, it is crucial to be able to predict the flow rate through a valve and hence the expected temperature drop of the fluid in the pipeline.

The NORDICCS report by Aursand [7] shows that volatile impurities such as CH_4, N_2 and O_2 have a positive effect on depressurization temperature, in the sense that they slightly increase the lowest temperature reached during a depressurization. On the other hand, the area of the valve has a large impact on this temperature. With a larger valve, the pipe will be emptied in a shorter time, leading to lower temperatures.

The assumptions used regarding equilibrium between the two phases in the flow through the valve can greatly influence the predicted flow rate. If equilibrium is assumed, the flow rate will be smaller than if the flow is out of equilibrium (or *frozen*). The actual flow rate is expected to be somewhere in between the frozen and equilibrium limits, but the actual values are hard to predict exactly. The valve flow model by Henry and Fauske [28] is a commonly used model that lies in between the two limits. However, even for oil–gas pipelines, for which there exists a lot of experience and experimental data, there are no models that are universally accepted to be the best.

More experimental data would be beneficial to properly characterize valve flow of CO_2. However, experimental data for depressurization of CO_2 pipelines is scarce. Clausen et al. [15] compared experimental data for depressurization of a 50 km onshore CO_2 pipeline with simulation data from OLGA. The results showed reasonable agreement for the pressure, while there were significant temperature discrepancies.

4.2.1 Recommendation

Since there are no universally correct valve models, and certainly not for CO_2 flow, it is recommended to make conservative choices depending on what parameters one is interested in. For example, if one wishes to estimate the lowest possible temperature during a depressurization, a frozen valve model could be used, since this gives the highest flow and the largest temperature drop. Conversely, if the aim is to find the maximum time it will take to empty a pipeline, an equilibrium model could be used, since this gives the lowest flow rate.

The ECCSEL gap analysis [58] lists a depressurization facility for CO_2-rich mixtures as one of the major gaps in the laboratory infrastructure. Similarly as for the viscosity apparatus mentioned in Section 3.2, funds have been allocated to construct such a depressurization facility as part of ECCSEL. Work is underway at SINTEF Energy Research to establish a project to realize this facility, collect experimental results and develop models. If the facility is built, it is expected that the resulting data will support the development of models predicting running-ductile fracture, as well as flow models for CO_2 transport, including valve models.

5 Simulation tools

For oil and gas pipelines, many simulation tools developed over several decades exist. However, CO_2 has properties that are significantly different from those of oil and natural gas, so it is not evident that existing tools are sufficient for simulation of CO_2 pipeline flow. In this section, we will mention the most common commercial tools and discuss their potential for simulating CO_2 pipelines. For a more comprehensive overview, the reader is referred to the work by Aursand et al. [8], which was published with support from the NORDICCS project.

5.1 OLGA

The dynamic two-fluid model OLGA has been developed since the 1980s [10], and has become the industry standard for simulating three-phase flow of oil, gas and water. A single-component two-phase module for CO_2 has recently been added [27], which does not include dry ice. However, this only handles pure CO_2, so CO_2 with impurities is not yet handled properly. The development of a new model formulation is underway, which is expected to improve the handling of CO_2 with impurities.

5.2 LedaFlow

This transient multiphase flow simulation tool was developed in the early 2000s by Total, ConocoPhilips and SINTEF. It is currently developed further for the commercial market by Kongsberg Oil & Gas Technologies. As with OLGA, LedaFlow was mainly developed for simulating three-phase oil–gas–water mixtures. The underlying mathematical model on which it is based can in principle be used for CO_2 flow, but this will require the implementation of thermodynamic models and closure relations for CO_2 flow.

5.3 Models at SINTEF Energy Research

At SINTEF Energy Research, a thermo- and fluid-dynamical modelling framework has been developed since 2007, in several projects, including CO_2 Dynamics [54], BIGCCS, IMPACTS, and NORDICCS. The main focus has been on resolving fast transients such as pressure waves, and on robust and accurate thermodynamics. To this end, a variety of flow models, equations of state and numerical methods have been studied. At present, the code can handle pure CO_2 with dry ice, as well as CO_2 mixtures with various impurities. It forms the thermo- and fluid-dynamical basis of the coupled model mentioned in section 4.1. The code undergoes continuous improvement in ongoing projects.

In a NORDICCS report, Morin [51] compared the SINTEF code to OLGA for some depressurization cases for pure CO_2. It was found that the numerical method used was not accurate enough to fully resolve the resulting liquid volume fractions. A more accurate higher-order method was therefore implemented, which lead to significant improvements [52]. However, there are still numerical challenges that should be investigated further.

5.4 Recommendation

No single tool stands out as the best choice for simulations of CO_2 pipeline transport. OLGA and LedaFlow both are widely used in the oil and gas industry, and are to a large extent based on experimental data, but are not yet fully capable of simulating CO_2 flow, especially not with impurities. The SINTEF model (above) has, for the moment, a narrower application range, but it does seem to handle impurities better.

6 Summary

The research on multiphase flow has a half-century long history, but due to the inherent complexity of such flow, there are still significant challenges to overcome. As long as computational resources limit us to using mostly one-dimensional models, we cannot expect to fully resolve all flow phenomena. There is a wide range one-dimensional models for multiphase flow available, which are in essence as valid for CO_2 as for any other fluid. However, the closure relations, e.g. models for viscosity, flow patterns, friction and thermodynamics, can be significantly different for CO_2. Due to lacking experimental data, many of these models have not yet been validated for CO_2 or CO_2 mixtures. This calls for more experiments to characterize CO_2 mixtures at conditions relevant for CO_2 transport.

More specifically, the following experiments are recommended:

- Depressurization of pipelines
- Phase equilibrium measurements
- Viscosity measurements
- Friction measurements for various flow patterns
- Measurement of density, heat capacity and speed of sound
- Full-scale running fracture tests

Complex phenomena like a running ductile fracture requires coupled models that include both thermodynamic, structure-mechanical and fluid-mechanical effects. Such models are still being developed, and their predictions will be crucial for determining the necessary pipe steel thickness.

When it comes to thermodynamic models, there seems to be a gap between accurate but slow models (such as EOS-CG or GERG-2008), and less accurate but fast models (such as cubic equations of state). For simulation purposes, it would be beneficial with an equation of state in between the two extremes, with sufficient speed but still close to the accuracy of reference equations of state.

Existing commercial simulation tools are typically aimed at flow in nuclear reactors or oil and gas pipelines, and have only limited support of CO_2. Presently, none of the commercial simulation tools can handle CO_2 mixtures with reasonable reliability and accuracy. These tools are also limited by the mentioned lack of experimental data for e.g. viscosity and thermodynamic properties for CO_2 mixtures.

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