Numerical and Analytical Study of Large Amplitude Shape Oscillations of Viscous Droplets

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Introduction

Droplet oscillations, despite being seemingly simple and inconspicuous, play a crucial role and significantly contribute to various natural and industrial processes. The mathematical foundation for understanding these oscillations was first theorized over 140 years ago by Lord Rayleigh [4] and has since become central to fluid dynamics research. Understanding droplet dynamics is crucial for optimizing many modern technical processes. Various theoretical models and experimental studies have investigated droplet oscillations across a range of conditions, from small deviations from the initial spherical shape with inviscid droplets to those with large amplitudes, high viscosity and nonlinear oscillation behavior [1, 3, 7, 9].
This study extends these seminal works by examining in detail the impact of the following three specific factors on droplet oscillations. First, large initial aspect ratios and amplitudes, denoted as $\varepsilon = R_{ax}/R_{rad}$. Second, it explores varying material properties, with particular focus on liquid viscosity characterized by the Ohnesorge number $Oh = \mu_l/\sqrt{\rho_l \sigma D_0}$. Finally, it investigates different initial droplet shapes, comparing ellipsoidal forms to spherical harmonics of order 2. The effects of these factors are analyzed in terms of oscillation frequency f, the time spent in prolate and oblate shapes t_p, t_o, and the total energy budget E_{tot} contained in these shapes. The primary goal is to present a novel methodology for analyzing data obtained from highly resolved direct numerical simulations (DNS) conducted with ITLR's Free Surface 3D (FS3D) multiphase flow solver, thereby facilitating the comparison and extension of existing analytical models and approaches.

Fundamentals and Computational Setup

This study utilizes the ITLR in-house multiphase code FS3D, which solves the incompressible Navier-Stokes equations via direct numerical simulations. The code employs a finite volume approach on a staggered Cartesian grid to conserve mass and momentum. The classical Volume-of-Fluid (VOF) method is used by introducing an additional scalar field denoting the volume fraction of the fluid in each computational cell to distinguish between the liquid (subscript l) and gaseous (subscript g) phases. An additional transport equation tracks the advection of the liquid phase. The Piecewise Linear Interface Calculation (PLIC) algorithm is applied to accurately capture the interface and minimize numerical diffusion. Complete volume conservation during advection is ensured by treating the dilatation term, which occurs due to the directional splitting of the transport equation, as proposed by Weymouth and Yu [8]. Both phases are treated as a single fluid in a one-field formulation, with physical properties calculated locally based on the local VOF-value of the scalar field. FS3D is fully parallelized with MPI and OpenMP, optimized to run efficiently on the HPE Apollo supercomputer *Hawk* at the High Performance Computing Center Stuttgart (HLRS), where all simulations for this study were performed. For additional details on the numerical methods and capabilities, see Eisenschmidt et al. [2].

For the numerical study of droplet oscillations in a gaseous surrounding environment, a three-dimensional cuboidal Cartesian grid is used. A single liquid droplet is centered in the domain, with boundary conditions set far from the droplet to avoid boundary effects. The droplet is resolved with 85 grid cells per diameter, as verified in Reutzsch et al. [5]. The boundary conditions are zero gradient, gravity is neglected and the balanced CSF (bCSF) surface tension model is employed. To induce oscillations, the droplet is initialized with shapes deviating from the spherical form, such as ellipsoids with aspect ratios $\varepsilon = R_{ax}/R_{rad}$ (where R_{ax} and R_{rad} are

the axial and radial radii, respectively) or higher-order Legendre polynomials. Material properties and parameter ranges for ε and Oh for the present study are given in Tab. 1.

The droplet shape oscillation data is analyzed by extracting the time spent in prolate (t_p, $\varepsilon > 1$) and oblate (t_o, $\varepsilon < 1$) shapes, as well as the oscillation frequency $f = 1/(t_o + t_p)$. Additionally, the energy budget, encompassing surface energy E_σ and kinetic energy E_{kin}, with total energy defined as $E_{tot} = E_\sigma + E_{kin}$, is tracked. Non-dimensional parameters are used for evaluation and plotting the results. These are for the time $\hat{t} = t/\tilde{t}$, for the frequency $\hat{f} = f/\tilde{f}$ and for the energy $\hat{E} = E/\tilde{E}$, using the following parameters for non-dimensionalization $\tilde{t} = \sqrt{\sigma/(\rho_l R_0^3)}$, $\tilde{f} = \sqrt{8\sigma/(\rho_l R_0^3)}/(2\pi)$ and $\tilde{E} = R_0^2\sigma$.

