Thermomechanical Hamilton's Equations for Colliding Particles at High Velocities

Kwon Joong Son, Jong Kyoo Park, Euigyung Jeong, Man Young Lee, Hee Keun Cho, and See Jo Kim

***Abstract*—**This paper presents the theoretical model for two particles colliding in the velocity range of ballistic impact. The equations of motion consist of the time-evolution equation for the thermodynamic state variable as well as the Hamilton's equations for the kinematic variables of motion. This model can account for the thermo-mechanical interaction between the elastic particles during the collision. Incorporation of the internal energy into the formulation of equations of motion results in a more general form of conservation of energy. The model can be adopted to extend further the existing numerical methods such as the discrete element method (DEM) to solve complex and large-scale particle interaction problems in mechanical, civil, aerospace, and architectural applications.

***Keywords*—**Ballistic impact, energy method, Hamilton's equations, particle method

I. Introduction

HIGH-VELOCITY impact problems are of great interests in many engineering applications such as crashworthiness of vehicles [1], bullet-proof body armor systems [2][3], meteorite impact protection for spacecraft [4] and so on. In general, the contact and impact of material bodies lead to the elastic-plastic deformation during impact. At high velocities, the large strain may cause a considerable change in the kinetic energy of molecules, which eventually leads to a significant change in the temperature and internal energy. Therefore, the associated energy conversion from the initial kinetic energy into the strain and thermal energies has to be considered for the analysis of high-velocity impact problems. This paper focuses on the thermo-elastic collision model for the spherical particles in the velocity range of 100-1000 m/s, which encompasses a wide variety of ballistic impact problems. The numerical calculation results are also given and discussed.

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II. System Hamiltonian

The kinetic energy $T^{(i)}$ of the i-th particle in a translational motion is

$$T^{(i)} = T^{(i)}\left(\mathbf{p}^{(i)}\right) = \frac{\mathbf{p}^{(i)T}\mathbf{p}^{(i)}}{2m^{(i)}} \tag{1}$$

where $\mathbf{p}^{(i)}$ linear momentum and $m^{(i)}$ the mass of the particle. Neglecting the gravitational potential energy, the potential energy that each mass particle can store is the thermodynamic internal energy due to the impact-induced compression. The Hamiltonian for the system of particles has the summation form,

$$H = \sum\left(T^{(i)} + U^{(i)}\right) \tag{2}$$

where $U^{(i)}$ is the internal energy of the i-th particle. The equation of state adopted in this study is in the Grüneisen form, and the associated expression for the pressure in a compressed state is given by

$$P(\mu, U) = \frac{\rho_0 C_{s0}{}^2\mu\left[1+\left(1-\frac{\gamma_0}{2}\right)\mu-\frac{b}{2}\mu^2\right]}{\left[1-(S_1-1)\mu-S_2\frac{\mu^2}{\mu+1}-S_3\frac{\mu^3}{(\mu+1)^2}\right]^2} + (\gamma_0 + b\mu)U \tag{3}$$

where ρ_0 is the reference density, C_{s0} is the reference bulk speed of sound, γ_0 is the initial Grüneisen's gamma, b is the coefficient of the volume dependence of gamma, S_i (i = 1,2, and 3) are the Hugoniot slope coefficients [5]. The variable μ in (3) is a measure of material compression expressed as

$$\mu = 1 - \frac{\rho_0}{\rho} \tag{4}$$

where ρ is the current material density. Equations (2) and (3) enable the Hamilton's equations to take the thermodynamics of colliding bodies into account.

III. Hamilton's Equations of Motion

Hamilton's equations of motion [6] for the two thermo-elastically interacting spherical particles can be written as

$$\dot{\mathbf{p}}^{(i)} = -\frac{\partial V^{(i)}}{\partial \mathbf{c}^{(i)}} + \mathbf{f}^{(i)}(t) \tag{5}$$

$$\dot{\mathbf{c}}^{(i)} = m^{(i)^{-1}}\mathbf{p}^{(i)} \tag{6}$$

where $V^{(i)}$is the potential energy stored in the i-th particle and $\mathbf{f}^{(i)}(t)$ is the non-conservative force associated with material compression. In the case where the gravitational potential energy is negligible compared to the total energy, $V^{(i)}$ can be approximated as the internal energy $U^{(i)}$. In addition to (5) and (6), an internal energy evolution equation in rate form is required for the complete description of the system dynamics.

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The power balance law leads to the necessary equation of holonomic constraint given by

$$U^{(i)} = \frac{m^{(i)}}{{\rho^{(i)}}^2}\dot{\rho}^{(i)} \quad (7)$$

where the current density $\rho^{(i)}$ is calculated based on the simple additive interpolation scheme in [6]. Equation (7) is just the first law of thermodynamics for the colliding particles without considering energy dissipation modes such as friction, plastic deformation, fracture, and so on. Integration of the first-order differential equations (5)–(7) produces an approximate solution for the problem. This solution enables us to predict the thermodynamic states (e.g., internal energy, pressure, entropy, and density) as well as the kinematic states (e.g. center of mass position and velocity) for each particle.

IV. Example Problem

Traditional central impact problem between two spherical particles was solved by the means of the Hamiltonian approach in the previous section. Fig. 1 shows the initial configuration of the two particles made of steel in a collinear motion condition.

