Nanotechnology-Based Performance Improvements For Portland Cement Concrete – Phase I

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ABSTRACT

A fundamental understanding of the nano-structure of Portland cement concrete (PCC) is the key to realizing significant breakthroughs regarding high performance and sustainability. MBTC-sponsored research (MBTC 2095/3004) using molecular dynamics (MD) provided new understanding of Calcium Silicate Hydrate (CSH) structure (the main component giving strength and durability to PCC); however, the study was limited, particularly regarding nano-level mechanical properties in the PCC due to number of atoms that could be considered in the MD approach. In this work discrete element method (DEM) for considering the CSH gel structure is proposed. The progress made in phase I out of three phases is reported. The review of DEM application in engineering and specifically for CSH study is reported. Existing free ware and commercial code available for DEM study is presented. An in house DEM code is developed to apply an indentor type load to a cohesive material. Sample model calculation reasonably illustrated the development and application of the DEM code.

Chapter 1: Introduction

Concrete is the most utilized construction material as well as least understood scientifically. The life of concrete is restricted due to shrinkage cracks, tensile cracks etc. This is mainly due to the complex amorphous structure of cement paste. For copper or iron it is very easy to find the atomic structure from experiment. Since more than five different atoms are combined together to form cement paste or CSH (Murray et al., 2010 & Janikiram Subramaniam et al., 2009), it is very difficult to know the atomic structure from experiment. A fundamental understanding of the nano-structure of concrete is the key to realizing significant breakthroughs regarding highperformance and sustainability. Recently through MBTC 2095/3004 project, some understanding of the atomic structure of CSH was brought out using molecular dynamics (MD). Selvam and his group (2009-2011) proposed possible atomic structure of CSH using molecular dynamics (MD) modeling. Further study to relate properties from nano level to macroscopic level is restricted due to limitations in considering number of atoms necessary to consider the changes in few nanometer lengths.

Nonat (2004) and Gauffinet et al. (1998) observed that C-S-H gels had lamellae-type morphologies with lamellae sizes of approximately 60 × 30 × 5 nm. From the AFM images taken from Dagleish as shown in Figure 1.1 the CSH fibers may be of the size of 60 nmx 300 μm. To understand the interaction between those fibers one need a computational size much larger than few nano meters. This can be done through discrete element modeling. Recently Chandler et al. (2010) and Fonseca et al. (2011) utilized DEM to understand the micro structure of CSH. But the particles considered where sperical in shape. The actual CSH fibers are long and thin. Further research is needed to consider proper CSH fibers in DEM modeling. Especially when the nano scale properties are investigated by nanoindentation experiment (Constantinides and Ulm, 2007), DEM model will be very useful by simulating the CSH properties through nanoindentation.

In this proposed work the change in the CSH structure in few nanometer length will be considered using the discrete element method (DEM). This will provide insight into the way the CSH structure is constructed and how the mechanical properties in the macroscopic level is contributed. Knowing the CSH structure through DEM, the structure of low density and high density CSH will be researched. The properties for the DEM will be taken from MD and other experimental observations.

