

24th COBEM - 2017



24th ABCM International Congress of Mechanical Engineering
December 3-8, 2017, Curitiba, PR, Brazil

COBEM-2017-6909

3D NUMERICAL SIMULATIONS OF RAYLEIGH-TAYLOR INSTABILITY

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Abstract. Film boiling represents an important physical phenomenon since it's present in several engineering applications. Film boiling on a horizontal surface is a typical example of the Rayleigh-Taylor instability in which during film boiling, phase changes takes place at the interface. Rayleigh-Taylor instability occurs when a heavy fluid initially lies above a lighter one in a gravitational field. Initially, the vapor is in equilibrium with the liquid at the interface, and the direction of thermal transfer is from the vapor side to the liquid side. Numerical simulations of film boiling were performed using a uniform grid; then simulations were conducted with adaptive mesh refinement (AMR). Flow visualization revealed the formation of Rayleigh-Taylor instability with its two coherent structures; namely, bubbles and spikes. Thermal transfer rate at the heated bottom wall was evaluated by mean Nusselt number and compared to an experimental correlation in literature. Efficiency of AMR simulations were compared to simulations with uniform grid. Good agreement was found between thermal transfer rate computed in the present work and literature. In addition, AMR simulations were more than 200% faster than simulations with uniform grid and relevant computational resources were spared.

Keywords: Nusselt number, thermal transfer, baroclinic torque, CFD

1. INTRODUCTION

A particular case of natural convection in two-phase flow which has great relevance in nature and in science, is the one that occurs when Rayleigh-Taylor instability takes place. Rayleigh-Taylor instability is the result of baroclinic torque created by the misalignment of the pressure and specific mass gradients at the interface (Sidharth et al., 1991). Baroclinic torque is mathematically represented by the transport equation of vorticity which can be obtained by taking the curl of momentum equation. Equation (1) presents the mathematical representation of the vorticity transport:

$$\frac{D\vec{w}}{Dt} = -\vec{w}(\vec{\nabla}\vec{v}) + \frac{(\vec{\nabla}\rho \times \vec{\nabla}p)}{\rho^2} + (\vec{w} \cdot \nabla)\vec{v} + \frac{1}{Re}(\vec{\nabla}^2\vec{w}) \quad (1)$$

This instability has a particularly important application in inertial confinement fusion (Roberts et al., 2016). Rayleigh-Taylor instability occurs when a heavy fluid initially lies above a lighter one in a gravitational field (Sharp, 1988). Although Rayleigh-Taylor instability is rarely observed in its authentic form, it plays an important role in various natural and technological processes. The formation of bubbles from a vapor film beneath a liquid in film boiling is a classic example of relatively authentic Rayleigh-Taylor instability (Tryggvason, 1988). Sharp (1988) enumerated some examples of Rayleigh-Taylor instabilities in nature and in technological fields, such as overturn of the outer portion of the collapsed core of a massive star; the formation of high luminosity twin-exhaust jets in rotating gas clouds in an external gravitational potential; Laser implosion of deuterium-tritium fusion targets; electromagnetic implosion of a metal liner and several others cases.

Numerical results from computational simulations depends on the quality of the employed spatial discretization. Accurate numerical solution from the partial differential equations rely on the discretization on a computational grid with sufficiently high resolution; however, simulations using uniform grids overly increase computational costs due to a large domain region unnecessarily refined. Then, a uniform and fine grid is associated with a high computational cost which may limit the applicability of solving several complex problems of interest. Conversely, adaptive mesh refinement (AMR) is a computational tool allowing a criteria definition to guide a spatially non-uniform mesh refinement according to an indicator function, such as vorticity, temperature gradient or interface presence.

AMR may provide a strategy to solve complex problems using lower computational resources compared to uniform

grids (Akhtar and Kleis, 2013) and it reduces computational power requirement without affecting precision (Ningegowda et al., 2014). The interest in using AMR in multiphase flows is particularly high since the interface region requires a fine grid due to high gradients calculations and the rest of the domain usually do not require a fine grid (Nikolopoulos et al., 2007).

