

A numerical strategy for investigating internal circulation in droplets

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The current study uses numerical approaches to investigate the effect of internal circulation on droplet dynamics. In jet atomization simulations, it is computationally expensive to track all droplets. A common way to reduce the computation expanse is to use Lagrangian strategy to treat small droplets. To better model Lagrangian-represented droplets in high temperature and pressure environment, the physical understanding of droplets need to be improved. In high temperature and pressure environment, the droplet shape and internal circulation should be considered. To study the mechanism on how droplet shape and internal circulation influence droplet dynamics, we will use direct numerical simulation (DNS) to simulate a droplet falling at its terminal velocity in high temperature and pressure air. An in-house code developed for interface-capturing DNS of multiphase flows will be employed for the computation.

I. Introduction

The combustion efficiency of a gas turbine is a major concern in industrial applications. The gas turbine combustion consists of a series of physical processes, including jet injection, jet atomization, droplet breakup, vaporization, and spray combustion, etc. In Figure.1, a 2D simulation using Herrmann's parameters [1] is performed to show the liquid jet atomization. A liquid jet is injected into a cross-flow, and the jet is atomized into large fragments. The action of surface tension is not enough to preserve these structures, and fragments will further breakup into small droplets to form spray. The total surface area of liquid phase will then be increased and enhance the combustion efficiency. To simulate droplet vaporization with high accuracy usually requires very fine mesh resolution, which is too computationally expensive in jet atomization simulations to track all droplets. One way to reduce the computation cost is to treat small droplets as Lagrangian particles. Therefore, we will need to improve the physical understanding of droplets to better predict the dynamics of droplets represented by Lagrangian particles. For gas turbine combustion, classical droplet models are incomplete, because in the high temperature and pressure environment, droplets are usually highly deformed, and the density of gas is significantly increased. As a result, the mass and heat diffusion timescales for the gas becomes comparable to that for the liquid, and the coupling between gas and liquid phases is enhanced. Therefore, a detailed

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study on droplet shape and internal circulation effect will be needed. To study their effect on droplet dynamics, we perform an in-house code developed by our group [2] for interface-capturing DNS of vaporization multiphase flows.

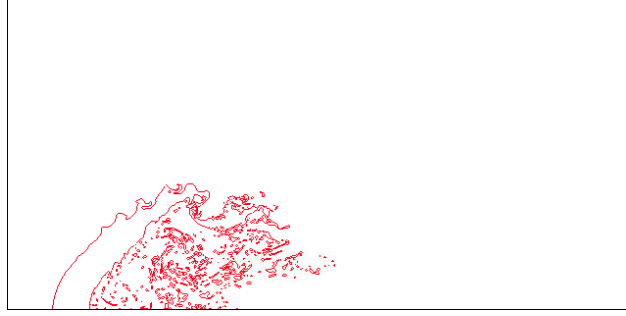


Fig. 1 2D jet cross-flow simulation using Herrmann's parameters [1]

II. Problem Formulation

To study droplet internal circulation, we consider an initially spherical droplet centered at a cubic computational domain $[8D]^3$, where D is the diameter of the droplet, and a uniform incoming gaseous flow will be entering the domain in a speed of U_{in} . By choosing the droplet's center of mass as the frame of reference, and utilizing an artificial gravity to balance the drag force, the droplet will be steady around the center of the computational box, and the velocity difference between the droplet and the gaseous inflow will be the terminal velocity of the droplet. The gas phase properties are chosen from dry air at an ambient gas temperature $T_{inf} = 1300K$, and the liquid phase properties at the phase interface is from n-decane at boiling temperature $T_{int} = 447.3K$. The mass fraction of the vapor is 1 at both the interface and the farfield. Constant thermophysical properties and unit Lewis number are assumed in the simulation.

III. Methodologies

A. Governing Equations

The governing equations for the conservation of momentum of both the liquid and gas phases used in our simulations are:

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \mu \mathbf{S} + \mathbf{f}, \quad (1)$$

where $\mathbf{S} = \nabla \mathbf{u} + \nabla \mathbf{u}^\top - \frac{2}{3} \nabla \cdot \mathbf{u}$, $\mathbf{f}$ is the external body force used for stabilizing the droplet in the frame of reference. The conservation of mass is guaranteed by solving the pressure term from the pressure Poisson equation.

