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A level set method for vapor bubble dynamics

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ABSTRACT

This paper describes a finite-difference computational method suitable for the simulation of vapor–liquid (or gas–liquid) flows in which the dynamical effects of the vapor can be approximated by a time-dependent, spatially uniform pressure acting on the interface. In such flows it is not necessary to calculate the velocity and temperature fields in the vapor (or gas). This feature simplifies the solution of the problem and permits the computational effort to be focussed on the temperature field, upon which the interfacial mass flux is critically dependent. The interface is described by a level set method modified with a high-order "subcell fix" with excellent mass conservation properties. The use of irregular stencils is avoided by suitably extrapolating the velocity and temperature fields in the vapor region. Since the accurate computation of momentum effects does not require the same grid refinement as that of the temperature field, the velocity field is interpolated on a finer grid used for the temperature calculation. Several validation and grid refinement axi-symmetric tests are described which demonstrate the intended first-order time, second-order space accuracy of the method. As an illustration of the capabilities of the computational procedure, the growth and subsequent collapse of a laser-generated vapor bubble in a microtube are described.

1. Introduction

Fixed grids are an attractive choice for the computation of free-surface flows due to their flexibility and efficiency, but they also give rise to very significant numerical problems which have generated a large literature.

In many of the proposed methods the interface is spread over a few computational cells (see e.g. [1,2]), or the density difference between the two fluids is artificially limited for numerical expediency [3]. Both features are undesirable in the case of flows in which vapor–liquid phase change processes are important as the accurate calculation of mass and heat fluxes at the interface is then of paramount importance. For this and other reasons several "sharp interface" methods have been devised such as the ghost-fluid method [4,5] and several variants of the volume of fluid (see e.g. [6–8]) and front tracking (see e.g. [9]) methods. In view of the connections with the present work, a particular mention is deserved by level-set methods implemented both with sharp (see e.g. [5,7,10]) and diffuse (see e.g. [2]) interfaces sometimes, as in the last paper cited, in combination with the volume-of-fluid method.

A central difficulty in the simulation of phase change processes stems from the small thermal diffusivity of liquids of common interest, in particular water, coupled with a large latent heat and a large difference between the liquid and vapor densities. Heat fluxes at the liquid–vapor interface are therefore large and capturing them correctly requires a very fine grid. For this reason, many of the available methods are illustrated with applications to fluids near the critical point, where the latent

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heat is smaller and the phase densities closer, or to model problems. Exceptions are Refs. [7,10,11] in which the actual properties of water at normal pressure are used. In its most recent work this group has returned to a moving mesh [12].

A feature common to all these methods is their insistence on solving the Navier–Stokes equations in both the liquid and the vapor or gas phases. While this strategy endows them with a great generality and renders them able to deal with the density differences that one may encounter at very high pressures or close to the critical point, it fails to take advantage of the very significant simplification that is available in the much more common case in which the vapor density is several orders of magnitude smaller than the liquid one. In these situations, when the extent of the vapor space is limited, such as in the case of vapor bubbles, the most significant dynamical effect of the vapor is to provide a time-dependent, spatially uniform pressure on the liquid while its inertia and viscous stresses play a negligible role. Furthermore, the vapor temperature can also be assumed spatially uniform due to the very fast time scales for phase change and acoustic propagation.

This paper presents a numerical method suitable for these situations. Other problems to which it is equally applicable are encountered in the dynamics of gas bubbles and in other situations in which the pressure in the vapor or gas space can be assumed to be uniform. While we limit ourselves to axi-symmetric problems here, the method is readily extendable to three dimensions as well.

While abandoning the attempt to solve the vapor momentum equation limits the applicability of our method, the simplification to which it leads permits us to devise a more accurate solution procedure than possible with other methods, and in this aspect resides the usefulness of this work.

This study arose from an interest in the numerical solution of vapor–liquid flows encountered in microfluidic devices in some of which one takes advantage of the rapid and violent dynamics provided by vapor bubbles created by the intense local heating of small liquid masses in a confined environment. A well known example is the ink-jet printing process, in which the fast expansion of a vapor bubble in a narrow flow channel results in the ejection of a droplet of ink [13–16]. Other potential uses of vapor bubbles in small devices without mechanical moving parts include actuation [17,18], pumping [19,20], surface cleaning [21] and others. The performance of such devices is critically dependent on the bubble behavior which therefore needs to be understood from a fundamental viewpoint.

In the method described in this paper the liquid mass, momentum and energy equations are solved in cylindrical coordinates by means of a standard projection method on a uniform staggered grid. The vapor is modeled as a region of spatially uniform temperature, computed from an energy balance at the interface, and accompanying uniform saturation pressure which serves as a boundary condition for the liquid. The phase boundary is captured implicitly by means of the level set method. Discretization near the interface requires ghost values for the velocity in the vapor region. These values are generated by a procedure originally suggested in [22] modified according to the ideas of [23], which enforce the incompressibility constraint and properly account for viscous stresses at the interface.

Another feature of the method is that the energy equation is solved on a much finer grid than the momentum equation. This feature permits the accurate evaluation of temperature gradients at the interface, which are of paramount importance in establishing phase-change mass fluxes, while at the same time limiting the overall computational cost. A more detailed description of this and other features can be found in [24].

2. Mathematical formulation

We assume that velocities and temperature differences are sufficiently small that the liquid density and thermal properties can be treated as constants. The equations expressing the conservation of its mass, momentum and energy are therefore

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot \tau, \tag{2}$$

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \alpha \nabla^2 T, \tag{3}$$

with $\mathbf{u}$, p, τ and T the liquid velocity, pressure, Newtonian viscous stress tensor and temperature fields, and ρ and α the liquid density and thermal diffusivity. Here and in the following liquid quantities are not subscripted; vapor quantities carry the subscript v, and quantities evaluated at the phase interface the subscript s.

Local temperature differences along the interface would give rise to evaporative or condensing mass fluxes able to equilibrate them on a smaller time scale than any other process under consideration. Furthermore, due to the very small vapor inertia, pressure gradients cannot persist beyond the acoustic time scale. The vapor phase is therefore modeled as a region with negligible inertia and spatially uniform pressure.

The balance of normal stresses at the interface is expressed by

$$p_v = p_s + \sigma\kappa - \mathbf{n} \cdot \tau_s \cdot \mathbf{n}, \tag{4}$$

where p_v is the vapor pressures, p_s the liquid pressure at the interface, σ the surface tension coefficient, κ the local curvature and $\mathbf{n}$ the unit normal directed into the liquid. Since the viscous stresses in the vapor are neglected, the liquid tangential stress at the interface must vanish: