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Discrete element simulation of granular particles and their Numerical simulation in a rotating cylinder

S.H. Oleena *

The objective of this contribution is to present a numerical simulation method to model the motion of a packed bed in a rotary kiln using object-oriented techniques. The method chosen is the Lagrangian time-driven method and it uses the position, the orientation, the velocity and the angular velocity of particles as independent variables. These are obtained by time integration of the three-dimensional dynamics equations which were derived from the classical Newtonian mechanics approach based on the second law of Newton for the translation and rotation of each particle in the granular material. This includes keeping track of all forces and moments acting on each particle at every time-step. Contact forces depend on the overlap geometry, material properties and dynamics of particles and include normal and tangential components of repulsion force. The resulting equations of particle motion are solved by the Gear predictor–corrector scheme of fifth-order accuracy.The back ground version of DEM and time integration algorithm are developed and implemented into C++ code. The implementation of time-integration algorithm is verified by simple test concerning particle-particle, particle-wall interaction for which analytical expression exist. In this paper particle force due to different material property are investigated.

Keywords:

DEM simulation;
Granular materials;

Author correspondence:

S.H.Oleena,
Research scholar, University Library
University of Kerala,Palayam, Thiruvananthapuram, Kerala - India

1. Introduction

Rotating Cylinder play a noticeable role in the processing of granular material in chemical industries in an extensive variety of physical processes, including size reduction, waste reclamation, agglomeration, solid mixing, drying, heating, cooling, etc. The general use of rotating cylinder is also caused by its ability to handle various feedstock, from slurries to granular materials, and to activate in distinct environments. Rotary cylinder are the most usually used mixing devices in metallurgical and catalyst industries. Rotary dryers play an important role in many industrial applications, such as chemistry, metallurgy and materials science, mineral industries, and food processing[19],[20]. It is important to recognize the mixing characteristics and heat transfer presentation. DEM models is the study of mixing in various amalgamation

* Doctorate Program, Linguistics Program Studies, Udayana University Denpasar, Bali-Indonesia (9 pt)

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systems including rotating drum [4]. Particle transport is vital and happens in two directions: transverse and axial. Particle transport in the transverse direction is comparatively uniform, while particle transport in the axial direction may diverge with different residence time.

The discrete element method (DEM), originally developedby Cundall and Strack [6],[7], has been used successfully to simulate chute flow [8], heap formation [16], hopper discharge[27],[22], blender segregation [30],[24],[17] and flows in rotating drums [21],[[30].

The DEM allows for the simulation of particle motion and interaction between the particles, taking into account not only the obvious geometric and material effects such as particle shape, material non-linearity, viscosity, friction, etc, but also the effect of various physical fields of surrounding media, even of chemical reactions (Kantor *et al*. 2000)Recently, DEM has been used for the solution of discrete and continuous problems including solid, fluid and molecular mechanics, heat transfer etc[26],[10],[12],[5],[15],[28],[1].

One of the most promising area of future applications of discrete element method seems to be geotechnical engineering. The discrete approach assumes the soil is an assembly of granules or discrete particles where micromechanical behavior of soil is pre-defined by micromechanical inter granular properties.

2. Discrete State formulation.

The granular media present a space filled by the particle termed here as discrete elements. The media are assumed to be composed of spherical particles with same radii R_i. The particles are assumed to be deformable bodies, deforming each other by normal and shear force.

The composition of media is time-dependent because distinct particle change their position by free rigid body motion or by contacting with neighbor particles or walls. Each particle may be in contact with other particles.

The visco-elastic material of granular media is defined by the modulus of elasticity, Poisson's ratio and damping coefficients in normal and shear directions. The boundary conditions of media are determined by planes and treated as particles with an infinite radius and mass. The external is induced with kinematic boundary conditions which are implemented by the walls movements.

The dynamic behaviour of media is considered as the dynamics of each particle. Consequently, the overall response of media is predicted by the behaviour of individual particles, the dynamics of which is evaluated by applying the second Newton's law. One of the most important issues considered by a discrete approach is the detection of interaction force between contacting particles. The interaction forces of each contacting pair are locally resolved on the basis of actual geometry of kinematic contact between two spherical particles, inter-particle contact forces and boundary conditions.