B. Interface Capturing

A volume-of-fluid method (VOF) is employed to solve the liquid-gas interface. In VOF method, a scalar field called the volume fraction ϕ is defined. For computational cells entirely within the liquid phase, $\phi = 1$, and for cells within the

gas phase, $\phi = 0$. When the phase interface crosses a cell, the volume fraction will be within the range of $[0, 1]$, and the effective density and viscosity can be defined as:

$$\begin{aligned}\rho &= \rho_l \phi + \rho_g (1 - \phi), \\ \mu &= \mu_l \phi + \mu_g (1 - \phi).\end{aligned}\tag{2}$$

The effective density and viscosity are used to solve the momentum conservation equations of the gas and liquid together [2]. In this way, the velocity fields of the gas and liquid are treated as a union, and Eq.1 can be solved only once for one union velocity field. But the energy equation is still solved for each phase separately [3].

The evolution of the volume fraction field can be described by an advection equation with the velocity field to be the gas/liquid velocity [4]:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0.\tag{3}$$

C. Artificial Gravity

The droplet in the computational domain will move due to the drag force. In the desire of studying a stationary droplet, Palmore and Desjardins [5] derived a method that mimics the flow over a falling droplet at terminal velocity. In this method, the gravity is fixed and the terminal velocity is converged. However, due to the uncertainty of the drag coefficient caused by droplet deformation, the velocity reached will still be lower than the terminal velocity. To ensure constant terminal velocity was reached, Setiya and Palmore [6] developed a gravity update scheme to balance the changing drag force. Since the drag force is unknown explicitly, their method is based on a feedback control loop:

$$g^{n+1} = g^n + \frac{\alpha U_d}{\tau_c},\tag{4}$$

where U_d is the droplet velocity, α is an arbitrary weighting constant, and τ_c is the capillary time defined as $\tau_c = \sqrt{\frac{\rho_l + \rho_g}{\sigma}} \left(\frac{D}{2\pi}\right)^{\frac{3}{2}}$, where σ is the surface tension. This approach has higher robustness on inflow boundary conditions compared to [5]. Setiya and Palmore's results suggest $\alpha \geq 0.5$ is practical to finally balance the droplet, while $\alpha \ll 0.5$ will lead to significant shift of the droplet. See Figure.2.

We further improved Setiya and Palmore's approach by taking the displacement of droplet into consideration [7]:

$$g^{n+1} = g^n + k_U U_d + k_X X_d,\tag{5}$$

where X_d is the displacement of droplet, and k_U and k_X are the control parameters to be determined. Since the motion in x-direction is the most dominant, we only consider the component of U_d and X_d in x-direction. For the current setting, we set $k_U = 1/(2\tau_c)$ and $k_X = 0$, which is equivalent to $\alpha = 0.5$ in Equation.4.

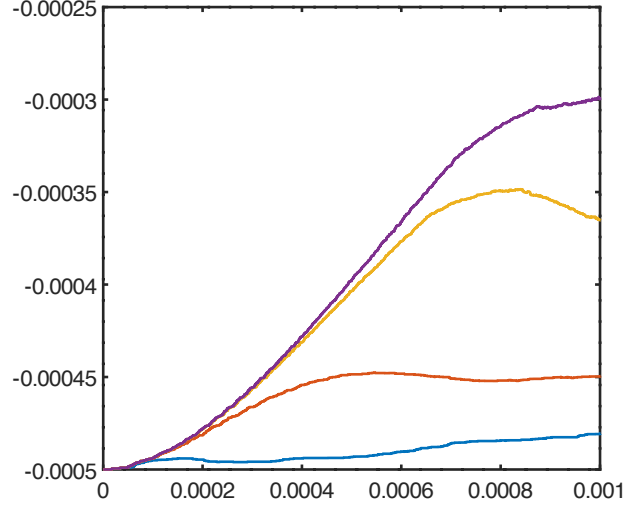


Fig. 2 X-position of droplet with time at $\alpha = 0.5$ (blue), 0.05 (orange), 0.005 (yellow), 0.0005 (purple); image courtesy from [6]

D. Controlling Parameters

The following non-dimensional groups in the following are the controlling parameters for this the problem we are investigating:

$$Re = \frac{\rho_G U_{in} D}{\mu_G}, \quad (6)$$

$$We = \frac{\rho_G U_{in}^2 D}{\sigma}, \quad (7)$$

$$\Lambda = \frac{\rho_L \mu_L}{\rho_G \mu_G}, \quad (8)$$

where Re is the Reynolds number of gas, We is droplet Weber number. For Λ , since we do not change viscosity in our simulations, it reduces to liquid-to-gas density ratio. The pressure of gas is proportional to its density through ideal gas law, therefore we control the pressure of gas by changing liquid-to-gas density ratio.

