Numerical simulation of explosion using Smoothed Particle Hydrodynamics with variable smoothing length

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1. Introduction

Explosion threatens Nuclear Power Plant component's safety, so explosion is an important issue in the nuclear engineering field. Some cases of explosion phenomena such as ex-vessel steam explosion need more verification to insure safety analysis.

Explosion phenomena involve special features such as large deformation, moving material interface. These features are generally difficult for traditional grid-based numerical methods. On the contrary, a Lagrangian based meshless method SPH is easy to express large distorted condition, adopting this method to simulate an explosion.

In addition, the accuracy of the explosion phenomenon analysis can be improved by adjusting the smoothing length according to particle's local condition adaptively. In order to confirm its simulation ability, observing and analyzing the results of the sod shock tube problem and underwater explosion problem.

In this study, the SOPHIA code with adaptive smoothing length algorithm was used. The SOPHIA code is a GPU-parallelized SPH solver developed by Seoul National University for analyzing complicated multi-physics problem associated with nuclear reactor safety.

2. SPH method

2.1 SPH basics

SPH is a Lagrangian based meshless method which first used for describing astrophysical motion. Because of SPH's feature, the SPH method expands to many fields [1].

The SPH method assumes fluid system as finite particle's collection. So, particle moves with their physical variables such as mass, velocity, pressure. Physical variables are derived by interpolation with neighbor particle.

Arbitrary function f 's SPH interpolation is represented by multiplying the kernel function and integrating over the computational domain for a function f . For calculating numerical approximated integral formation in computer, discretized formulation is used in SOPHIA code.

$$f_i(r) = \sum_j \frac{m_j}{\rho_j} f_j W(r_i - r_j, h_i) \tag{1}$$

$$\nabla f_i(r) = \sum_j \frac{m_j}{\rho_j} f_j \nabla W(r_i - r_j, h_i) \tag{2}$$

Where i connotes center particle, j connotes neighbor particle which used in SPH interpolation and m is mass, ρ is density. W is the kernel function which is a function of distance between particles and smoothing length.

The SPH derivative approximation of a function is in the similar way by multiplying kernel function's derivative instead of kernel function.

2.2 SPH governing equation with variable smoothing length

Smoothing length h decides the range of interaction for each particle. General SPH uses a constant smoothing length for all particles, but in some case particle need to have longer smoothing length if they don't have enough particle in their domain or need to have shorter smoothing length if they have so many particles in their domain. So deciding appropriate smoothing length increases accuracy and efficiency of SPH method [2].

$$h_i \propto \left(\frac{1}{\rho_i}\right)^d \tag{3}$$

Smoothing length of each particle is determined by using a Newton-Rapson method which is one of iterative method. This method includes smoothing length correction factor term as follows.

$$\Omega_i = 1 - \frac{\partial h_i}{\partial \rho_i} \sum_j m_j \frac{\partial W_{ij}(h_i)}{\partial h} \tag{4}$$

The governing equation for hydrodynamics are the conservation equations of continuum mechanics.

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v} \tag{5}$$

$$\frac{d\vec{v}}{dt} = -\frac{1}{\rho} \nabla \mathrm{p} \tag{6}$$

$$\frac{dE}{dt} = -\frac{p}{\rho} \nabla \cdot \vec{v} \tag{7}$$

Where $\vec{v}$ is velocity, p is pressure and E is internal energy.

The discretized SPH formulation has various forms of governing equation.

In mass conservation (5), there are two approaches to calculate density in the SPH method, mass summation (8) and continuity (9). In this study, the mass summation approach is used.

In momentum conservation (6) and energy conservation (7), these equations choose symmetric form (10), (11) and adapt search range to bigger smoothing length to obey Newton's third law.

Equation of state is a function of density and internal energy. It is different from each simulation.

Table I: SPH formulation for governing equation

Governing equation	SPH formulation
Mass conservation	$\rho_i = \sum_j m_j W(h_i)$ (8) $\frac{d\rho_i}{dt} = \frac{1}{\Omega_i} \sum_j m_j \overrightarrow{v_{ij}} \nabla_i W_{ij}(h_i)$ (9)
Momentum conservation	$\frac{d\vec{v_i}}{dt} = -\sum_j m_j \left[\frac{p_i}{\Omega_i \rho_i^2} \nabla_i W_{ij}(h_i) + \frac{p_j}{\Omega_j \rho_j^2} \nabla_i W_{ij}(h_j) + \Pi_{ij} \cdot \overline{\nabla_i W_{ij}} \right]$ (10)
Energy conservation	$\frac{dE_i}{dt} = \frac{1}{2} \sum_j m_j \overrightarrow{v_{ij}} \left[\frac{p_i}{\Omega_i \rho_i^2} \nabla_i W_{ij}(h_i) + \frac{p_j}{\Omega_j \rho_j^2} \nabla_i W_{ij}(h_j) + \Pi_{ij} \cdot \overline{\nabla_i W_{ij}} \right]$ (11)
Equation of state	$p_i = f(\rho_i, E_i)$ (12)

