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MULTIPHASE MICROFLUIDICS:
THE DIFFUSE INTERFACE MODEL

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This volume contains 35 illustrations

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PREFACE

The aim of this text is to review the theory and describe some relevant applications of the interface diffuse model for one-component, two-phase fluids and for liquid binary mixtures, to model multiphase flows in confined geometries.

In classical models, multiphase flows are described assuming that the different phases are separated by a sharp interface, with appropriate boundary conditions. Imposing that the condition of local equilibrium is satisfied, physical properties such as density and composition are allowed to change discontinuously across the interface, so that one of the main difficulties of this approach consists in solving the free boundary problem and determine the position of the interface. In fact, interface tracking breaks down whenever the real interface thickness is comparable with the lengthscale of the phenomenon that is being studied, as it happens, naturally, in micro-devices. This problem arises elsewhere as well, such as in modeling drop coalescence and break up and in describing the wetting and de-wetting of solid surfaces. In these cases, it is more reasonable to use a different approach, as was proposed at the end of the 19th century by Rayleigh and Van der Waals, where interfaces have a non-zero thickness, i.e. they are diffuse, so that all quantities can vary continuously.

In the first chapter of this text, Lamorgese, Molin and Mauri review extensively the diffuse interface approach. The equations of motion are derived, showing how additional stresses, the so called Korteweg stresses, arise naturally as reversible body forces that tend to minimize the free energy of the system, acting exclusively in the interface region. Several case studies will be presented to demonstrate the advantages of the diffuse interface method in modeling multiphase flows in microdevices, as compared to the classical two-phase flow approach. Among the examples that will be presented, here we mention the following problems: a) mixing, spinodal decomposition and nucleation of macroscopically quiescent regular binary liquid mixtures; b) vapor-liquid phase separation of a single component fluid; c) heat transfer enhancement due to phase change; g) spontaneous emergence of complex structures during growth far from equilibrium.

This model is further extended in the second chapter by Park, Mauri and Anderson, to analyze the phase separation of regular ternary

liquid mixtures. Unlike critical binary mixtures, which during spinodal decomposition evolve into bicontinuous structures, ternary mixtures seem to lose such symmetry and therefore exhibit different scalings. A considerable emphasis is devoted to the advanced numerical modeling schemes that have been developed so far, stressing the computational difficulties encountered in implementing the diffuse interface method.

The third chapter consists of Thiele's account of the continuum approaches to thin films of liquid mixtures and, in particular, of recent studies of dewetting films for simple and complex liquids. After describing the basic dewetting models for one-layer single-phase liquid films, the case of binary mixtures undergoing both dewetting and decomposition processes is discussed, assuming that the films first decompose into stratified films and then evolve into lateral structures. Two approaches are presented: a two-layer sharp-interface theory in the form of coupled evolution equations for the layer thickness profiles and a diffuse-interface short-wave one-domain model, with boundary conditions at the sharp liquid-solid and liquid-gas interfaces. After describing the linear stability of stratified films, advantages and disadvantages of the diffuse interface model are analyzed as compared to the sharp interface approach.

Finally, in the fourth chapter, Plapp generalizes the diffuse interface approach to cases in which the phase field cannot be identified (as in the diffuse interface approach) with a physical quantity (coarse-grained on a mesoscopic scale), and instead can only be interpreted as a smoothed indicator function. In particular, a phenomenological phase-field model for solidification is introduced, showing that, with a proper choice of some interpolation functions, surface and bulk properties can be adjusted independently. The link between this phase-field model and the classic free-boundary formulation of solidification is established by the use of matched asymptotic analysis. As examples of applications of this approach, the solidification of alloys and the advected field model for two-phase flows are briefly discussed.

The text is addressed to doctoral students, young researchers as well as practicing R&D engineers, who are interested in microfluidics and, in general, with multiphase flows.

Roberto Mauri

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