E. Internal Circulation

Because the gas and liquid phases are coupled through the continuity of velocity and shear stress at the phase interface [8], we choose the gas density to be the controlling parameter for changing the strength of internal circulation. To quantify the strength of internal circulation, several common physical quantities are considered, including the maximum liquid velocity, the maximum and mean vorticity of the droplet, and the droplet enstrophy. The definition of

vorticity ω and enstrophy $\mathcal{E}$ is:

$$\omega = \nabla \times U_L, \quad (9)$$

$$\mathcal{E} = \frac{1}{2} \omega^2, \quad (10)$$

where U_L is the liquid phase velocity field, ω is vorticity, and $\mathcal{E}$ is enstrophy. In addition, the Hill's constant is used to as a measure of internal circulation strength as well. The Hill's spherical vortex [9] is the simplest modelling to the droplet internal circulation, and the Hill's constant is a quantity derived from Hill's solution to represent the internal circulation strength. The vorticity magnitude of Hill's vortex is given by [10]:

$$|\omega| = 5A |\mathbf{r}| \sin \theta, \quad (11)$$

where $\mathbf{r}$ is any vector within the droplet from the droplet center, θ is the angle enclosed by $\mathbf{r}$ and the x-axis, and A is the Hill's constant representing the vortex strength. Its first approximation is given by Harper and Moore [11]:

$$A = \frac{3U_{in}}{2R^2}, \quad (12)$$

where U_{in} is the inflow velocity, R is the radius of the spherical droplet. In our code, the local Hill's constant is calculated by using the following expression:

$$A = \frac{\omega \cdot \mathbf{r}_t}{r \sin \theta}, \quad (13)$$

where $\mathbf{r}_t$ is the unit vector normal to $\mathbf{r}$ in y-z plane. When calculating the mean vorticity, enstrophy and Hill's constant, we will implement a volume integration over the droplet:

$$\bar{\psi} = \frac{1}{V} \iiint_V \psi dV, \quad (14)$$

where V is the volume of the droplet, ψ is any variable that need to be volume-averaged, and $\bar{\psi}$ is the volume-averaged variable. A limitation of numerical strategy for momentum solution is that liquid and gas velocity are solved on one field. For cells near the phase interface, large velocity difference might occur if gas velocity is included. To avoid including gas velocity in the calculation of circulation variables, we uses extrapolation method [12] to extend the liquid velocity to the whole domain, such that the velocity field used for calculation will be smooth.

IV. Results and Discussions

Various numerical simulations on droplet falling at its terminal velocity have been performed. The simulation parameters are listed in Table.1. Based on these parameters explored, we investigated the effect of liquid-to-gas density ratio and Weber number on the strength of internal circulation, as well as the correlation between droplet deformation and internal circulation.

Case	ρ_L/ρ_G	$P^* = P/P_{atm}$	Re	We
a1~a5	20	38.2	70	1,3,6,9,12
b1~b5	40	19.1	70	1,3,6,9,12
c1~c5	20,40,60,160,765	38.2,19.1,9.56,4.78,1.0	70	6

Table 1 Properties of the gas and liquid

1. Quantification of Droplet Internal Circulation

The aforementioned variables have been investigated in this section to see if they are appropriate for quantifying droplet internal circulation strength. Figure.3 shows how their behavior evolve over time when the droplet is deforming. For maximum values, as can be seen from Figure.3a-3b, they are not good choices for the quantification of internal circulation strength. The curves of maximum variables are not smooth and are deviating frequently. Numerical errors and the recognition of the phase interface will easily affect maximum values. Compared with maximum variables, volume-averaged variables are more suitable to quantify the strength of internal circulation, see Figure.3c-3e.

