



EDEM Contact Model: Timoshenko Beam Bond Model

Authors:

Nick J. BROWN

John P. MORRISSEY

Jin Y. OOI

*School of Engineering,
University of Edinburgh*

Jian-Fei CHEN

*School of Planning, Architecture and Civil Engineering,
Queen's University, Belfast*

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v1.0

June 4, 2015

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PREFACE

This reference manual provides the key information regarding an bonded beam contact model for EDEM that has been developed over many years at the University of Edinburgh. The contact model has been implemented as a User Defined Library (UDL) through the API capabilities of EDEM.

This phenomenologically based contact model has evolved over many years of use and development to capture the key bulk behaviour of cohesive powders and granular solids. This guide is written to accompany the contact model and provide the details regarding the motivation and implementation of the contact model. An example problem and description is also provided as an accompanying standalone guide for use with the contact model.

While this version of the contact model has been used and tested extensively, no piece of code is ever completely bug free and, as such, the user should remain vigilant for unexpected outcomes. All efforts have been made to ensure all information is correct at time of writing. The contact model is provided with no explicit guarantee of accuracy or results.

Development never ceases so all further comments, queries or bug reports can be reported to the author or DEM Solutions Ltd.

Please cite the contact model as:

1. Brown, N. J., Chen, J. F. & Ooi, J. Y. A bond model for DEM simulation of cementitious materials and deformable structures. *Granul. Matter* 16, 299–311 (2014).
2. Brown, N. J. *Discrete Element Modelling of Cementitious Materials*. (2013).

ACKNOWLEDGEMENTS

To acknowledge everyone who contributed to the work over the last few years is not a straight forward task.

The input of other colleagues has also played a role in the continual development of the contact model.

A further acknowledgement and thank you is required for the DEM Solutions team who were always willing to help out and answer the difficult questions when something was not working!

1 INTRODUCTION

The failure of cemented granular materials is highly influenced by the initiation and propagation of cracks that occur at cemented grain interfaces (cement joint). In the Discrete Element Method (DEM) the representation of a cemented joint can be achieved by inserting bonds between elements (particles) at contacts. Each bond is capable of resisting the relative displacement of the two particles it connects in at least one degree of freedom. In this manner a collection of particles can be transformed into a heterogeneous macroscopic granular solid through the introduction of bonds [9]. Fracture and progression of damage in the granular solid is introduced by including a failure criterion for each bond; when this criterion is reached the bond is removed from the contact and the subject material degrade from macroscopic solids to being more particulate in nature. Bonded contacts differ from cohesive contacts as the resisting forces that exist at a bonded contact cannot be reformed once a bond has failed.

From fundamental mechanics either a strut (spring) element or a beam element may be used to define the constitutive relationship of a bond. A strut only resists the axial force, but is simple to implement and fast for computation; beams are more computationally expensive but provide more realistic representations of the bond mechanism as they can take into account axial, bending, shear and torsion behaviour at a cemented joint e.g. [1; 4; 7; 14]. It has been shown [14] that beam models provide a good compromise between computational time and accuracy.

A novel bonded contact model [2; 3] based on the Timoshenko beam theory, which will be referred to as the Timoshenko Beam Bond Model (TBBM), has been implemented in the software EDEM[®] through the API functionality. The model has been shown to be suitable for modelling the behaviour of cemented granular materials [2; 3].

NOTE 1: COMPILED VERSIONS

The compiled User Defined Library (UDL) is available for both 64-bit Windows and Linux based operating systems.

- The Windows version has been compiled in Visual studio 2013 and is compatible with EDEM 2.6. Earlier versions of EDEM may require the [Visual Studio 2013 Redistributable package](#) to be installed first.
- The Linux version has been compiled with gcc on Scientific Linux 6. This should be compatible with all 64-bit Linux systems and all versions of EDEM.

2 MODELLING APPROACH

In the TBBM cemented granular materials are represented by an assembly of spherical particles which may interact at either bonded or non-bonded contacts. Due to their spherical nature, only one contact can exist between any two particles.

NOTE 2: LIMITATIONS

It should be noted that it is not currently possible to use the model with non-spherical particles.

