



Thermodynamic interpolation for the simulation of two-phase flow of non-ideal mixtures

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ABSTRACT

This paper describes the development and application of a technique for the rapid interpolation of thermodynamic properties of mixtures for the purposes of simulating two-phase flow. The technique is based on adaptive inverse interpolation and can be applied to any Equation of State and multicomponent mixture. Following analysis of its accuracy, the method is coupled with a two-phase flow model, based on the homogeneous equilibrium mixture assumption, and applied to the simulation of flows of carbon dioxide (CO₂) rich mixtures. This coupled flow model is used to simulate the experimental decompression of binary and quinary mixtures. It is found that the predictions are in good agreement with the experimental data and that the interpolation approach provides a flexible, robust means of obtaining thermodynamic properties for use in flow models.

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1. Introduction

The modelling of compressible two-phase or flashing flows is commonplace in a wide range of areas in engineering. For example, cavitation in automotive fuel injection systems (Martynov, 2006), flash boiling of water during loss-of-coolant accidents in nuclear reactors (Blinkov et al., 1993) and liquid boiling and expansion in refrigeration systems and heat pumps (Simões-Moreira and Bullard, 2003). Whilst various approaches are available to model the dynamics of two-phase flow, the accuracy of simulations for flashing two-phase flows to a large extent depends on the accuracy of the physical properties data in use. This particularly applies to multicomponent mixtures, which are commonly found as working fluids in the above systems.

In practice, complex mathematical formulas known as Equations of State (EoS), are used to provide the thermodynamic properties for both vapour and liquid phases. As a result, a prac-

tical problem arises when pressure explicit EoS are coupled with flow models. In these EoS, the thermodynamic properties are predicted as a function of pressure, temperature and composition while phase equilibria, at a given system pressure and temperature (P - T), is determined using a variety of isothermal 'flash' algorithms (Michelsen, 1982a,b). This formulation contrasts with the fluid-dynamics models, where the conservation laws governing are naturally posed in terms of density and internal energy (ρ - e). To overcome this problem, one possible solution is to use the so-called isochoric-isoenergetic flash (Castier, 2009; Michelsen, 1999). However, existing isochoric-isoenergetic flash algorithms are neither robust nor computationally efficient in the context of flow simulation because they either rely on an internal iterative loop over the P - T variables (Michelsen, 1999; Saha and Carroll, 1997) or on the direct minimisation of total entropy (Castier, 2009; Munkejord and Hammer, 2015).

The problem of computational inefficiency is exacerbated by the complexity of modern EoS. In the oil and gas industry, fluid flow simulators almost exclusively use cubic EoS (such as Soave-Redlich-Kwong, Peng-Robinson, etc., Zaydullin et al., 2014). Cubic EoS can be solved relatively at low computational cost; however, the higher order EoS developed in the last two decades provide

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improved accuracy in physical property estimations, though this is at slightly higher computational cost. For example, for the case of CO₂ and its mixtures, high accuracy is provided by the Statistical Associating Fluid Theory (SAFT) EoS (Diamantonis and Economou, 2011) or by the “reference” EoS (Span and Wagner, 1996) and both EoS have a large number of relatively complex terms. As a result, application of these EoS to flow simulations not only increases the computational cost, but also the susceptibility to numerical instabilities in the underlying isothermal flash algorithms.

This is a particular problem in the simulation of flows associated with Carbon Capture and Storage (CCS), where the CO₂ stream may contain a number of impurities and vary in composition (Porter et al., 2015). Indeed, it is well established that the presence of these impurities has important impacts on many aspects where the modelling of two-phase flow is relevant, including ductile fracture (Mahgerefteh et al., 2012a) and the release rate in the case of loss of containment (Brown et al., 2013).

Previous work to address this issue has focused on producing tables of thermodynamic properties from isenthalpic or isentropic flash calculations (Mahgerefteh et al., 2006), which are facilitated by changing the variables with which the flow is resolved; however, this means that alternative numerical techniques must be applied to the fluid flow equations and that conservation of mass, momentum and energy is not ensured. Similarly, isothermal tables to replace the isothermal flash in the iterative loop described above have been widely applied (for example Andresen, 2009; Zaydullin et al., 2014); in particular, Zaydullin et al. (2014) extended the compositional space adaptive tabulation (CSAT) technique of Iranshahr et al. (2010) and applied it to compositional and thermal reservoir simulations of multicomponent multiphase systems. In this case, the generalised negative flash approach (Iranshahr et al., 2010) was used to first establish and then extend the set of tie-simplexes for the CSAT procedure. These tie-simplexes were then used to look up, for a particular pressure and temperature, the phase state of the mixture. Dumbser et al. (2013) presented a method of building an interpolating function in terms of density and internal energy using adaptive mesh refinement for a single component fluid; however, this relied on the ability to calculate isochoric-isoenergetic flashes which cannot be done efficiently for mixtures.