It should be noted that the Weber number will influence the shape of droplet. For $We \leq 6$, the droplet will deform to an ellipsoidal shape gradually. For $We = 9$, a thin flat disk will finally form. For $We = 12$ (which is not shown on the plot), the droplet will breakup at last.

After the internal circulation is fully established, case a4-a5 with larger We will decay immediately, while case a1-a3 with smaller We keep steady for a period of time and then decay. We found for $We = 9$, compared to cases with smaller We , its deformation is much stronger, see Figure.4. It indicates that the droplet deformation could be an explanation for the quick decay in internal circulation strength for $We = 9$. Therefore, both Weber number and droplet shape will influence the internal circulation strength.

2. The Effect of Pressure

We are concerned with what would happen on droplets under high pressure conditions, since such conditions resemble the high temperature environment in gas turbine combustion. To investigate the effect of pressure on droplet internal circulation, we fix $We = 6$, and vary liquid-to-gas density ratio ρ_L/ρ_G from 765 to 20, corresponding to change the pressure P^* from 1 to 38.2. As shown in Figure.5, for all of the three variables, higher pressure of the gas will have a stronger internal circulation strength. It indicates an enhancement of the coupling between the gas and liquid phase in

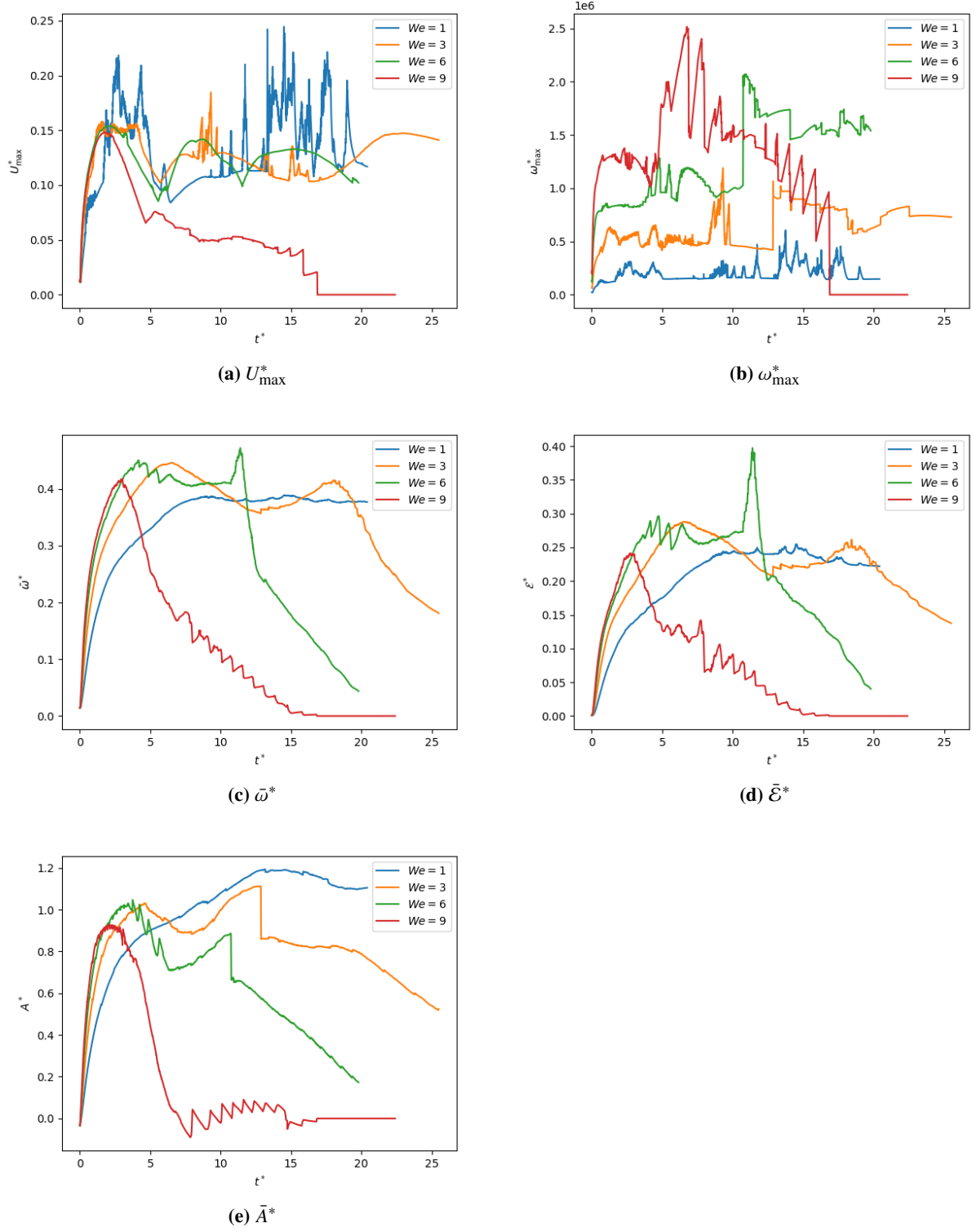


Fig. 3 Variables used for quantification of the strength of droplet internal circulation; $\rho_L/\rho_G = 20$. Asterisk means the variable is non-dimensionalized. $U_{\max}^* = U_{\max}/U_{in}$, $\omega^* = \omega/(U_{in}/D)$, $\mathcal{E}^* = \mathcal{E}/(0.5 (U_{in}/D)^2)$, $A^* = A/(U_{in}/D^2)$, $t^* = t/\tau_c$.

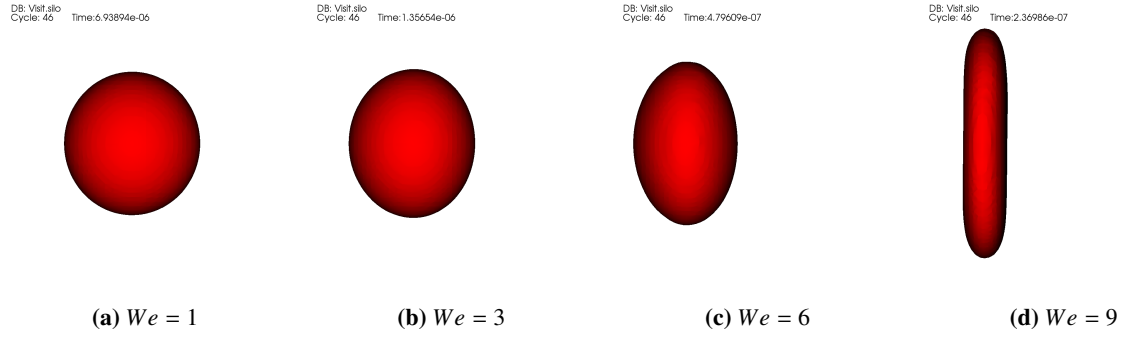


Fig. 4 Droplet deformation for case a1-a4 with $P^* = 38.2$ at $t^* = 15$. t^* is the non-dimensional time normalized by the capillary time τ_c .

