Numerical study of shock waves attenuation by a polydispersed water spray

C. Siddappa[1], O. Thomine[1], A. Hadjadj[1], M. S. Shadloo[1], and G. Gai[2]

[1]INSA Rouen, Normandie University, CNRS, CORIA-UMR 6614, 76000 Rouen, France
[2]Department of Mathematics, University of British Columbia, Vancouver, BC, Canada

1 Introduction

The purpose of this paper is to study the attenuation of shock waves through a cloud of scattered particles or droplets, as found in water spraying systems. This type of system has a range of industrial applications, including reducing the risk of explosions in nuclear reactor containment buildings. In such cases, a water spray can help to prevent the acceleration of flames and the formation of subsequent blasts. Numerical and experimental studies have been conducted in the past to improve our understanding of the physics of shock-spray or shock-droplets/particles interaction in nuclear systems [1] [2] [3]. Despite the multitude of theoretical and experimental investigations, the physical mechanisms underlying shock-droplets interaction have not yet been fully explained, both quantitatively and qualitatively. Further well-designed experiments and/or numerical modeling are needed, particularly in high-Mach number regimes.

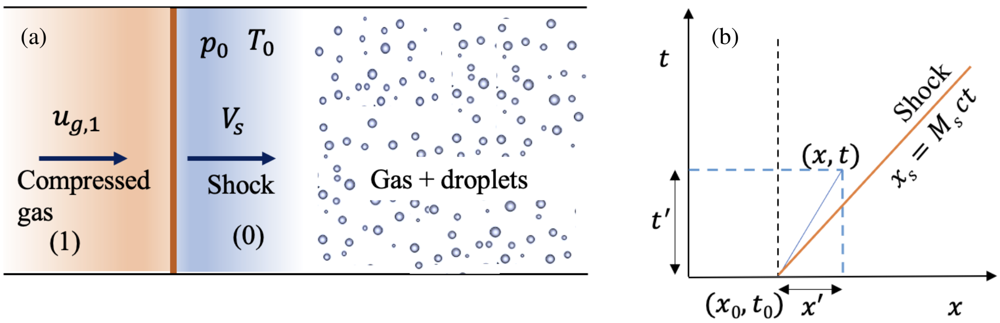

Figure 1: (a) Schematic representation of shock-spray interaction, where $u_{g,1}$ is the gas velocity, and V_s is the shock velocity, and (b) space-time (x,t) diagram, where x_0 is the initial position of shock-spray interaction, x' is the distance covered by droplets after interaction, t' is the duration of the interaction, and x_s is the shock position.

In this paper, we conduct a series of one- and two-dimensional numerical simulations to investigate the interaction between a planar shock wave and a cloud of suspended particles/droplets. The goal is to improve our understanding of shock attenuation/amplification in a two-phase flow, specifically in the context of hydrogen explosion. The flow configuration is depicted in Fig.1 (a). A shock wave travels at a velocity V_s, initiated by a moving piston travelling at a speed of $u_{g,1}$, through a cloud of particle-laden gas with zero-initial velocity. The droplets are assumed to be spherical and solid, with a small initial volume fraction $\tau_{v,0}$ so that collisions between particles are neglected. The physical parameters of key interest in this study are the incident shock Mach number, M_s, the volume fraction, τ_v, the particle response time, τ_p, and the standard deviation σ in the log-normal distribution of droplet size. The main focus of our study is to extend the model originally developed by *Gai et al.* [4] for monodisperse particle to polydisperse particle cloud.

Correspondence to: chethan.siddappa@insa-rouen.fr

2 Numerical tool

To study the shock-spray interaction, we use the *in-house* compressible direct-numerical simulation Navier-Stokes solver, Asphodele [6], on a Cartesian grid. We adopt the Eulerian-Lagrangian approach, using an Unresolved Discrete Particle Model (UDPM) to handle the particle dynamics. For space discretization of the transport equations, we employ a fifth-order WENO (weighted essentially non-oscillatory) scheme with global Lax–Friedrichs splitting, while a third-order Runge–Kutta method is used for time marching.

