Validation DualSPHysics code for liquid sloshing phenomena

*Sergei.K. Buruchenko¹, Alejandro J.C. Crespo²

¹South Ural State University, Snezhinsk, Russia. ²Universidade de Vigo, Spain.

*Corresponding author: askskb@gmail.com

Abstract

The DualSPHysics code is proposed as a numerical tool for the simulation of liquid sloshing phenomena. A particular type of sloshing motion can occur during the core meltdown of a liquid metal cooled reactor (LMR) and can lead to a compaction of the fuel in the center of the core possibly resulting in energetic nuclear power excursions. This phenomenon was studied in series of "centralized sloshing" experiments with a central water column collapsing inside the surrounding cylindrical tank. These experiments provide data for a benchmark exercise for accident analysis codes. To simulate "centralized sloshing" phenomena, a numerical method should be capable to predict the motion of the free surface of a liquid, wave propagation and reflection from the walls. The DualSPHysics code based on the smoothed particle hydrodynamics method was applied to the simulation of "centralized sloshing" experiments. Simulation results are compared with the experimental results. In a series of numerical calculations it is shown that overall motion of the liquid is in a good agreement with experimental observations. Dependence on the initial and geometrical symmetry is studied and compared with experimental data.

Keywords: ICCM2014, Computational method, Sloshing Experiment, Smoothed Particle Hydrodynamics

Introduction

The problem of safety in nuclear reactors has been intensively studied from the time of the development of the first reactor designs. Over time, several severe accidents occurred at nuclear reactors, but without dangerous consequences for the environment, until the accident at Chernobyl Nuclear Power Plant (NPP) occurred in 1986 and massive severe accident at Fukushima NPP (2011), where four units were seriously damaged by a tsunami wave. Today it is clear that further successful development of the nuclear energy industry is impossible without deeper knowledge of severe accidents and without the provision of safety guarantees to the public, based on comprehensive analyses of nuclear reactor safety.

One of the current problems in severe accident analysis is the problem of molten corium motion, which could possibly result in a recriticality event. The movement of the corium during an accident involving melting of the reactor core may be initiator of a recriticality event with dangerous high power excursions.

Simulation with Eulerian methods is difficult, since special treatments are required for capturing the indicated phenomena. To be more specific, the treatments required are the Volume Of Fluid (VOF) method, combined with mesh refinement, for tracking the free-surface, and sliding meshes, for the connection between the moving and stationary meshes. The above treatments increase the computational cost and requirements of the simulation considerably. An alternative way of simulating the flow is the Smoothed Particle Hydrodynamics (SPH) method which will be used in the present work for the simulations.

The SPH method was initially developed by [Lucy (1977)], [Gingold & Monaghan (1977)] and has been used for modeling astrophysical problems. The application of SPH to a wide range of scientific areas has led to significant extensions and improvements of the original method [Monaghan (2005)], [Liu(2003)]. SPH is a Lagrangian, particle, mesh-less method and has the

advantages of tracing and resolving the free-surface without any special treatment and describing moving/deforming boundaries easily.

The DualSPHysics code [Gomez-Gesteira et al. (2012a, 2012b)] is proposed as a numerical tool for the simulation of liquid sloshing phenomena. A particular type of sloshing motion can occur during the core meltdown of a liquid metal cooled reactor (LMR) and can lead to a compaction of the fuel in the center of the core possibly resulting in energetic nuclear power excursions. This phenomenon was studied in series of "centralized sloshing" experiments [Maschek et al. (1992a, 1992b)] with a central water column collapsing inside the surrounding cylindrical tank. These experiments provide data for a benchmark exercise for accident analysis codes. To simulate "centralized sloshing" phenomena, a numerical method should be capable to predict the motion of the free surface of a liquid, wave propagation and reflection from the walls.

