The Extension of PHOENICS VOF to Three Phases

1.Introduction

This article reports on the extension of the existing PHOENICS VOF (volume of fluid) option to simulate three phase flows, such as those encountered in applications involving three different immiscible fluids. Examples include systems involving combinations of liquids and gases with differing densities, like those found in the water/oil/air interfaces of an oilfield separator and the liquid-steel/liquid-slag/gas interfaces of a gas-stirred metallurgical ladle. The extension to three fluids involves the solution of a conservation for an additional colour (or indicator) function, C_3, to represent the third phase; and a modification of the surface-tension force in the mixture momentum equation to handle the three distinct fluids.

2.Theoretical Considerations

The transport equation for C_3 has the same form as the existing colour function C_1 used in two-phase VOF simulations, i.e.:

$$\frac{\partial C_3}{\partial t} + \nabla \cdot V C_3 = 0 \qquad (1)$$

The option exists in PHOENICS to solve this equation in conservative or in non-conservative form, depending on the physical problem. The following algebraic equation enforces volume continuity and links the two colour functions: $\sum_{n=1}^{3} C_n = 1$, where C_n is the colour function of phase n.

The **physical properties** of the resulting mixture are computed under the above constraint by using equations of the form: $\phi = \sum_{n=1}^{3} C_n \phi_n$, where ϕ denotes the density, kinematic viscosity, specific heat capacity, thermal conductivity and volumetric expansion coefficient

3. Surface Tension Effects

The PHOENICS two-phase VOF method uses the standard continuous surface force (CSF) approach of Brackbill et al (1992) to introduce **surface-tension forces** into the momentum equations in form of an equivalent body force, which in case of a two-phase system, takes the following form: $\mathbf{f}_{cap} = \sigma \kappa_i \delta \mathbf{n}_i$, where σ is interfacial tension, $\mathbf{n}_i = -\nabla C_i / |\nabla C_i|$ is unit normal vector at the interface pointing out of the i-phase, with C_i the colour function of the i-phase, $\delta = |\nabla C_i|$ is the Dirac delta function centred at the interface and $\kappa_i = -(\nabla \cdot \mathbf{n}_i)$ is the interface curvature.

The drawback of the CSF approach is that for different densities of adjacent phases, the capillary force introduced into the momentum equations produces an unsymmetrical distribution of the acceleration field relative to the interface location. For example, the acceleration $\mathbf{f}_{cap}/\rho$, where ρ is the local VOF phase density, is much higher in a less dense phase and vice versa. The CSF

approach will lead to a thinning or thickening of the smooth transitional region between phases, depending on the direction of the vector $\mathbf{f}_{cap}$. If $\mathbf{f}_{cap}$ is pointing into a less dense phase, then the interface tends to thicken with time, whereas if it is pointing into a denser phase, the interface will become thinner with time. This problem has been resolved by Brackbill et al (1992) for two-phase systems by using density scaling of the CSF (DS-CSF), as follows:

$$f_{cap} = -\sigma\kappa_i \nabla C_i \frac{\rho}{\langle\rho\rangle} \qquad (2)$$

where $\langle\rho\rangle = (\rho_1 + \rho_2)/2$ is the average density between adjacent phases 1 and 2. This practice results in a symmetric distribution of the acceleration with respect to the interface.

In this work, by following Tofighi and Yildiz (2013), the DS-CSF has been extended to three phases by splitting the resulting capillary force into three constituents, one per phase. Each of these phase-specific forces is given by equation (2) above, but instead of using interfacial surface tensions, three phase-specific surface tensions σ_n (where n = 1,2, 3) are used in these forces. This approach is valid only for three-phase systems, as will be discussed later. When focusing on a given phase n, the idea of density scaling is to treat the two others as a single n-adjacent phase with spatially varying density.

By analogy with a two-phase system, but using now the density of the n-adjacent phase for the DS-CSF, the capillary force for a three-phase system can be computed as:

$$f_{cap} = \sum_{n=1}^{3} f_{ncap} = -\sum_{n=1}^{3} \sigma_n \kappa_n \nabla C_n \frac{\rho}{\langle\rho\rangle_\alpha} \qquad (3)$$

where $\mathbf{f}_{n,cap}$ is the equivalent of $\mathbf{f}_{cap}$ for phase n with $\langle\rho\rangle_n = (\rho_n + \rho_{n\text{-adjacent}})/2$. This formulation redistributes the surface forces across interfaces in such a way as to produce a symmetric acceleration. It remains to define the values of phase-specific surface tensions. The idea is based on the decomposition of the resulting force vector into three constituent phase-specific forces (see Tofighi and Yildiz (2013)). These phase-specific forces are then treated individually in the same manner as surface forces in two-phase systems, where only one type of interface is possible. For this purpose, the interfacial tension between phases n and β is expressed through artificially introduced phase-specific surface tensions, so that $\sigma_{n\beta} = \sigma_n + \sigma_\beta$ where:

$$\begin{cases} \sigma_1 = 0.5(\sigma_{12} + \sigma_{13} - \sigma_{23}) \\ \sigma_2 = 0.5(\sigma_{12} + \sigma_{23} - \sigma_{13}) \\ \sigma_3 = 0.5(\sigma_{13} + \sigma_{23} - \sigma_{12}) \end{cases} \qquad (4)$$

One difficulty in three phase systems is the possibility of direct contact between all phases. However, these situations are accounted for automatically by the foregoing capillary-force decomposition into the sum of phase-specific capillary forces.

4. References

J.U.Brackbill, D.B.Kothe, C.Zemach, ”A continuum method for modeling surface tension”, J. Comp. Physics 100, 335-354 (1992).

N. Tofighi, M. Yildiz, “Numerical simulation of single droplet dynamics in three-phase flows using ISPH”, Computers & Mathematics with Applications 66 (2013) 525–536, (2013).