Numerical Study on Liquid-Vapor Phase Change with Applications in Vapor Bubble Dynamics

By

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Abstract

This thesis presents a detailed analysis of vapor bubble dynamics and the interfacial process of liquid-vapor phase change. A spherically symmetric model for single vapor bubble is employed to present a numerical and theoretical analysis of the intermediate bubble collapse, where in contrast to the thermally induced or inertia dominated collapse, both the effects of liquid-vapor interfacial heat transfer and the advection of the surrounding liquid play an important role. The contrast in thermal, intermediate, and inertial behavior of collapse is represented in the form of a regime map defined by two non-dimensional quantities, $B_{sat}$ and $\xi$, which can be directly evaluated from the initial system conditions of collapse.

The same model is also used to simulate a spherically symmetric bubble growth configuration to assess the physical validity of a constant interface temperature assumption made by Highly-Resolved Simulation (HRS) studies aimed at solving flows undergoing phase change. Results show that HRS predictions are inaccurate during the initial period of bubble growth, which coincides with the inertial growth stage. A closed-form expression for a threshold time is derived, beyond which the commonly employed HRS assumptions hold.

Forgoing the limitation of spherical symmetry, the second theme of this thesis is on the development of a general two-phase flow solver that can handle the phase change process. Under a finite volume framework using a geometric Volume of Fluid (gVoF) approach, two key challenges with phase change flows have been addressed in this work, namely, (i) added deformation of the interface, and (ii) capture of velocity and pressure gradient discontinuity at the interface, both caused due to phase change. To track the interface in the gVoF scheme, an effective flux is defined that captures the effect of phase change on interface motion. This
method improves upon the source term approach used in other studies. For the solution of velocity, and pressure, a ghost fluid approach has been implemented, which is the first of its kind in a VoF-based phase change solver.
Chapter 1

Introduction

Bubble dynamics refers to the motion of an enclosed gas-filled entity present inside a liquid phase. Gas inside the bubble can be the vapor phase of the liquid that surrounds the bubble or a non-condensable gas, like air in water. The focus of this study is on the former, pure vapor bubbles. Such bubbles are oftentimes a point of interest in the context of boiling \([4–7]\) or cavitation \([8–11]\) phenomenon. Boiling refers to the process of vapor formation that occurs when liquid is heated beyond its saturation temperature (or boiling point); while cavitation is a term used for vapor formation due to sudden decrease in local pressure below its saturation value (de-pressurization) at the local temperature \([12]\). These phenomenon are important for several applications \([13]\), such as,

- for heat and mass transfer processes \([14, 15]\) in the power, electronics, and chemical industries,

- in dispersion processes \([16, 17]\) in petroleum industry and atmospheric processes, and

- in surface erosion \([18]\) processes for medical applications and in naval industry.
With such a wide range of applications, understanding the physics of bubbles has remained an active field of research in the past century.

Early research on vapor bubbles mainly relied on experiments [9, 19–31], and theoretical models that were essentially a reduced form of the Navier - Stokes equations [8, 10, 30, 32–40] under strict, simplifying assumptions. It has been well-established that vapor bubbles have a short length scale, and a small lifetime in physical processes, which implies clear limitations for experiments used to study bubble dynamics. Yet, excellent experimental works have provided insightful photographic evidence for bubble growth and collapse under various conditions that allowed for the validation or improvement of existing theoretical models [41]. While experiments have the factor of uncertainty, the theoretical analysis also tends to be impractical for realistic systems due to the departure from sphericity, presence of a multitude of bubbles, presence of multiple species/components, and a wide range of initial thermo-physical conditions. Nonetheless, they have provided a strong fundamental basis related to the governing mechanisms, and the relative importance of various physical factors in the process of bubble growth or collapse.

More recently, with the advancement in computing power, direct numerical simulations (DNS) have gained importance [11, 42–55]. Such analysis employs a solution for the numerically discretized form of the partial differential equations governing the coupled behavior of flow dynamics and energy transfer in a system of vapor bubbles. These methods are referred to as DNS methods with the underlying assumption that all time and length scales associated with the physical process are resolved in these simulations. However, to avoid ambiguity with different simulations, we prefer to refer to these methods as Highly Resolved Simulation methods or HRS methods. While powerful, the development of a robust and stable technique
using this method is not straightforward. Besides, there is a rapid increase in the computational cost for even moderately complex applications. Each mode of research must synergize with another, to provide meaningful insights about any process involving vapor bubbles.

This dissertation provides a numerical and theoretical take on the analysis for two of the most common phenomenon associated with vapor bubbles, namely, bubble growth and collapse. Furthermore, new ideas have been proposed as part of this thesis for the development of a generalized HRS method that can simulate the phenomenon of the phase change (boiling or condensation associated with vapor bubbles). Notably, the methods developed in this dissertation are not specific to any particular application and can be used to study any thermo-physical condition for vapor bubbles or phase change that satisfy the underlying assumptions of the proposed method.

The research work has been divided into three chapters:

- The work in chapter 2 is a detailed analysis of the physics of bubble collapse (Bardia and Trujillo [3]). At first, the existing literature about the physics of bubble dynamics is reviewed. Based on that, a numerical model is developed for a canonical system of single, spherical vapor bubbles from the two-phase momentum and energy equations. This model is then employed to obtain a bubble collapse rate for a range of system conditions. A closer look at the results revealed that certain cases of collapse had useful similar characteristics, and hence, a novel categorization for the process of vapor bubble collapse has been proposed.

- In chapter 3, the same model developed in chapter 2 is employed to study the limitations in existing HRS methods (Bardia and Trujillo [1]). These limitations are associ-
ated with the assumptions used to simplify the complex 3-D, coupled two-phase flow equations. An analytical expression is also proposed to circumvent these limitations.

- The third aspect of this research presented in chapter 4 describes the development of an in-house numerical solver for highly resolved simulations of vapor bubbles. The development focuses on the specific physical process of the phase change (evaporation or condensation), which is a critical surface phenomenon governing the behavior of vapor bubbles. The code has been developed using C++ within the OpenFOAM-v1706+ framework and builds upon the pre-existing two-phase fluid flow solver, *interIsoFoam*. Two key components have been completed and presented as part of this thesis:

  - A scalable and physically accurate tracking of the liquid-vapor interface, which deforms under the effect of bulk flow as well as phase change, and
  - A finite-volume Ghost Fluid Method (GFM) implementation to capture pressure gradient, and velocity discontinuities at the liquid-vapor interface arising due to phase change.

The novelty in this method especially stems from the enforcement of a jump in pressure gradient often ignored in older works [54, 56–60] of phase change numerical methods.

These modifications have been tested without the solution of an energy equation.

Remaining aspects of the proposed phase change solver related to the temperature equation and evaluation of the rate of phase change will be points of future work as described in chapter 5.