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Simulation of Dam Break Flow Using Quasi-Molecular Modelling

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ABSTRACT

We developed a new method based on quasi-molecular modelling to simulate dam break flow. Each quasi-molecule was a group of particles that interacted in a fashion entirely analogous to classical Newtonian molecular interactions. The tank had a base length of 58.4 cm. A water column with a base length of 14.6 cm and a height of 29.2 cm was initially supported on the right side by a vertical plate drawn up rapidly at time t = 0.0 s. The water fell under the influence of gravity acting vertically downwards. The numerical results were validated by quantitative comparison with a previous study. The predicted height and leading edge of the water column corresponded very well with experimental measurements from a previous study. Therefore, our new method based on quasi-molecular modelling showed its ability to adequately simulate a free surface problem.

Keywords: Quasi-molecular modelling, particle modelling, molecular aggregate approach, dam break flow, dam collapsing

INTRODUCTION

Dam break flow has been the subject of intensive research for a long time [1,2]. Dam break flow includes several features of existing problems in the area of fluid mechanics, environment protection, marine hydrodynamics, and coastal engineering. The breaking wave phenomena often observed in dam break flow allows it to be included into a class of complex applications such as tank sloshing [3], the transportation of sediment [4], the interaction of extreme waves with floating structures and the green water on deck simulation [5].

Dam break flow represents the sudden release of fluid from behind a vertical barrier. Some experimental measurements (i.e. time evolution of the breaking water wave, and the position of the wave front on the vertical and horizontal walls) are performed on the dam break flow or collapse of a liquid column problem [2,6]. Photographs showing the time evolution of the collapsing column as well as the wave returning after hitting a wall on the opposite side are available for the purpose of evaluating the numerical methodology on the basis of flow visualisation. Measurements of the exact interface shape are not available, but some secondary data such as the reduction of the water column height [6] can be employed for quantitative comparison of the obtained results. Dam break flow is widely used as a classical test case for numerical simulation of free surfaces and moving interfaces [7-13]. The computation of highly nonlinear free surface flows is difficult because neither the shape nor the position of the interface between air and water is known a priori; on the contrary, it often involves unsteady fragmentation and merging processes.

In this paper, we propose an alternative modelling approach by considering the flow of the free surface (i.e. moving interface and deformable boundaries). This approach is based on classical molecular mechanics using molecular aggregates (i.e. lumped masses) called quasi-molecules or particles, and resulted in an N-body problem which must be solved numerically [14]. Quasi-molecular or particle modelling is a new numerical approach developed by Greenspan [14]. In this quasi-molecular modelling, the number of molecules is scaled down from their actual values ($\sim 10^{24}$) to smaller sizes (i.e. a small set of quasi-molecular particles which is approximately $10\text{-}10^2$ particles), while the intermolecular forces are correspondingly adjusted to approximate the correct hydrodynamic situation in order to agree with classical molecular-type formulas and conserve both mass and normalised energy. Unlike the continuum and statistical mechanics approaches, this approach concerns non steady state phenomena and variations in dynamical responses due to the variation of system parameters.

This study aimed to develop a new method based on quasi-molecular modelling to simulate 2-D dam break flow, and test the capability of the model with a free surface problem. Due to some limitation in computation power, the discussion is restricted to two dimensions, although the concepts and techniques could also be applied to three dimensions. Throughout the paper, cgs units are used.

METHODOLOGY

Quasi-molecular Modelling

We used quasi-molecular modelling to simulate dam break flow. The physical response of the fluid was caused by external forces (i.e. gravity). Gravity acted uniformly on all molecules in the fluid. In quasi-molecular modelling, interaction forces were considered only between nearest-neighbour particles and assumed to be of the same form as in molecular dynamic (MD) modelling. The interaction force was represented by Eq. (1):

$$F(R) = \frac{G}{R^p} + \frac{H}{R^q} \tag{1}$$

where G, H are parameters in the particle structure
p, q are exponential parameters in the particle structure
R is equilibrium position in the particle structure

G, H, p, q were positive constants with $q > p$ in order to obtain the repulsive effect that was necessarily stronger than the attractive one. Molecular interaction forces had two components: attraction and repulsion. The four parameters G, H, p and q were yet to be determined. If p, q and R_0 (R_0 is the equilibrium distance of the quasi-particle structure) were given, then by conditions of mass and energy conservation, G and H may be derived.