Π_{ij} is the artificial viscosity which prevents unphysical oscillations in the numerical results, especially modeling shock wave simulation and it uses average kernel gradient [3].

$$\overline{\nabla_i W_{ij}} = \frac{1}{2} \{ \nabla_i W_{ij}(h_i) + \nabla_i W_{ij}(h_j) \} \tag{13}$$

3. SPH simulation of Sod Shock Tube

3.1 Geometry and condition of Sod Shock Tube

The sod shock tube problem is a representative problem of a Riemann solver. A tube filled with gas which is separated by a wall into two parts, high pressure (1Pa) / density (1kg/ m^3) region and low pressure (0.1795Pa) / density (0.25kg/m^3) region. When the wall is taken away quickly, a shock wave, a contact discontinuity and a rarefaction wave appear. The shock wave propagates to low density region, while the rarefaction wave propagates to high density region. The contact discontinuity also propagates behind the shock wave [4].

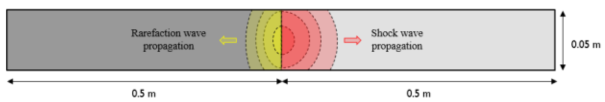

Fig. 1. Sod shock tube geometry

In this problem, the following equation of state for the ideal gas (14) is used in the simulation

$$p = (\gamma - 1)\rho \tag{14}$$

Where γ=1.4 is the ratio of specific heat.

4.2 SPH simulation results of Sod Shock Tube

After 0.2 second, the shock is observed around x=0.3m, the rarefaction wave is located between x=-0.3m and x=0m and the contact discontinuity is between x=0.1m and x=0.2m.

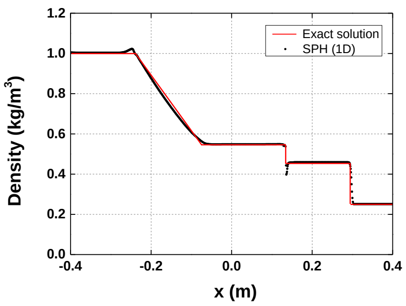

Fig. 2. Sod shock tube density profile

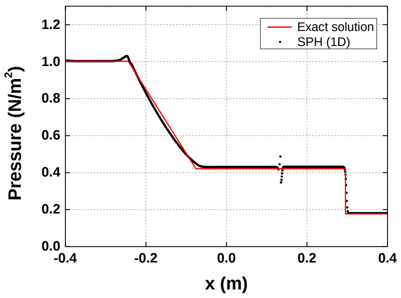

Fig. 3. Sod shock tube pressure profile

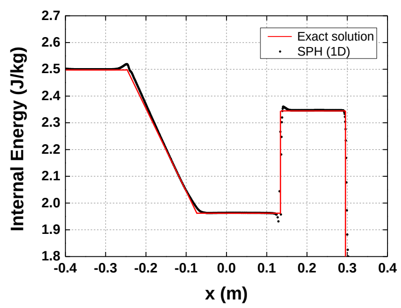

Fig. 4. Sod shock tube internal energy profile

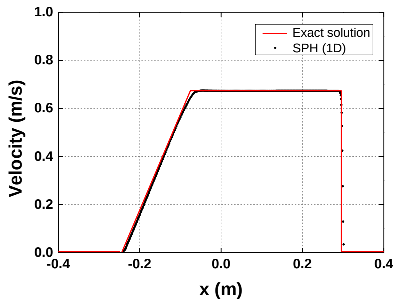

Fig. 5. Sod shock tube velocity profile

4. SPH simulation of Underwater Explosion

4.1 Geometry and condition of UNDEX

The underwater explosion problem is very expensive and dangerous to experiment, so the analytic solution of the underwater explosion problem is limited to simple case.

Special difficulties such as large deformations, moving material interfaces and a detonation process of high explosive in the whole underwater explosion process make more challenges for numerical methods due to its complexity.

In this study, a square shaped TNT charge (0.1m × 0.1m) explodes in water confined in a rigid square wall (1m × 1m) as described in Fig. 6.

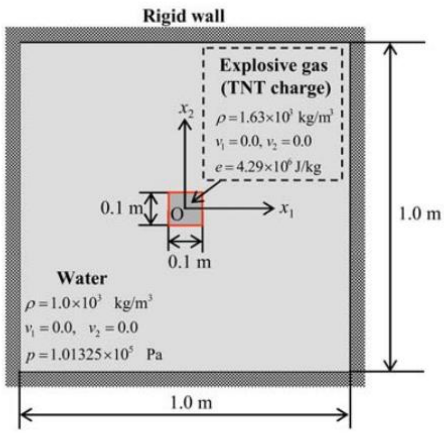

Fig. 6. Confined underwater explosion geometry [5]

In this problem, TNT use JWL equation of state which is used for explosive gas (15)

$$p = A\left(1-\frac{\omega\eta}{R_1}\right)e^{-\frac{R_1}{\eta}} + B\left(1-\frac{\omega\eta}{R_2}\right)e^{-\frac{R_2}{\eta}} + \omega\eta\rho_0 E \quad (15)$$