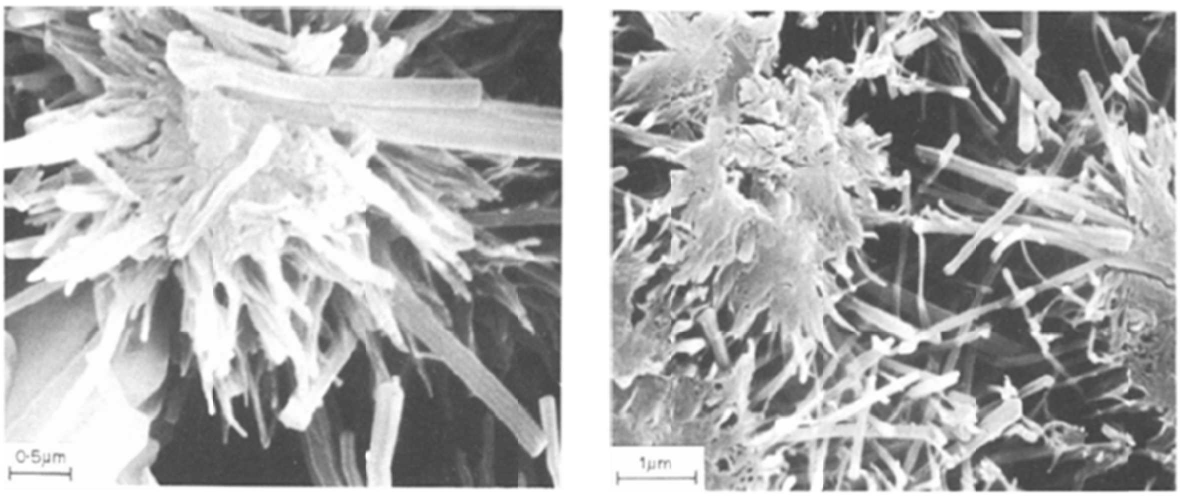

Figure 1.1 C-S-H and Spherulites micro particles as seen by Atomic Force Microscopy (AFM). Reproduced from Dagleish et. al (1982).

Project Objectives

The overall objective is to apply nano-science-based principles to improve the performance, and ultimately the life cycle of transportation construction materials. Specific objectives include:

1. Develop DEM to study the low density and high density configuration of CSH (Phase 1)
2. Compare modeled cement properties with experimental observations (Phase 2).
3. Using the refined Portland cement concrete (PCC) nano-structure model, investigate additional material modifications to improve the mechanical properties of PCC (Phase 3).
4. Identify and define procedures necessary to implement next-generation PCC materials in field applications (Phase 3)

The proposed project is for three years. This report is the progress for the first year. Hence progress made in DEM application to CSH is documented in this report.

Chapter 2: DEM Applications in Engineering

In engineering applications most of the computer modeling in industry and research is done using continuum based methods like finite element (FEM), finite difference (FDM) and boundary element (BEM) methods. There are situations where in the continuum based methods are not applicable as in stability of rocks in a slope, failure of brittle materials like ice and ceramics, transport of solids in chutes and hoppers etc. In these situations discontinum methods are applicable. Discrete element method is the first one to evolve in this area. Cundall (1971) developed this method to study the dynamics of granular particles and blocks. Other methods are evolving as a combination of FEM and DEM. For further status one can refer to recent reviews by Bobet (2010), Jing (2003), Cundall and Hart (1992), Donze et al. (2008) and Lemos (2010) from rock mechanics to architecture. Recent books in this area are Jing and Stephansson (2008), O'Sullivan (2011), Mohammadi (2003) and Munjiza (2004).

DEM is similar to MD (Allen & Tidsley, 1991) where in Newtonian dynamics of particle is considered between particles. In MD only forces due to atomic potentials are considered. In DEM normal and tangential forces due to contact and corresponding damping forces are considered mainly. Depending upon the problems other forces are considered. In Chandler et al. (2010) to study the properties of CSH through nanoindentation they considered Van der Waals forces and electric double layer force in addition to normal and tangential contact forces. The contact forces can be calculated as soft or hard contact. In most of the work soft contact is considered.

2.1 DEM Application in Various Engineering Discipline

The application of DEM and related discontinua methods are very extensive. Some of the applications of DEM and DEM+FEM in engineering are as follows:

1. Nanoindentation of CSH modeling (Chandler et al. 2010 & Fonseca et al. 2011)

2. Wave propagation in soil and rock media: explosion ground fall in jointed rock, caving in confined environment, fault slip induced by mining (Cundall and Hart, 1992)
3. Underground structures like tunnel subjected to dynamic loading (Bobet, 2010)
4. Brick and masonry structure modeling. Strength of joints in bridges and arches (Lemos, 2010)
5. Application in soil, rock and concrete. Triaxial test simulation, Saturated and unsatrurated soil, fractured rock with circulating fluid and micro mechanics of concrete (Donze et al. 2008)
6. Bin flow of granular material, Couette and Channel flow (Babic, 1988)
7. Ice mechanics: Ice sheet impacting offshore platform (Pande et al. 1990)
8. Impact effect on structures using FEM+DEM (Munjiza, 2004)
9. Delamination of composites and crack propagation using FEM+DEM (Mohammadai et al.1998 & Mohammadi, 2003)
10. Modeling continuum mechanics problems using DEM (Liu et al, 2004; Liu and Liu, 2006, Li et al. 2009 and Cheng et al. 2009)
11. Predicting the granular material property using DEM for continuum mechanics modeling

2.2 Area of Expertise Needed for DEM

Depending on the application DEM modeling needs some or all of the following area of expertise:

1. Rigid body dynamics (Cundall & Strack, 1979)
2. Contact dynamics considering normal and frictional contact for impact and other loads- penalty method is generally preferred (Munjiza 2004 & Mohammadai, 2003)
3. Contact detection techniques: Neighbourhood list & Box method (Allen and Tidesley, 1991 & Babic, 1988)
4. Constitutive law to calculate the contact forces

5. Nonlinear FEM modeling and Updated Lagrangian technique (Owen and Hinton, 1980, Smith, 1982, Munjiza, 2004)

2.3 Different Shapes Used in DEM Modeling

Cundall (1971 and 1979) used cylindrical balls and rectangular blocks for his modeling. In the above work the particles are considered to be rigid and the contact is considered to be soft. Cundall and Hart (1992) used spherical particle to any polyhedral shape for 3D modeling. Developing computer codes for cylindrical and spherical particle is much easier than blocks and polyhedral. In the 1992 work they also considered the deformation in 2D and 3D bocks by performing FEM analysis. For 2D cylinders and 3D spherical particles only one value the radius is required to define the geometry and also there is only one possible type of contact between any two particles. Hence coding is much easier than other shapes. But these particles tend to roll or rotate and hence they don’t reflect the behavior of many granular materials.

Other shapes like ellipses (Ting et al 1993), ellipsoids (Ling and Ng, 1997), polygons (Feng and Owen 2004) and polyhedral (Ghaboussi and Barbosa, 1990) and superquadrics (Williams and O’Connor) are used. These shapes can represent much better the granular materials but they take more computer time in detecting the contact. Anandaraja (1994) used stick type DEM particles to simulate cohesion materials like clay. These particles can represent much better than disc/spheres. In the future any of these shapes will be considered in modeling CSH.

Chapter 3: DEM Model Development

3.1 DEM and CSH Modeling

Only few researchers investigated the nano level behavior of concrete. Selvam and his group () investigated the atomic structure of CSH using MD. This is also a discontinua method but the scope of application is limited by few nanometers and pico seconds. On the other hand the visualization of CSH using AFM images shows that they are thin and long in μm length. Hence DEM type discontinua may be very useful for CSH understadning. Few researchers like Chandler et al. (2010) and Fonseca et al. (2011) used DEM for CSH modeling and they used spherical particle of the size of 5 nm to predict the load deflection curve of the nanoindentation from experiment. Chandler et al. (2010) considered both normal and tangential forces and moments due to contact where as Fonseca et al. (2011) considered only forces. Both considered Van der Waals attractive forces. For the electric double layer force chandler et al. considered a relation from Monte Carlo study where as Fonseca et al. considered a fixed attractive force within certain distance. They both considered different compaction of the particles in the computational domain and compared the nanoindentation load deflection curve with experimental measurements and macro properties of concrete.

The actual CSH is long and thin fibers as shown in Figure 1 from AFM images. Hence particles whose shape is more like thin ellipsoid or stick may represent much better as discussed in section 2.3.

3.2 Available Computer Models

There are several computer models available in the commercial market for granular materials and rock mechanics applications as discussed in Jing and Stephansson (2008), and O'Sullivan (2011). Few of the open source and commercial codes available in the literature are listed below. Most of the details are obtained from Wikipedia.:

Open Source Codes:

1. **BALL & BLOCK** code listed in Cundall (1971) and described with some detail of implementation in Cundall and Strack (1979). These are 2D DEM code written in FORTRAN for disc and block. These are the first DEM code developed in the literature. Further developments were discussed and the new version of the code is listed in Strack and Cundall (1978).
2. **TRUBAL** is a 3D code. Discussed and listed in Strack and Cundall (1978).
3. **ESyS-Particle**: HPC Discrete Element Modelling Software: Available from: https://launchpad.net/esys-particle/ . This a 3D spherical particle code written in C++ and can also run under MPI for parallel computing.
4. **LAMMPS**: Code developed from Sandia. It is started as a MD code and has some features of DEM for spherical particles. Fonseca et al. (2011) used this code for their CSH modeling. The code is available from http://lammps.sandia.gov/ .
5. **LIGGGHTS**: This is an extension of LAMMPS and has more features of DEM. Available from http://www.liggghts.com/
6. **LMGC90:** Code is available from: **http://www.lmgc.univ-montp2.fr/~dubois/LMGC90/index.html .** The details and application of code is not clear
7. **PASIMODO:** Pasimodo is a spherical particle code written in C++. The code is available from: . http://www.itm.uni-stuttgart.de/research/pasimodo/pasimodo_en.php
8. **YADE:** Yade is written in C++. Available from https://launchpad.net/yade/ .Several researchers used it. Need to get more description.
9. **CHANNEL code:** This is a FORTRAN code used by Prof. Hayley Shen for a DEM class. The theoretical details (Babic, 1988) and the code can be downloaded from: http://people.clarkson.edu/~hhshen/Courses%20Page/Courses/Course5/course5.html .