Just as in MD modelling, the dynamic equation of motion for each particle P_i of the system was given by Eq. (2):

$$m_i \frac{d^2 \vec{R}_i}{dt^2} = -980 m_i \vec{\delta} + \alpha \sum_{\substack{j=1 \\ j \neq i}}^{N} \left(\frac{G}{R_{ij}^p} + \frac{H}{R_{ij}^q} \right) \frac{\vec{R}_{ij}}{\left| R_{ij} \right|}, \; i \neq j \tag{2}$$

where m_i is mass of P_i
$\vec{R}_{ij}$ is the vector form of P_j to P_i

α is a normalising constant for P_i
N is the number of particles

α was obtained from Eq. (3):

$$\alpha \left| -\frac{G_i}{(\frac{3R_0}{2})^p} + \frac{H_i}{(\frac{3R_0}{2})^q} \right| < 980 m_p \tag{3}$$

where m_p is the mass of the particle [11]

α was used to normalise the interaction force between two particles. After normalisation, the interaction force between two particles was less than the gravitational force (i.e. < 9.81 cm/s^2).

For the simulation of dam break flow by particle modelling, we chose $p = 1$, $q = 3$, $R_0 = 1.12391$ cm and the distance of local interaction $D = 1.5$ cm, so the motion of particle P_i was determined by the dynamic Eq. (4).

$$\frac{d^2\vec{R}_i}{dt^2} = -980\vec{\delta} + \alpha \sum_{\substack{j=1 \\ j\neq i}}^{964} \left(\frac{101.1250}{R_{ij}} - \frac{145.6190}{R_{ij}^3} \right) \frac{\vec{R}_{ij}}{|R_{ij}|} \tag{4}$$

where vector $\vec{\delta} = (0,1)$, and the first term on the right-hand side (i.e. $-980\vec{\delta}$) was the gravity term. The normalising constant for P_i was $\alpha = -1.2777 \times 10^{-6}$.

For computational convenience, we used the time transformation $T = 10t$ (t in seconds). Eq. (4) was reformed as Eq. (5).

$$\frac{d^2\vec{R}_i}{dT^2} = -9.8\vec{\delta} + \sum_{\substack{j=1 \\ j\neq i}}^{964} \left(\frac{28.616}{R_{ij}} - \frac{36.147}{R_{ij}^3} \right) \frac{\vec{R}_{ij}}{|R_{ij}|} \tag{5}$$

Our model solved this equation simultaneously with a leapfrog numerical scheme.

Numerical Solution

In general, $F_i = m_i \ddot{r}_i$ $i = 1,2,3, \ldots, N$ could not be solved analytically from the given initial data and had to be solved numerically. The choice of a numerical method was simplified by the physics of quasi-molecular modelling in small time steps. The reason was that the repulsive component H/R^q in Eq. (1) could only be treated accurately with small time steps for small R, since

H/R^q was unbounded as R went to zero. Therefore, the advantages of using a high order numerical method, which allowed the choice of large time steps in obtaining a high degree of accuracy, were not applicable in quasi-molecular modelling. The leapfrog formulas relating position, velocity and acceleration for particle P_i are shown in Eq. (6) - (8).

$$\vec{v}_{i,1/2} = \vec{v}_{i,0} + \frac{\Delta t}{2}\vec{a}_{i,0}, \text{ (starter formula)} \tag{6}$$

$$\vec{v}_{i,k+1/2} = \vec{v}_{i,k-1/2} + (\Delta t)\vec{a}_{i,k}, \; k = 1,2,3,\ldots \tag{7}$$

$$\vec{r}_{i,k+1} = \vec{r}_{i,k-1/2} + (\Delta t)\vec{v}_{i,k+1/2}, \; k = 0,1,2,\ldots \tag{8}$$

where $\vec{v}_{i,k}$, $\vec{a}_{i,k}$ and $\vec{r}_{i,k}$ were the velocity, acceleration and position vectors of particle P_i at time $t_k = k\Delta t$, Δt was the time step, $\vec{v}_{i,k+1/2}$ was the velocity of particle P_i at $t_k = (k+1/2)\,\Delta t$, and so on.