At a non-bonded contact a spring-dashpot configuration is assumed with the contact behaviour described using the well-used Hertz-Mindlin (no slip) contact law [8; 10]. At a bonded contact a beam element is assumed to rigidly connect the two particles. Each bond element is assumed to be circular and straight in three dimensional space at formation. The behaviour of this bond is assumed to follow the Timoshenko beam theory [13], and as described in Section 4. For simplicity, it is assumed that the beam element connects to the centres of the two particles, so that each end of the bond shares the same six degrees of freedom as the particle. Both contact types resist compressive and shear forces, but bonded contacts can also resist tensile forces as well as bending and twisting moments.

In the material assembly particles and bonds do not directly represent individual grains and cement interfaces, but rather represent the constituent parts of the subject material and their interactive properties at the mesoscopic scale. Representing each grain on the microscopic scale would be too computationally expensive and require extensive information for calibration.

3 MODEL IMPLEMENTATION DETAILS

The TBBM has been implemented in the three-dimensional discrete element software EDEM through an Application Programming Interface (API). Verification of the TBBM in EDEM is presented in Brown [2] with a summary provided in Section 5. It should be noted that there are three steps involved in the preparation of a material model that is to be tested using the TBBM:

1. Particle Generation (can be in EDEM or third party software)
2. Bond parameter selection (this needs to happen before the simulation file is opened in EDEM and subsequent bond initialisation)
3. Bond initialisation (this happens in EDEM simulator and although may be part of the same simulation file as the loading, it should be considered as a separate process)

The TBBM is only compatible with spherical particles which can be generated either using EDEM or third party software.

3.1 BOND NETWORK FORMATION

When using the TBBM to bond particles that are not in physical contact it is necessary for the contact radius of those particles to be set to a value greater than their physical radius. In the example shown in Figure 3.1 although particles A and B are not in physical contact they can be bonded together as their contact radii overlap. The contact radius parameter, for each particle, can be found in the creator section of EDEM, as highlighted in Figure 3.2. It should be noted that contact radius is scaled with physical radius when a size distribution is used in EDEM for particle generation. Like other particle properties, the contact radius of a particle can't be changed in EDEM after it has been generated.

