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Three-dimensional modeling of fluid dynamics and heat transfer for two-fluid or phase change flows

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A numerical algorithm based on the VOF method was proposed to solve two-phase/two-fluid flow problems by the authors recently. Different from other surface reconstruction approaches, the interface between the two fluids is represented by a continuous surface as the contour surface of the VOF function. It is robust and easy to implement. In this article, the method is extended to deal with three-dimensional flows. Also considered in the study is the heat transfer in the flow with or without phase change. In order to validate the method, a variety of flow problems are under consideration and comparison with empirical correlations is made. The method is first tested by considering a benchmark case with prescribed 3-D velocity field. It is then applied to the problem of bubble rising in a quiescent liquid, followed by investigating the splashing of a drop impacting on a liquid film. To assess the heat transfer model for phase change, the boiling flow emerging from a superheated planar film is under investigation. The last one considered is a jet flow caused by injection of high-temperature octane into a water container.

1. Introduction

Two-phase/two fluid flows can be found in a variety of applications in industrial processes. Earlier studies on this subject heavily rely on experiments. The fast advancement in numerical techniques has made accurate simulation of these flows feasible in the past two decades. Unlike single-fluid flows, there is an interface between the two fluids across which thermophysical properties suffer significant changes, making the mathematical problem more stiff to be solved. The situation becomes even worse by understanding that the position of the interface requires to be solved as part of the solution.

To solve the multi-fluid problems, a widely adopted approach is to treat the fluids as a single fluid with variable thermal properties and use an Eulerian grid to allow the interface to move around in the grid. Therefore, one of the most important issues in this modeling is to track the interface accurately. Owing to the jump of the thermal properties, the methods similar to the shock-capturing schemes employed in high-speed, compressible flows will inherently suffer diffusion at the fluid surface [1,2]. To avoid this problem, various methods have been developed. In the front tracking method [3–5], the interface is represented by a surface grid moving with local velocities. It is obvious that this kind of method is difficult to implement because it needs to deal with interaction between the two grids.

An alternative is to use indicator functions to distinguish different fluids in the flow field. In level set methods [6], the LS function represents a signed distance function which is positive on one fluid side and negative on the other side. The major drawback of the methods is lack of mass conservation, though the problem can be partially relieved by a reinitialization procedure [7,8].

VOF is another popular indicator function representing the fraction of one fluid occupying the control volume. Unlike other methods, conservation of mass can easily be attained in this approach. Among a variety of options, the one with interface reconstruction using a piecewise linear plane (PLIC) [9,10] is most favored. However, the reconstruction process and the calculation of flux across cell faces are complicated, especially serious in 3-D problems [11]. Unlike the LS function which is continuous, the VOF is a step function, i.e. discontinuous across the interface, which results in difficulties calculating geometric properties, such as interface normal or curvature. This leads to inaccurate calculation of the surface tension and, thus, unphysical spurious currents near the interface when the continuous surface force model (CSF) is incorporated in the VOF approach [12]. Several methods have been proposed to improve the estimation of surface tension and reduction of spurious currents. In the study of Francois et al. [13], a height function is reconstructed locally as an approximation of the interface location. The curvature is then estimated from this height function.

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Nomenclature

C	specific heat
C_i	volumetric flux through the ith face
e	specific energy
Eo	Eovots number $(= \Delta\rho g d^2/\sigma)$
$\vec{f}_\sigma$	surface tension force
$\vec{g}, g$	gravitational acceleration
Gr	Grashof number $(= \rho_v \Delta\rho g \lambda^3/\mu_v^2)$
h	film thickness
h_{12}, h_{lv}	latent heat of evaporation
Ja	Jacob number $(= C_v(T_w - T_{sat})/h_{lv})$
k	thermal conductivity
$\dot{m}$	mass flux
Mo	Morton number $(= g\mu_l^4/\rho_l\sigma^3)$
$\vec{n}$	unit normal vector
Δn	normal distance away from the interface
Nu	Nusselt number
$\overline{Nu}$	space and time averaged Nusselt number
Oh	Ohnesorge number $(= \mu_l/(\sigma\rho_l d)^{1/2})$
P	pressure
Pr	Prandtl number $(= C_v\mu_v/k_v)$
Re	Reynolds number $(= \rho_l U d/\mu_l)$
$\dot{q}$	heat release rate
$\vec{s}_f$	surface vector of cell face
$\vec{s}_f^w$	surface vector of wetted area on cell face
S_{int}	interface surface in cell
S_M, S_α	source terms in continuity and VOF equations
t	time
Δt	time step size
T	temperature
ΔT	superheat temperature
U	terminal velocity of rising bubble
V	drop impact velocity
$\vec{V}$	velocity vector
Δv	cell volume
We	Weber number $(= \rho_l V^2 d/\sigma)$