Results and Discussion

The left graphs of Fig. 1-3 quantify the investigated effects on the evolution of the nondimensional oscillation frequency $\hat{f}$ as a function of the droplet's instantaneous aspect ratio $\varepsilon > 1$. The top row illustrates the impact of increasing elongation/amplitude ε, the second row shows the influence of viscosity through the Ohnesorge number Oh and the third row compares the initial shapes of an ellipsoid with those of a spherical harmonic of order 2.

As ε decreases over time due to viscous damping, the oscillation period shortens, leading to an increase in frequency. Consequently, $\hat{f}$ increases and eventually converges non-monotonically towards $\hat{f} = 1$, aligning with predictions by [3, 9]. While this method of analyzing and plotting $\hat{f}$ over ε is well-established in literature, novel observations emerge in cases of large amplitudes, high viscosities and varying shapes. Specifically, for large amplitudes $\varepsilon > 1.5$, an spreading of curves and increase in frequency is observed, which deviates from predictions by linear theory or conventional models. Additionally, increasing Oh, which corresponds to higher liquid viscosity, results in a decreased oscillation frequency, particularly in the later stages of oscillation for $\varepsilon < 1.3$. When comparing a regular ellipsoid with a droplet initialized as a second harmonic, differences arise, with the second-order harmonics case displaying higher frequencies for the same initial elongation, particularly for $\varepsilon > 1.3$. This may be explained by nonlinearities and mode coupling between higher and lower oscillation modes.

Given that droplet oscillation dynamics are governed by the interplay of kinetic energy, surface tension and viscosity, which together dictate the droplet's shape and stability, analyzing this interaction by plotting the energy at specific phases (e.g., oblate or prolate) is insightful. This is illustrated in the right plots of Fig. 1-3, where the total nondimensional energy $\hat{E}_{tot}$ is plotted against $\hat{t}_o$ and $\hat{t}_p$. Remarkably, all cases (varying ε, Oh and initializations) consistently collapse onto a single curve. During the prolate phase ($\hat{t} > 1.12$), the time spent in this shape increases linearly with total energy $\hat{E}_{tot}$, correlating with an increase in droplet elongation ε. Conversely, in the oblate shape, $\hat{t}_o$ asymptotically approaches ≈ 0.98 as $\hat{E}_{tot}$ increases. Notably, for higher viscosities ($Oh \gtrsim 0.006$) and larger elongations for different initial shapes, deviations from this curve occur, which are not predicted by analytical models.

The right plot of Fig. 1 additionally shows results from an analytical model recently proposed in [6] that predicts the dynamics of an oscillating droplet in an immiscible fluid, by solving the mechanical energy balance over the droplet using a generalized curvilinear coordinate system. The model assumes irrotational potential flow in both the inner and outer fields, accounting

Table 1. Material properties of the liquid and the gaseous phase with the investigated ranges from the conducted simulations.

Liquid Properties				Gaseous Properties		Investigated Range	
ρ_l	μ_l	σ	D_0	ρ_g	μ_g	ε	Oh
$\mathrm{kg\,m^{-3}}$	$\mathrm{mPa\,s}$	$\mathrm{mN\,m^{-1}}$	mm	$\mathrm{kg\,m^{-3}}$	$\mathrm{mPa\,s}$	$-$	$-$
998.2	1.00153	72.75	1.000	1.204	0.01821	$1.05 - 2.5$	$5.9 \cdot 10^{-4} - 5.9 \cdot 10^{-2}$