3 Theoretical modeling of particle dispersion using a one-way formalism

In this study, we develop a new reduced-order model to investigate the impact of polydisperse particles on shock waves using a one-way formalism. Our model is an extension of a previously developed model for monodisperse particles [4]. Consider a shock-spray interaction, as shown in Fig.1 (b), where the contact surface is initially at x_0. The distance traveled by a particle as a result of this interaction is denoted by x', and the duration of the interaction is denoted by t'. The key parameters that differ in this study are the size distribution of the droplets and their response time, which are not constant. In the case of polydisperse particles, there are N particles, each with its own diameter $d(n)$ and response time $\tau_p(n)$. By applying the equation of motion and the planar shock wave relation, we can obtain the particle velocity v_p as:

$$v_p(x,t,\tau_p(n),u_{g,1}) = \; u_{g,1}\left[1-\exp\left(-t'(x,t)/\tau_p(n)\right)\right] \tag{1}$$

where,

$$t'(x,t,\tau_p(n),u_{g,1}) = \tau_p(n)\,\mathscr{W}\left(\frac{u_{g,1}e^{\eta}}{M_s c-u_{g,1}}\right)+\frac{M_s ct-u_{g,1}\tau_p(n)-x}{M_s c-u_{g,1}}, \qquad \eta=\frac{u_{g,1}\tau_p(n)-M_s ct+x}{\tau_p(n)(M_s c-u_{g,1})}$$

where c is the sound speed, $\mathscr{W}$ is the Lambert function, μ_g is the viscosity of gas. The spray characteristics can be determined by the conservation of mass. Assuming the particles to be solid, we can calculate the cloud density (particle volume fraction) τ_v as follows:

$$\frac{\tau_v(t',\tau_p(n),u_{g,1})}{\tau_{v,0}} = \left[\left(1-\frac{u_{g,1}}{M_s c}\right)+\mathscr{T}\right]^{-1} \tag{2}$$

where,

$$\mathscr{T} = \sqrt{\frac{\rho_p}{18\mu_g\tau_p(n)}}\sqrt[3]{\frac{6\tau_v}{\pi}}u_{g,1}\tau_p(n)\exp\left(\frac{-t'}{\tau_p(n)}\right)\left[\exp\left(\sqrt{\frac{18\mu_g\tau_p(n)}{\rho_p}}\sqrt[3]{\frac{\pi}{6\tau_v}}\frac{1}{M_s c\tau_p(n)}\right)-1\right]$$

3.1 One-dimensional free-piston shock tube

We perform a one-dimensional numerical simulation of a free-piston shock tube to analyze the interaction between a shock wave and polydisperse particles. A shock tube facility produces fast and relatively high-temperature flows by driving a single shock wave into a quiescent gas. Using a simple piston theory, it is possible to obtain the jump conditions across a shock at different flow regimes by varying the shock strength and thereby the shock velocity. In this study, we assume that the flow is inviscid and follows the perfect-gas law, and we do not account for heat transfer between the gas and droplets. Initially, we compute average quantities of the droplet cloud such as the mean volume fraction and the mean diameter, which is, $\widetilde{d}=\frac{1}{N}\Sigma_{n=1}^{N}d(n)$. This approach is based on the work of *Beetstra et al.* [7]. The particles involved in the flow have a mass density of $\rho_p = 1000\,kg/m^3$ under ambient temperature and pressure conditions, corresponding to a gas that is considered to be water. The piston tube domain has a length L_0 of 1 m and is discretized with 1000 points. The initial shock-spray contact surface is located at 0.5 m. To confirm the accuracy of the model and gain a deeper understanding of the physical processes involved, numerical simulations are carried out with initial conditions of M_s = 1.1 and $\tau_{v,0} = 5.2 \times 10^{-4}$ (using one-way formalism) and compared with theoretical predictions. After the shock wave passes, the velocity of the particles increases towards that of the gas, with larger particles accelerating gradually and smaller ones responding quickly, as illustrated in Fig. 2 (a) and (b). The theoretical model takes into account both σ and $\widetilde{d}$ and shows good agreement with the numerical simulations.

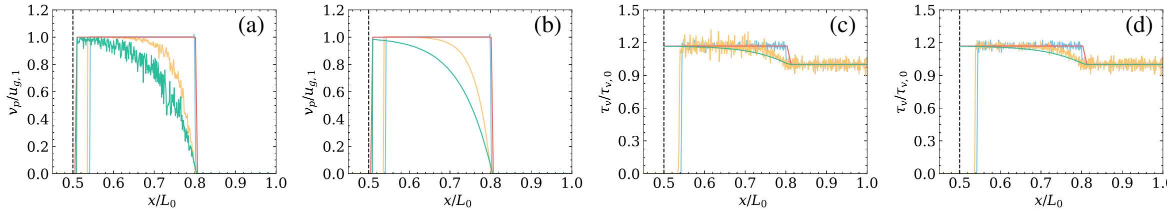

Figure 2: Spatial evolution of normalized particle mean velocity for (a) σ = 0.1, (b) σ = 0.001 and normalized particle volume fraction for (c) σ = 0.1, (d) σ = 0.001 at $t = 800\,\mu s$. Curves: numerical results for $\widetilde{d} = 1\,\mu m$ (blue) and $\widetilde{d} = 10\,\mu m$ (orange), theoretical results for $\widetilde{d} = 1\,\mu m$ (red) and $\widetilde{d} = 10\,\mu m$ (green).

