EXTENSIBLE VOLUME-OF-FLUID SOLVER FOR PHASE-CHANGE HEAT TRANSFER

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Phase-change heat transfer occurs in critical stages in most energy intensive technologies, and is often a bottleneck for efficiency and system intensity. Robust simulation tools are thus needed to investigate underlying phase-change transport processes and to inform device engineering. While mature software is available for adiabatic two-phase flow analysis, phase-change simulation approaches are still in their infancy. In most prior studies, investigators have extended adiabatic volume-of-fluid (VOF) solvers with thermal energy transport equations and coupled source terms for phase-change. Few of these codes are interoperable, publicly available, or actively maintained, leading to a great deal of repeated development and validation effort. Many different models have been proposed for these source terms (*e.g.*, [1]–[4]), each best suited to specific phase change processes. Here, we present a new extensible open-source VOF phase-change solver, *interThermalPhaseChangeFoam* (https://github.com/MahdiNabil/CFD-PC/), that supports run-time selection from multiple phase-change models (analogous to selection of turbulence models). Validated tutorial cases are provided for horizontal film condensation, smooth and wavy falling-film condensation/evaporation, nucleate boiling, and rising bubble condensation. With multiple implemented phase-change formulations and these demonstration cases, users can rapidly select a model and apply the solver to new applications of interest.

interThermalPhaseChangeFoam is based on the adiabatic two-phase VOF solver: interFoam [5]. The fluid is assumed to have constant density in each phase, yielding the continuity constraint with a phase-change dilatation source term ($\dot{v}_{\mathrm{pc}}$, Eqn. 1). The standard momentum equation is applied (Eqn. 2). The solver supports use of either hydrostatic-corrected-pressure ($p' = p - \rho g h$, $c_{\mathrm{hsp}} = 0$), or static pressure ($p' = p$, $c_{\mathrm{hsp}} = 1$). Additionally, support is provided for run-time selection of surface tension force models (from the formulations of [6]–[8]). The phase-fraction transport equation is employed (Eqn. 3), with a source term ($\dot{\alpha}_{1,\mathrm{pc}}$) for liquid-vapor phase change. A compressive velocity field (u') is employed here to counteract numerical diffusion of α_1. A thermal energy transport equation is specified with a phase-change heating term, neglecting pressure work and viscous dissipation (Eqn. 4). By default, fluid transport properties in each cell (μ, k) are evaluated as α_1-weighted arithmetic averages of phase values. The code also supports improved blending based on the relative orientation of the interface to cell faces (*i.e.*, whether phase-resistances act in serial or parallel [9]).

$$\frac{\partial u_i}{\partial x_i} = \dot{v}_{\mathrm{pc}} \tag{1}$$

$$\frac{\partial(\rho u_{\mathrm{i}})}{\partial t} + \frac{\partial}{\partial x_{\mathrm{j}}}\left(\rho u_{\mathrm{i}} u_{\mathrm{j}}\right) = -\frac{\partial p'}{\partial x_{\mathrm{i}}} + \frac{\partial \tau_{\mathrm{ij}}}{\partial x_{\mathrm{j}}} + c_{\mathrm{hsp}} \rho g_{\mathrm{i}} + f_{\sigma,i} \tag{2}$$

$$\frac{\partial \alpha_{1,\mathrm{pc}}}{\partial t} + \frac{\partial(u'_i \alpha_i)}{\partial x_i} = \dot{\alpha}_{1,\mathrm{pc}} \tag{3}$$

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial}{\partial x_{\mathrm{j}}}(\rho u_{\mathrm{i}} h) = -\frac{\partial}{\partial x_{\mathrm{i}}}\left(k_{\mathrm{eff}} \frac{\partial T}{\partial x_i}\right) - \dot{q}_{\mathrm{pc}} \tag{4}$$

Phase-change source terms ($\dot{v}_{\mathrm{pc}}$, $\dot{\propto}_{1,\mathrm{pc}}$, $\dot{q}_{\mathrm{pc}}$) are evaluated with run-time selected closure models that extends the abstract *thermalPhaseChangeModel* class. Each phase-change model must define a method for evaluating the thermal source term ($\dot{q}_{\mathrm{pc}}$). Overloadable default virtual methods are also provided for $\dot{v}_{\mathrm{pc}}$ and $\dot{\propto}_{1,\mathrm{pc}}$ (Eqn. 5, as defined in [4]).

$$\dot{v}_{\mathrm{pc}} = \frac{\dot{q}_{\mathrm{pc}}}{h_{\mathrm{LV}}}\left(\frac{1}{\rho_{\mathrm{V}}} - \frac{1}{\rho_{\mathrm{L}}}\right) \qquad \dot{\alpha}_{1,\mathrm{pc}} = -\frac{\dot{q}_{\mathrm{pc}}}{\rho_{\mathrm{L}} h_{\mathrm{LV}}} \tag{5}$$

The current solver release includes a number of phase-change models, including:

