Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Benchmark solutions

Numerical investigation on the mechanism of ligament formation aroused by Rayleigh–Taylor instability

Fushui Liu^a, Ning Kang^a, Yikai Li^{a,b,*}

^a School of Mechanical Engineering, Beijing Institute of Technology, Beijing 100081, China
^b State Key Laboratory of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, China

ARTICLE INFO

Article history: Received 1 March 2017 Revised 12 June 2017 Accepted 14 June 2017 Available online 16 June 2017

Key words: Interfacial dynamics Ligament formation Rayleigh–Taylor instability CLSVOF method

ABSTRACT

Ligament formation aroused by the Rayleigh–Taylor (R-T) instability is crucial to the secondary atomization of fuel drops in the internal combustion engine because it is a transition stage for a continuous bulk liquid to generate discrete droplets. In this paper, based on the detailed numerical data on the pressure and velocity fields, we investigated the mechanisms of how a ligament is generated from the interface due to a constant external acceleration. It is found that the maximum pressure location, which is formed due to the horizontal colliding flow from the trough portions, is a typical nonlinear characteristic and plays an essential role in ligament generation. The ligament above the maximum pressure location grows freely from the bottom bulk fluid region. In the nonlinear development of the interface deformation, the flow near the ligament root region reaches a steady state, in which the trough interface is discovered to retain a sinusoidal shape with a constant amplitude and descend at a constant velocity. The steady quantities, such as the dimensionless trough bottom descending velocity, U^* , amplitude of the trough surface, δ_0^* , and the distance between the maximum pressure location and the trough bottom point, ξ^* , are demonstrated. The effects of the Bond number and Reynolds number on the nonlinear dynamics during the ligament formation process are also discussed in this paper.

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1. Introduction

Liquid atomization [1,2] plays an essential role in the combustion efficiency and emission performance for the internal combustion (IC) engine (including Diesel engine and Gasoline Direct Injection engine, etc.) [3]. High quality of the liquid fuel atomization leads to small droplets, which favors fuel evaporating and air/fuel mixing process and eventually improves the combustion efficiency and emission performance. The size of the atomized fuel droplets directly depends on the secondary atomization, during which the droplets and ligaments are atomized through several breakup mechanisms [4–8]. With the increase of the injection pressure and the engine speed, the Weber numbers between the parent drops and gas flow become high and the Rayleigh-Taylor (R-T) instability tends to be predominant in the breakup process [9–12]. Thus, the research on the dynamics associated with the R-T instability becomes more and more imperative to better understand the fundamental mechanisms of atomization in the IC engine and to construct more precise atomization models for the industrial application.

http://dx.doi.org/10.1016/j.compfluid.2017.06.011 0045-7930/© 2017 Elsevier Ltd. All rights reserved.

R-T instability is aroused on the interface between two immiscible fluids if an external constant acceleration directs from the heavy fluid to light fluid. This phenomenon was first theoretically studied by Lord Rayleigh [13]. Taylor [14] then developed a linear analysis on the R-T instability without consideration of the capillary and viscous forces. They concluded that the linear R-T unstable wave amplitude grows exponentially with the growth rate $\alpha = \sqrt{ka_cAt}$, where k is the wave number, a_c is the net acceleration acted on the system, and $At = (\rho_H - \rho_L)/(\rho_H + \rho_L)$ is the Atwood number, where ρ_H and ρ_L are the densities of the heavy and light fluid, respectively. Later, Bellman and Pennington [15] and Piriz et al. [16] further developed the linear theory to incorporate the impacts of surface tension and viscosity, both of which play stabilizing or damping effects on the growth rate of the amplitude of the unstable wave. The comprehensive review on the effects of other physical properties, such as the density gradients, compressibility, etc., can be found in [17].

The linear analysis for the R-T instability is no longer valid when the amplitude of the unstable wave grows to be comparable with its own wavelength $\lambda = 2\pi/k$ [18–20]. The nonlinear effects aroused by the large surface deformation must be considered to accurately predict the dynamic behaviors of the R-T waves. Lewis [18] proposed an experimental apparatus for accelerating







^{*} Corresponding author. E-mail address: liyikai@bit.edu.cn (Y. Li).

small quantities of various liquids vertically downwards to study the R-T instability of a liquid-air system, which validated the linear theory until the surface wave amplitude reaches about 0.4λ . After a short transition stage, the air columns (or referred to as the bubbles) eventually penetrate through the liquid with a constant velocity *U* proportional to $\sqrt{a_c r}$, where *r* is the radius of curvature of the tip of the air column. This saturation behavior of the bubble penetration at the late-time stage is attributed to the nonlinear dynamics associated with the large surface deformation, which attracts great academic attentions of subsequent researchers. Based on the approximate potential flow analysis, Alon et al. [21], Goncharov [22] and Sohn [23] derived an expression of the constant bubble penetrating velocity of the R-T instability for arbitrary Atwood numbers, *i.e.*,

$$U = \sqrt{\frac{2At}{1+At} \frac{a_c}{C \cdot k}},\tag{1}$$

where C = 3 for the two-dimensional (2D) case and C = 1 for the three-dimensional (3D) cases. Instead, a simple drag-buoyancy model was proposed by Oron et al. [24] to study the nonlinear dynamics of the R-T instability, which gives the same constant bubble penetrating velocity as that derived by the potential flow model (Eq. (1)). Liu [20,25] investigated the cylindrical and spherical effects on the R-T instability in weakly nonlinear regime using the method of the parameter expansion up to the third order. They elucidated the interaction between different harmonic components of the R-T unstable waves. Waddell [26] performed an experiment in which a tank containing different fluids was accelerated downwards on a linear rail system to study the single-mode R-T instability at low Atwood numbers. The measurements showed that both the gas bubble and liquid spike velocities approach constant values at low Atwood numbers, which agree well with the analytical results derived by Oron et al. [24] and Goncharov [22]. In addition to the single-mode instability, numerous research groups have performed experiments on the multi-mode R-T instability in which an arbitrary disturbance is initially imposed on the interface [27–31].