Standart SPH formalism

The SPH formalism relies on the use of kernel approximation of field functions for the calculation of the operators appearing in the discretization of the flow equations, instead of using a computational grid. In this way it is able to approximate derivatives or functions from unconnected and randomly scattered computation points. The basis of the SPH approximations originates from the following identity:

$$f(x) = \int f(x')\delta(x - x')dx'$$
⁽¹⁾

where f(x) is a function of three dimensional position vector **x**, $\delta(x - x')$ is the Dirac delta distibution and Ω is the volume of the integral that contains **x**. The above relation can be approximated using a smoothing kernel function W(x - x', h):

$$\langle f(x) \rangle = -\int_{\Omega} f(x')W(x-x',h)dx'$$
 (2)

A similar equation can be derived for the gradient of a function:

$$\left\langle \nabla f(x) \right\rangle = -\int f(x') \nabla W(x - x', h) dx'$$
(3)

In order the above approximations to be valid,² the kernel function W(x - x', h) has to fulfill certain requirements. such

as:

•Unity or normalization condition : $\int W(x - x', h) dx = 1$ •Dirac distribution property : $\lim W(x - x', h) = \delta(x - x')$ •Compact condition : W(x - x', h) = 0, for $|x - x'| > k \cdot h$, where $k \cdot h$ is the kernel's support domain •Also the kernel function has to be even, positive and monotonically decreasing function.

There are many types of kernel functions. In the present work the quintic kernel is used [Monaghan (2005)]

$$W(q) = \frac{21}{16\pi\hbar^3} \left(1 - \frac{q}{2}\right)^4 (2q+1) \quad 0 \le q \le 2$$
(4)

where q = |r|/h, with |r| the distance between two computational points and h a characteristic smoothing length.

In the SPH method the entire system is represented with a finite number of particles that carry individual mass, occupy individual space and the characteristic quantities of the flow (e.g. velocity, density, pressure etc.). Thus the continuous integral relations can be written in the following form of discretized particle approximation:

$$\left\langle f(x_i) \right\rangle = \sum_{j=1}^{\infty} \frac{m_j}{\rho_j} f(x) W_{ij}$$
(5)

$$\left\langle \nabla f(x_i) \right\rangle = \sum_{j=1}^{\infty} \frac{m_j}{\rho_j} f(x) \nabla W_{ij}$$
(6)

In the above equations $W_{ij} = W(x_i - x_j, h)$, m_j is the *j* particle's mass and p_j is the *j* particle's density.

Using the above approximations for a function and the derivative of a function, one can derive the SPH flow equations [Monaghan (2005)]:

Momentum equation:

$$\frac{dV_i^{\alpha}}{dt} = -\sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij}\right) W_{ij,\alpha} + g$$
(7)

Continuity equation:

$$\frac{d\rho_i}{dt} = \rho_i \sum_j \frac{m_j}{\rho_j} \left(V_i^{\alpha} - V_j^{\alpha} \right) W_{ij,\alpha}$$
(8)

where g-gravity acceleration, Π_{ij} is the viscosity term suggested by [Monaghan (2005)], V_i^{α} is velocity, P_i is pressure, *latin* indexes denotes particles number, *greek* index denote coordinate direction.

$$\frac{\partial W_{ij}}{\partial x_i^{\alpha}} = W_{ij,\alpha} \tag{9}$$

Pressure is calculated from an equation of state, thus the method is weakly compressible. The Tait equation of state is commonly used .

$$p = \frac{\rho_0 c_0^2}{\gamma} \left[\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right]$$
(10)

In the above equation $\gamma = 7$, ρ_0 is the reference density and c_0 is an artificial speed of sound, since the real speed of sound would require a very small time step. In order to keep density variations less than 1%, the value of c_0 is chosen ~10 V_{max}, according to [Monaghan (2005)].

The dynamic boundary conditions described in [Crespo et al., (2007)] are used in this work. The boundary particles satisfy the same continuity equation as the fluid particles, therefore, their density and pressure also evolve. Hence, when a fluid particle approaches a boundary particle, and they are at the interaction distance defined by the kernel range, the density of the boundary particles increases giving rise to an increase distance of the pressure and the force exerted on the fluid particle also increases due to the pressure term in the momentum equation creating a repulsive mechanism between fluid and boundary.