Commercial Codes

1. **Applied DEM**: Bulk flow analysis 3D DEM software. Available from: http://www.applieddem.com/default.aspx
2. **EDEM**: Developed by DEM Solutions Ltd. Available from: http://www.dem-solutions.com/ . This also a bulk material software application.
3. **ELFEN**: ELFEN is a 2D/3D FEM+DEM code. This can model crack initiation and crack propagation. Developed by Rockfield Software. For further details: www.**rockfield**.co.uk/**elfen**
4. **PFC3D:** Developed by ITASCA. Details are available from: http://www.itascacg.com/pfc3d/ . This is the company started by Cundall. They have several software for different applications. Distinct element modeling for geotechnical analysis of rock, soil, and structural support in two and three dimensions. They are FLAC, UDEC and PFC.FLAC & FLAC3D: Advanced continuum modeling for geotechnical analysis of rock, soil, and structural support in two and three dimensions. UDEC & UDEC3D: Distinct element modeling for geotechnical analysis of rock, soil, and structural support in two and three dimensions

DEM Visualization

1. **VisPartDEM**: VisPartDEM is a opensource code. It is available from: http://lsl.vgtu.lt/vispartdem/en/About_149 . Some write up from the web page is as follows: "VisPartDEM is an open source distributed visualization tool for large particle systems simulated by the Discrete Element Method. VisPartDEM performs intensive post-processing necessary for visualization of derived variables. Discrete element computations are based on particle positions, forces acting between particles and Newton's laws. Particle systems have no permanent connections or usual grid that can be applied for spatial discretization or visualization purposes. Advanced algorithms based on surface extraction and Voronoi diagrams are implemented in order to obtain geometric representation of propagating cracks. VisPartDEM is designed as grid visualization tool, but it is ported on the other infrastructures"

2. **DEV_KM**: Kostek and Munjiza (2009) discussed above this visualization code and they said it is available in the open source.
3. **TECPLOT**: Tecplot is commercial visualization software that is extensively used for CFD applications. Using the 2D/3D scatter form one can visualize the disc/sphere and quadrilaterals and cuboids one can visualize similar to FEM data format.

3.3 Computer Model for the Current Study

Since the project is a pioneering work commercial codes cannot be used directly. Hence it is decided to develop in house research program. In addition the code will be useful for other research work in the department. At this stage we found a 2D DEM code for the flow application that has been used as a teaching material by Prof. Shen of the Clarkson University. A modified version of the BALL code reported in Cundall (1971) is also used to understand the DEM technique. Both codes uses disc or cylindrical particle for DEM study. Both codes were implemented in our system and sample problems were run. The computed results using the modified version of the code will be reported in the coming sections.

In addition we also got a 3D DEM code from Dr. John Peters and Mr. Wayne Hodo, Waterways Experimental Station, Vicksburg, Mississippi. This code is little complex and it is yet to implement in our system. Work is underway to install properly so that we can run it in our system. This code has ellipsoid type shapes that can be considered for modeling CSH.

All the above codes have contact forces but not Van der Waals and electric double layer attractive forces. Currently work is underway to include the attractive force and nanoindentor form of load applying procedure in 2D model. Later the same procedure will be tried in the 3D DEM code. Also the effect of elliptic and ellipsoidal shape will be included in the model.

Chapter 4: Results from DEM Modeling

4.1 Study Using BALL Code Considering Only Contact Forces

The BALL code from Cundall (1971) is used to study the equilibrium position of 100 balls due to gravity. The initial positions of the balls are shown in Figure 4.1. The position of the balls after 11000 time step is shown in Figure 4.2. The angle of inclination is about 10 degrees which is what expected for the data given for the code. Since these are mainly to test the code the input data and other details are not given. The detail can be found from Cundall (1971) and Cundall and Strack (1979).