4 Mono- *vs* polydispersed particles using a two-way formalism

This section compares one-dimensional numerical simulations of polydisperse and monodisperse particles. The simulations are conducted with the following initial conditions: initial pressure p_0 = 1 atm, temperature T_0 = 298 K, standard deviation $\sigma = 0.25$, M_s = 1.1, and $\tau_{v,0} = 5.2 \times 10^{-4}$, for various mean droplet diameters $\widetilde{d}$.

4.1 Influence of the particle response time

The particle response time τ_p is defined as the time required by the particle to respond to the carrier flow.

$$\tau_p = \frac{\rho_p \widetilde{d}^2}{18\,\mu_g\, f(Re_p)} \tag{3}$$

where ρ_p is the mass density of the particles, $\widetilde{d}$ is the mean diameter of particles, μ_g is the dynamic viscosity of the gas, Re_p is the particle Reynolds number, and $f(Re_p)$ = 1.0 + 0.15$(Re_p)^{0.687}$. As in the monodisperse case studied by *Gai et al.* [5], we observe that small particles have a greater attenuation effect than large particles in polydisperse flow. Additionally, the polydisperse spray exhibits more attenuation effects than the monodisperse spray, as shown in Figure 3.

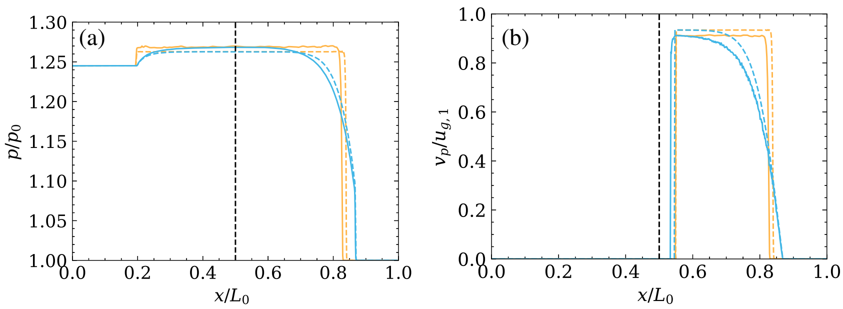

Figure 3: Spatial evolution of (a) normalized pressure and (d) normalized particle mean velocity for different droplet diameters: $\widetilde{d} = 1\,\mu m$, $\tau_p = 2.3\,\mu s$ (orange) and $\widetilde{d} = 10\,\mu m$, $\tau_p = 100\,\mu s$ (blue) at $t = 1\,ms$ (polydispersed: solid-line and monodispersed: dashed-line).

4.2 Criteria for particle number-density peak

The compressed region can result in a particle number-density peak, which can alter the spray dispersion topology. Previous work [5] observed the peak under certain flow conditions, when the time required for compressed gas zone formation τ_c was much larger than the particle response time τ_p, and the peak intensity increased at high Mach numbers. However, in the polydispersed case with $\widetilde{d} = 10\,\mu m$, $\tau_{v,0} = 5.2\times10^{-4}$, and $\sigma = 0.25$, as shown in Fig.4 (a), there was no density peak observed due to the presence of small droplets in the polydisperse cloud. A parametric study was conducted for different $\widetilde{d}$ and σ, and it was found that the peak density was observed at a particular condition of $\sigma = 0.001 \ll 1$, with a droplet diameter of the order of $\mathscr{O}(10\,\mu m)$, that satisfies $\tau_c \gg \tau_p$, and increases with the Mach number, as shown in Fig. 4 (b). This phenomenon can only be observed using the two-way formalism, which accounts for the mutual interaction between the shock and droplets.