Coordinate-System Setup

Dam break flow of a liquid column was simulated in 2-D. The dimension of the reservoir and the water column corresponded with those used in the experiment carried out by Martin and Moyec [2] and Koshizuka et al. [6]. The reservoir had a base length of 58.4 cm and the water column a base length (a) of 14.6 cm and a height (n^2a) of 29.2 cm, where a was the width of the liquid column and n was defined as a constant such that n^2a was the height of the column (**Figure 1a**). The water column was initially supported on the right side by a vertical plate drawn up rapidly at time, $t = 0.000$ s (**Figure 1a**).

The position of the water wave front and the height of the residual water column were plotted as functions of elapsed time and compared with experimental data from references [2] and [6]. Horizontally, the distance travelled by the water front from its initial starting point was defined as X_{front}, where $X_{front} = x/a$. Vertically, the quantity H represented the residual height (i.e. in comparison to the original starting state) and was defined by $H = y/(n^2a)$. Time was defined in two separate units, depending upon the direction of motion under consideration. Horizontally the unit was T, where $T = nt\sqrt{g/a}$ and vertically t^*, where $t^* = t\sqrt{g/a}$. All values have been rescaled to the appropriate dimensionless units described therein. In columns of water, we constructed a regular triangular grid of $N = 964$ points with the recursion formula (**Figure 1b**).

$$
\begin{array}{llll}
x_1 = 0\,,\ y_1 = 0\,, & x_{32} = 0.365\,, & y_{32} & = 0.63219 \\
x_{i+1} = 0.73 + x_i\,, & y_{i+1} = y_1\,, & i & = 1,2,...,22 \\
x_{i+1} = 0.73 + x_i\,, & y_{i+1} = y_{24}\,, & i & = 24,25,...,44 \\
x_i = x_{i-45}\,, & y_i = 1.2644 + y_{i-45}\,, & i & = 46,47,...,964
\end{array}
$$

The edge length of each triangular building block was 0.73 cm. At each grid point (x_i, y_i), we set a particle P_i, that is, an aggregate of water molecules or a water particle (**Figure 1b**). Water particles were distributed uniformly throughout the interior of the cavity. We assigned an initial random velocity over the interval [0,0] to each particle in order to complete the initial data condition.

