The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5-9 June 2022, Oslo, Norway

A volume-of-fluid method for multicomponent evaporating two-phase flow

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Keywords: *Phase change, Multicomponent evaporation, Volume-of-Fluid*

Pure fluids are rarely encountered in nature and working fluids that are used in industry are no exception. For instance, liquid fossil fuels and renewable liquid biofuels are mostly multicomponent mixtures of organic compounds such as hydrocarbons or alcohols. To illustrate the role of multiple chemical compositions in evaporation we extended our previously developed VoF-based numerical method for weakly compressible phase-changing flows [1, 2] to the case of multi-component evaporation. Compared to the single-component counterpart, the presence of N evaporating species requires to solve N transport equations in the gas phase imposing a Dirichlet boundary condition at the moving interface, while $N-1$ transport equations are solved in the liquid phase imposing a Robin boundary condition at the interface. This strategy ensures not only the conservation of the transported species in both phases, but also the correct estimation of the mass fluxes (both the overall and the contribution from every species).
The resulting approach is built on top of a second-order accurate two-fluid Navier-Stokes solver coupled with an algebraic volume of fluid method (MTHINC) and extended with one equation for the thermal energy and the required number of transport equations for the vaporized liquid species. The method is first tested against the canonical benchmark of static and isolated droplet neglecting thermal effects. Moreover, the complex cases of non-isothermal evaporation both in laminar and turbulent conditions will be addressed and discussed. Finally, we will examine the influence of turbulence on evaporation and compare evaporation rates to the laminar case.

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