2. MATHEMATICAL MODEL

Since phase change is occurring at the interface, a source term at the interface is required to account mass balance. Then, continuity equation is given by the following expression (Akhtar and Kleis, 2013):

$$\vec{\nabla} \cdot \vec{v} = \int S \frac{1}{\rho} (\vec{x} - \vec{x}_k) \quad (2)$$

where the source term S is given by eq. (3):

$$S = \frac{\rho C_p (T - T_r)}{L} \quad (3)$$

where T_r is the reference temperature which was considered the temperature in saturation condition. Momentum equation is shown in eq. (4):

$$\rho \frac{D\vec{v}}{Dt} = -\vec{\nabla} p + \vec{\nabla} \cdot [\mu (\vec{\nabla} \vec{v} + (\vec{\nabla} \vec{v})^T)] + \rho \vec{g} \quad (4)$$

Finally, energy equation presents an additional source term to account the energy employed in phase change which is presented in eq. (5):

$$\rho C_p \frac{DT}{Dt} = k \nabla^2 T - \int S C_p (T - T_{ref}) (\vec{x} - \vec{x}_k) \quad (5)$$

3. COMPUTATIONAL PROCEDURE

Rayleigh-Taylor instability is simulated in non-isothermal two-phase flow in a cubic cavity with height aspect ratio of one. Null velocities and null pressure gradient were imposed to all the domain faces. The bottom and top walls have, respectively, a uniform high and low temperature. The south, north, west and east walls were considered adiabatic. Uniform grid simulations were conducted using 128^3 cells and AMR simulations were performed considering the most refined level with the same spatial discretization employed in the uniform grid simulation.

Computational simulations of film boiling were performed considering Jakob number of 1.0, Prandtl of 1.0 and Grashof number of 11200. A thin layer of superheated vapor lies under a saturated liquid and phase change occurring at the interface promotes the production of vapor from the saturated liquid. In addition, the baroclinical torque induces the formation of a mushroom-shaped bubble and spikes.

In order to simulate Rayleigh-Taylor instability, a numerical perturbation was applied to the physical model to promote the development of this flow instability. Then, the interface was initialized with trigonometric functions in order to create an initial perturbation, as proposed by Akhtar and Kleis (2013). The interface was initialized with a function that combines a reference height with trigonometric functions. Simulations were performed using a three-dimensional cubic cavity with flow subjected to gravity acceleration action, as shown in Fig. 1.

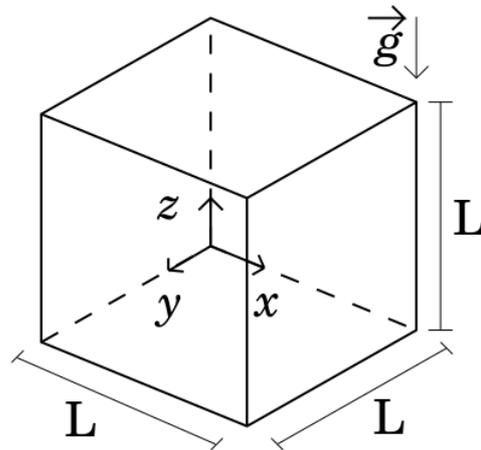


Figure 1. Physical model employed in the present paper

Domain boundaries were named according to geographic orientation which is illustrated in Fig. 2. The east and west walls have, respectively, a uniform high and low temperature. The south, north, bottom and top walls are adiabatic.