Greek symbols

α	VOF function
α^*	smoothed VOF function
κ	mean curvature
λ	characteristic length for film boiling
λ_d	most dangerous Taylor wavelength
μ	viscosity
ρ	density
$\Delta\rho$	density difference between the fluids
σ	surface tension
$\tilde{\tilde{\tau}}$	viscous stresses

Subscripts

C	neighboring cell
f	cell face
fj	jth cell face
int	interface
l	liquid phase
o	octane
P	primary cell
sat	saturation state
v	vapor phase
w	water or wall value
$1, 2$	fluids 1 and 2

Superscripts

n	new time step
o	old time step

In the PROST method of Renardy and Renardy [14], a least-squares fit of a quadratic surface to the VOF for each interface cell and its neighbors is calculated. Another option, which was developed by Sussman and Puckett [15] and gradually draws popularity recently, is to combine the advantages of both VOF and LS. This coupled LS and VOF method is achieved by advecting the interface using the conservative VOF function and estimating the interface normal and curvature using the continuous LS function. Modifications and applications of this CLSVOF method can be found in a number of studies [16–20].

Numerical analyses using the VOF and LS methods have been applied to various flow systems. Chen et al. [21] investigated the deformation of gas bubbles rising in a viscous liquid. The effects of density, Reynolds number, and surface tension on the formation of toroidal bubbles were examined. Another study on bubble rising was reported by Hua and Lou [22]. The comparison of simulations with experiments shows satisfactory agreement. Wide ranges of Reynolds number, Bound number, density ratio and viscosity ratio were under consideration. The study was extended by Hua et al. [23] to simulate fully 3-D bubble flows. Good agreement with experiments in terms of terminal speed and bubble shape was obtained. Also considered in this study is the interaction of two rising bubbles.

Boiling is an important thermal process due to its capability to convert large quantity of thermal energy from liquid to vapor phase. Son and coworkers conducted pioneer works to study bubble growth and release from a planar film [24] or a nucleate [25]. Esmaeli and Tryggvason [26] studied multi-mode film boiling on a plane sufficiently large to allow formation of bubbles of different sizes and spacings. Comparison of the overall mean Nusselt number with empirical correlation at different wall superheats showed reasonably good agreement. Film boiling on a horizontal cylinder was investigated by Son and Dhir [27]. The effects of cylinder diameter and gravity on the flow and heat transfer were quantified. Tsui et al. [28] studied the effects of superheat on the bubble formation in planar film boiling. Five distinct regimes of bubble patterns were identified.

Temperature distribution during manufacturing process is crucial to the product quality of mold casting and injection molding processes. Modeling of the heat transfer in two-fluid flows without phase change has been made by Davidson and Rudman [29]. The heat transfer across the faces of the interface cell is obtained by considering the heat fluxes of individual fluids after the interface is reconstructed from the VOF distribution. In the study of Tsui et al. [30], satisfaction of the continuity condition for temperature and heat flux at the interface gives the interface temperature. This temperature is implemented as an internal Dirichlet condition for energy calculations.

As addressed above, the VOF-based PLIC method is popular among a variety of choices. In this method, the interface is rebuilt as a plane in the cell where the interface is located. The resulting interface is discontinuous across the common face shared by the neighboring cells. During the reconstruction process, iteration is usually required such that the wetted volume fraction in the cell