Implenmentation details

The SPH scheme presented in the previous section is implemented in the DualSPHysics code. The code is implemented using both the C++ and CUDA programming languages. The code can then be executed either on the CPU or on the GPU since all computations have been implemented both in C++ for CPU simulations and in CUDA for the GPU simulations. The philosophy underlying the development of DualSPHysics is that most of the source code is common to CPU and GPU which makes debugging straightforward as well as the code maintenance and new extensions. This allows the code to be run on workstations without a CUDA-enabled GPU, using only the CPU implementation. On the other hand, the resulting codes should be necessarily different since code developers have considered efficient approaches for every processing unit.

Computational runtime increases dramatically with the number of particles in the SPH simulations. Hence, parallelisation methods are essential to run simulations with a huge number of particles in a reasonable execution time. GPUs constitute a suitable hardware for scientific tasks where mathematical calculations are carried out using large sets of data.

Optimization strategies for CPU and GPU implementations of a smoothed particle hydrodynamic method [Gomez-Gesteira et al. (2012a, 2012b)] introduced the framework to implement SPH codes using the best techniques and performance optimizations on GPU. That work focused on identifying suitable algorithms for efficient parallelization since a proper and full use of all the capabilities of the GPU architecture is not straightforward. As an initial step, the implementation focused on solving the particle interactions on a GPU using CUDA and the next step was the implementation of the neighbour list and the time integration in order to develop an entire GPU-SPH model.

Experiment description

The DualSPHysics code described in the previous sections, has been applied to the numerical simulation of the three-dimensional sloshing liquid motion problems. These problems has been experimentally studied in KfK (presently KIT) in the framework of the safety analysis of fast nuclear reactors [Maschek (1992a)].

The sloshing experiments had two main objectives. The first was to obtain a better understanding of centralized sloshing phenomenon. In a hypothetical severe accident of a fast nuclear reactor, a possible recriticality may occur following core melting and relocation of the fissile materials.

The second purpose of the sloshing liquid motion experiments was to provide data for a benchmark exercise for reactor accident analysis codes [Maschek(1992b)]. These data were subsequently used to verify and validate the SIMMER-III/IV reactor safety analysis code [Shirakawa (2008)], [Yamano et. Al (2008)].

Experiments were performed with water under normal conditions. The experimental installation consists of a cylindrical container separated by a membrane into two coaxial parts. The container was opened, so that the environment is air under atmospheric pressure. At the initial moment, the membrane is quickly moved up, resulting in the water column collapsing under the force of gravity.



Fig. 1 Central sloshing experiment geometry.

In Fig.1 (a) and Fig.1 (b), the different experimental configurations at the beginning of the experiments are presented:

- (a) a fully symmetrical configuration with no obstacles in the flow
- (b) an asymmetrical configuration with no obstacles
- (c) a symmetrical configuration with a rod bank installed around the liquid column.

For the asymmetrical case, the same experimental and computational domain geometry is used, but the position of the water column is shifted by an offset of 8.25 cm from the container center.

The parameters of the numerical model used in the calculations for the symmetrical geometry are: container diameter D = 0.44 m, diameter of water column d = 0.11 m, height of water column h = 0.2 m, water density 1000 kg/m³.

The geometry of the numerical model for the test cases with rod imitators is the same as for the experimental series without rods. The difference is the presence of twelve vertical rods equidistantly positioned around the water column. Their distance from the center is $R_c = 17.6$ cm . The rod diameter (d_{rod}) in the experiments was 2 cm, to simulate a blockage ratio similar to that in a real reactor pool. The same value for the rod diameter has been used in the numerical model. An overview and sketch of the experimental setup, with geometrical sizes, for these test series are given in Fig. 1 (b).