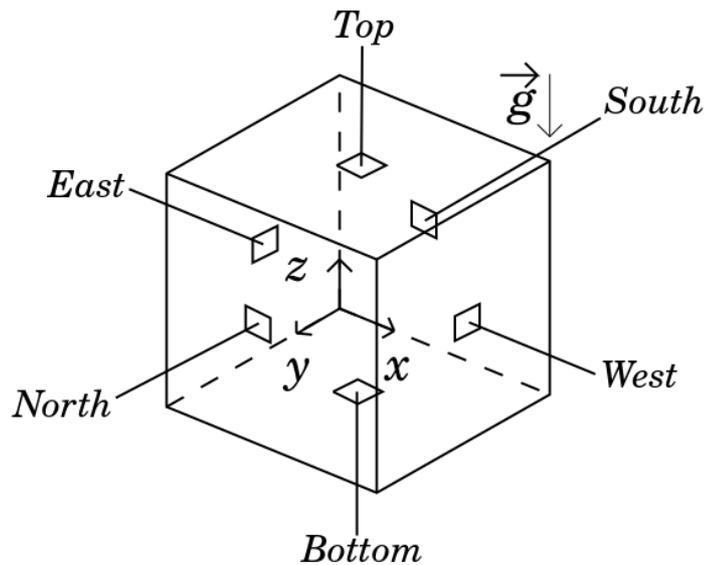


Figure 2. Domain boundaries names according to geographic orientation

4. RESULTS AND DISCUSSION

The two coherent structures that compose Rayleigh-Taylor instability are evident of identification in Fig. 3. Firstly, there are four noticeable spikes (fluid structure of heavy fluid growing into light fluid) and, secondly, one bubble (fluid structure of light fluid growing into heavy fluid) mushroom-shaped.

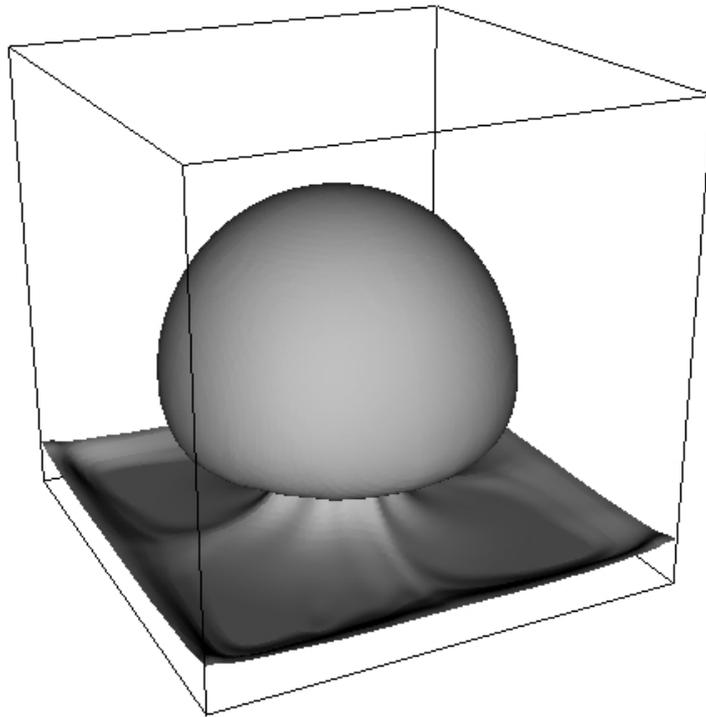


Figure 3: Rayleigh-Taylor at the final time of the simulation.

Rayleigh-Taylor instability is developed more slowly at the beginning of the simulation. The instability is developed in a faster mode when the velocity vectors, that promotes the baroclinic torque at the interface, increases in module. In addition, the mushroom-shaped bubble became more evident at the final stage of the simulation.

According to the simulations using AMR, regions away from the interface were solved with a relatively course grid. At the beginning of the simulation, the number of cells needed in the simulation with adaptive mesh refinement is more than 8 times lower than simulations using a uniform grid and, at the end, is more than 4 times lower.

Figure 4 shows mesh configuration at the initial time of the simulation, where a large region of the domain consist of a course grid and only a small portion of the computational domain comprises a fine mesh.

