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A Particle-Based Computational Framework for a Newtonian Fluid Drop Impact on a Rigid Surface

Tapan Jana[1], Amit Shaw[1], L. S. Ramachandra[1]
[1]Department of Civil Engineering, Indian Institute of Technology
Kharagpur, West Bengal, India
tapan.jucivil@gmail.com; abshaw@civil.iitkgp.ac.in; lsr@civil.iitkgp.ac.in

Abstract - The study of drop impact on solid surfaces is a fascinating and multifaceted field that delves into the intricate interplay of fluid dynamics, material science, and surface interactions. A plethora of intricate physical processes emerge in the drop impact phenomena within fractions of a second. In the present work, a numerical framework based on smoothed particle hydrodynamics is developed to simulate a Newtonian fluid drop impact over a rigid surface. A suitable boundary condition is considered for numerical stability and accuracy. The numerically obtained results are compared with the available results from the literature.

***Keywords*:** Newtonian fluid, Drop impact, Particle-based method, Smoothed particle hydrodynamics, Weakly compressible fluids

1. Introduction

Several crucial phenomena, with profound consequences in several fields, arise when liquid droplets collide with solid surfaces. The most important of them is the possibility of splashing, which is a major concern in situations when the substrate or liquid might be fragmented, such as in soil erosion or when coating faults manifest. Assessing the ultimate spread radius is another crucial step since it affects the quality and efficiency of coatings in industrial operations and has vast repercussions for many coating applications. Applications such as ink-jet printing, spray coating, and microelectronics manufacturing also heavily rely on the maximum spread radius, which determines the area that a drop covers. Results pertaining to solidification, liquid absorption into porous surfaces, and liquid retention within regions delineated by surface roughness are affected by this maximum spreading factor. Advancements in several sectors, such as agriculture, environmental science, and cutting-edge manufacturing processes, are facilitated by a comprehensive understanding of these phenomena.

The exploration of droplet impact dynamics, encompassing natural events like rainfall and industrial processes in manufacturing, printing, spraying, and pharmaceutical coating, had been the focus of interdisciplinary research by past researchers [1]-[3]. Earlier investigations relying on high-speed photography [4]-[7] paved the way for diverse strategies, including the use of viscoelastic surfactants [8] and the correlation of droplet spreading with crucial parameters like the Weber number [9]. These insights, applicable across industries, contributed to the experimental understanding and the development of theoretical models for predicting droplet behaviour [10]. Researchers extensively investigated droplet impact numerically, with notable contributions from Harlow and Shannon [11] in 1967 using the finite difference method. To emphasize the impact of factors on spread dynamics, Fukai et al. [12] included surface tension effects in a finite element model. Subsequent studies improved the models by including the effects of surface tension, inertia, and the body together. The boundary integral method [13], the coupled finite-volume technique and level set approach [14], the finite element approach (FEM) [15], and the volume of fluid method (VOF) [16] [17] were adopted by past researchers to get through understanding of the behaviour of droplets upon impact.

Simulating large deformation issues is a major barrier for FEM due to mesh distortion. When materials exhibit fluid-like behaviour, this problem gets much worse in the instances of large deformation. The inherent limitations of FEM continue to be a problem, despite the use of adaptive meshing methods to solve these concerns. In recent years, SPH has emerged as a leading numerical technique in issues characterized by large deformation, where severe material flow also exists. With its meshless approach and adaptive nature, SPH is the go-to method for faithfully capturing the intricacies of large deformation phenomena and material behaving as fluid. The present work aims to test how effectively an SPH-based framework could model the impacting Newtonian fluid drop problem onto a rigid wall.

2. Governing equations and their discretized forms

SPH, a leading mesh-free approach, was first introduced by Lucy [18] and Gingold [19] for astrophysical simulations, and since then, it has emerged as a powerful tool across a variety of scientific problems. Its applicability spans impact problems [20]-[23], fluid flow modelling [24], as well as damage assessment in a concrete dam [25]. This exemplifies the remarkable impact and wide-ranging utility of SPH in diverse scientific investigations. The conservation equations for mass, momentum, and energy, based on Lagrangian description, are represented in Einstein's indicial notations as,

$$\frac{d\rho}{dt} = -\rho \frac{\partial v^{\beta}}{\partial x^{\beta}} \tag{1}$$

$$\frac{dv^{\alpha}}{dt} = \frac{1}{\rho}\frac{\partial \sigma^{\alpha\beta}}{\partial x^{\beta}} + g^{\alpha} \tag{2}$$

$$\frac{de}{dt} = \frac{\sigma^{\alpha\beta}}{\rho}\frac{\partial v^{\beta}}{\partial x^{\beta}} \tag{3}$$