- **HiLoRelaxed** – This model applies phase-change source terms on the two-mesh-cell layer around threshold values of α_1 (different thresholds for evaporation and condensation). The phase-change rate is specified to return interface cells to T_{sat} at each time step ($\dot{q}_{\mathrm{pc}} = \rho c_{\mathrm{p}}(T - T_{\mathrm{sat}})/\Delta t$). Under-relaxation is supported to improve numerical stability.
- **HiLoRelaxedSplit** – This is a modified version of the above solver that shifts the liquid and vapor components of $\dot{v}_{\mathrm{pc}}$ slightly away from the interface cells to reduce interface smearing and improve conservation of each phase.
- **Yang** – This implements the model of Yang *et al*. [1] which specifies phase-change rates based on empirical constants (r_{L}, r_{V}) multiplied by the relative temperature difference from T_{sat} (*e.g.*, $\dot{q}_{\mathrm{pc,evap}} = r_{\mathrm{L}} \alpha_1 \rho_{\mathrm{L}} (T - T_{\mathrm{sat}})/T_{\mathrm{sat}}$).
- **None** – This model sets the phase-change source terms to 0, yielding sensible-only heat transfer. It is useful for debugging new case setups, and evaluating the significance of phase-change effect.

New phase change models are currently under development to account for interfacial resistance effects in small-scale flows and microlayer evaporation during boiling.

The solver is packaged with tutorial cases and mesh independence studies that demonstrate simulation of horizontal film condensation, smooth laminar falling-film condensation/evaporation, wavy falling-film condensation, nucleate boiling, and rising bubble condensation. As an example, results from the axisymmetric rising bubble condensation tutorial are presented in Fig. 1. Here, the liquid is initially subcooled by 1 K, the bubble is initially D = 460 µm, and fluid properties are: ρ_L = 900 kg m^{-3}, ρ_V = 10 kg m^{-3}, μ_L = 4.5E-3 kg m^{-1} s^{-1}, μ_V = 5.0E-4 kg m^{-1} s^{-1}, k_L = 1.0 W m^{-1} K^{-1}, k_V = 0.02 W m^{-1} K^{-1}, $c_{p,L}$ = 2.0 kJ kg^{-1} K^{-1}, $c_{p,V}$ = 2.5 kJ kg^{-1} K^{-1}, σ = 5E-3 kg s^{-2}, and h_{LV} = 2000 kJ kg^{-1}. At each time step, the domain velocity is corrected by the average gas-phase rise velocity, setting the simulation in the frame of reference of the bubble. The average condensation heat flux is presented in Fig. 1c, and compared with results from the correlation of Ranz and Marshall [10]. After start up (from t = 0.05 to 0.15 s), the average heat flux deviation is 5.6%. Varying the mesh resolution from Δr = 5.0 – 11.0 µm (over four cases) leads to a 6% variation of heat fluxes, which oscillate slightly with grid size.

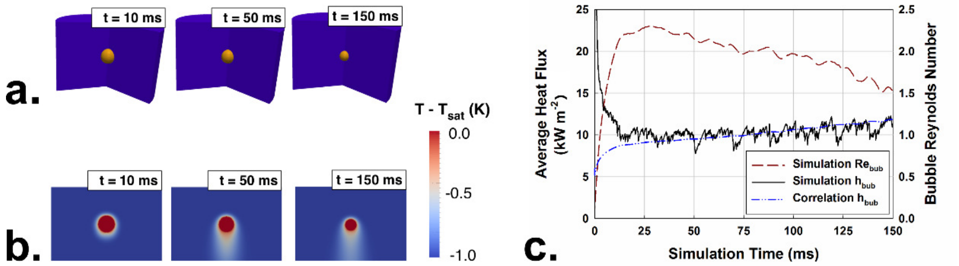

Figure 1: Condensing bubble (a) interface and (b) temperature profile. (c) Heat flux comparison with analytical correlation.

interThermalPhaseChangeFoam enables simulation of a broad range of condensation, boiling, and evaporation processes in a single environment. It includes multiple phase change models suited to different applications. One limitation of this solver is that it does not support geometric interface reconstruction. This limits the potential accuracy of surface tension force calculations. The VOF formulation conserves phase masses well, but the slightly smeared interface (typically ~3 cells) may be unacceptable for cases with thin boundary layers near the interface. Such interface-resolving limitations can be overcome with a sufficiently fine mesh near the interface. However, users must be careful, as extremely fine grids can amplify spurious currents. Thus, the current solver is best suited to cases where bulk liquid- and vapor-domain transport is important, as opposed to cases with dominant interface dynamics. The solver also assumes uniform densities in the two phases. This approximation is common for thermally driven phase change processes, but should be assessed for cases with large pressure or temperature variations. In ongoing work, this solver is being applied to study dropwise condensation and flow boiling. For the dropwise condensation problem, a new phase change model is being implemented framework that captures both macroscale and sub-grid scale heat transfer contributions (available in the *DropwiseSGS* git branch). This software is hoped to enable and accelerate the simulation of phase-change heat transfer, and serve as an asset to the thermal sciences and energy engineering communities.

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