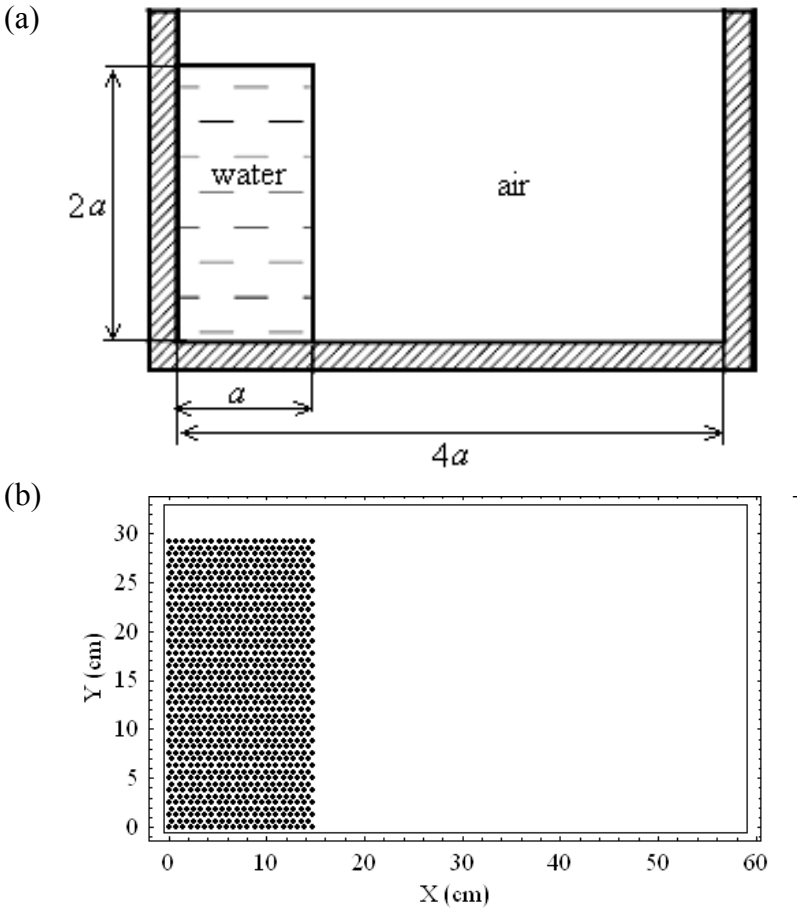

Figure 1 (a) General layout of the dam break flow problem and boundary condition and (b) configuration of 964 water particles of water column.

After all initial data were determined, we allowed each of the 419 water particles P_i interact with all other particles in accordance with Eq. (5). The numerical solution was generated by the leap-frog formulae with $\Delta t = 0.001$. We imposed a local interaction distance $D = 1.5$ cm.

NUMERICAL RESULTS AND DISCUSSION

Time sequences of evolution of the dam break flow from time $t = 0.00$ to $t = 1.20$ s are shown in **Figures 2a-h**. A non-dimensionalised time, $t^* = t\sqrt{g/a}$, was used for explaining different stages of the problem. At time $t^* = 0.00$ s, the water column was allowed to flow. A relatively high velocity and shallow water depth flew in the x-direction quickly formed (e.g. $t^* = 0.16$ s). As time progressed, the flow impacted on the vertical wall at the opposite side of the tank. An upward water jet was suddenly formed that rose until gravity overcame the upward momentum ($t^* = 3.50$ s). At this moment, the jet became thicker and the flow started to reverse. Due to the oncoming flow, an adverse momentum gradient was created that resulted in an overturning wave ($t^* = 4.00$ s). This wave formation continued until the wave tip reconnected with the incident shallow water flow that now had less forward momentum. A sudden rise in pressure occurred at the reconnection point that was of the same order of magnitude as the pressure on the impact wall. This was due to the existence of high relative momentum between the fluid at the wave tip and the free-surface just before the attachment. At this stage, the flow became complicated as several big and small pockets of entrained air were created due to the first and subsequent impacts on the free-surface. For $t^* > 5$, the overall momentum of the flow had reduced considerably, therefore, analysis of the flow beyond this point was of no practical significance.

Gravity (i.e. $g = 9.81$ cm/s^2) caused the water column on the left of the reservoir to seek the lowest possible level of potential energy (**Figures 2a-h**). Thus, the water column would collapse and eventually come to rest. The initial stages of the flow were dominated by inertia forces with viscous effects increasing as the water came to rest.

The height of the collapsing water column decreased rapidly as time increased (**Figure 3a**). The leading edge of the collapsing water column increased as time increased (**Figure 3b**). Data available from the experiments in references [2] and [6] consisted of pictures which showed the time evolution of the breaking water wave, and secondary data such as the position of wave front on the vertical and horizontal walls. Comparisons between the numeric and experimental data are presented in **Figures 3a** and **b**. The results from the simulation were in good agreement with the experimental ones.

