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Numerical Modeling of Shock Induced Aerobreakup of a Droplet at High Reynolds and Weber Number

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Shock/droplet interactions have been the focus of numerous experimental and numerical investigations due to the importance of understanding droplet physics in many aerospace engineering applications. This paper presents a status update on current modeling efforts for simulating shock/droplet interactions (primarily in 2D) using the open-source NGA2-MAST framework (https://github.com/desjardi/NGA2). 2D simulation results using NGA2 are compared to previously published numerical and experimental results for shock Mach numbers ranging from 1.18 to 2.50. This work will provide the foundation for future 3D modeling efforts of shock/droplet interactions with higher shock Mach numbers.

I. Introduction

The behavior of multiphase flow is an area of interest for many engineering disciplines. The interaction between a shock wave and a water droplet is an important problem that influences the design of supersonic and hypersonic vehicles [1, 2]; during flight, a shock-processed droplet can impact a vehicle and cause damage. Many experimental and numerical studies have been conducted investigating this interaction under a variety of conditions (e.g. [3–7]). As described in [8], this phenomenon is classified into two stages: stage 1) wave dynamics, and stage 2) droplet breakup. The droplet breakup has been observed to be primarily composed of two instability modes: 1) shear-induced entrainment (SIE) caused by the Kelvin-Helmholtz Instability (KHI), and 2) Rayleigh-Taylor Piercing (RTP) caused by the Rayleigh-Taylor instability (RTI) [8].

The first instability mode, related to the Kelvin-Helmholtz Instability, occurs at the interface of two fluids of different tangential velocities. Since there is a discontinuity between the gas and liquid velocities, vorticity is non-zero (often described as a vortex sheet). The vorticity of each phase then induces an angular velocity field that will continue to grow in an oscillatory nature until mixing of both phases occurs [9]. This instability is referred to as shear-induced entrainment in which particles of each phase are transported across the interface by the induced velocity [10]. The second instability mode, related to the Rayleigh-Taylor Instability, occurs between two fluids of different densities undergoing an acceleration. When the lighter fluid pushes against the heavier fluid the two phases begin to mix, with ripples and bubbles starting to form at the interface [11, 12]. As the interface pressure shifts towards equilibrium, the heavier fluid pushes back on the lighter fluid causing a wave-like, oscillatory instability at the fluid interface.

In this work, we use the open-source NGA2 Multiphase All-Mach Semi-Lagrangian Transport (NGA2-MAST)¹ computational framework [13], to simulate shock-induced aerobreakup of a two-dimensional water cylinder. For brevity, NGA2 will be used to refer to the solver for the rest of this paper. Multiple verification and validation cases have been conducted by the code developers, and results and detailed information about the solver are presented in [13]. Results from a detailed validation effort of a jet in a supersonic crossflow are presented in [14]. In this work, numerical results using NGA2 will be compared to results presented in [15], which uses the solver described in [16, 17]. Results will also be compared to experimental data presented in [18]. Quantities of interest (QOIs) to be compared to other works primarily include the droplet center of mass (COM) drift and velocity.

II. Numerical Methods

The NGA2-MAST framework is an all-Mach, multiphase, volume-of-fluid (VOF) flow solver [13]. A 6-equation model is used in which the energy of each phase is solved separately. The NGA2 framework was chosen to study this

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¹https://github.com/desjardi/NGA2

phenomenon for several reasons. First, the VOF scheme is robust and ensures consistent computations of conservative flow properties while limiting numerical dissipation. Secondly, it uses the open-source Interface Reconstruction Library (IRL) which provides efficient tools for tracking the liquid-gas interface. Third, the solver utilizes a hybrid approach where a semi-Lagrangian transport scheme [13, 19, 20] is used in proximity to sharp interfaces and shocks. In smooth regions of the flow, a centered scheme is used. A dilatation-based shock sensor and the volume fraction field are used to identify shocks and material interfaces [13, 21]. NGA2 also enables the inclusion of surface tension, viscosity, and multiple equations of state (EOS). For the work presented in this paper, we use a stiffened gas EOS for the liquid phase and the ideal gas EOS. The energy of each phase is solved separately as discussed in [13]. Finally, NGA2 is designed to be an all-Mach solver, allowing for the analysis of flows at multiple shock Mach numbers.