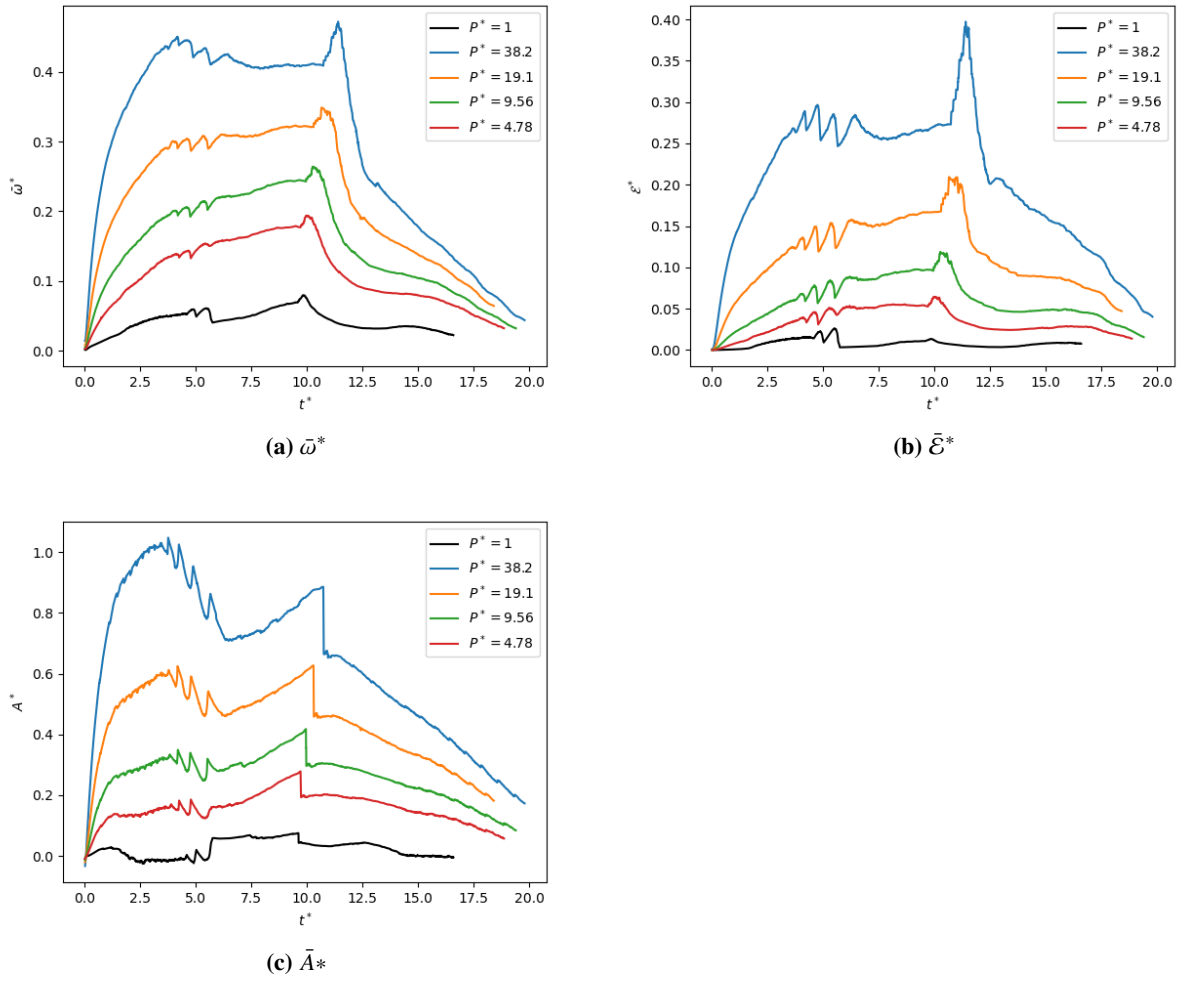


Fig. 5 Effect of pressure on the strength of droplet internal circulation at $We = 6$.

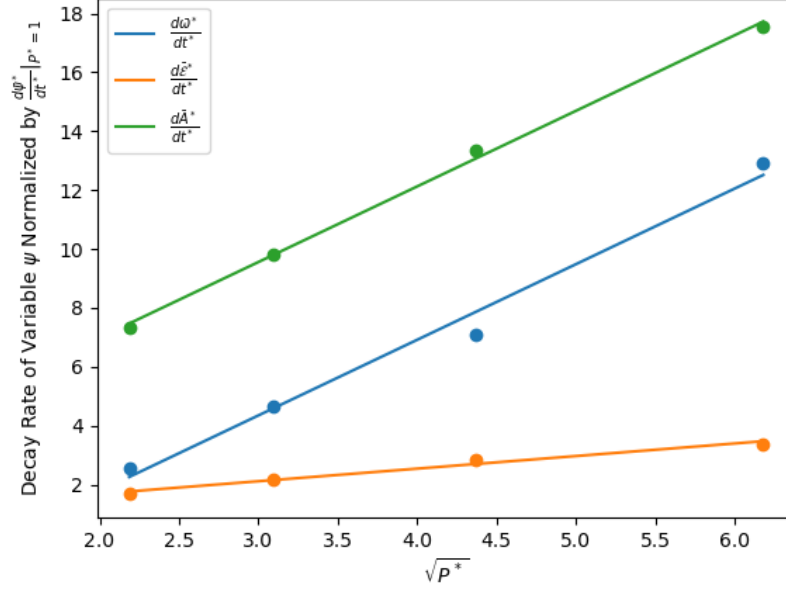


Fig. 6 Decay rate correlation with $\sqrt{P^*}$; the decay rate of each variable is normalized by its decay rate at atmospheric pressure; straight lines are fitted results, and points are data from simulations.

high pressure conditions. For $P^* = 1$, the internal circulation strength is close to 0, corresponding to a case that the interaction between the gas and liquid is negligible under atmospheric pressure.