With the development of computer speed and capacity, numerical simulations, which can exactly control the initial status and provide detailed information on the velocity and pressure fields, are usually used to study the dynamics associated with the R-T instability. With the inviscid and incompressible assumption, Baker et al. [32,33] simulated a 2D single-mode RT instability by a vortex numerical method to investigate the influence of the liquid depth on the surface dynamics, which is found to be changed significantly when the liquid depth is smaller than half the imposed unstable wavelength. Ramaprabhu et al. [34–36] carried out a series of simulations on the 3D single-mode R-T instability at different Atwood numbers ranging from 0.005 to 1. Their calculation results showed that when the densities of two fluids are on the same order, the bubble does not penetrate through the liquid with a constant velocity but undergoes a reacceleration process at very latetime stage because the secondary Kelvin-Helmholtz (K-H) instability is aroused on the liquid spike surface. To investigate the effect of the Reynolds number on the interfacial dynamics in R-T instability, Liang et al. [37] conducted a 3D simulation to track the interface behavior until the amplitude of the bubble reaches as high as $H = 5.5\lambda$ with the lattice Boltzmann method (LBM) at At = 0.15. Ramaprabhu et al. [38] and Li et al. [19,39] numerically studied the influence of time-dependent accelerations on the evolution of the single-mode Rayleigh-Taylor instability. Yang et al. [40] conducted a numerical study on the R-T instability in the presence of an external electric field for a wide range of fluid flow and electric field conditions. The turbulent mixing process and dynamics associated with the R-T instability was also numerically studied by Yongs and Zhang et al. [41,42] by imposing an initial disturbance consisting of different modes.

As shown above, there have been many theoretical, experimental and numerical works to study the nonlinear dynamics of the R-T instability, most of which focused mainly on the gas bubble dynamics. However, for the application of R-T instability to the secondary atomization in IC engines, the dynamics associated with the formation of the elongated liquid surface deformation (ligament) and its resultant breakup due to the R-T instability is of more importance. The mechanism of the latter process does not mainly depend on the way of the ligament formation, which has been extensively studied through the liquid column disintegration research [43–45]. On the other hand, previous studies lack detailed analysis on the velocity and pressure fields in the R-T instability, thus the microscopic mechanism on how the constant inertial force acted on the liquid and gas phases produces liquid ligament is still unclear. In this paper, we employed the coupled level-set and volume-of-fluid (CLSVOF) method [46-48] to study the nonlinear dynamics associated with the ligament formation process aroused by the R-T instability in 2D configuration, which shares the same fundamental mechanism of the ligament formation as the 3D case [19]. The numerical results of the velocity and pressure fields are analyzed in detail to elucidate the fundamental dynamics associated with the ligament formation. The effects of Reynolds number and Bond number are also systematically discussed.

The rest of this paper is organized as follows. In §2, the numerical methodology, including the physical model and the numerical solver adopted in this paper are described. Based on the detailed information on the velocity and pressure fields, the overall nonlinear dynamics associated with the ligament formation process induced by the R-T instability, as well as the effects of Bond number and Reynolds number, are discussed in §3. Finally, the conclusions drawn from this paper are given in §4.

2. Numerical methodology

2.1. Physical model

In this numerical study, as shown in Fig. 1, we considered a container filled with one fluid of density ρ_H lying on the horizontal bottom and the other overlying fluid of density ρ_L , where ρ_H $> \rho_L$. Both fluids are assumed to be Newtonian and incompressible since the characteristic velocities in both phases considered in this study are far smaller than the sound speeds. The two fluids are immiscible and the surface tension coefficient on the interface between them is σ . The whole system was accelerated downwards with a_c+g (where g is the gravitational acceleration) in the laboratory reference frame. Then in the reference frame attached with the container, an apparent upward inertial acceleration a_c would act on the heavy fluid towards the light fluid. Additionally, we assumed that only a single-mode R-T instability is aroused and the dimension of the container is far larger than the wavelength of the R-T waves, which means that the effect of container side-wall is negligible and the behaviors of the unstable R-T waves are repeated for each wavelength. Thus, only the dynamics occurring in one wavelength is needed to explore with appropriate boundary conditions.

The equations governing the motion of the fluids in the frame referring to the container bottom can be written as

$$\begin{cases} \nabla \cdot \mathbf{u} = 0\\ \rho(\phi) \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \rho(\phi) a_c \mathbf{e}_y + \mu(\phi) \nabla \\ \cdot \left[\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}} \right) \right] + \mathbf{F}_{\mathrm{s}} \end{cases}$$
(2)

where **u** is the velocity vector whose horizontal component is u and vertical component is v, p is the pressure, $\mathbf{e}_{\mathbf{y}}$ is the unit vertical vector, and μ is the dynamic viscosity. In this study, the surface tension force was modeled by the continuum surface force (CSF)

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