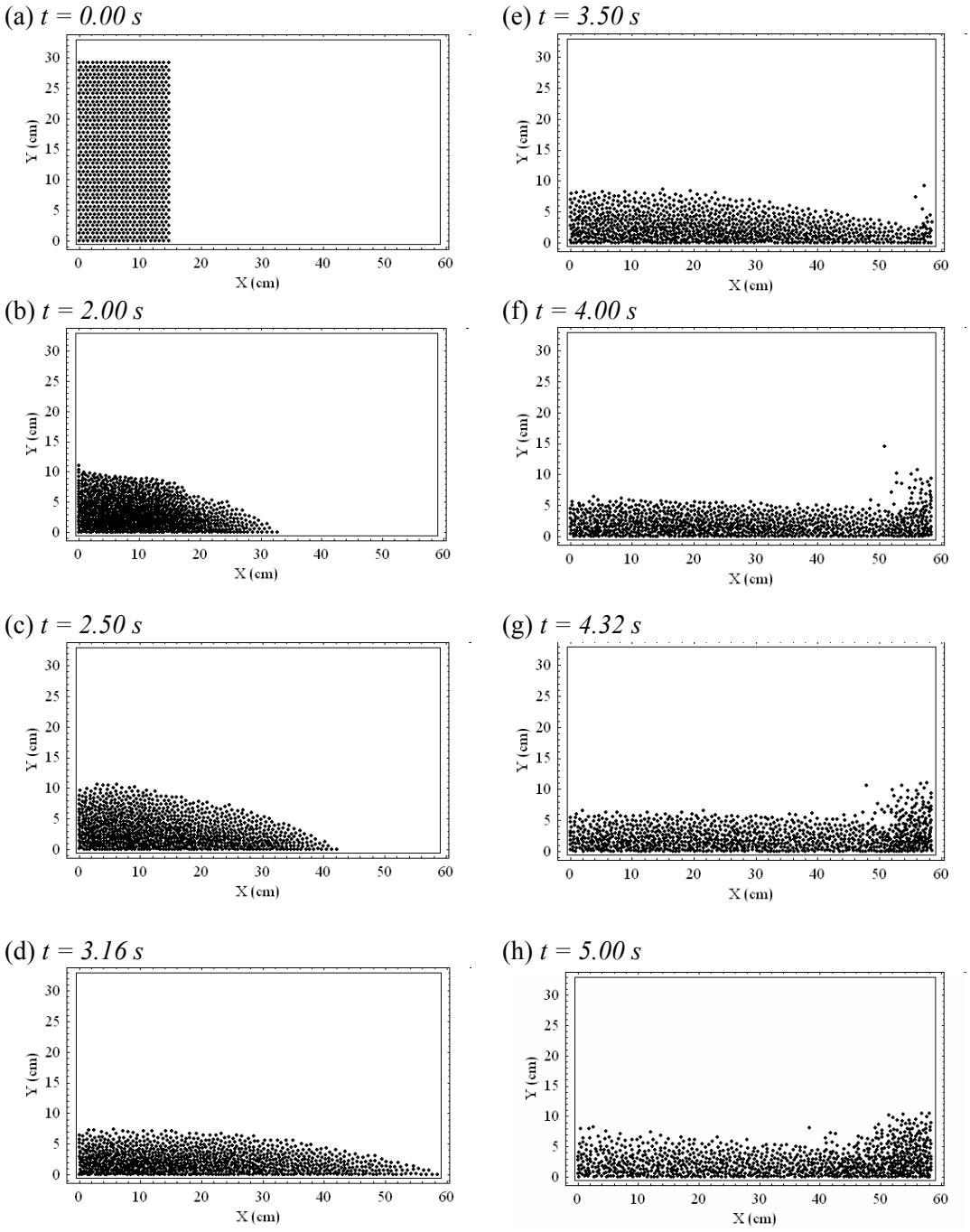

Figure 2 Time evolution of the dam break flow. (a) *t = 0.00* (s), (b) *t = 0.16* (s), (c) *t = 2.26* (s), (d) *t = 3.12* (s), (e) *t = 3.50* (s), (f) *t = 4.00* (s), (g) *t = 4.32* (s) and (h) *t = 5.00* (s)