SPH represents the computational domain using particles, employing a particle-based discretization method. With N particles distributed across the discretized domain, the discrete form of conservation equations is expressed as

$$\frac{d\rho_i}{dt} = \sum_{j\in N} m_j (v_i^{\beta} - v_j^{\beta}) W_{ij,\beta} \tag{4}$$

$$\frac{dv_i^{\alpha}}{dt} = \sum_{j\in N} m_j \left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} - \Pi_{ij}\delta^{\alpha\beta}\right) W_{ij,\beta} + g^{\alpha} \tag{5}$$

$$\frac{de_i}{dt} = -\frac{1}{2}\sum_{j\in N} m_j \left(v_i^{\beta} - v_j^{\beta}\right)\left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} - \Pi_{ij}\delta^{\alpha\beta}\right) W_{ij,\beta} \tag{6}$$

The stress tensor is composed of hydrostatic pressure and deviatoric stress. In the case of visco-elastic fluid, the deviatoric stress consists of a solvent contribution (τ_s) and a polymeric contribution (τ_p). The stress can be represented as,

$$\sigma^{\alpha\beta} = -P\,\delta^{\alpha\beta} + \tau_s^{\alpha\beta} + \theta.\tau_p^{\alpha\beta} \tag{7}$$

Now, for Newtonian fluid, the polymeric contribution is zero. The solvent contribution (τ_s) can be expressed as

$$\tau_{s,i}^{\alpha\beta} = \eta_s \left(k_i^{\alpha\beta} + k_i^{\beta\alpha}\right) \tag{8}$$

$$\text{where, } k_i^{\alpha\beta} = \frac{dv_i^{\alpha}}{dx^{\beta}} = \sum\nolimits_{j\in N} m_j/\rho_j (v_i^{\beta} - v_j^{\beta}) W_{ij,\beta} \tag{9}$$

and η_s is solvent viscosity. In Equations (5), and (6), Π_{ij} is artificial viscosity. The hydrostatic pressure (P) is calculated using an equation of state, and its expression is

$$P = \frac{\rho_0 c_0^2}{\gamma}\left(\left(\frac{\rho}{\rho_0}\right)^\gamma - 1\right) \tag{10}$$

Here, c_0 is the sound speed, ρ_0 is the initial density, and γ is a parameter considered 7 here.

3. Impacting drop configuration

This study utilizes SPH for extensive simulations in an effort to delve into the complex dynamics of droplet impact. In this section, the initial configuration of the impacting droplet, a key component that greatly affects the behaviours that follow is shown. The basic elements of the initial condition of the droplet are the diameter, velocity, and release height, which provide a solid foundation for understanding the complexities of impact dynamics. Figure 1(a) shows a vertical cross-section of the impacting drop, as described in Tomé et al. [26].

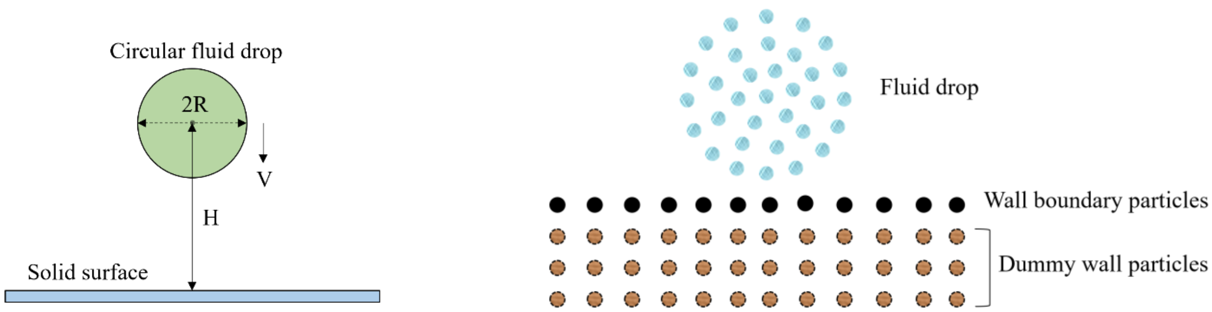

Fig.1. (a) Initial configuration of the impacting drop; (b) Implemented boundary condition for wall

