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# Hybrid SPH-MD two-phase modelling of 3D free-surface flows introducing double K-H instability

Jafar Ghazanfarian*, Mahshid Moradi

*Department of Mechanical Engineering, Faculty of Engineering, University of Zanjan, University Blvd., Zanjan 45371-38791, Iran*

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ABSTRACT

This paper studies multi-dimensional free-surface problem using a hybrid method combining the particle-based Smoothed-Particle Hydrodynamics (SPH) and atomistic Molecular dynamics (MD) techniques. In order to verify/validate the accuracy of the numerical solver, several cases including the 2D single-phase and two-phase dam break flows with dry bed, the 2D dam break flow over a layer of sand, the 3D broken dam flow, and the standard Kelvin–Helmholtz instability have been considered. After performing the particle-independence test, numerical results have been produced for several cases including the energy dissipation in 2D dam break flow with the fluidized bed, the interaction of 3D breaking dam flow with an obstacle of various heights and locations, exhaustive investigation of air particles for 2D and 3D cases, and the effect of surface tension by changing the container size and water temperature. Finally, a new version of the Kelvin–Helmholtz instability has been proposed, in which three layers of parallel flow (2 water layers and 1 air layer) including an interface and a free-surface become unstable. It is found that the water-water interface is more unstable than the air-water contact surface, and the amplified waves on the air-water interface are traveling standing waves with sharp tips.



## 1. Introduction

Two-phase flows including free-surface are important in various industrial applications including offshore and arctic structures, and in nature such as natural hazards, floods, Tsunami waves, and the melt flow from volcano. On the other hand, the development of mesh-free particle-based Lagrangian computational methods such as smoothed-particle-hydrodynamics (SPH) has accelerated the growth of our knowledge about processes involving boundary deformation, boundary motion, and free-surface.

The broken dam flow is a famous hydraulic problem in which a huge amount of water discharges at a short period of time, and creates a flood flow at the downstream. This sudden fall of water generates large surface waves and may be so hazardous from structural and environmental aspects. So, the analysis and prediction of the breaking dam flow and its consequences is a critical issue.

The first study of the broken dam flow goes back to the nineteenth century. Ritter [1] theoretically considered the problem of falling a column of water over a horizontal dry bed. The effect of friction with the bed was ignored in this study. Dressler [2] completed the wok of Ritter by adding the friction effects to the analysis. The experimental data were reported about the front of advancing wave, returning wave, and the wave shape in three channels with various roughnesses.

Chang et al. [3] investigated the surface waves created from the breaking of a dam with dry and fluidized beds. They presented results for 4 cases including a rough flat channel, a rough bumpy channel with various downstream boundary conditions, a non-prismatic channel, and a realistic scale model of the Toce River in Italy. Lo and Shao [4] used the SPH method with the LES model to simulate the near-shore solitary wave mechanics. Their results contain cases of a solitary wave against a vertical wall and running up a plane slope. Wang et al. [5] simulated the movement of the river flow by a particle recycling method (PRM) under the framework of smoothed particle hydrodynamics (SPH). The discontinuous deformation analysis (DDA) was used to model the landslide movement, and the interaction between the solid and fluid phases is achieved by the coupled DDA-SPH method.

Ghadimi et al. [6] examined the numerical simulation of fluid flow phenomena, including complicated free surface deformation, a two dimensional solitary wave on a beach, the effect of various wave heights to water depth ratios on solitary wave generation, and condition in which wave breaking occurs. Frazao and Zech [7] presented experimental study of a dam-break flow in an initially dry channel with a 90 degrees bend, with refined measurements of water level and velocity field. Pahar and Dhar [8,9] presented a modified incompressible smoothed particle hydrodynamics (MISPH) method for fluid-porous media interaction problems. They validated the model by using existing

* Corresponding author.
*E-mail address:* j.ghazanfarian@znu.ac.ir (J. Ghazanfarian).

