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Multiphase flows of N immiscible incompressible fluids: An outflow/open boundary condition and algorithm

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A B S T R A C T

We present a set of effective outflow/open boundary conditions and an associated algorithm for simulating the dynamics of multiphase flows consisting of N ($N \geqslant 2$) immiscible incompressible fluids in domains involving outflows or open boundaries. These boundary conditions are devised based on the properties of energy stability and reduction consistency. The energy stability property ensures that the contributions of these boundary conditions to the energy balance will not cause the total energy of the N-phase system to increase over time. Therefore, these open/outflow boundary conditions are very effective in overcoming the backflow instability in multiphase systems. The reduction consistency property ensures that if some fluid components are absent from the N-phase system then these N-phase boundary conditions will reduce to those corresponding boundary conditions for the equivalent smaller system. Our numerical algorithm for the proposed boundary conditions together with the N-phase governing equations involves only the solution of a set of de-coupled individual Helmholtz-type equations within each time step, and the resultant linear algebraic systems after discretization involve only constant and time-independent coefficient matrices which can be pre-computed. Therefore, the algorithm is computationally very efficient and attractive. We present extensive numerical experiments for flow problems involving multiple fluid components and inflow/outflow boundaries to test the proposed method. In particular, we compare in detail the simulation results of a three-phase capillary wave problem with Prosperetti's exact physical solution and demonstrate that the method developed herein produces physically accurate results.

1. Introduction

In this work we focus on the dynamics and interactions of a system of N ($N \geqslant 2$) immiscible incompressible fluids in an unbounded flow domain. In order to numerically simulate such problems it is necessary to truncate the domain to a finite size. Consequently, part of the boundary in the computational domain will be open, in the sense that the fluids can freely leave (or even enter) the domain through such boundaries, and appropriate boundary conditions will be required on the open (or outflow) portions of the domain boundary. We are particularly concerned with situations in which the multitude of fluid interfaces formed in the system will pass through the open domain boundaries. Following the notation of our previous works [11,14,15], we refer to such problems as N-phase outflows. Here N denotes the number of different fluid components in the system, not necessarily the number of material phases.

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N-phase outflows and open boundaries pose a number of issues to numerical simulations. First, the problem involves multiple fluid interfaces at the open/outflow boundary, which are associated with multiple surface tensions and the contrasts in densities and viscosities of these fluids. How to deal with the surface tensions, and the density and viscosity contrasts in the N-phase open/outflow boundary conditions (OBC) poses the foremost issue. Second, backflow instability is another crucial issue confronting N-phase outflow simulations. Backflow instability refers to the numerical instability associated with strong vortices or backflows at the open/outflow boundary, which causes computations to blow up instantly when strong vortices or backflows occur at the outflow boundary. The backflow instability issue is not unique to multiphase flows. This issue is well-known in single-phase outflow problems [16,18,13], but it becomes much worse for two-phase [12,19] and multiphase outflows because of the density contrasts and viscosity contrasts at the outflow boundary. Third, N-phase problems with $N \geqslant 3$ pose the so-called reduction consistency issue on the design of outflow/open boundary conditions [15]. Reduction consistency refers to the property that, if only M $(2 \leqslant M \leqslant N-1)$ fluid components are present in the N-phase system (while the other fluid components are absent), the governing equations and the boundary conditions for the N-phase system should reduce to those for the corresponding smaller M-phase system [15]. The reduction consistency of N-phase outflow/open boundary conditions is an issue unique to multiphase outflow and open-boundary problems.

The development of effective outflow/open boundary conditions is an important problem in computational fluid dynamics. For single-phase problems, this has been under intensive investigations for decades and a large volume of literature exists; see e.g. [20,36] for a comprehensive review of related literature and [16,13] and the references therein for a sample of more recent works. On the other hand, for two-phase $(N = 2)$ outflows and open boundaries the existing work in the literature is very limited, and for multiphase outflow and open-boundary problems involving three or more $(N \geqslant 3)$ fluid components, there is no existing work available in the literature to the best of our knowledge. The zero-flux (Neumann) and extrapolation boundary conditions from single-phase flows have been used for the two-phase Lattice-Boltzmann equation in [29]. The zero-flux condition has also been employed for the outflow boundary with a level-set type method in [2,38]. The outflow condition for two immiscible fluids is considered for a porous medium in [26], and for one-dimensional two-phase compressible flows in [31,9]. In [12,19] we have developed a set of two-phase open boundary conditions having the attractive property that these conditions ensure the energy stability of the two-phase system, which is therefore effective for dealing with two-phase open boundaries.

In the current paper we consider the multiphase outflow and open-boundary problem with N $(N \geqslant 3)$ immiscible incompressible fluid components in the system, and present a set of effective outflow/open boundary conditions and an associated numerical algorithm for such problems within the phase field framework. The proposed open boundary conditions are designed based on considerations of two properties: energy stability and reduction consistency. By looking into the energy balance of the N-phase system, we design the open boundary conditions in such a way to ensure that their contributions shall not cause the total energy of the N-phase system to increase over time, regardless of the flow state at the outflow/open boundary. This energy-stable property holds even in situations where strong vortices or backflows occur at the open boundary. As a result, these boundary conditions are very effective in overcoming the backflow instability. We then look into the reduction consistency of these boundary conditions, and study how these conditions transform if some fluid components are absent from the N-phase system. The reduction consistency property limits the choice and the form of those boundary conditions that ensure the energy stability. The N-phase outflow/open boundary conditions and also the inflow boundary conditions proposed herein satisfy both the energy stability and the reduction consistency.

The outflow/open boundary conditions proposed herein are developed in the context of an N-phase physical formulation we developed recently in [15]. This formulation is based on a phase field model for the N-fluid mixture that is more general than a previous model [11]. The thermodynamic consistency and the reduction consistency of this formulation have been extensively studied in [15]. The formulation rigorously satisfies the mass conservation, momentum conservation, the second law of thermodynamics, and the Galilean invariance principle. This formulation is fully reduction consistent, provided that an appropriate potential free energy density function satisfying certain properties is employed for the N-phase system [15]. The reduction consistency of a set of Cahn–Hilliard type equations for a three-component and multi-component system (without hydrodynamic interactions) has previously been considered in [6,8]. The thermodynamic consistency of two-phase and multiphase systems has also been considered in [30,25,1,21,11,27,14,39]. We refer the reader to e.g. [4,28,41,7,24,42,5, 40,43] for other contributions to two-phase and multiphase flow problems.

We further present an efficient numerical algorithm for the proposed outflow and inflow boundary conditions together with the N-phase governing equations. This is a semi-implicit splitting type scheme. Special care is taken in the numerical treatments of the open/ouflow boundary conditions such that the computations for different flow variables and the computations for the $(N-1)$ phase field functions have all been de-coupled. The algorithm involves only the solution of a set of individual de-coupled Helmholtz-type equations (including Poisson) within each time step. The resultant linear algebraic systems after discretization involves only constant and time-independent coefficient matrices, which can be pre-computed during pre-processing, even when large density contrasts and large viscosity contrasts are involved in the N-phase system.

The novelties of this paper lie in two aspects: (i) the set of N-phase energy-stable and reduction-consistent outflow/open boundary conditions and inflow boundary conditions, and (ii) the numerical algorithm for treating the proposed set of outflow and inflow boundary conditions.

The rest of this paper is structured as follows. In the rest of this section we provide a summary of the general phase field model developed in [15] for the N-fluid mixture. This model provides the basis for the N-phase energy balance relation and the development of energy-stable boundary conditions. In Section 2 we propose a set of outflow and inflow boundary