PHASE FIELD MODELING OF MULTIPHASE SYSTEMS

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EXTENDED ABSTRACT

Research on multiphase flows is very active, even if its beginning dates back in the 19th century, when Young, Laplace and Gauss developed the first theory of multiphase flow, assuming that different phases are separated by a sharp interface, that is a surface of zero thickness. At the end of the 19th century, though, another approach was proposed by Van der Waals [1], who assumed that interfaces have a non-zero thickness, i.e. they are "diffuse" over a region where the interfacial forces are smoothly distributed. Later, in 1901, Korteweg continued this work and proposed an expression for the capillary stresses, which are generally referred to as Korteweg stresses, showing that they reduce to surface tension when the region where density changes from one to the other equilibrium value shrinks on to a sharp interface (see review articles in [2]).

We can appreciate the importance of the phase field, or diffuse interface, method when we compare it to traditional multiphase flow modeling. In classical multiphase fluid mechanics, we assume that each phase is at chemical equilibrium (i.e. its density and composition correspond to their equilibrium value at the given pressure and temperature) and are separated from each other by a zero thickness interface, where appropriate boundary conditions are imposed. On the other hand, in the phase field method the interface consists of a transition zone between the phases, of finite thickness, where all the properties of the mixture vary continuously. Clearly, the classical model ceases to apply when the lengthscale of the phenomenon is comparable with the interface thickness, as it happens in the motion of contact lines along solid surfaces, in the breakup and coalescence of bubbles and droplets, and, of course, in multiphase flows in micro devices. Instead, the phase field approach remains valid in all these cases and therefore, in particular, can describe microfluidic phenomena, which the classical multiphase approach cannot model. In addition, because the composition of the mixture is a continuous function, no separate description of the time evolution of the sharp interface is required, thus avoiding mathematical complexities and numerical instabilities typical of interface tracking.

Perhaps the best-known example of phase field model is the Cahn-Hilliard equation [3], that is used for modeling the phase separation of binary alloys that are quenched into the unstable region of their phase diagram. Here, the relaxation of the order parameter (i.e. the mixture composition) is driven by local minimization of the free energy, subjected to phase field conservation and as a result, the interface layers do not deteriorate dynamically. Other applications for which phase field models are particularly well suited are structure formation and evolution in flow systems, an area of technological impact in soft materials processing. There, hydrodynamics can be introduced by coupling the convective Cahn-Hilliard equation of mass transport to a modified Navier-Stokes equation of momentum transport, that includes a phase field-dependent body force, which is generally referred to as Korteweg force. This latter is proportional to the chemical potential gradients and, accordingly, since at thermodynamic equilibrium the chemical potentials are uniform, it can be seen as a non-equilibrium body force that tends to restore chemical equilibrium. [4]

The main drawback of the phase field approach is that its characteristic length coincides, approximately, with the interface thickness. Accordingly, even introducing corrections (which however are rigorously correct only for regular mixtures) to increase the size of the computing domain, we can simulate volumes of, at most, one millimeter size. Therefore, we can simulate the whole domain only when we are dealing with microfluidic problems. Unfortunately, though, fully implicit numerical treatment of interfacial terms yields expensive schemes while explicit discretization quickly lead to numerical instability or impose impractical time-stepping constraints. Here, we would like to propose an efficient and robust numerical method for the coupled Cahn-Hilliard/Navier-Stokes system.

REFERENCES

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