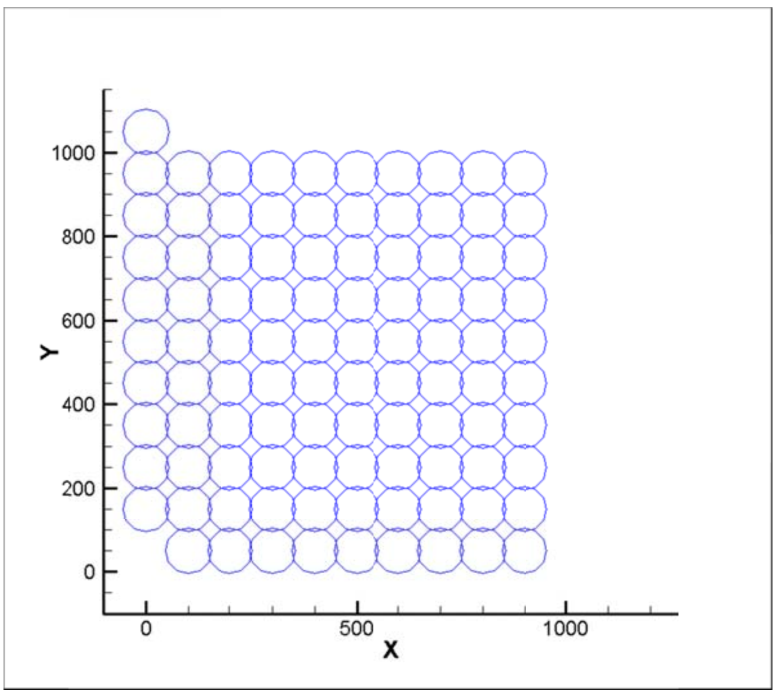

Figure 4.1 Initial positions of the 10x10 cylinders including gravity effect

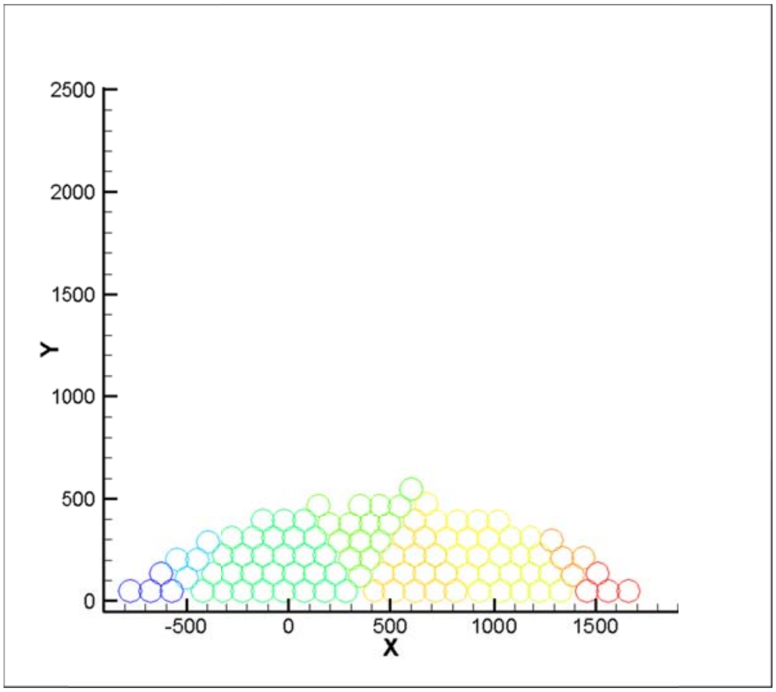

Figure 4.2 Position of the cylinders after 11,000 time steps including gravity effect

4.2 Modifications to the BALL Code to Consider Moving Wall and Cohesive Forces

The BALL code considers the fixed wall at the bottom by using a dummy ball at the bottom of the wall as shown in Figure 4.5. In addition to the fixed wall, to consider the load application similar to indentation, two moving walls are introduced at the top of the 20x10 balls as shown in Figure 4.5. The code is modified to consider moving walls. The detail of the theory is discussed in Babic (1988). The main difference from their work to this work is considering the directions of normal and tangential directions in the disc. In the current model the directions are similar to Cundall and Strack (1979) which is opposite to Babic (1988) as shown in Figure 4.3. When considering the walls the angle has to be given counter clockwise as shown in Figure 4.5. One wall starts at the middle point at angle of 135 degrees and the other is little above the surface with an angle of 225 degree as shown in Figure 4.4. Since the contact is on one side the angle has to be chosen properly so that proper side becomes active.

