Capturing Liquid Thermodynamics in Bubble Collapse Using Tabulated Data

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**Abstract.** This study aims to improve the Kapila model, a mechanical equilibrium multiphase method, by incorporating complex equations of state for liquid and gas phases to accurately simulate realistic thermodynamics. While our previous research has explored the effects of real gas thermodynamics with a similar diffuse interface method, this study focuses on the limitations of simplified equations of state in capturing liquid thermodynamics. The authors argue that the use of a real liquid model such as International Association for the Properties of Water and Steam (IAPWS) database is necessary to avoid the temperature overprediction. This is further investigated in a bubble collapse case, revealing the importance of advanced liquid thermodynamics. Specifically, the study demonstrates a spurious liquid temperature jump near the bubble interface when a simplified equation of state is utilized.

1. Introduction

The detrimental effects of bubble collapse due to high velocities, pressures, and temperatures have long been recognized as a ubiquitous engineering challenge [1]. While prior research has primarily focused on the extremely high temperature of the bubble contents and its associated air dissociation and chemical reactions, the role of surrounding liquid thermodynamics in influencing the collapse phenomena has not been comprehensively elucidated. Nonetheless, it is well-established that the initial liquid temperature has a significant impact on both the dynamics and lifetime of the bubble [2], as well as its shape stability [3]. Additionally, experimental findings have demonstrated that cavitation damage to materials is influenced by liquid temperature through variations in the impact force of the liquid jet [4].

Numerical investigations have been conducted to explore the effects of liquid temperature on cavitation. In addition to prior studies utilising zero-dimensional models, such as Rayleigh-Plesset, several multidimensional CFD studies have been conducted on the thermal effects of liquid assuming both incompressibility and compressibility, along with the use of stiffened gas or Tait equations of state (EoSs). However, these EoSs fail to accurately represent the thermodynamic behaviour of liquids. In the present study, we draw attention to the thermodynamic errors associated with these simplified EoSs and investigate their impact on bubble collapse. It is noteworthy that the gas phase is elegantly modelled utilizing the Redlich-Kwong-Soave equation of state (RKPR EoS) that was previously introduced in our work [5]. Therefore, the present solver is capable of accurately capturing full real thermodynamic behaviour, thereby enhancing the fidelity of the simulation results.

1. Numerical method

In the present study, a 5-equation mechanical equilibrium multiphase model known as Kapila model [6] is employed to simulate bubble collapse. This model is derived from the full disequilibrium model of Baer-Nunziato [7] and is characterized by a zero relaxation time for velocity and pressure. Neglecting the effects of viscosity, heat conductivity, surface tension, and phase transition, we implement the Kapila model in both spherical and Cartesian coordinates to achieve a more comprehensive solver:

|  |  |
| --- | --- |
| $$\frac{∂q}{∂t}+\frac{∂F}{∂r}+\frac{∂G}{∂z}=s\_{nc}\left(q\right)+s\_{g}\left(q\right),$$ | (1) |

where:

$q=\left[\begin{matrix}α\_{1}\\α\_{1}ρ\_{1}\\\begin{matrix}α\_{2}ρ\_{2}\\\begin{matrix}ρu\\\begin{matrix}ρE\end{matrix}\end{matrix}\end{matrix}\end{matrix}\right], F=\left[\begin{matrix}α\_{1}u\\α\_{1}ρ\_{1}u\\\begin{matrix}α\_{2}ρ\_{2}u\\\begin{matrix}ρu^{2}+p\\\begin{matrix}\left(ρE+p\right)u\end{matrix}\end{matrix}\end{matrix}\end{matrix}\right],s\_{nc}=\left[\begin{matrix}(K+α\_{1})\left(\frac{∂u}{∂r}+\frac{∂w}{∂z}\right)\\0\\\begin{matrix}0\\\begin{matrix}0\\\begin{matrix}0\end{matrix}\end{matrix}\end{matrix}\end{matrix}\right]$, $s\_{g}=-\frac{β}{r}\left[\begin{matrix}-Ku\\α\_{1}ρ\_{1}u\\\begin{matrix}α\_{2}ρ\_{2}u\\\begin{matrix}ρu^{2}\\\begin{matrix}u\left(ρE+p\right)\end{matrix}\end{matrix}\end{matrix}\end{matrix}\right],$

in which parameter $β=2,0$ corresponds to the 1D spherical and Cartesian coordinates, respectively. The solver is developed in AMReX platform [8] using a FV Godunov method with MUSCL scheme for face reconstruction and HLLC solver for solving the Riemann problem at cell boundaries.

1. Results

The setup for a 1D spherical bubble collapse with $R\_{0}=1 $mm with domain length $L\_{0}=20 $mm using $2000$ cells is shown in Table 1. The RKPR equation of state has been used for air. For water, however, IAPWS and stiffened gas EoSs are utilised to make the comparison. The latter has been widely used in the literature due to its simplicity and capability to represent compressibility of water.

**Table 1**. Initial conditions for the collapse case with real thermodynamics

|  |  |  |  |
| --- | --- | --- | --- |
| $p\_{air}$ **(Pa)** | $p\_{f}$ **(Pa)** | $$ρ\_{air}\left(\frac{kg}{m^{3}}\right)$$ | $T\_{water}$ **(K)** |
| $$10^{5}$$ | $$8.7×10^{6}$$ | 1.225 | 288 |

In Figure 1(a), it is observed that the bubble dynamics obtained with both EoSs are in an excellent agreement with Keller-Miksis. However, the temperature prediction at the collapse moment in the vicinity of the bubble interface is different as shown in Figure 1(b). The stiffened gas EoS results in a of 30% temperature overprediction compared to the IAPWS EoS. Our analysis reveals that the stiffened gas EoS fails to accurately capture liquid thermodynamic behaviour, primarily due to the use of an unphysically large polytropic exponent of 4.4, as well as the simplified physical modelling, such as the neglect of molecular repulsive forces.

|  |  |
| --- | --- |
| (a) | (b) |

**Figure 1.** (a) Bubble dynamics and (b) water temperature predicted by IAPWS and stiffened gas EoSs.

This has been further depicted in Figure 2 where spatio-temporal change of the temperature is plotted. In Figure 2(b), the fake temperature front during the collapse only with the stiffened gas is evident.

|  |  |
| --- | --- |
| Chart, histogram  Description automatically generated(a) | Chart, histogram  Description automatically generated(b) |

**Figure 2.** Spatio-temporal change of the mixture temperature when using (a) IAPWS (b) stiffened gas EoSs for liquid.

Our future research identifies the shortcoming of the simplified liquid EoSs through a more concrete analysis of various thermodynamic models and their impacts on simulation of more complicated cases.

**Acknowledgments**

This work was supported by the European Union Horizon-2020 Research and Innovation Programme (UCOM Project), Grant Agreement No. 813766. Additional funding has been received by the UK’s Engineering and Physical Sciences Research Council (EPSRC) through grant EP/K020846/1. The authors would like to thank Prof. Stéphane Zaleski for the fruitful discussions and comments on this research.

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