4. Boundary condition

This research presents a novel approach for simulating a rigid wall, which helps with particle insufficiency problems at SPH boundaries. Inspired by Xu et al. [27], our method involves employing two distinct particle types - boundary particles aligned along solid walls and dummy particles packed into a grid just outside (Figure 1(b)). The wall particles are kept fixed throughout the whole simulation. The pressure of each wall particle is calculated using an extrapolation formula, and dummy particles adopt the pressure of the nearest wall particle. This approach, distinct from traditional repulsive forces, integrates wall and dummy particles into continuity and linear momentum equations. The combination resolves particle deficiency near boundaries, enforcing a no-slip boundary condition for improved accuracy and stability.

5. Numerical simulation

This section presents a detailed analysis of the simulated impacting drop problem employing SPH. Our study focuses on understanding the complex dynamics of drop impact by looking at the distribution of velocities and the development of pressures in the simulation. A detailed investigation of fluid-solid interactions is made possible by SPH, which elucidates how a Newtonian droplet reacts when it hits a hard surface. By looking into the temporal evolution of both drop impact velocity and pressure distribution, we aim to demonstrate key findings that contribute to the understanding of impact dynamics and further enhance the applicability of SPH in simulating such complex fluid phenomena. The scenario involves a 2D simulation where a disc with an initial radius of 1 cm falls from a height of 4 cm onto the rigid surface. The droplet is assigned a downward velocity of 1 m/s. Total number of particles is 7957, considering the inter-particle spacing between particles as 0.02 cm. The time step is taken as $4\text{x}10^{-6}$ s after fulfilling CFL criteria. Here, the solvent viscosity of fluid is 4.0 Pa-s.

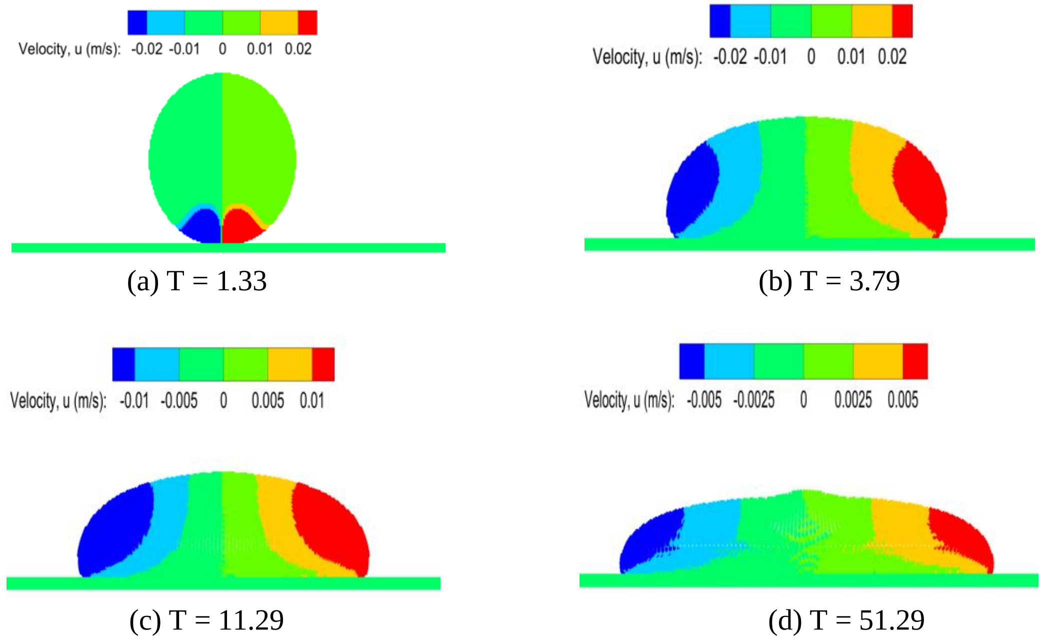

Fig.2. Horizontal velocity (u) contour plot of impacting drop at different values of non-dimensional time, T

Figure 2 shows the horizontal velocity contour for the Newtonian drop impact on the rigid wall at different non-dimensional time T = tV/2R. The contour plot shows that the horizontal velocity decreases after hitting the rigid surface as it flows slowly on the top of the rigid surface. The results also show that particles on the left and right sides of the drop are moving with the same velocity but along opposite horizontal directions. Symmetry in the results proves that the developed framework based on SPH correctly simulates the impacting drop problem.