III. Problem Setup

The shock-water cylinder interactions presented in this paper are studied in a two-dimensional computational domain as shown in Fig. 1. A water cylinder with an initial diameter of $d_o = 4.8$ mm is impacted by a shock moving from left to right. The computational domain (Fig. 1) is $15d_o$ in the x-direction and $6d_o$ in the y-direction. The computational grid contains 1500 cells in the x-direction and 600 cells in the y-direction (constant dx and dy), corresponding to 100 cells across the cylinder diameter. Extending downstream of the domain of interest is a region with stretched mesh cells in the x-direction, extending the domain so that flow features are not reflected towards the droplet. This region contains 75 cells in the x-direction with a constant geometric stretching ratio of 1.1, which extends the domain by approximately $149d_o$. The boundary condition at the inlet of the domain is set to a constant velocity based on the calculated analytical post-shock velocity. The shock is initialized using numerical values extracted from a single-phase simulation which uses the same timestep and mesh as the full two-phase simulations.

The water cylinder and air downstream of the shock start at rest with $\rho_g = 1.204 \text{ kg/m}^3$, $\rho_l = 1000 \text{ kg/m}^3$, and $P_g = P_l = 101.325 \text{ kPa}$, where ρ_g is the gas density, ρ_l is the liquid density, P_g is the gas pressure, and P_l is the liquid pressure. The liquid phase is modeled using the stiffened gas equation of state(Eq. 1) with the ratio of specific heats set to $\gamma_l = 6.12$ and the reference pressure at $P_{\infty} = 343.44$ MPa. The values used in these simulations are different than those used in [13, 14] but are the same as those used in [15] (derivation of these values is discussed in [22]). The gas phase is modeled using the ideal gas equation (Eq. 2) with the ratio of specific heats for air at $\gamma_g = 1.4$. The center of the water cylinder is initially located 0.048 m from the left of the domain boundary and on the horizontal center line of the domain (y = 0). The shock is initialized 0.01 m upstream from the leading edge of the water cylinder. Surface tension has been neglected to match the conditions found in [15] except for three out of the nine simulations presented which have a surface tension coefficient of $\sigma = 0.0757$ N/m, and correspond to shock Mach numbers of 1.18, 1.47, and 1.73. All simulations presented in this work are inviscid. The shock-Mach numbers under investigation and the flow properties for each simulation are summarized in Table 1.

$$p = (\gamma - 1)\rho e - p_{\infty} \tag{1}$$

$$p = (\gamma - 1)\rho e \tag{2}$$



Fig. 1 Schematic of computational domain of interest.

M_s	Post shock u (m/s)	Post shock $\rho_g \ (\text{kg/m}^3)$	Post shock P_g (kPa)	Free stream Re	Free stream We
1.18	95.11	1.57	147.7	3.6 <i>e</i> 4	9e2
1.30	151.82	1.82	182.9	6.42 <i>e</i> 4	2.6e3
1.47	226.14	2.18	238.56	1.07e5	7e3
1.73	329.61	2.704	336.92	1.77 <i>e</i> 5	1.86 <i>e</i> 4
2.00	429.02	3.21	455.85	2.48 <i>e</i> 5	3.75 <i>e</i> 4
2.50	600.7	4.01	721.9	3.73 <i>e</i> 5	9.2 <i>e</i> 4

 Table 1
 Shock-Mach Numbers Under Study

The two primary QOIs reported in this work are the water cylinder COM drift and velocity. These values, ($\bar{\mathbf{x}}$ and $\bar{\mathbf{u}}$), respectively, are calculated using Eqs. 3 and 4, where α_l is the volume fraction of the liquid phase, ρ_l is the liquid density, X_{COM} is x-coordinate the center of mass of the water cylinder, and u_{COM} is the x-component of velocity of the center of mass. The volume integral is calculated over the entire computational domain

$$\overline{\mathbf{x}} = \frac{\int \alpha_l \rho_l \mathbf{x} d\mathbf{V}}{\int \alpha_l \rho_l d\mathbf{V}}$$
(3)

$$\overline{\mathbf{u}} = \frac{\int \alpha_l \rho_l \mathbf{u} d\mathbf{V}}{\int \alpha_l \rho_l d\mathbf{V}} \tag{4}$$

The same temporal non-dimensionalization as [15] is used, where the non-dimensional time, t^* (Eq. 5), is defined using the free stream velocity behind the shock, the original droplet diameter, and the square root of the ratio of the free stream gas density to the liquid density.

$$t^* = t \frac{u_g}{d_o} \sqrt{\frac{\rho_g}{\rho_l}} \tag{5}$$

IV. Results and Discussion

A. Center of Mass Drift and Velocity

To compare to the results presented in [15], six separate two-dimensional inviscid simulations with a shock Mach number ranging from 1.18 - 2.5 were studied. Results presented in [15] do not account for surface tension, while some results presented in this work do include surface tension, namely cases with shock mach numbers of 1.18, 1.47, and 1.73. The droplet center of mass (COM) drift and COM velocity were calculated and plotted against non-dimensional time, and compared to the results presented in [15] in Figs. 2 and 3.