3. Geometry of Kinematic contact of spherical particles.

Let any two particles i and j be in contact with position vectors x_i and x_j with center of gravity lying at O_i and O_j having linear velocities v_i and v_j, angular velocities ω_i and ω_j respectively [1].

The contact point c_{ij} is defined to be at the center of the overlap area position vector x_{cij} .The vector x_{ij} of the relative position point from the center to gravity of particle i to that of particle j is defined as $x_{ij} = x_i - x_j$. The depth of overlap is h_{ij}. Unit vector in the normal direction of the contact surface through the center of the overlap area is denoted by n_{ij}. It extends from the contact point to the inside of the particle i as $n_{ij} = n_{ji}$

The vector d_{cij} and d_{cji} are directed towards the contact point from the centers of particle i and particle j respectively and are represented as

$$d_{cij} = x_{cij} - x_i$$
$$d_{cji} = x_{cji} - x_j$$

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Since the particle shape is assumed to be spherical, for sphere of any dimension the contact parameters can be written as follows:

$$h_{ij} = \begin{cases} R_i + R_j - |x_{ij}|, |x_{ij}| < R_i + R_j \\ 0, |x_{ij}| \geq R_i + R_j \end{cases}$$

$$d_{cij} = -\left(R_i - \frac{h_{ij}}{2} \right) n_{ij}$$

Where R is the radius of the particle. The relative velocity of the contact point is defined as

$$v_{ij} = v_{cij} - v_{cji}$$

In case of contact with partial slip, particles may slip relative to the distance $\delta_{t,ij}$ is the integrated slip in tangential direction after particles i and j came into contact and can be defined by the equation,

$$\delta_{t,ij} = \left| \int v_{t,ij}(t) dt \right|$$

Here $\delta_{t,ij}$ is allowed to increase until the tangential force exceeds the limit imposed by static friction. The vector of tangential displacement $\delta_{t,ij}$ is defined to be perpendicular to the normal contact direction and located on the same line as $v_{t,ij}$. If the tangential component of the contact velocity $v_{t,ij}$ is not equal to zero, then the unit vector t_{ij} of the tangential contact direction is directed along $v_{t,ij}$. If $v_{t,ij}$ is equal to zero, t_{ij} has the same direction as that of the slip. Otherwise t_{ij} is equal to zero, if $v_{t,ij}$ and $\delta_{t,ij}$ are equal to zero, then

$$t_{ij} = \begin{cases} \frac{v_{t,ij}}{|v_{t,ij}|}, v_{t,ij} \neq 0 \\ \frac{\delta_{t,ij}}{|\delta_{t,ij}|}, v_{t,ij,} \delta_{t,ij} \neq 0 \end{cases}$$

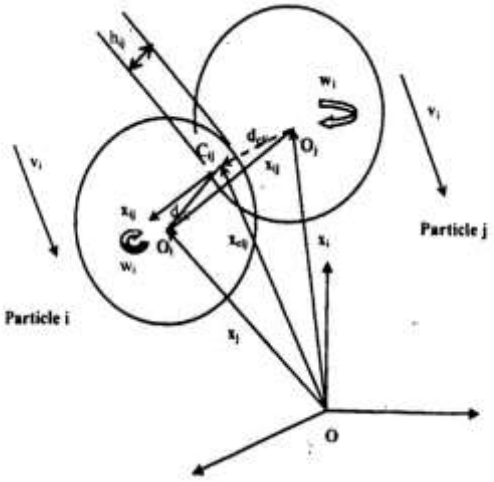

Figure 1.Contact between two particles i and j.

4. Inter particle contact force.

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The contact force can be expressed as the sum of normal and tangential components;

$$F_{ij} = F_{n,ij} + F_{t,ij}$$

Contact force between the spherical particles are modeled as spring, dash-pots and a friction slider. The contact forces between them depend on the overlap geometry, the properties of the material and the relative velocity between the particles in the contact area. Hence in the perfect contact model, it is required to describe the effects of elasticity, energy loss through internal friction and surface friction and attraction on the contact surface for describing the contact force calculations.