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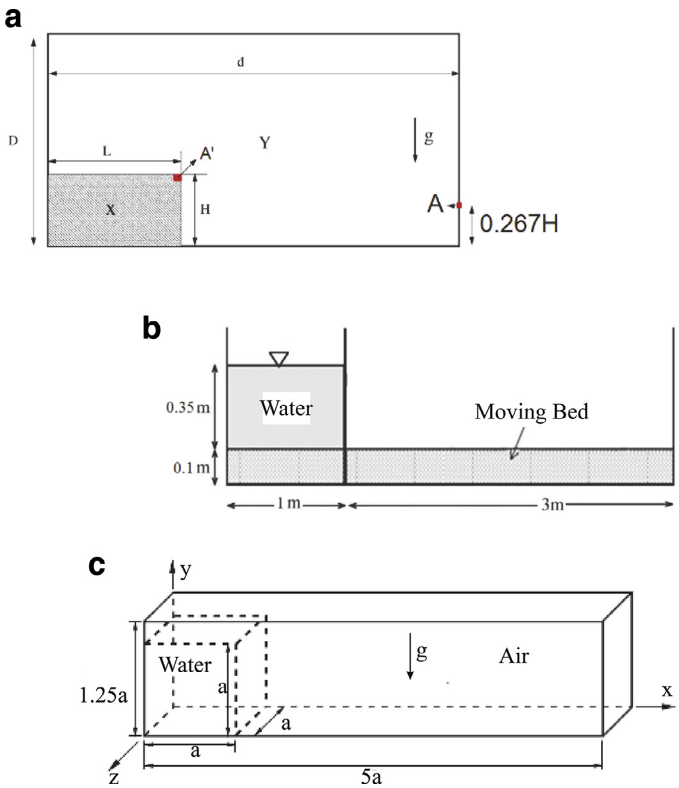


**Fig. 1.** Schematic geometry of free-surface flows used for the validation of the solver, (a) 2D dam break flow, (b) 2D dam beak flow with the moving bed, (c) 3D dam break flow.

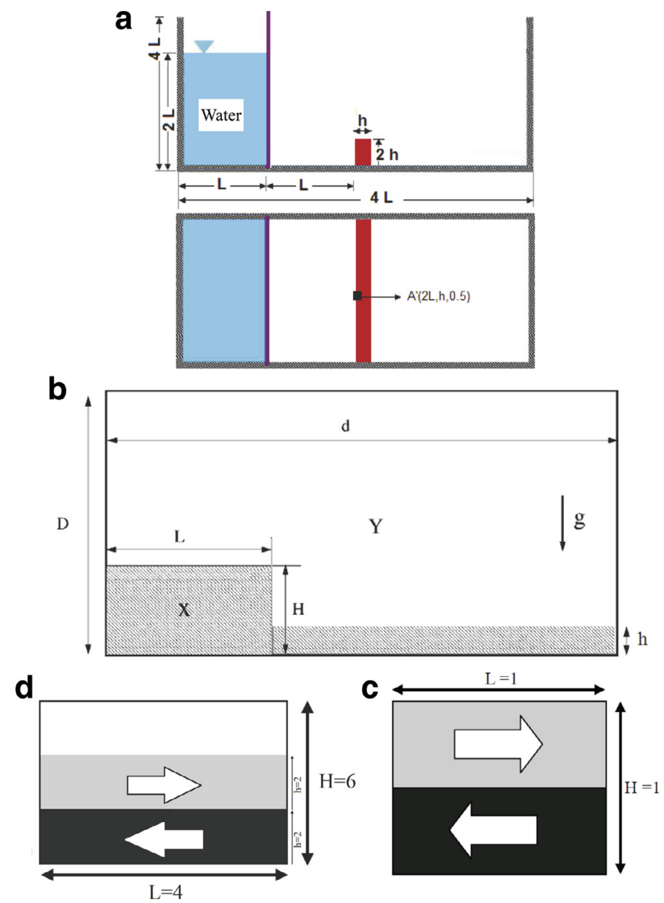


**Fig. 2.** Schematic geometry of the free-surface flows used to generate numerical results, (a) the side-view and the front-view of 3D dam break flow interaction with a bump, (b) 2D flow with the fluidized bed, (c) the traditional Kelvin–Helmholtz instability, (d) the double Kelvin–Helmholtz instability with a layer of air on top of water.

