

Evaporation of a Suspended Droplet Using a Space-Time Least-Squares Spectral Element Method with C1 Hermite Elements for the Navier-Stokes-Korteweg Equations

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The evaporation of liquid droplets is a ubiquitous problem found in many engineering applications such as spray combustion and chip cooling. Due to experimental limitations to study such systems, numerical methods have been proposed to investigate the evaporation mechanism. However, the numerical methods can encounter some challenges related to the dynamics of the interfaces during phase change, in which mass transfer boundary conditions need to be specified. These heat and mass boundary conditions at the interface remain under scrutiny. To overcome this issue, diffuse-interface approaches based on the Navier-Stokes-Korteweg (NSK) equations have been proposed as an alternative. The NSK equations are a phase field model based on a constitutive law to represent the capillary stress acting in the interface region. The model is a set of third order PDEs derived from van der Waals theory of capillarity and uses the mass density as the parameter to distinguish the different phases so that the fluid properties vary continuously between phases. The NSK model presents an intrinsic thermodynamic consistency and is expected to provide a unified predictive capability for thermal phenomena. Numerical difficulties on the implementation of the NSK model arise due to the high gradient of the solutions within the interface region along with stability and accuracy issues. The non-monotone constitutive relation for the pressure may lead to unphysical behaviour in the phase mixture region. Also, the discretization of the system in conservative form leads to the occurrence of parasitic velocities inside the interface between the phases. A well-balanced scheme can be obtained by discretizing the system in a non-conservative fashion. Provided a sufficiently smooth solution, the construction of higher order schemes leads to more efficient algorithms. To that extent, the use of C1 continuous basis functions in the discretization of the domain has gained attention among practitioners. In this work, we describe a space-time formulation of the least-squares spectral element method for the NSK equations to simulate the evaporation of a suspended droplet in 2 dimensions. C1 Hermite elements are used for the domain discretization and a quantitative comparison with available solutions to the problem is carried out. Performance tests concerning grid resolution, time, accuracy and computational costs of the solutions are executed.

REFERENCES

- [1] A.Y. Snegirev, *Transient temperature gradient in a single-component vaporizing droplet*. Int. J. Heat and Mass Transf., Vol. 65, pp. 80-94, 2013.
- [2] L. Zhang, M.R. Tonks, D. Gaston, J.W. Peterson, D. Andrs, P.C. Millet and B.S. Biner, *A quantitative comparison between C0 and C1 elements for solving the Cahn-Hilliard equation*. J. Comp. Phys., Vol. 236, pp. 74-80, 2013.
- [3] M. Gumulya, R.P. Utikar, V. Pareek, R. Mead-Hunter, S. Mitra and G.M. Evans, *Evaporation of a droplet on a heated spherical particle*. Chem. Eng. Journal, Vol. 278, pp. 309-319, 2015.
- [4] K. Park, M. Gerritsma and M. Fernandino, *C1 continuous h-adaptive least-squares spectral element method for phase field models*. Comput. Math. Appl., Vol. 75(5), pp. 1582-1594, 2018.
- [5] K. Park, M. Fernandino and C.A. Dorao, *Thermal two-phase flow with a phase-field method*. Int. J. Multiphase Flow, Vol. 100, pp. 77-85, 2018.
- [6] E.J. Gelissen, C.W.M. van der Geld, M.W. Baltussen and J.G.M. Kuerten, *Modeling of droplet impact on a heated solid surface with a diffuse interface model*. Int. J. Multiphase Flow, Vol. 123, 2020.
- [7] S. Prasanna Raj Yadav, C.G. Saravanan, S. Karthick, K. Senthilnathan and A. Gnanaprakash, *Fundamental droplet evaporation and engine application studies of an alternate fuel produced from waste transformer oil*. Fuel, Vol. 259, 2020.
- [8] J. Lemoine and A. Münch, *A fully space-time least-squares method for the unsteady Navier-Stokes system*. J. Math. Fluid Mech., Vol. 23, issue 102, 2021.