4.1 Normal Force

The normal component of contact force between particles can be expressed as the sum of elastic repulsion, internal friction and the surface attraction forces.

$$F_{n,ij} = F_{n,ij,elastic} + F_{n,ij,viscous}$$

Normal elastic repulsive force is based on the linear Hooke's law of a spring with a spring stiffness constant $k_{n.ij}$ and is given by the expression,

$$F_{n,ij,elastic} = K_{n,ij} h_{ij} n_{ij}$$

Normal energy dissipative force is dissipated during real collisions between particles and, in general, it depends on the history of impact. A very simple and popular model is based on the linear dependency of force on the relative velocity of the particles at the contact point with a constant normal dissipation coefficient γ_n and is expressed as

$$F_{n,ij,viscous} = -\gamma_n m_{ij} v_{n,ij}$$

4.6.2 Tangential force

The tangential component force model depends on the normal force and normal displacement. Further the model for static friction must include energy dissipation, because perpetual oscillations in tangential direction will be obtained during the time of static friction. In the literature two major approaches can be found to represent tangential contact forces namely; global and complex models. Global models describe all the phenomena of the tangential force through a single expression. Complex models describe static and dynamic friction by separate equations and the Coulomb criteria. Of course, the continuous particle interaction models require special models for tangential forces. The tangential force $F_{t,ij}$ being divided into parts of static friction or dynamic friction. When the tangential force $F_{t,ij}$ is larger than the Coulomb-type cut-off limit, dynamic friction predominates. When $F_{t,ij}$ is lower than the limit, the model of static friction force $F_{t,ij,static}$ must be implemented. Such an approach can be modeled by

$$F_{t,ij} = -t_{ij} \min\left(\left| f_{t,ij,static} \right|, \left| f_{t,ij,dynamic} \right| \right)$$

Where $F_{t,ij}$ is the unit vector in the tangential direction of the contact point.Dynamical frictional force can be described as.Static frictional force is the sum of the tangential spring and energy dissipation force

$$F_{t,ij,static} = F_{t,ij,spring} + F_{t,ij,dissipation}.$$

Tangential spring forcecan be described as $F_{t,ij,spring} = -k_{t,ij} \delta_{t,ij} t_{ij}$. Friction model for energy dissipationin the tangential direction can be used in the energy dissipation in normal direction

$$F_{t,ij,dissipation} = -\gamma_t m_{ij} v_{t,ij}$$

Governing equation for the motion of granular material inside a rotating cylinder.

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$$m_i \frac{d^2 x_i}{dt^2} = m_i a_i$$
$$= F_i$$
$$v_i = \frac{dx_i}{dt}$$

Force acting on i^{th} particle F_i is,

i.e., sum of gravitational force and contact force

$$F_i = m_i g + \sum_{\substack{j=i \\ j \neq i}}^{N} F_{n,ij} + \sum_{\substack{j=i \\ j \neq i}}^{N} F_{t,ij}$$

Torque acting on the particle

$$I_i \frac{d^2 \theta_i}{dt^2} = T_i$$
$$\omega_i = \frac{d\theta_i}{dt}$$
$$T_i = \sum_{\substack{j=i \\ j \neq i}}^{N} d_{cij} \times F_{ij}$$

The contact forces between them depend on the overlap geometry, the material of the particles, and the relative velocity of the particles in the contact area.

5. Boundary Conditions

The properties of granular flow are strongly dependent on the boundary conditions at the wall. Therefore the boundary conditions are very important for an adequate simulation of the granular material behavior. Several types of boundary conditions can be employed:

(a) Walls that may be moving or stationary
(b) Inflow and outflow
(c) Periodic

Walls can be constructed using planes, spheres, cylinders or any other shape as big particles or by an array of small particles. In general, boundaries of the system such as walls are required for the motion of granular material or particles within enclosures, where the wall may have an important influence on the motion of a granular material due to wall-particle interaction. Furthermore, walls can move and rotate around a point of rotation. The rotation of wall particles, in particular is unavoidable in the present study, in which the motion of granular material on the rotating cylinder solely depends on the moving wall. A rotating cylinder can be constructed by a cylinder or sphere with a negative radius. Collisions between particles and walls are defined by the material and geometry of the particles and walls, as in the case of collisions between particles. It is convenient to construct rough walls by an array of particles [27]. For the present formulation the following methodology is adapted; the systemunder consideration has been modelled by an ensemble of spheres possessing thesame material constants as that of the grains inside the container. The motion ofthe wall spheres is not affected by the impacts but is, strictly governed by thecontinuous rotation of the cylinder. The calculation of contact forces between theparticles and wall are defined in the same way as between particles.