In this work a robust technique for efficiently performing isochoric-isoenergetic flashes, for the purposes of two-phase flow calculations, is presented. The technique is based on adaptive inverse interpolation and can be applied independently of the EoS and the specific mixture under consideration. The technique is intended for the application of the complex, computationally heavy EoS that are required for the accurate prediction of the thermodynamic properties and phase equilibria of CO₂ mixtures. For this study, the Perturbed Chain-SAFT (PC-SAFT) is selected for this purpose (Gross and Sadowski, 2001); however, any other EoS can be used. PC-SAFT is an accurate EoS rooted in statistical mechanics that has gained significant interest by oil and gas and chemical industries in recent years for the calculation of thermodynamic properties. This is the first attempt, to our knowledge, to use PC-SAFT for compressible fluid flow simulations, although it has been applied to multiphase flows in other contexts such as within hydrocarbon reservoirs (see for example Mohebbinia, 2013; Yan et al., 2015). The new method is then coupled with a two-phase flow model based on the homogeneous equilibrium mixture assumption (Brown et al., 2015a; Mahgerefteh et al., 2012b) and applied to the simulation of CCS relevant two-phase flows.

This paper is structured as follows: Section 2 firstly presents the fluid flow model applied in this study (Section 2.1) followed by a description of the interpolation scheme developed based on well-established and widely adopted techniques (Section 2.2). The section ends with an overview of the PC-SAFT EoS used in this work.

Section 3 provides an analysis of the interpolation technique’s consistency with the EoS (Section 3.1). Next, the method is coupled with the two-phase flow model and a number of tests are performed to establish the robustness and computational efficiency of the method in the presence of rapid transients (Section 3.2). This coupled flow model is then used to predict the decompression of binary and quaternary mixtures and the results are compared against experimental data, which in the case of the binary data is previously unpublished (Section 3.3). Conclusions and suggestions for future work are discussed in Section 4.

2. Methodology

2.1. The homogeneous equilibrium model (HEM) flow model

The model applied in this study is based on the assumptions of one-dimensional, unsteady flow and, in the case of two-phase flow, thermodynamic and mechanical equilibrium, i.e. a single temperature, pressure and velocity, between the saturated vapour and liquid phases. In this case the respective continuity, momentum, and energy conservation equations are given by (see for example Zucrow and Hoffman, 1975):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial z} = 0 \quad (1)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial z} = -2f_w \frac{\rho u^2}{D_p} \quad (2)$$

$$\frac{\partial E}{\partial t} + \frac{\partial u(E + P)}{\partial z} = -2f_w \frac{\rho u^3}{D_p} \quad (3)$$

where ρ , u , P are respectively the mixture density, velocity and pressure, which are functions of time, t , and spatial coordinate, z ; D_p and f_w , are the pipeline diameter and Fanning friction factor, calculated using Chen’s correlation (Chen, 1979), and E is the total mixture energy defined as:

$$E = \rho \left(e + \frac{1}{2} u^2 \right) \quad (4)$$

where e is the mixture specific internal energy:

$$e = x_{eq} e_v + (1 - x_{eq}) e_l \quad (5)$$

x_{eq} is the equilibrium vapour quality, and ρ is the mixture density defined as:

$$\frac{1}{\rho} = \frac{x_{eq}}{\rho_v} + \frac{(1 - x_{eq})}{\rho_l} \quad (6)$$

In Eqs. (5) and (6) the subscripts v and l refer to the vapour and liquid phases respectively.

To solve Eqs. (1)–(3) numerically, a finite volume method is used (Leveque, 2002), where, following Brown et al. (2015b), the conservative left-hand-side of Eqs. (1)–(3) are solved using the AUSM+ flux vector splitting scheme (Liou, 2006).

2.2. Interpolation technique

As described previously, the coupling of the EoS described in Section 2.3 with the flow Eqs. (1)–(3) where the fluid is two-phase is complicated by the fact that the free variables are the density, ρ , and internal energy, e , with which we must compute the system P and temperature, T , while the computation of the phase equilibria using an EoS (in this case PC-SAFT as described in Section 2.3) is most commonly performed using the P and T of a mixture for a fixed given total composition. To overcome this, we introduce the construction of two interpolant grids, one of which is constructed using the P and T as free variables, denoted $\{P, T\}$, and the other

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