The initial velocity field in water is zero. The initial pressure field is hydrostatic:

$$p = \rho g h \tag{11}$$

Experiment and numerical results

In this section the results of the simulation of the centralized sloshing experiment in the symmetrical geometry, the asymmetrical geometry and experiment geometry with 12 rod bank are presented.

The main quantitative parameters for the symmetrical case are the arrival time of the liquid at the wall, the time and height of the maximal wave at the wall, and the time and height of the central peak. The central peak height is the most important of these for the recriticality analysis, and, as has been found, the peak height is difficult to reproduce in the numerical simulation.



Figure 2. Experiment and simulation result for symmetrical case.

Furthermore, a correct definition and measurement of the central peak height is not very obvious. In the applied experimental technique, large drops on top of the peak moving with the same velocity as the bulk flow were included in the height measurement (see the more detailed discussion of the definition of the central peak value in the following subsection).



Figure 3. Experiment and simulation result for asymmetrical case. T=0 sec, T=0.25 sec, T=0,47 sec, T=0.75 sec

For the asymmetrical case, only the timing of the maximum height at the walls and the height of the maxima were measured in the experiments.

Fig. 2-4 shows a visualization of the results of the simulation in comparison with the experimental observations of the liquid sloshing motion.



1 0 7 100

Figure 4. Experiment and simulation results with 12 rod bank. T=0 sec, T=0.21 sec, T=0.36 sec, T=0.86 sec.

The results are summarized in Table 1-3. Most of the quantitative simulation results are in a good agreement with both experimental data and the numerical results predicted by the reactor safety analysis code SIMMER-IV, although some deviations in the central peak value are observed. Also, for the asymmetrical case, a lower value of the height of the right-hand slosh is predicted. A similar value was obtained using the SIMMER-IV code. For the asymmetrical geometry, the lower values may be due to the relatively low resolution of the numerical model.

	Slosh at outer container wall			Slosh at pool center	
Symmetrical	Arrival time	Time of	Maximum	Time of	Maximum
case	at wall [s]	maximum	heights [cm]	maximum	height [cm]
		heights [s]		height [s]	
Experiment	0.20±0.02	0.42 ± 0.02	16±1.0	0.88 ± 0.04	40±5
SPH result 2.8	0.21	0.30	14	0.88	0.33
M particles	0.21	0.37	14	0.00	0.33
SIMMER-IV					
(coarse mesh -	0.20	0.40	17.25	0.88	36
44×44×100)					
SIMMER-IV					>50
(fine mesh -	0.20	0.38	18.75	-	/JU (overestimated)
92×92×100)					(overestimated)

Table 1. 3D Central Sloshing: Symmetrical Case

Table 2. 3D Central Sloshing: Asymmetrical Case

A symmetrical Case	Slosh at po	ol center	Slosh at right wall		
Asymmetrical Case	Time of maximum height [s]	Maximum height [cm]	Time of maximum height [s]	Maximum height [cm]	
Experiment	0.36±0.02	14.0 ± 2.0	0.48 ± 0.02	24±2.0	
SPH result 2.8 M particles	0.36	14.5	0.48	21.5	
SIMMER-IV	0.36	17.25	0.48	21	

Table 3. 3D Central Sloshing: Symmetrical Case. Vertical Rod Bank

Vertical Rod	Slosh at outer wall			Slosh at pool center	
Bank	Arrival time	Time of	Maximum	Time of	Maximum
	at wall [s]	maximum	height [cm]	maximum	height [cm]
		heights [s]		height [s]	
Experiment	0.20 ± 0.02	0.42 ± 0.02	15±1.0	0.88 ± 0.04	15±3
SPH result 2.8 M particles	0.21	0.39	16	0.86	0.12

The comparative snapshots from the experiment and numerical simulation for the test cases with 12 rod bank are presented in Fig. 4.