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7. Time integration scheme

Various time integration schemes can be used to solve the equations. The main requirements for a good scheme are given below:

- It should be stable
- It should satisfy the required accuracy
- It preferably should satisfy energy and momentum conservation
- It should not require excessive memory

Time consuming calculation of inter-particle forces should be carried to the minimum possible extent-ideally, once per time step, Δt

Some of the most popular schemes used in DEM by various authors include; first order Euler's scheme, Fourth-order RungeKutta method [2] velocity verlet scheme [3],[11],[23], second order AdamsBashforth scheme [25] and predictor-corrector schemes [18],[27],[[9],[13].

Van Gunsteren and Berendsen [29] compared the Gear predictor-corrector, Runge-Kutta and verlet schemes for macromolecular simulations and concluded that Gear scheme is the best for small time steps and verlet algorithm for larger time steps.Hence the 5thorder Gear predictor-corrector scheme [2]is used in this work to solve the equations, which is stable for second-order differential equations with global truncation error of $O\left(\Delta t^{q+1-2}\right)=O\left(\Delta t^{q-1}\right)$

$$x_i(t+\Delta t)=x_i(t)+\dot{x}(t)\Delta t+\ddot{x}_i(t)\frac{(\Delta t)^2}{2!}+\dddot{x}(t)\frac{(\Delta t)^3}{3!}+x_i^{(iv)}(t)\frac{(\Delta t)^4}{4!}+x_i^{(v)}(t)\frac{(\Delta t)^5}{5!}$$

$$\dot{x}_i(t+\Delta t)=\dot{x}_i(t)+\ddot{x}_i(t)\Delta t+\dddot{x}(t)\frac{(\Delta t)^2}{2!}+x_i^{(iv)}(t)\frac{(\Delta t)^3}{3!}+x_i^{(v)}(t)\frac{(\Delta t)^4}{4!}$$

$$\ddot{x}_i(t+\Delta t)=\ddot{x}_i(t)+\dddot{x}_i(t)\Delta t+x_i^{(iv)}(t)\frac{(\Delta t)^2}{2!}+x_i^{(v)}(t)\frac{(\Delta t)^3}{3!}$$

$$\dddot{x}_i(t+\Delta t)=\dddot{x}_i(t)+x_i^{(iv)}(t)\Delta t+x_i^{(v)}(t)\frac{(\Delta t)^2}{2!}$$

$$x_i^{(iv)}(t+\Delta t)=x_i^{(iv)}(t)+x_i^{(v)}(t)\Delta t$$

$$x_i^{(v)}(t+\Delta t)=x_i^{(v)}(t)$$

Then the inter particle forces acting on each particle at time $(t+\Delta t)$is evaluated using the predicted particle positions. Applying the obtained evaluated forces at time $(t+\Delta t)$and Newton's second law, the particle accelerations $\ddot{x}(t+\Delta t)$ can be determined. The difference between the predicted accelerations and evaluated accelerations is then computed;

$$\Delta\ddot{x}_i=\ddot{x}_i(t+\Delta t)-\ddot{x}_i^{p}(t+\Delta t)$$

The predicted particle positions and their derivatives are corrected using the difference, $\Delta\ddot{x}$,obtained between the predicted accelerations and that given by the evaluated force. In the Gear's Predictor Corrector algorithm, this difference term is used to correct all the predicted tparticle positions and their derivatives. The correction terms are given by;

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$$x_i = x_i^p + \alpha_0 \Delta R_2$$

$$\dot{x}_i \Delta t = \dot{x}_i^p \Delta t + \alpha_1 \Delta R_2$$

$$\frac{\ddot{x}_i (\Delta t)^2}{2!} = \frac{\ddot{x}_i^p (\Delta t)^2}{2!} + \alpha_2 \Delta R_2$$

$$\frac{\dddot{x}_i (\Delta t)^3}{3!} = \frac{\dddot{x}_i^p (\Delta t)^3}{3!} + \alpha_3 \Delta R_2$$

$$\frac{x_i^{(iv)} (\Delta t)^4}{4!} = \frac{x_i^{(iv)p} (\Delta t)^4}{4!} + \alpha_4 \Delta R_2$$

$$\frac{x_i^{(v)} (\Delta t)^5}{5!} = \frac{x_i^{(v)p} (\Delta t)^5}{5!} + \alpha_5 \Delta R_2$$

Where,

$$\Delta R_2 = \frac{\Delta \ddot{x}_i (\Delta t)^2}{2!}$$

Values of parameters α_i [2] for second order differential equations of predicting order q are presented in table 7.1.