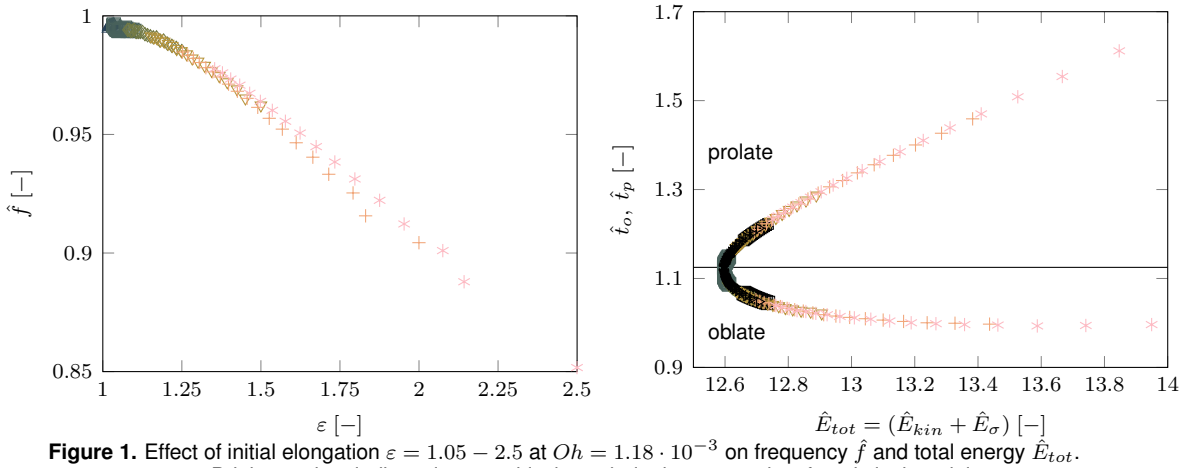

Figure 1. Effect of initial elongation $\varepsilon = 1.05 - 2.5$ at $Oh = 1.18 \cdot 10^{-3}$ on frequency $\hat{f}$ and total energy $\hat{E}_{tot}$. Brighter colors indicate larger ε, black symbols denote results of analytical model.

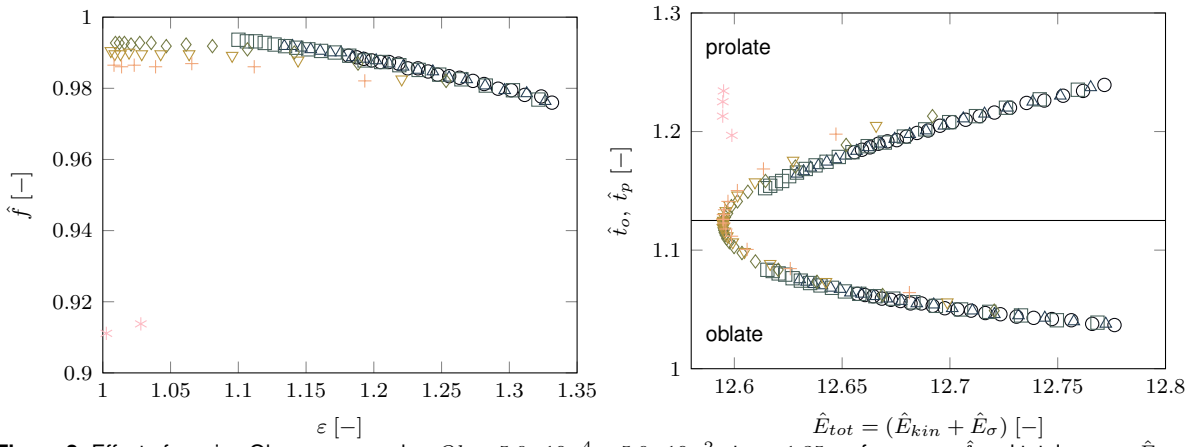

Figure 2. Effect of varying Ohnesorge number $Oh = 5.9 \cdot 10^{-4} - 5.9 \cdot 10^{-2}$ at $\varepsilon = 1.35$ on frequency $\hat{f}$ and total energy $\hat{E}_{tot}$. Brighter colors indicate larger Oh.

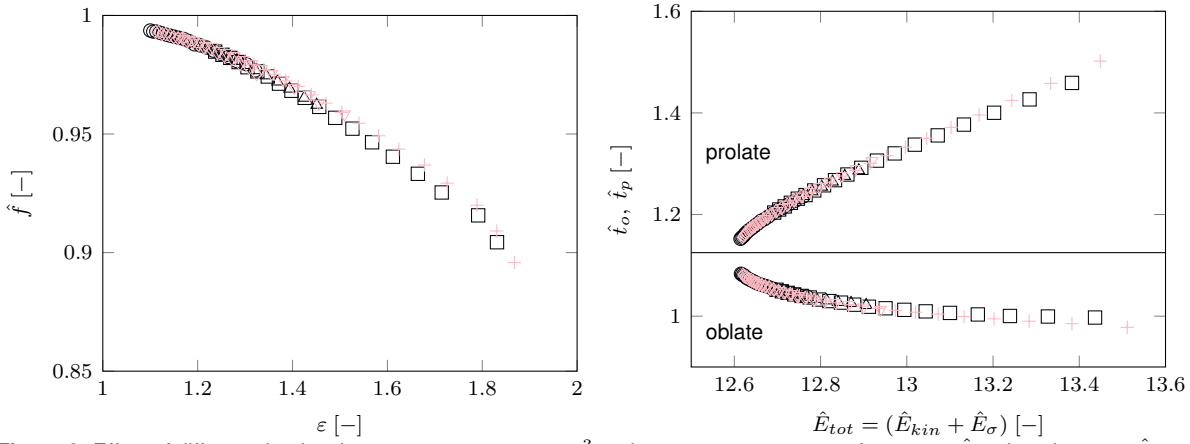

Figure 3. Effect of different droplet shapes at $Oh = 1.18 \cdot 10^{-3}$ and $\varepsilon = 1.35, 1.50, 2.00$ on frequency $\hat{f}$ and total energy $\hat{E}_{tot}$. The dark color indicates the initial ellipsoidal form, the bright color indicates the initial spherical harmonic of order 2.

for viscous dissipation. For small ε and Oh, the model agrees well with the results. However, deviations at larger amplitudes and viscosities may arise from mode coupling, where energy is transferred from higher modes to lower ones rather than being damped, leading to different energy distributions and, consequently, different prolate and oblate oscillation times.

Conclusion and Outlook

Analytical modeling often falls short in accurately predicting non-linear behavior or only capturing weakly non-linear phenomena. This study demonstrates that highly resolved numerical simulations, combined with appropriate data analysis, can effectively address these limitations, offering significant enhancements and extensions to available models methods. This study

introduced a novel approach for the detailed investigation of oscillating droplets, specifically focusing on cases with large amplitudes, highly viscous liquids and varying initial droplet shapes. The analysis revealed that by appropriately nondimensionalizing the data, a consistent collapse of data points is achieved when plotting the time droplets spend in prolate and oblate shapes against their total energy, encompassing both kinetic and surface energy. This collapse was observed across both numerical and analytical results within a specific range of conditions.

Nevertheless, several open questions remain that warrant further study, including a deeper investigation into the effects and discrepancies of varying initial droplet shapes (such as ellipsoids versus higher harmonics) on frequency variation and total energy, as well as a thorough exploration of the observed oblate/prolate asymmetry. Another important area for investigation is to uncover the underlying physical mechanisms that explain the observed patterns and the consistent collapse of data points in the plots of oscillation times versus total energy across different conditions. Additionally, it is crucial to reassess the assumption of potential flow within droplets in the analytical model, by using highly resolved DNS for comparison and flow visualization, as this can provide a more accurate depiction of the flow dynamics.

Nomenclature

D_0	droplet equivalent diameter [m]	ε	initial aspect ratio [$-$]
E	energy [(kg m^2)/s^2]	μ	dynamic viscosity [mPa s]
f	frequency [1/s]	ρ	density [kg/m^3]
Oh	Ohnesorge number [$-$]	σ	surface tension [N/m]
R_{ax}, R_{rad}	droplet (axial, radial) radius [m]	$\tilde{}$	non-dimensionalization factor
t_o, t_p	oblate, prolate time [s]	$\hat{}$	non-dimensional parameter

Acknowledgments

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