The values calculated using NGA2 match well with the results presented by Meng [15] in the early stages of the interaction. However, as t^* approaches ~ 0.4, differences are observed between the simulation results. In general, for the simulations performed in this work, the droplet center of mass moves further downstream compared to the simulations presented in [15]. Simulations that include surface tension agree with the results in [15] for a longer amount of time than those that neglect surface tension effects, though then the results still diverge. Further discussion of the effects of surface tension can be found in Sec. IV.B.

B. Surface Tension Effects

A comparison between the NGA2 results and the experimental data presented in [18] can be seen in Fig. 4. The cylinder drift was measured from the front stagnation point, as described in [15]. To determine this drift, the interface location of the liquid and gas phases was determined by using a liquid volume fraction threshold of $\alpha_T = 0.99$. The simulation results presented in Fig. 4 correspond to a shock Mach number of 1.47 with surface tension included. The observed discrepancies between the numerical results and experimental data are still under investigation.



Fig. 2 Normalized droplet center of mass location for a variety of different shock Mach numbers, with and without surface tension included. Meng et al. results taken from [15].



Fig. 3 Normalized *x*-component of droplet center of mass velocity for a variety of different shock Mach numbers, with and without surface tension included. Meng et al. results taken from [15].

Figure 5 shows a side-by-side visualization of a snapshot of a shock/droplet interaction simulated in NGA2 with and without surface tension included for a shock Mach number of 1.18. Colored contours refer to velocity magnitude, and



Fig. 4 Comparison of front stagnation point drift of shock Mach 1.47 case (blue) from NGA2 and experimental data (red) - experimental data taken from [18].

the droplet VOF is shown in black with a liquid volume fraction threshold of $\alpha_T > 0.99$. When the surface tension is not included (Fig. 5a), the droplet deformation at the leading edge starts to form a jetting feature at the front of the droplet at approximately $t^* = 0.85$. When the surface tension is included (Fig. 5b), this structure is no longer observed. In addition, when surface tension is not included, larger amounts of droplet stripping is observed numerically. This may contribute to the discrepancies observed between the current simulation results and those presented in [15]. It is also consistent with the results shown in Figs. 2 and 3 where surface tension decreases both the motion and velocity of the center of mass of the droplet for a given shock Mach number.



(b) With surface tension

Fig. 5 Water Cylinder deformation of the shock Mach 1.18 case at $t^* = 0.853$. VOF (black) and velocity magnitude contour plot (red/blue). a) neglects surface tension b) includes surface tension.

V. Future Work

To fully simulate a more realistic shock-droplet interaction, the phenomenon should be solved in 3D (as stated in [12], interface instabilities are heavily influenced by three-dimensional effects). As a proof-of-concept and demonstration of future work, coarse 3D simulation results are shown in Fig. 6. The shock Mach number for this simulation is 1.47. The computational grid was set to be uniform within the entire domain, with 256 cells in the *x*, *y*, and *z* directions corresponding to approximately 12 cells across the droplet diameter. The domain length was set to $12d_o$ in each direction with the droplet being centered in the domain. The specific heat ratios for the gas and liquid phases were set to $\gamma_g = 1.4$ and $\gamma_l = 4.4$ respectively, with a reference pressure of $P_{\infty} = 600$ MPa. The gas phase pre-shock pressure and density were set to $P_g = 101.325$ kPa and $\rho_g = 1.204$ kg/m³. Surface tension was included in this case and was set to $\sigma = 0.0757$ N/m and viscosity for both phases was neglected. The results presented in this section are preliminary and future 3D simulations will use a finer mesh resolution.



Fig. 6 3D (coarse) demonstration simulation. Numerical Schileren (center-plane) and VOF (blue) are shown.

Furthermore, we are working towards simulating the shock/droplet interactions based on the experimental conditions presented in [6, 8]. A sample experimental shock/droplet interaction image from a test performed in [6] is shown in Fig. 7.

VI. Conclusion

The deformation and breakup of a water cylinder under shock loading have been simulated and compared to published numerical and experimental data. Six cases with varying shock Mach numbers were investigated. Our simulation results using the NGA2 solver [13] compared well for early times when compared to the results from the



Fig. 7 Sample visualization for a shock/droplet experiment described in [6].

Harten-Lax van-Leer Contact (HLLC) solver used in [15]. NGA2 simulations with surface tension have been observed to be closer to results presented in [15] and experimental data in [18]. An unresolved 3D shock-droplet simulation was presented as a proof-of-concept demonstration for future work. Future research also includes the validation of copmutational results against experimental data, and further investigation into the effects of viscosity and surface tension.

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