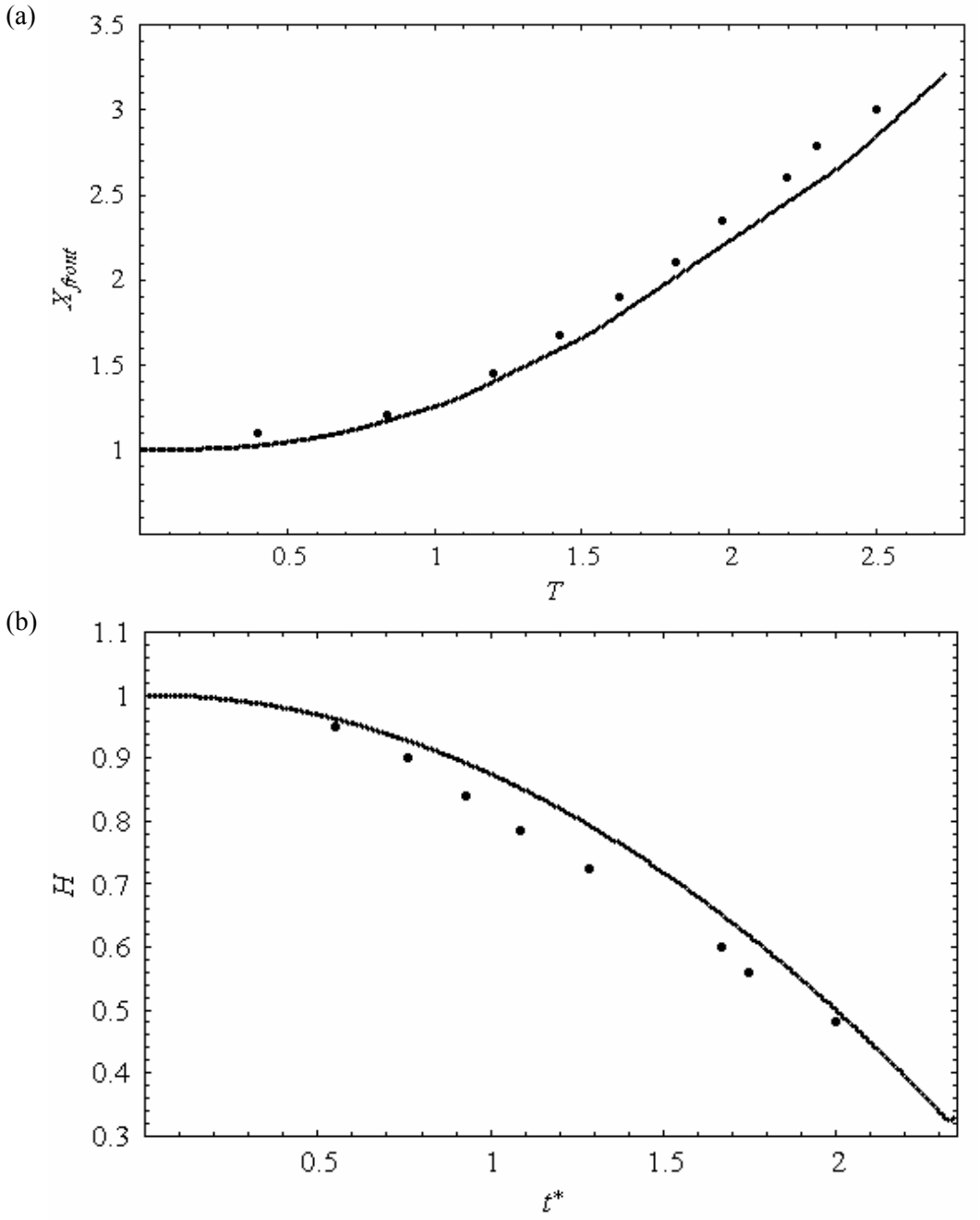

Figure 3 Quantitative comparison of the numerical results (–) and experimental measurement (•). (a) non-dimensional wave front (X_{front}) of the collapsing water column versus non-dimensional time. (b) non-dimensional height (H) at the left wall positions of the collapsing water column versus non-dimensional time.

CONCLUSION

Many researches have been done on dam break flow. However, this is the first to use Quasi-molecular or particle modelling simulating the dam break flow. The simulation of dam break flow starts with a high velocity, shallow water depth flowing in the *x*-direction quickly, the flow impacting on the vertical wall at the opposite side of the tank, the upward water jet forming on the vertical wall and then the jet reversing. The simulated position of the wave front on the horizontal wall and non-dimensional height at the left wall positions of the collapsing water column are in good agreement with the experimental ones.

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REFERENCES

[1] JJ Stoker. *Water Waves*. John Wiley & Sons, New York, 1958, p. 415.

[2] JC Martin and WJ Moyce. An experimental study of the collapse of liquid columns on a rigid horizontal plane. *Phil. Trans. Roy. Soc. Lon. A. Math. Phys. Sci.* 1952; **244**, 312-24.

[3] JH Hwang, IS Kim, YS Seol, SC Lee and YK Chon. Numerical simulation of liquid sloshing in three-dimensional tanks. *Comput. Struct.* 1992; **44**, 339-42.

[4] D Pritchard and AJ Hogg. On sediment transport under dam-break flow. *J. Fluid Mech.* 2000; **473**, 265-74.