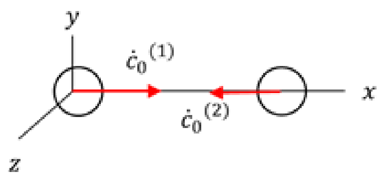

Fig. 1 The collinear motion and central impact of two identical spheres

Table 1 lists the materials parameters and properties of the two-particle system shown in Fig. 1. The initial velocity of 250 m/s for each particle was chosen so that the relative impact velocity should go beyond the bulk speed of sound of steel. Therefore, instead of the constitutive equation of an isotropic linear elastic material, the shocked equation for steel in (3) was used to compute the hydrostatic stress in compressed steel. The initial center-to-center distance is 4.5 cm so that the particle interaction begins at 10 µs. The first-order nonlinear ordinary differential equations (5)–(7) were numerically integrated using an explicit fourth order Runge-Kutta method for initial 25 µs. Numerical calculation results show that the time duration of impact is 4.4 µs, and the total energy is conserved.

TABLE I
GEOMETRIC, KINEMATIC, AND MATERIAL PROPERTIES OF PARTICLES

Symbol	Description	Quantity
r	particle radius	2 cm
c_0	initial velocity	250 m/s
d_0	initial center-to-center distance	4.5 cm
ρ_0	reference density (steel)	7810 kg/m^3
C_{s0}	bulk speed of sound	457.8 m/s
γ_0	initial Grüneisen's gamma	1.67
b	EOS coefficient	0.43
S_i	Hugoniot slope constants	S_1 = 1.33, S_2 = S_i = 0
c_p	specific heat	448 J/kg°C

Fig. 2 shows the velocity versus time graph for two particles. It also shows a linear momentum exchange between two identical particles without energy loss.

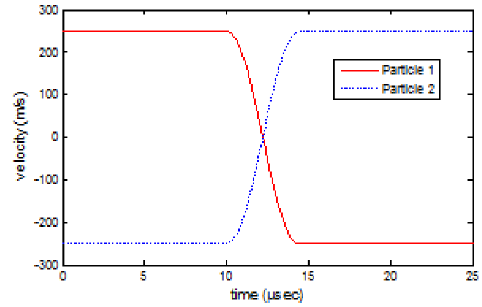

Fig. 2 The velocity versus time curves during 25 microseconds

Fig. 3 shows the pressure versus time graph for two particles. The peak pressure of 97.9 kbar occurs when the particles are the most compressed up to the density of 8237 kg/m^3.

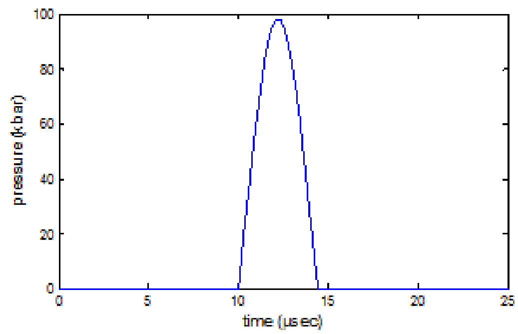

Fig. 3 The pressure-time curve for the colliding particles

Fig. 4 shows the temperature versus time graph that is identical for both particles. The temperature is computed using the specific heat

$$T^{(i)} = \frac{U^{(i)}}{c_p^{(i)} m^{(i)}} + T_0^{(i)} \quad (8)$$

where $c_p^{(i)}$ is the specific heat and $T_0^{(i)}$ is the reference temperature of the i-th particle before impact. The maximum temperature of 95.9 °C is observed at the end of the collision. The temperature remains constant after the collision because an adiabatic process is assumed to due to the lack of convective heat transfer during a very short period of simulation time.

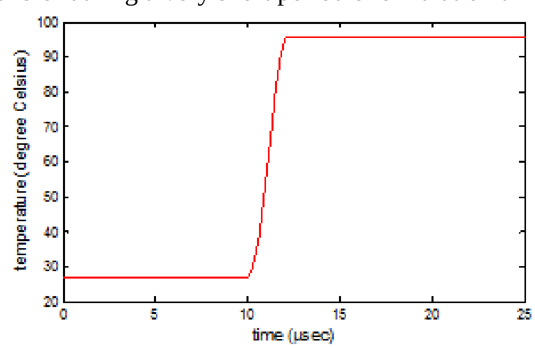

Fig. 4 The temperature evolution for the particle due to impact

Fig. 5 shows the conservation of the total energy consisting of the kinetic energy and the international energy of two particles. It also shows a seamless process of the transformation of energy from one form to another. This approach is more physical than the approach using the coefficient of restitution in that the state variables are continuously varying with time.

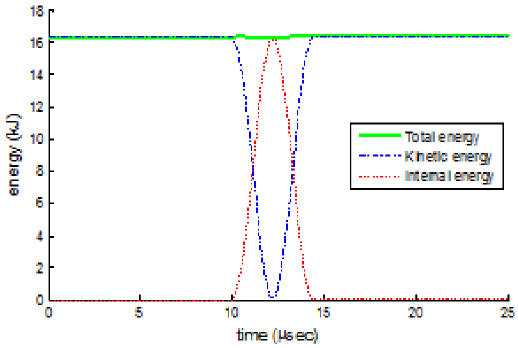

Fig. 5 Three types of energy versus time plot

V. Conclusion and Future Work

While the momentum equations in other conventional methods like discrete element method (DEM) only describe the time evolution of kinematic variables, the thermomechanical equations of motion modeled in this paper can also predict the time evolution of thermodynamic states. This approach can contribute to the advancement of current discrete element method in simulating the impact behavior of granular materials. The future work may include the multi-particle problems, non-spherical particles, solid-fluid interaction problems, and so on.

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