Pseudo-boiling of supercritical water

R. Barney[a]*, R. McCallen[a], and J.P. Delplanque[b]
Corresponding author: rebecca.barney@ll.mit.edu

[a] Lawrence Livermore National Laboratory †
[b] University of California, Davis

Abstract: Supercritical fluid presents highly varying properties which contribute to an unstable fluid dynamics and interesting heat transfer characteristics. At different isobaric pressures above the critical pressure the property variations induce fluid to transition from liquid-like to gas-like. This research studies a natural convection cavity to simulate supercritical water, water above the critical temperature and pressure of 647K and 22.1MPa. Results show that a high-fidelity code developed at LLNL can capture the highly varying properties, unstable structures, and transition from liquid-like to gas-like in the supercritical fluid regime.

Keywords: Supercritical fluid, Computational Fluid Dynamics, Heat transfer, Pseudo-boiling, high-fidelity

The behavior of fluids at supercritical thermodynamic conditions is inherently complex due to large variations in thermodynamic and transport properties. Recent numerical and experimental investigations for a variety of applications illustrate ongoing interest for these fluids, especially for supercritical CO_2 and supercritical water. For example, supercritical water reactors (SCWR) operate in this extreme condition of high-pressure and temperature, resulting in highly dynamic flow fields and unexpected heat transfer characteristics. Heat transfer with the use of supercritical fluids is directly associated with the large property variations, like the thermal diffusivity, viscosity, and specific heat. The property changes through increasing/decreasing temperatures greatly affect the heat transfer from what is normally expected with single-phase fluids.

A natural convection cavity in a pseudo-two-phase flow regime is the focus of this research. The pseudo-two-phase flow in the supercritical hydrodynamic regime is a prominent area of research [1, 2, 3, 4, 5]. In the supercritical thermodynamic regime a gas-like and a liquid-like region are separated by the Widom line that is the locus of the maxima of the specific heat [6]. Along this Widom line the thermodynamic properties change drastically, as seen in Figure 1, where the density decreases 6-fold, viscosity drops by a factor of 2, while the specific heat spikes by an order of magnitude. The variations in density and viscosity, produce a thick pseudo-interface, and flow dynamics akin to film boiling.

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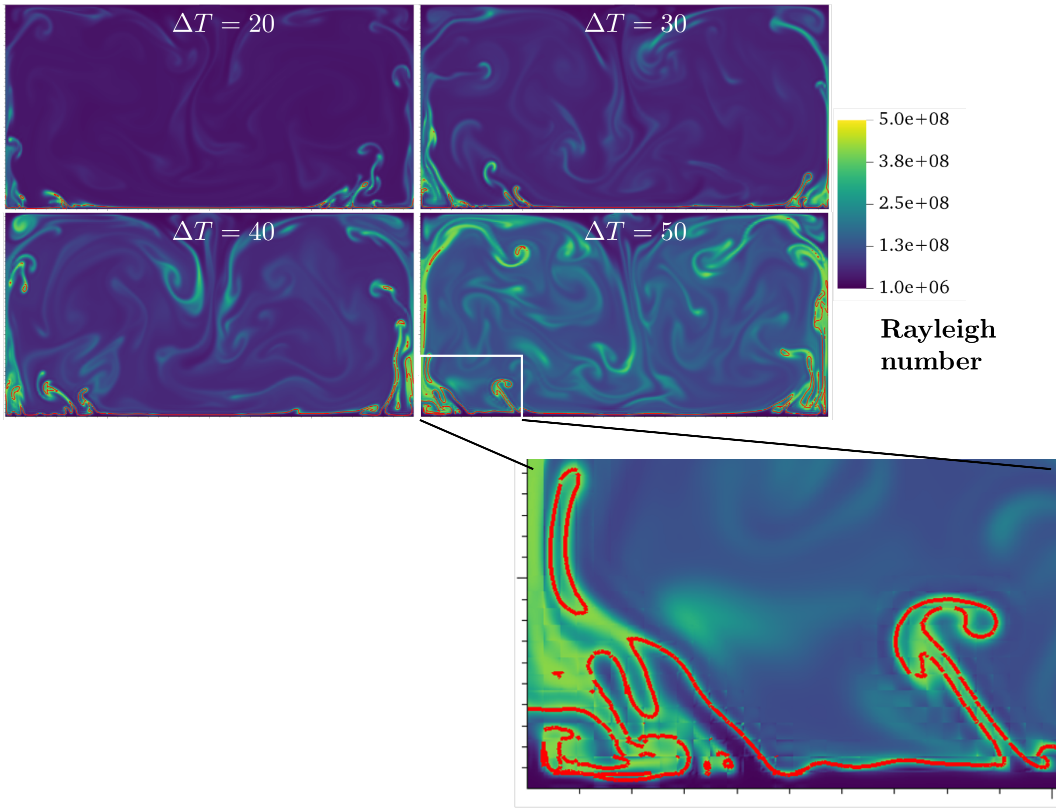

Figure 1: Colormap of Rayleigh number with the Widom line drawn in red. The wall temperature is increased from 660 K to 700 K.

To investigate the thermally driven hydrodynamic instabilities using supercritical water, a high-order fully-implicit numerical method is used. Such strong variations in thermophysical properties (in particular, density) are difficult to simulate and an altogether compressible framework is needed. Therefore, the compressible Navier-Stokes equations are solved without any additional assumptions. The fully implicit, high-order in space and time, reconstructed discontinuous Galerkin (rDG) method as implemented within the multi-physics code called ALE3D (Arbitrary Lagrangian and Eulerian in 2D and 3D), developed at Lawrence Livermore National Laboratory (LLNL), is used [7, 8]. This fully implicit, L-stable method accurately captures the compressible nature of the flow in the limit of very low Mach number. The rDG method solves for the lower order degrees of freedom and reconstructs, within each element, the higher order degrees of freedom.

Results demonstrate the ability of the simulation method to capture the pseudo-two phase regime, and Widom line accurately. Simulations results in Figure 2 show a pseudo-film at the heated wall of the cavity can be seen. The heated fluid at the bottom of the cavity is driven upwards by buoyancy forces and causes mixing in the cavity. The local Rayleigh and Richardson numbers can provide a map of the flow field and buoyancy forces, which drive mixing. The boiling curve is studied as well, showing an increase in heat flux with an increase in temperature differential between the wall and initial temperatures, similar to what is observed below the critical point.

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