Conclusion

The DualSPHysics computer code based on the SPH method has been applied to the numerical simulation of the three-dimensional sloshing liquid motion problem. A number of numerical models have been created to reflect different configurations of the experimental installations. These are as follows:

- Fully symmetrical configuration: the liquid column is symmetrically located at the container center.
- Asymmetrical configuration: the liquid column is located with an offset from the container center.
- Symmetrical configuration with obstacles: rod imitators are installed around the liquid column.

The quantitative parameters of the flows predicted by the numerical algorithm have been compared with the available results of the simulations performed with the SIMMER-III/IV reactor safety analysis code and with experimental data. These measured flow quantities, such as the heights of the wall sloshes and the central peak, and the timings of these events, are accurately predicted with high resolution simulations. At the same time, the present algorithm based on the SPH method is capable of resolving the high central peak in the fully symetrical case, which was an issue for the SIMMER code.

A sensitivity study for the value of the central peak height in the symmetrical configuration has also been performed. The study showed the convergence of the central peak height value with an increase in the number of particles used for modeling.

In analyzing for a possible recriticality event, the height values of the central peak calculated for the different experimental configurations and different resolutions of the numerical model were compared. The highest peak, corresponding to the maximal volume of the fissile materials compacted in the center of the pool, is observed in calculations of the fully symmetrical configuration with the fine numerical resolution. Thus conclusion demonstrates the experimentally observed sensitivity of the liquid flow to the geometrical asymmetries of the vessel.

References

Lucy L., (1977) "A numerical approach to the testing of the fission hypothesis", Astron. J. Vol. 82, pp. 1013–1024.

- Gingold R.A., Monaghan J.J. (1977) "Smoothed particle hydrodynamics: theory and application to non- spherical stars", *Mon. Not. R. Astr. Soc.*, Vol. 181, pp. 375–389.
- Monaghan J.J., (2005) "Smoothed Particle Hydrodynamics", Rep. Prog. Phys. Vol. 68, pp. 1703–1759.
- Liu G.R., Liu M.B., (2003), "Smoothed particle hydrodynamics: a meshfree particle method", World Scientific Publishing Company, December 2003.
- Gómez-Gesteira M., Rogers B.D., Crespo A.J.C., Dalrymple RA, Narayanaswamy M and Domínguez JM. (2012a). SPHysics - development of a free-surface fluid solver- Part 1: Theory and Formulations. Computers & Geosciences, 48: 289-299.
- Gómez-Gesteira M., Crespo A.J.C., Rogers B.D., Dalrymple R.A., Domínguez J.M. and Barreiro A., (2012b). "SPHysics - development of a free-surface fluid solver- Part 2: Efficiency and test cases", *Computers & Geosciences*, Vol. 48, pp. 300-307.
- Maschek W., Munz C.D., Meyer L., (1992a) "Investigations of sloshing fluid motions in pools related to recriticalities in liquid-metal fast breeder reactor core meltdown accidents", *Nucl. Techn.*, 1992. Vol. 98(1), p. 27.
- Maschek W., Roth A., Kirstahler M., Meyer L., (1992b) "Simulation experiments for centralized liquid sloshing motions", Karlsruhe Research Centre Report KfK 5090, Dez. 1992.
- Crespo, A.J.C., Gómez-Gesteira, M., Dalrymple, R.A. (2007) "Boundary conditions generated by dynamic particles in SPH methods", *CMC: Computers, Materials, & Continua*, Vol. 5(3), pp. 173–184.
- Shirakawa N., (2008)"R&D of the next generation safety analysis methods for fast reactors with new computational science and technology", Proc. of 14th JAEA-FZK/CEA/IRSN/ENEA SIMMER-III/IV Review Meeting. Karlsruhe, Germany, September 9–12, 2008.
- Yamano H., Hosono S., Sugaya M., (2008)"Analysis of sloshing experiments", *Proc. of 14th JAEA-FZK/CEA/IRSN/ENEA SIMMER-III/IV Review Meeting*, Karlsruhe, Germany, September 9–12, 2008.