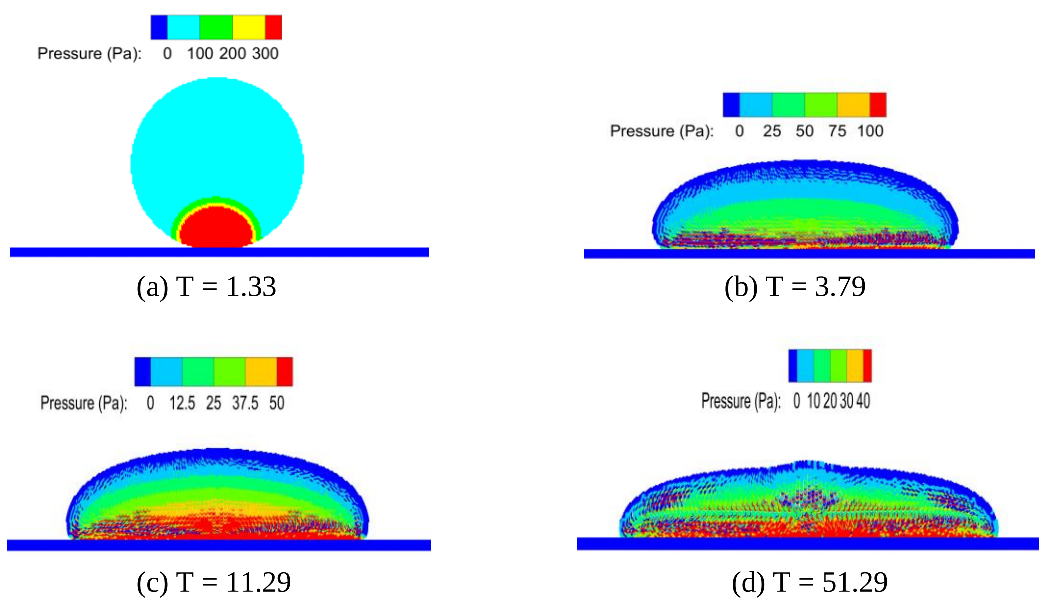

Fig.3. Pressure contour plot of impacting drop at different values of non-dimensional time, T

Figure 3 shows the pressure distribution of the drop. Initially, the pressure will be of higher value as the drop hits the rigid surface with a higher velocity. As the velocity decreases with time passes, the kinetic energy of the drop decreases also. Due to the dissipation of the kinetic energy, the pressure of the drop also decreases. Our simulations affirm the absence of tensile instability throughout the simulation. Figure 4 shows the time history of the fluid drop's width. It is compared with the FDM simulations of Tomé et al. [26], demonstrating good agreement with the existing literature. The results indicate that the Newtonian droplet undergoes uniform spreading post-impact, providing valuable insights for understanding and predicting fluid behaviour in various scenarios.

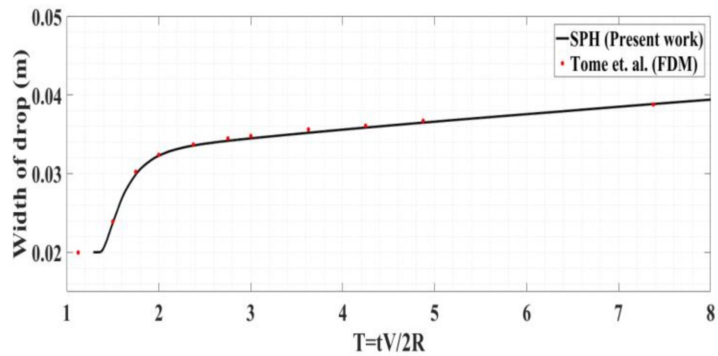

Fig.4. Comparison of drop width time histories in a Newtonian fluid: SPH (Present work) vs. FDM simulations (Tomé et al. [26]).

5. Conclusion

This study successfully employed SPH based framework to explore the intriguing phenomenon of the impacting drop problem, a major real-world issue. The investigation included the visualization of horizontal velocity and pressure contours at various time instances, providing insightful knowledge about the dynamic behaviour of the droplet upon impact. The impacting drop width variations were thoroughly examined with the literature and found to be in good agreement with the findings. This work contributes to the understanding of droplet impact dynamics and demonstrates the capability of the SPH approach in capturing critical features of the phenomenon. Validation against literature results strengthens the proposed computational framework, ensuring an invaluable tool for subsequent studies in fluid dynamics and related fields.

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