The water's behavior is very different in the case of compression and expansion, so water uses Mie-Gruneisen equation of state which depends on the states of water. The pressure of water in compressed state is (16) and in expanded state is (17)

$$p = \frac{\rho_0 C^2\mu\left[1+\left(1-\frac{\gamma_0}{2}\right)\mu-\frac{a}{2}\mu^2\right]}{\left[1-(S_1-1)\mu-S_2\frac{\mu^2}{\mu+1}-S_3\frac{\mu^3}{(\mu+1)^2}\right]} + (\gamma_0 + a\mu)E \quad (16)$$

$$p = \rho_0 C^2\mu + (\gamma_0 + a\mu)E \quad (17)$$

Where ρ_0 is the initial density, η is the ratio of the density to initial density and $\mu = \eta - 1$. When $\mu > 0$, water is in the compressed state and when $\mu < 0$, water is in the expanded state.

Table II: Material parameters and coefficients in the JWL EOS for TNT

Symbol	Meaning	Value
ρ_0	Initial density	1630 kg/m^3
A	Fitting coefficient	371.2 GPa
B	Fitting coefficient	3.21 GPa
R_1	Fitting coefficient	4.15
R_2	Fitting coefficient	0.95
ω	Fitting coefficient	0.3

Table III: Material parameters and coefficients in the Mie-Gruneisen EOS for water

Symbol	Meaning	Value
ρ_0	Initial density	1000 kg/m^3
C	Sound speed	1480 m/s
γ_0	Gruneisen coefficient	0.5
a	Volume correction coefficient factor	0
S_1	Fitting coefficient	2.56
S_2	Fitting coefficient	1.986
S_3	Fitting coefficient	1.2268

Underwater explosion includes two particles with a large difference in properties. The material interface treatment is needed to prevent unphysical penetration between TNT gas and water. In this study, interface sharpness force (18) is added on condition of near interface to treat this problem [6].

$$\frac{d\bar{v}_i}{dt} = -\frac{0.08}{m_i}\sum_j\left\{|p_i|\left(\frac{m_i}{\rho_i}\right)^2\nabla_i W_{ij}(h_i) + |p_j|\left(\frac{m_j}{\rho_j}\right)^2\nabla_i W_{ij}(h_j)\right\} \quad (18)$$

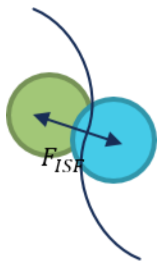

Fig. 7. Interface sharpness force at interface

4.2 SPH simulation results of UNDEX

At the beginning, a shock wave propagates outward and a rarefaction wave propagates inward after TNT detonation. When the shock wave reaches the wall, then the shock wave reflects from the wall and reflection wave come inward. The continuous process of shock reflection, explosive gas contraction and gas expansion and later compression make gas bubble pulse [7].

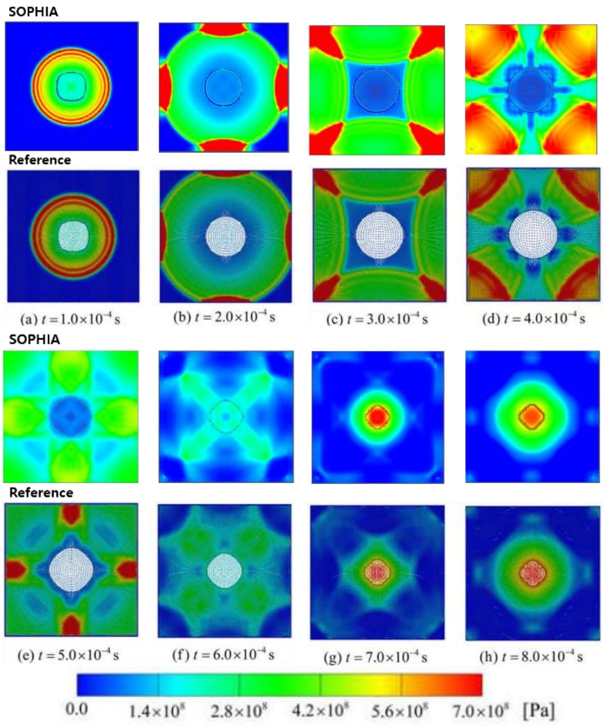

Fig. 8. Particle distributions and pressure distributions comparison with SOPHIA code results and reference results [5]

Excluding the results at t = 0.5ms and t = 0.6ms SOPHIA code is well suited to Reference underwater explosion simulation [5]. These errors expected to minimized by finding appropriate interface sharpness force model in underwater explosion simulation.

5. Summary

SPH has an advantage over the existing Eulerian method in analyzing problems accompanied by large deformations such as explosions. In addition, the accuracy of the analysis can be further improved by adjusting the smoothing length to suit the particle's local condition and using the governing equation that adopt variable smoothing length. The SOPHIA code which is developed by Seoul National University demonstrates that the shock wave caused by the explosion and the underwater explosion phenomena are well analyzed. Furthermore, it can be helpful in simulating the explosion phenomena inside and outside the reactor vessel.

ACKNOWLEDGEMENT

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