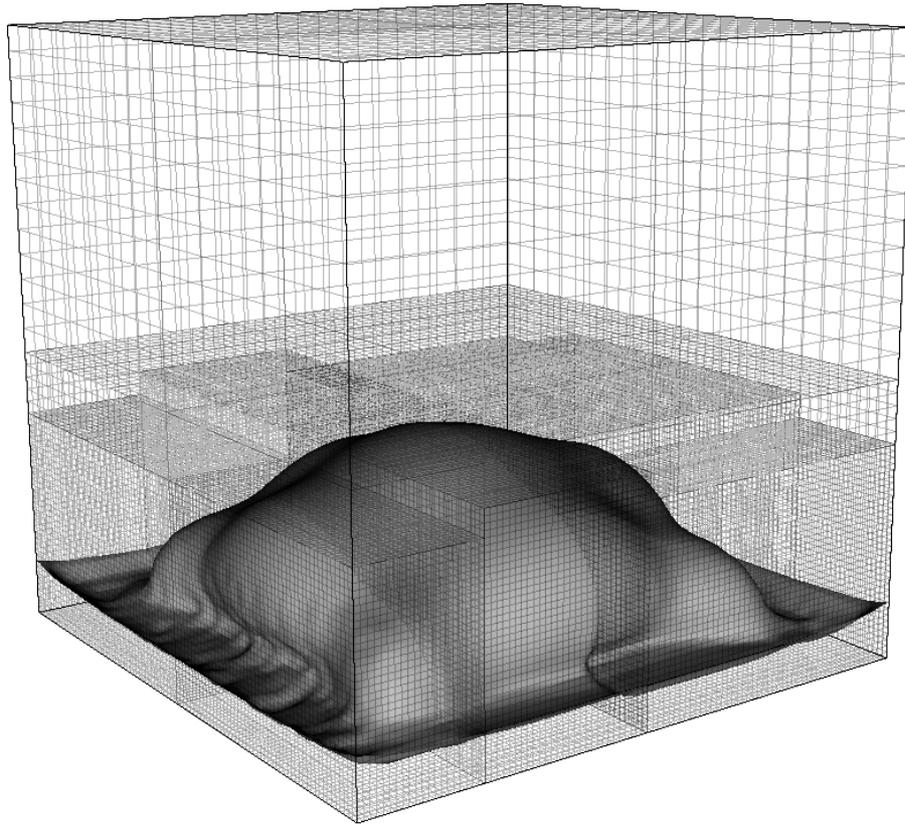


Figure 4: Rayleigh-Taylor with the mesh configuration at the initial time of the simulation.

Figure 5 shows the mesh configuration at the simulation's final time. At this moment, a large region of the domain requires a fine mesh due to the emergence of the interface in mushroom shape; however, it still requires much less cells compared to the uniform grid.

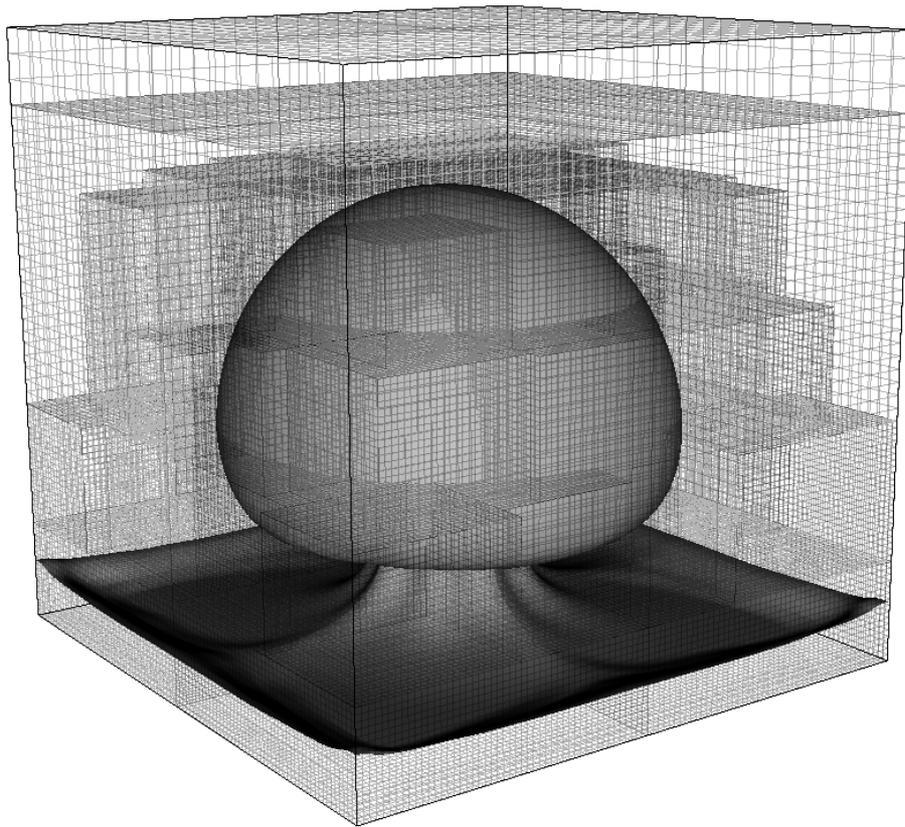


Figure 5: Rayleigh-Taylor with the mesh configuration at the final time of the simulation.

