The 18th International Conference on Finite Elements in Flow Problems (FEF2015)
16-18 March 2015, Taipei, Taiwan

Liquid-Vapor Phase Transitions: Thermomechanical Theory, Entropy Variable Formulation, and Boiling Simulations

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Key Words: *Phase-field model, Microforce theory, Van der Waals fluid, Entropy variables, Temporal scheme, Isogeometric analysis, Boiling flows.*

The Navier-Stokes-Korteweg equations were introduced as a phase-field model to describe liquid-vapor phase transitions. To date, there have been few numerical simulations performed for this system of equations, most of which focus on bubble dynamics and free surface problems. The full capability of this model has not been fully realized by the multiphase flow community.

In this work, we first derive a new modeling framework for multiphase flows, using the celebrated microforce theory developed by Gurtin [2]. Within this framework, once the explicit form of the thermodynamic potential is given, the model is closed and the second law of thermodynamics is satisfied automatically. In particular, by choosing the Helmholtz free energy function as the one given by van der Waals, the thermal Navier-Stokes-Korteweg equations derived by Dunn and Serrin are recovered, and their mysterious "interstitial working flux" [1] finds a new rational mechanics explanation.

In addition to the modeling, novel numerical technologies are developed for the thermal Navier-Stokes-Korteweg equations [3]. In the presence of a nonlocal surface energy term, the entropy variables are defined as functional derivatives of the mathematical entropy. This fact suggests that the entropy variables should not be looked upon as an algebraic change-of-variables but rather as a mapping from the conservation variables to their dual spaces. A weighted residual formulation based on the functional entropy variables leads to an unconditionally entropy-stable spatial discretization. Based on a family of new quadrature rules, a novel temporal scheme is developed. This scheme can be viewed as a second-order perturbed mid-point rule such that the temporal approximation is provably entropy dissipative. In contrast to the space-time formulation, this temporal scheme does not require

convexity for the entropy. This appealing property suggests that the new temporal scheme is applicable to a wide class of nonlinear problems.

The thermodynamically consistent algorithm is then applied to numerically investigating boiling phenomena by making appropriate assumptions on transport parameters and boundary conditions. Compared with traditional boiling models, the dependency on empirical knowledge is significantly reduced and there is no artificial modeling procedure involved. It will be demonstrated that this approach provides a unified predictive tool for both nucleate and film boiling. Two and three-dimensional simulation results will be provided and discussed.

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