[5] KS Varyani, XP Pham and P Crossland. Green water investigation onboard high-speed container shipsusing non-linear method. *Ship Tech. Research.* 2004; **5i**, 1-11.

[6] S Koshizuka and Y Oka. Moving particle semi-implicit method: Fully lagrangian analysis of incompressible flows. *In*: Proceedings of the

European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Barcelona, Spain. 11-14 September 2000.

[7] JV Soulis. Computation of two-dimensional dam break flood flows. *Int. J. Numer. Meth. Fluids.* 1992; **14**, 631-64.

[8] FH Harlow and JE Welch. Numerical calculation of time-dependent viscous incompressible flow. *Phys. Fluids.* 1965; **8**, 2182-89.

[9] CW Hirt and BD Nichols. Volume of fluid (VOF) method for the dynamics of free boundaries. *J. Comp. Phys.* 1981; **39**, 201-25.

[10] P Brufau and P Garcia-Navarro. Two-dimensional dam break flow simulation. *Int. J. Numer. Meth. Fluids.* 2000; **33**, 35-57.

[11] B Buchner. 2002, *Green water on ship-type offshore structures*. Ph.D. thesis, Delft University of Technology, the Netherlands.

[12] A Colagrossi and M Landrini. Numerical simulation of interfacial flows by smoothed particle hydrodynamics. *J. Comp. Phys.* 2003; **191**, 448-75.

[13] M Greco, OM Faltinsen and M Landrini. Basic studies of water on deck. *In*: Proceedings of the 23rd Symposium on Naval Hydrodynamics, Val de Reuil, France, 2001, p. 126-41.

[14] D Greenspan. *Quasi-molecular modelling*. JBW Printers and Binders, Singapore, 1991, p. 1-212.

บทคัดย่อ

สิทธิชัย กุลศรี มัลลิกา เจริญสุธาสินี และ กฤษณะเดช เจริญสุธาสินี

การจำลองการแตกของเขื่อนโดยใช้แบบจำลองควาซิโมเลกุล (Quasi-molecular)

เราได้พัฒนาวิธีการจำลองการไหลของน้ำจากเขื่อนแตกโดยใช้แบบจำลองควาซิโมเลกุล (Quasi-molecular) แบบจำลองนี้ในแต่ละควาซิโมเลกุลประกอบด้วยกลุ่มอนุภาคที่มีอันตรกิริยากันในรูปแบบของโมเลกุลที่ทำอันตรกิริยาแบบนิวโตเนียน (Newtonian molecular interaction) ในการจำลองการไหลของน้ำจากเขื่อนแตกในตู้สี่เหลี่ยมซึ่งมีฐานยาวเท่ากับ 58.4 เซนติเมตร, ความสูงของน้ำเริ่มต้นเท่ากับ 29.2 เซนติเมตรและฐานของน้ำเริ่มต้นเท่ากับ 14.6 เซนติเมตรซึ่งน้ำถูกคั่นด้วยแผ่นสี่เหลี่ยมเอาไว้ในระยะแรกของการจำลอง หลังจากนั้นน้ำจะถูกปล่อยออกมาอย่างรวดเร็ว ณ เวลา $t = 0$ วินาที น้ำเมื่อถูกปล่อยน้ำจะไหลลงสู่ที่ต่ำเนื่องจากการกระทำของแรงโน้มถ่วงของโลก ผลการจำลองเชิงตัวเลขถูกเปรียบเทียบกับผลที่ได้จากการทดลอง พบว่าผลที่ได้จากการจำลองเชิงตัวเลขของตำแหน่งความสูงของน้ำและตำแหน่งการไหลของน้ำในแต่ละช่วงเวลาใกล้เคียงกับค่าที่ได้จากการทำการทดลอง ดังนั้นจึงแสดงได้ว่าวิธีการแบบใหม่ของเราที่ใช้แบบจำลองควาซิโมเลกุลสามารถใช้จำลองปัญหาที่เกี่ยวกับผิวอิสระ (free surface problem) ได้

สำนักวิชาวิทยาศาสตร์ มหาวิทยาลัยวลัยลักษณ์ อำเภอท่าศาลา จังหวัดนครศรีธรรมราช 80161