Table 7.1: Values of the parameter *a*,

α_i	*q=3*	*q=4*	*q=5*
α_1	$\frac{1}{6}$	$\frac{19}{12}$	$\frac{3}{16}$
α_2	$\frac{5}{6}$	$\frac{3}{4}$	$\frac{251}{360}$
α_3	1	1	1
α_4	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{11}{18}$
α_5	-	$\frac{1}{12}$	$\frac{1}{6}$
α_6	-	-	$\frac{1}{60}$

The parameter, $\alpha_i$promotes numerical stability of the algorithm. The time step Δt of thex integration was chosen such that the entire contact between the particles was resolved within 10 time steps at least.

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The time step Δt, for the time integration of the particle position, velocity, orientation and angular velocity depends on the time of contact T_c, which can be expressed as

$$T_c = \lambda\sqrt{\frac{m}{k}}$$

Which is estimated based on the single degree of freedom system of mass m connected to the ground by a spring of stiffness *k*. Hence the time step must be sufficiently small to ensure a stable numerical scheme of time integration and Cundall and Strack [6] proposed that the time step must be smaller than the critical time step

$$\Delta T_c = \sqrt{\frac{m}{k}}$$

8. Computer Implementation

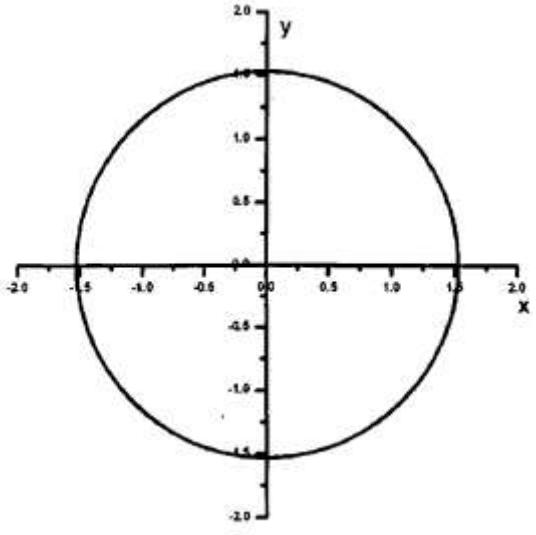
The major computational tasks of DEM at each time step can be summarized as follows*:*

- Finding the neighbour list for each particle
- Detection of contacts between a particle *i*and its neighbours
- Computation of contact forces from relative displacement between particles
- Summation of contact forces to determine the total unbalanced force
- Computation of acceleration from force
- Velocity and displacement by integrating the acceleration
- Updating the position of particles

9. Result and Discussion

9.1. Initial Condition.

The transverse plane of a horizontal cylinder is a circle. This is represented as a set of spherical particles at a distance equal to the cylinder radius from the origin of the Cartesian coordinate system chosen. The origin of the coordinate system is at the center of the circle as shown in Figure 2.



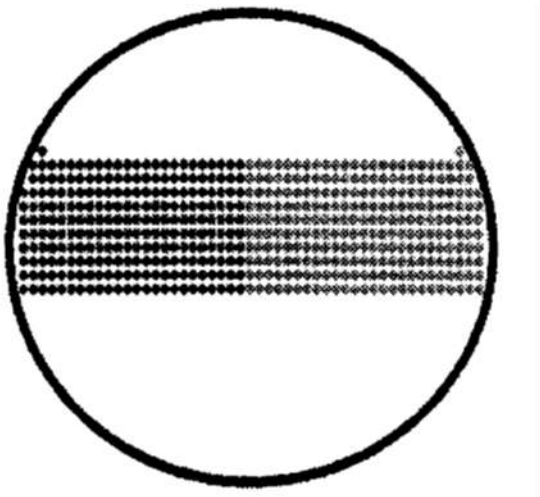


Figure 2: Coordinate system chosen for simulation.**Figure 3:** Initial Distribution of the particles.

