Erratum: Lattice-Boltzmann algorithm for simulating thermal two-phase flow [Phys. Rev. E 61, 5295 (2000)]

Bruce J. Palmer and David R. Rector
(Received 24 January 2004; published 16 April 2004)

DOI: 10.1103/PhysRevE.69.049903 PACS number(s): 47.55.Kf, 47.11.+j, 02.70.−c, 05.70.Fh, 99.10.Cd

In this paper we presented a lattice-Boltzmann algorithm for simulating thermal two-phase flow in a fluid. An error in reducing the data from some of the simulations reported in our paper led us to conclude that the algorithm could successfully model evaporation of a fluid. A more careful analysis has forced us to conclude that the lattice Boltzmann algorithm cannot be used for quantitative simulations of evaporation or other thermally driven phase changes, except possibly under very limited circumstances. The results on evaporation, summarized in Fig. 4 of the original paper, are incorrect. These results were intended to show that the evaporation rate and thermal flux into the boundary are related to the standard boundary condition that links two fluid domains in a classical continuum formulation of evaporation. However, recent efforts to repeat these calculations show that there are large discrepancies between the simulations and the classically expected result. After discovering the mistake, we investigated this issue extensively and found that a major problem was that the continuum equations that the lattice-Boltzmann algorithm was designed to reproduce are, themselves, incapable of reproducing this boundary condition. Direct simulation of the continuum equations using standard finite difference methods showed that while the lattice Boltzmann and continuum results were in reasonable agreement with each other, neither was capable of reproducing the classical boundary condition. For most conditions, the errors between the enthalpy of vaporization calculated from the equation of state and the enthalpy calculated from the thermal and mass fluxes at the interface were between 20% and 50%. The addition of the pressure and viscosity terms to the continuum equations (which are missing in the lattice-Boltzmann formulation) did not improve agreement; in fact, the discrepancy got worse. The continuum equations used in this study are similar to other diffuse interface formulations of two-phase flow [1–3] and our results suggest that although the diffuse interface approach has been used successfully for isothermal modeling of two-phase systems, more care will be needed in formulating diffuse interface approaches to thermally driven phase changes. Current approaches, which rely on replacing the scalar pressure with the pressure tensor in the hydrodynamic equations, do not appear to be sufficient.

Another numerical error led us to overestimate the time step that can be used in simulations and resulted in quantitative changes in some of the results reported, but not qualitative changes. In particular, the use of Eq. (3.19) for the thermal conductivity did not work for systems containing both liquid and vapor phases (it does work for single phase simulations). The alternative method discussed in the paper, of fixing the value of τ_ϵ and k independently, does work and was used to redo the remaining simulations. The value of τ_e was set equal to 1.0. The single sided difference approximations to the numerical derivatives were also abandoned and conventional second order finite difference approximations were used. Generally, we found that once the error had been removed, it was necessary to use time steps that were about a factor of two smaller than those originally reported. Qualitatively, the results were similar to those in our original paper, the most significant differences are shown below for Fig. 5. The temperature profile in the new version of Fig. 5 appears to relax more quickly than in the original calculation, but qualitatively remains the same. The temperature profile for an equilibrium drop (Fig. 1 of our original paper) was no longer completely flat but the deviations remained quite small relative to the average temperature. The magnitude of the deviations appeared to decrease as the values of the grid spacing and time step decreased. Overall, our conclusions are that the algorithm is still useful for single-phase-flow simulations and is an improvement over an earlier two-distribution model [4], but cannot be used for quantitative simulations of thermally driven phase change, except in limited cases.

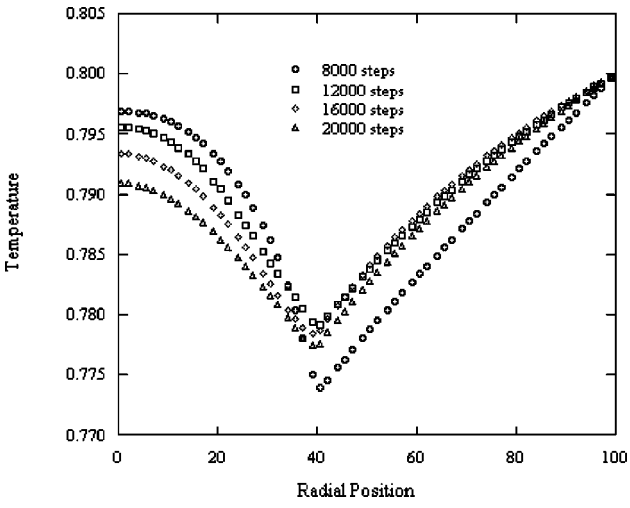

FIG. 5. Temperature profile for an evaporating drop at different times. The grid spacing is 0.5 and the time step is 0.05. These values are, respectively, one half and one quarter the values used in the original calculation.

[1] D. M. Anderson, G. B. McFadden, and A. A. Wheeler. Annu. Rev. Fluid Mech. **30**, 139 (1998).
[2] B. Ndiga and S. Zaleski Eur. J. Mech. B/Fluids **15**, 885 (1996).
[3] C. Denniston and J. M. Yeomans. Phys. Chem. Chem. Phys. **1**, 2157 (1999).
[4] B. J. Palmer and D. R. Rector, J. Comput. Phys. **161**, 1 (2000).