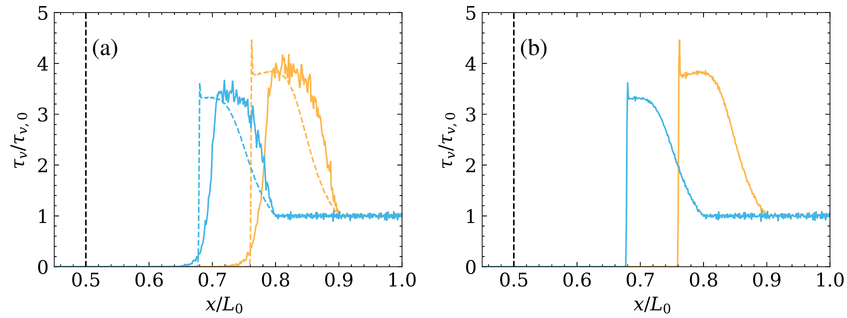

Figure 4: Particle volume fraction evolution for $M_s = 3$ (blue) and $M_s = 4$ (orange) at $t = 300\,\mu s$, (a) comparison of polydispersed (solid line) and monodispersed (dashed line) with σ = 0.25 and (b) Polydispersed case with σ = 0.001.

5 Two-dimensional shock-spray interaction

Following this study, 2D simulations are conducted in a rectangular piston tube with dimensions of $1\,m$ length and $0.1\,m$ width. The pressure distribution is measured at two locations: $\mathscr{L}_1 = 0.80\,m$ and $\mathscr{L}_2 = 0.96\,m$. Given that the shock-spray interaction is a complex phenomenon, determining an optimal cell size is essential to ensure accurate numerical simulations. As depicted in Fig. 5 (a), simulations are performed for various cell numbers with an initial condition of $M_s = 3$ and for $\widetilde{d} = 1\,\mu m$, $\tau_{v,0} = 5.2\times10^{-4}$, and $\sigma = 0.25$. The pressure peak is more distinct with a 1000×100 cell configuration than with other cell configurations. As a result, all subsequent simulations are conducted with this cell size.

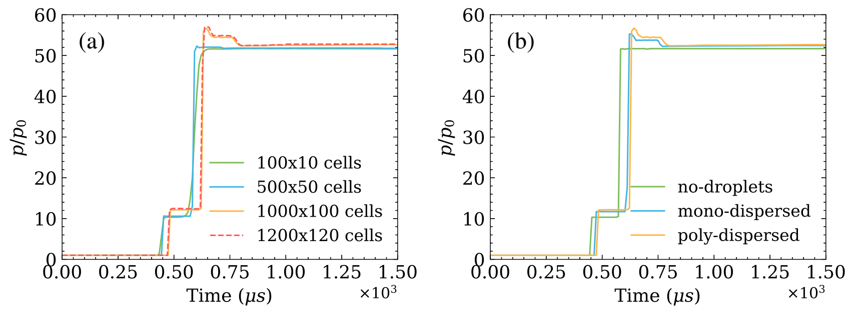

Figure 5: Time evolution of the normalized pressure profile located at $\mathscr{L}_2$ (a) grid independence analysis, (b) comparison between polydispersed, monodispersed, and free-droplet cases.

5.1 Comparison of polydispersed, monodispersed, and free-droplet cases

Simulations are performed for various cases with an incident-shock Mach number of $M_s = 3$, considering $\widetilde{d} = 1\,\mu m$ and $\tau_{v,0} = 5.2 \times 10^{-4}$. We investigated the shock propagating without droplets, shock propagating into a monodispersed phase, and shock crossing a polydispersed cloud of droplets. In Fig.5 (b), the pressure profile at location $\mathscr{L}_2$ is presented for all three cases. The results indicate that the attenuation effect is more pronounced in the polydispersed case compared to the other two cases.

5.2 Effect of particle mean diameter

Figure 6 (a) presents the pressure profiles at two different locations, $\mathscr{L}_1$ and $\mathscr{L}_2$, for two distinct droplet sizes, $\widetilde{d}$, of $1\,\mu m$ (orange) and $50\,\mu m$ (blue), using the same initial conditions as previously stated. After the interaction of the reflected shock with the droplets, a pressure peak is observed only for the case with small particles, while no peak is seen for the larger particles. This suggests that small particles respond more quickly to the shock passage than large particles, as confirmed by the velocity profile presented in Fig. 6 (b). Figure 7 illustrates the instant gas density plots with droplet volume fraction iso-contour for different $\widetilde{d}$ at $t = 300\,\mu s$. Consistent with the 1D results, small particles exhibit the most significant attenuation effect, which slows down the transmitted shock wave. Moreover, Figs. 7 (a) and (c) indicate that the contact surface of small particles moves faster than that of larger ones due to their lower τ_p. Finally, Fig. 7 (b) and (d) show numerical schlieren images that illustrate the flow structure, including the shock wave, the contact surface between the droplets and gas.