Figure 6 shows the temperature field and velocity vectors at simulation's final time. Velocity magnitude was higher at the mushroom neck where the baroclinic torque is more significant.

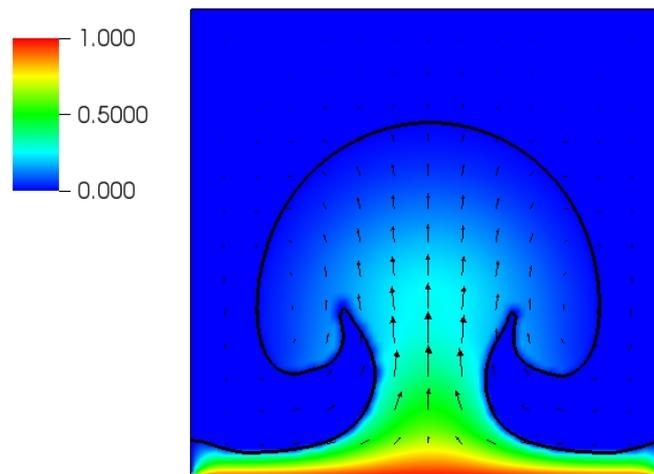


Figure 6: Rayleigh-Taylor temperature field and velocity vectors at simulation's final time.

Phase change at the interface considering Jakob number of 1.0 was confirmed by the formation of vapor from the saturated liquid. Mean thermal transfer rate at the heated wall (bottom wall) becomes nearly constant after the initial formation of the mushroom-shaped bubble, as seen in Akhtar and Kleis (2013).

Mean Nusselt number calculated at the bottom wall presented good agreement according to Klimenko's experimental correlation (Klimenko, 1981) with difference of about 3.5%. Klimenko's correlation (Klimenko, 1981) is given by eq. (6):

$$Nu = 0.425 \left(\frac{Gr Pr}{Ja} \right)^{\frac{1}{4}} \quad (6)$$

According to the numerical results obtained, adaptive mesh refinement was an important numerical strategy to simulate film boiling and particularly modelling the development of Rayleigh-Taylor instability since it saved significant computational resources and reduced the time required to perform the simulations of phase change.

Table (1) presents the computational time and the mean number of cells employed in the simulations. Since Rayleigh-Taylor instability develops more slowly at the beginning, only a small region of the domain required a fine grid for a large period of total time from the simulation process.

Table 1. AMR efficiency in the simulation of film boiling with Rayleigh-Taylor instability

Grid configuration	Number of cells	Time (h)
Uniform grid	2,097,152	76
AMR	295,000	32

The number of cells used in the uniform grid simulation was about 6 times larger than the mean number of cells used in the AMR simulation. Time needed to accomplish the simulation process was severely reduced; namely, it had reduced in 230%. Therefore, the employment of AMR allowed accurate numerical results in much less time and using smaller computational resources compared to simulations with the uniform grid.

5. CONCLUSIONS

Simulations of film boiling with a Rayleigh-Taylor instability were performed and validated with literature according to an experimental correlation of thermal transfer rate. The two typical structures (bubble and spike) from Rayleigh-Taylor instability were evidently seen.

AMR simulations provided great reductions in time and computational power required. Interface presence as refinement criteria was considered an adequate parameter to guide mesh refinement since the development of Rayleigh-Taylor and phase change process occurs at the interface between the two fluids.

6. ACKNOWLEDGEMENTS

The authors gratefully acknowledge financial support from Petrobras, CNPQ, Fapemig and Capes. The authors are also grateful to the Mechanical Engineering Graduate Program from the Federal University of Uberlândia (UFU).

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