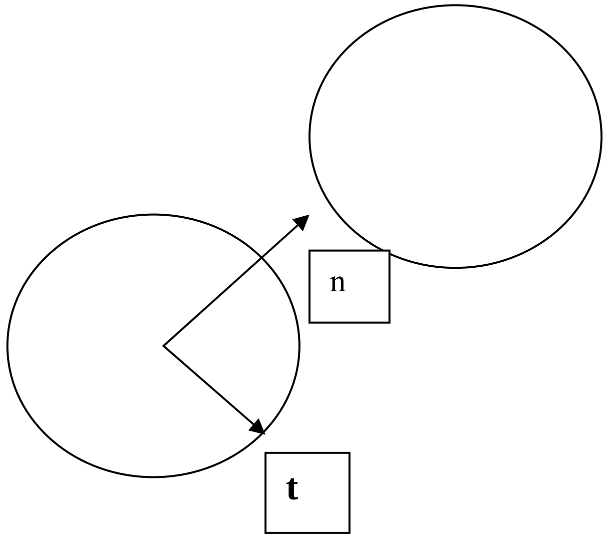

Figure 4.3 Direction of normal (n) and tangential (t) direction in a cylinder of the developed DEM code

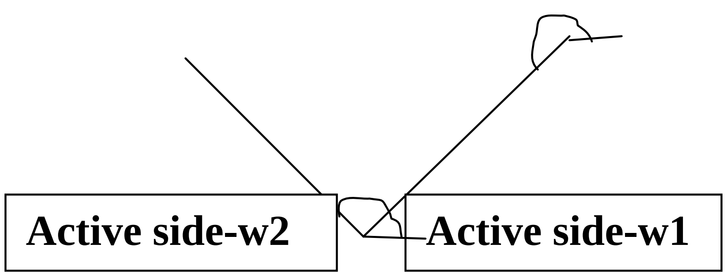

Figure 4.4 Angle measurements for the two walls.

The BALL code considers only the contact forces. But in our work of modeling CSH, in addition to contact forces there is also cohesive forces as reported by Chandler et al. (2010) and Fonseca et al. (2011). A constant attractive force is introduced in the model similar to Fonseca et al. (2011). At this time it is considered that there is cohesive force if the distance between cylinders where between d and 1.05d where d is the diameter of the cylinder. Also the gravity force is neglected in the current work.

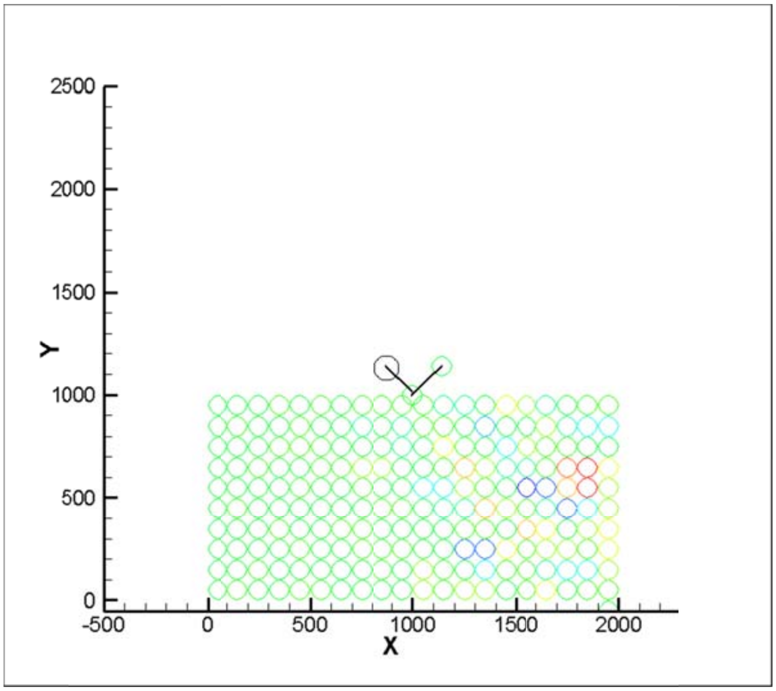

Figure 4.5 Initial positions of the 20x10 cylinders when an indentor is moving at a speed of u=1m/s

The final position of the balls when the indentor is coming down at a speed of 1units/s is shown in Figure 4.6. The position reported is after 8000 time steps.