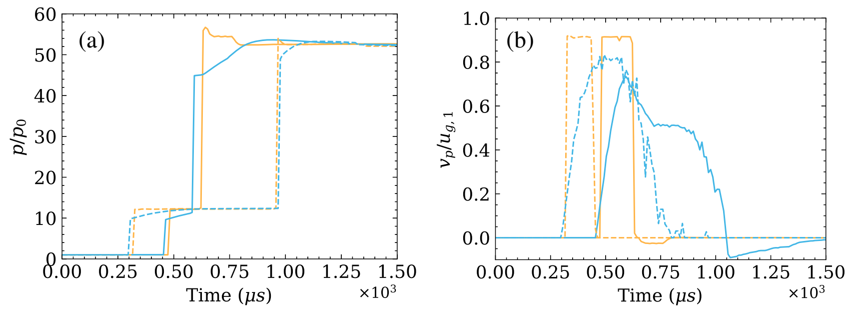

Figure 6: (a) Pressure and (b) particle mean velocity profile for different $\widetilde{d} = 1\,\mu m$ (orange) and $\widetilde{d} = 50\,\mu m$ (blue) at two different locations $\mathscr{L}_1$ (dotted-line) and $\mathscr{L}_2$ (solid-line).

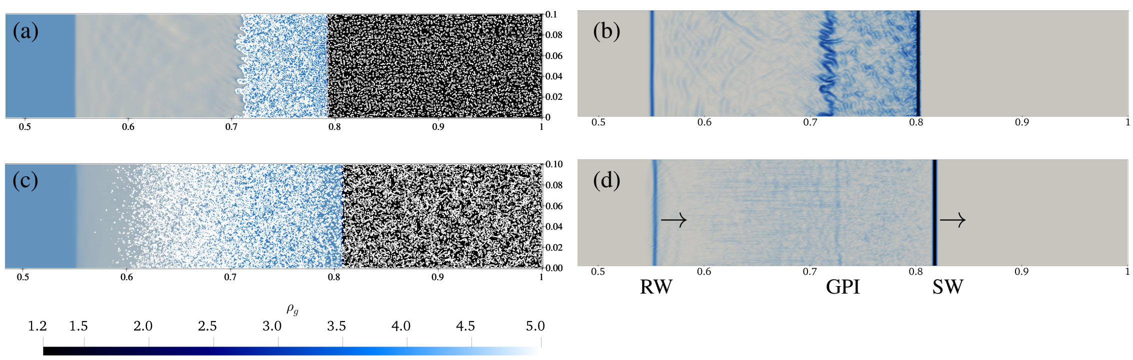

Figure 7: Color plots of gas density at $t = 300\,\mu s$ for cases with (a) $\widetilde{d} = 1\mu m$, and (c) $\widetilde{d} = 50\,\mu m$ (white-line: the particle volume fraction iso-contour) and corresponding numerical schlieren pictures for case with (b) $\widetilde{d} = 1\mu m$, and (d) $\widetilde{d} = 50\,\mu m$. RW: Reflected wave, GPI: gas-particle interface, SW: Shock wave

6 Summary

Sprayed water droplets are commonly utilized in the nuclear industry to prevent potential disasters caused by deflagration-to-detonation transition (DDT) and explosions. In this regard, understanding the physical mechanisms of shock-water spray interaction is crucial, especially when dealing with a cloud of polydispersed particles. This article addresses the canonical problem of a planar shock interacting with a polydispersed cloud of particles/droplets in a free-piston shock tube. A mixed Euler-Lagrange approach is employed to solve the governing equations for modeling the particle motion in one- and two-dimensional flow configurations. Furthermore, a theoretical model using a one-way formalism is developed to study the cloud dispersion topology, and the obtained results match well with the numerical simulations. To assess the effect of polydispersion on shock mitigation, the computational results obtained using the two-way formalism are compared with the monodispersed and droplet-free cases. Our findings demonstrate that the polydispersion of the cloud particles has a more significant attenuation effect than the monodispersed case. Additionally, small particles are more sensitive to the post-shock gas and have more attenuation effects, regardless of their dispersion characteristics. Moreover, the topological heterogeneity of droplets is an essential ingredient that needs to be included in the modeling of such phenomena. This study contributes to understanding how topological heterogeneity affects the evaporation dynamics of water droplets by shock waves.

7 Acknowledgement

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