The decay rate of vorticity, enstrophy and Hill's constant is estimated by fitting the data ranging from $t^* \in [16, 20]$, and the results can be seen in Figure.6. A linear correlation of decay rate to the square root of pressure can be found:

$$\frac{d\bar{\omega}}{dt}, \frac{d\tilde{E}}{dt}, \frac{d\tilde{A}}{dt} \sim \sqrt{P^*} \quad (15)$$

3. Droplet Drag Coefficient

We are also interested in how the drag coefficient C_d is correlated to the shape of droplet. For simplicity, we consider the Weber number to be the parameter that represents the droplet shape, and then examine its effect on drag coefficient. The drag coefficient is computed from the following expression:

$$\frac{1}{2} C_d \rho_L U_{in}^2 \pi \left(\frac{3V}{4\pi} \right)^{2/3} = (\rho_L - \rho_G) g V \quad (16)$$

As shown in Figure.7, a higher Weber number corresponds to a larger drag coefficient. Look back to Figure.4, the drag coefficient on a more deformed and flattened droplet will be higher. Besides, the steadiness of the drag coefficient also proves that our gravity update scheme works well.

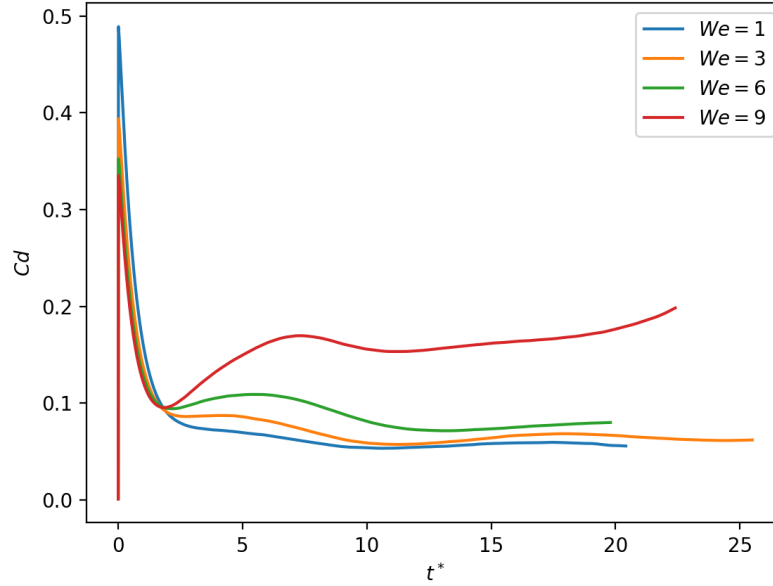


Fig. 7 Drag coefficient C_d on different We at $P^* = 38.2$ versus t^*

V. Conclusions

In this work, the strength of the internal circulation of a droplet falling at its terminal velocity has been studied. A control-loop based gravity update scheme is developed to keep the droplet balanced in the simulation. We select several variables to represent the internal circulation strength, and it comes out that volume-averaged variables, such as mean vorticity, enstrophy and Hill's constant, are more suitable for the quantification. We have found that the droplet Weber number and droplet shape will influence the internal circulation strength, but it should also be noted that the shape of droplet is also affected by the Weber number. At $We = 6$, we found the droplet internal circulation would be enhanced with higher pressure of gas. The drag coefficient is found to be positively correlated to the Weber number.

Acknowledgements

This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1548562.

The authors acknowledge the Texas Advanced Computing Center (TACC) at The University of Texas at Austin for providing HPC, visualization and storage resources that have contributed to the research results reported within this paper. URL: <http://www.tacc.utexas.edu>

The authors acknowledge Advanced Research Computing at Virginia Tech for providing computational resources and technical support that have contributed to the results reported within this paper. URL: <https://arc.vt.edu>

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