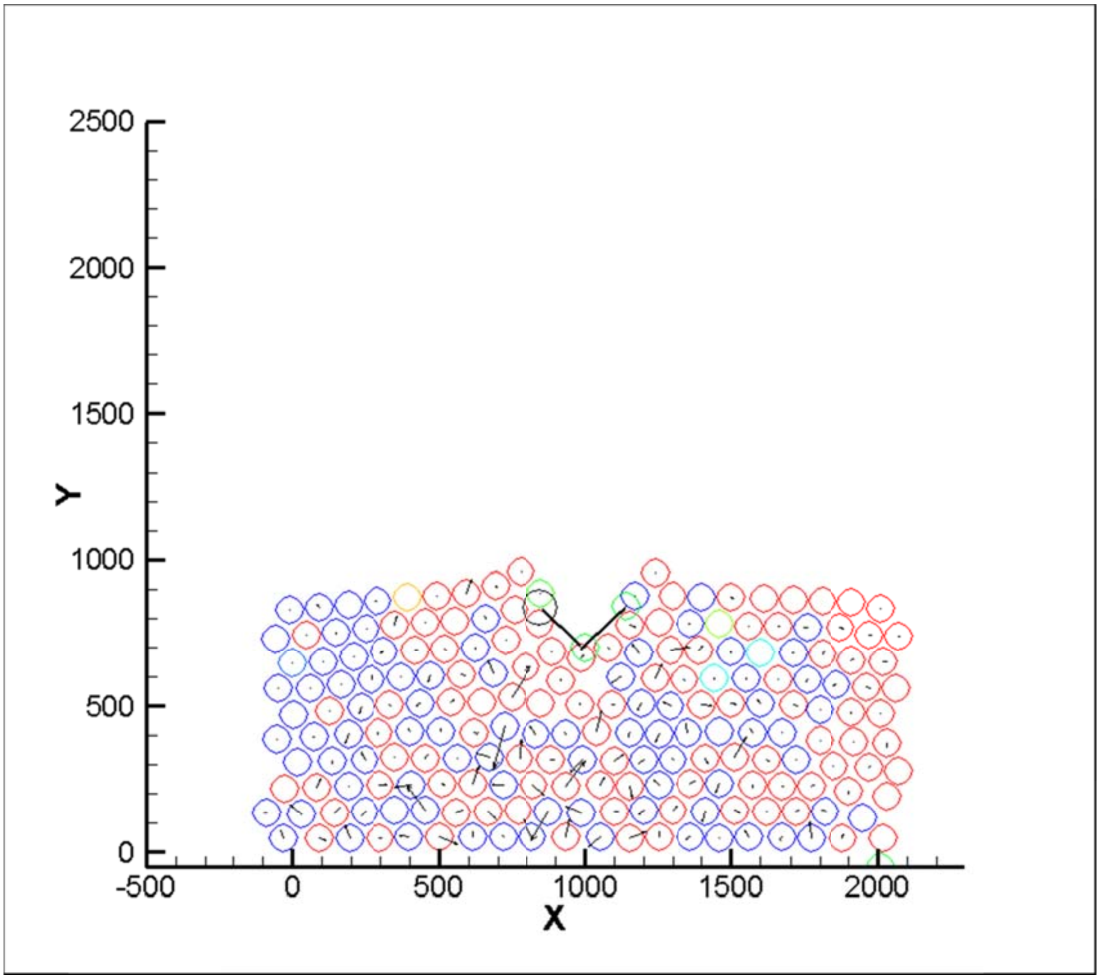

Figure 4.6 Position of the 20x10 cylinders after 8000 time steps when an indentor is moving at a speed of u=1m/s.

Chapter 5. Conclusions and Further Study

This research work was proposed for three years and the progress made for the first year as Phase I is reported here. The importance of using discrete element method (DEM) for nano science study of cement and concrete is discussed. The difficulty in using molecular dynamics (MD) to study the structure of CSH is also discussed. The current status of DEM application in understanding concrete is reviewed. Existing free ware and commercial codes based on DEM are reviewed. Different DEM codes that are available for this research and the difficulty in using those codes are also discussed.

The results computed from the in house DEM code when an indentor type load is applied to a cohesive material are presented. The developed code paves ways for further modification to consider shapes other than balls for future CSH study. The code needs to be modified for shapes similar to CSH which are long and thin. This can model the CSH much close than ever. The code also needs to be modified to have a better search algorithm to reduce computer time.

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