experimental results of dam break flow through a homogeneous porous block in a wet bed. Ataie-Ashtiani and Farhadi [10] developed a numerical method based on moving-particle semi-implicit method (MPS) for simulating incompressible inviscid flows with free surfaces. They introduced a kernel function that improves the stability of the MPS method. Staroszczyk [11] proposed the SPH model to simulate a two-dimensional problem of the collapse of a water column inside a rectangular tank. Their simulations illustrated the formation and subsequent propagation of a wave over the horizontal plane.

Ritchie and Thomas [12] adapted the SPH technique to allow a multiphase fluid in which SPH particles of widely differing density may be freely intermixed with applications involving galaxy formation and cooling flows. Church et al. [13] predicted the onset of mass transfer in eccentric binaries, and developed a two-phase SPH technique. Zainali et al. [14] presented a multi-phase incompressible SPH method with an improved interface treatment procedure. They demonstrated the effectiveness of the interface treatment that can handle multi-phase flow problems with high density and viscosity ratios, and modelled single vortex flow, square droplet deformation, droplet deformation in shear flow, and the Newtonian bubble rising in viscous and viscoelastic liquids.

Xiong et al. [15] proposed the SPH method for solving two-fluid model of dense particlefluid fluidizations by considering two types of SPH particles, where the interactions between particles of the same type constitute the inner-phase stress while those between particles of different types result in the drag force. Ghadampour et al. [16] examined the SPH method to simulate free-surface mud flow for two case studies, including the dam break and flow under a gate. They treated the mixture of water and sediment in the mud flow as a non-Newtonian fluid. Wu and Wang [17] established a one-dimensional model to simulate the fluvial processes under dam-break flow over movable beds by considering the effects of sediment transport and bed change on the flow. Bui et al. [18] presented an application of the SPH method to simulate the soilwater interaction. They modelled water as a viscous fluid with week compressibility and the soil as an elasticperfectly plastic material. Razavitotoosi et al. [19] described the application of SPH method for modelling two-dimensional waves caused by dam break over a movable bed in two dimensions. They modelled both fluid and sediment phases by particles as weakly compressible fluids.

Adami et al. [20] proposed a new surface tension formulation for multi-phase SPH scheme. They derived a new reproducing divergence approximation for drop-collision case without the need for a matrix inversion to obtain a stable and accurate scheme for surface curvature. Kordilla et al. [21] used a three-dimensional multi-phase SPH model to simulate surface tension dominated flow on smooth fracture surfaces. They modelled the droplet and film flow over a wide range of contact angles and Reynolds numbers encountered in such flows on rock surfaces. Zhang et al. [22] developed the method for simulation of surface tension-driven interfacial flow with the SPH model based on the interface reconstruction. Their cases include the drop deformation in shear flow, oscillation of square drop, head-on binary collision, and off-center binary collision.

Shadloo and Yildiz [23] presented a SPH solution for the Kelvin–Helmholtz Instability problem of an incompressible two-phase immiscible fluid in a stratified inviscid shear flow with interfacial tension over a wide range of Richardson number (Ri) and for three different density ratios. Tartakovsky and Meakin [24] developed a numerical model based on the SPH method to simulate the classical two-dimensional RayleighTaylor instability and three-dimensional miscible flow in fracture apertures with complex geometries. Price [25] discussed the treatment of discontinuities in the SPH simulations, the difference