The initial condition, *r*=0 of granular solids in the transverse plane of the rotating cylinder is assumed to be a packed bed of granular solids. Since the initial conditions of granular particles in a packed bed cannot be

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specified a priori. The calculations were carried out at two stages. Given the fill fraction, particle sizes and their distribution, the number of particles for each size range was determined using equation

$$np(i) = \frac{4\,fw_i A}{\lambda d_p(i)^2}$$

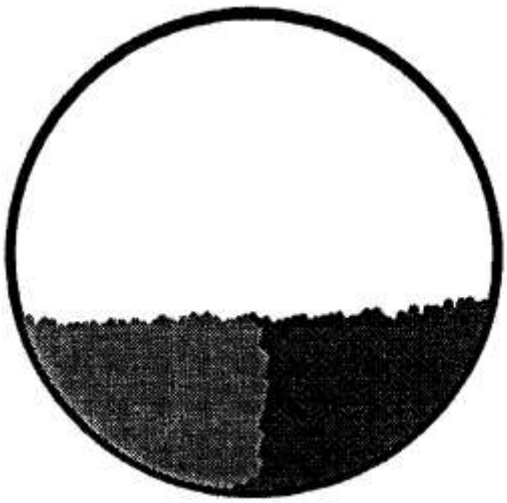
Where fw_i is the percentage of fraction of the particles of size $d_p(i)^2$ and A is the cross sectional area of the bed. An orthogonal grid is then generated with the size of the grid equal to the diameter of the largest particle and the particles are placed at the center of these grids so that they don't overlap over each other. Uniform sized particles are given a particular colour. Figure 3 shows one such initial distribution generated for two different sized particles at equal number concentrations.The initial velocities of individual particles were chosen randomly and the force of gravity is allowed to act on each particle.

9.2. Force due to gravity.

Initially the particles fall under gravity since there is no contact force, but after some time the contact forces also come into play. The bordering shape of the rotating cylinder, which first stops the pure vertical motion and secondly causes the particles to interact with each other, limits the motion of the particles. The total kinetic energy of the system is calculated as follows;

$$KE = \frac{1}{2}\sum_{i=1}^{N_p} m_i v_i^2$$

Where *mi* is the mass, v_i is the velocity and $N_p$is the total number of particles in the system The simulation was continued till all the particles came to rest; that is until the total kinetic energy of the system becomes negligible as shown in Figures 5 and 6. The location and linear and rotational velocities of particles at this stage are chosen as the initial conditions for the next stage of simulation.



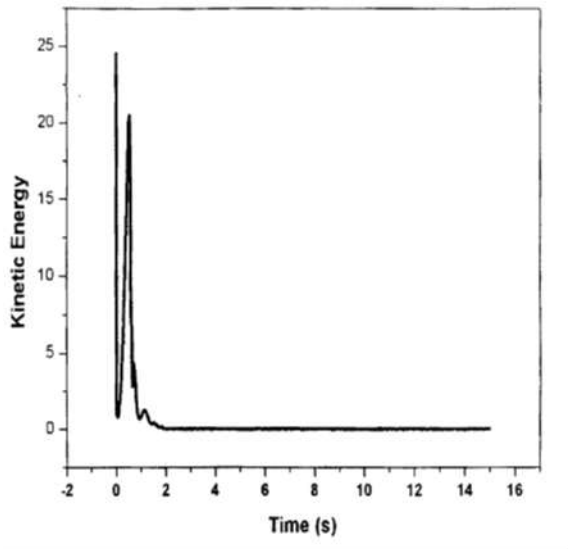


Figure 5: Initial packed bed**Figure4.4:** Total kinetic energy with respect to time

10. Conclusion

The result obtained in the present investigation may be generally described as follows:

1. The described discrete element model composed of visco-elastic spherical particles is implemented into the developed C++ code. This code open for new elements and interaction models may be considered as the first step in the development of an advanced simulation tool for granular and other inhomogeneous materials and is intended for modelling more complex geotechnical problems.
2. The time integration tests conducted with particle-particle and particle-wall interaction have proved that the performance of 5^{th} order Gear predictor corrector scheme is the better compared to the integration methods. This scheme is implemented into the code.

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