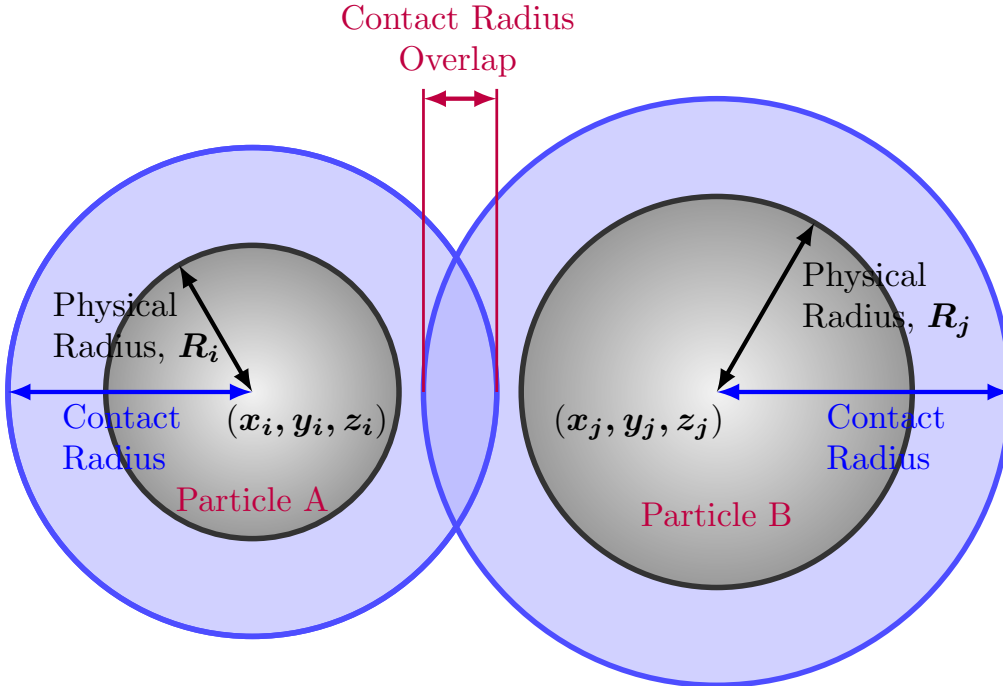


FIGURE 3.1: Particles A and B are in contact for the purposes of bonding

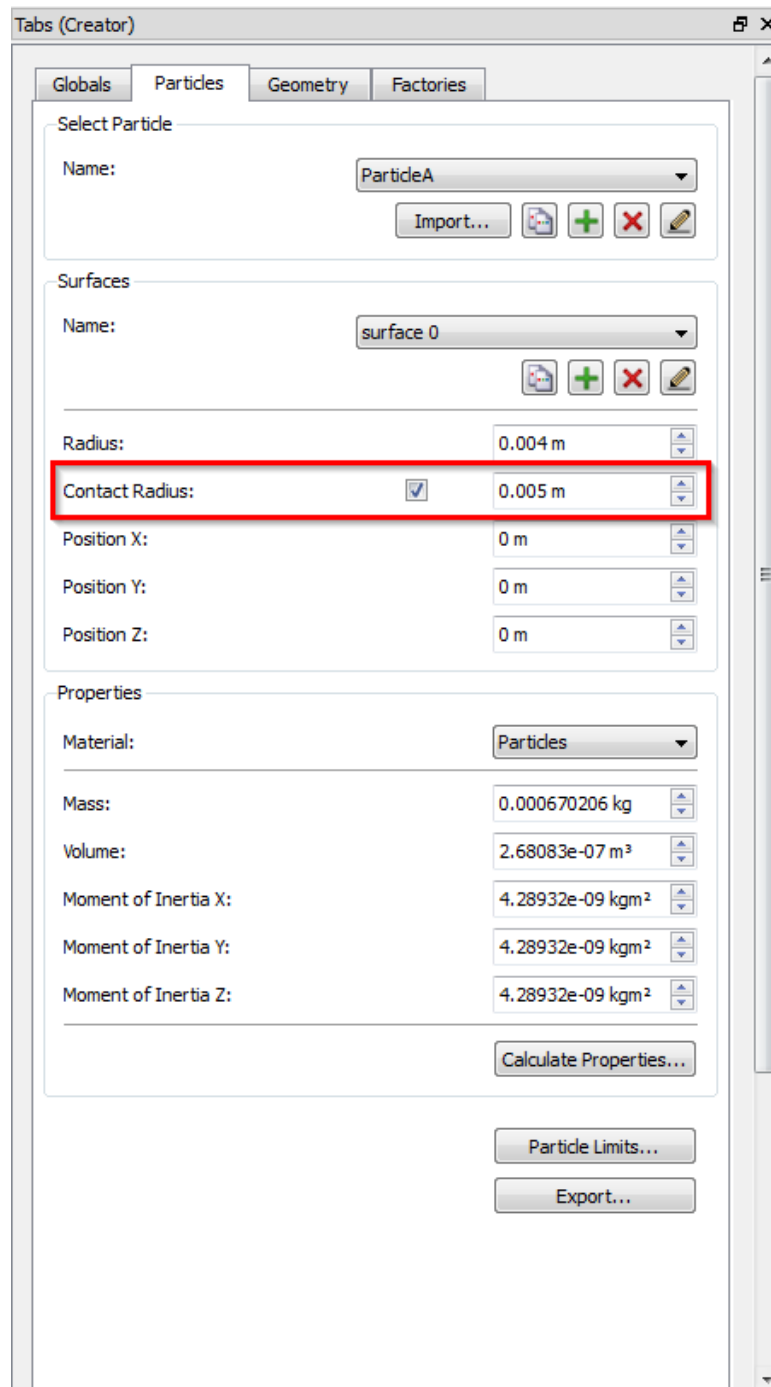


FIGURE 3.2: Contact radius and physical radius in EDEM creator

Other than the contact radius, the TBBM does not place a spatial restriction on where bonds are formed. As such, bond formation is not restricted to just being between nearest neighbours and therefore bonds can also be formed through other particles, as shown in Figure 3.3. It is therefore important to ensure the contact radius is sensibly chosen such that excessive bonding is prevented.

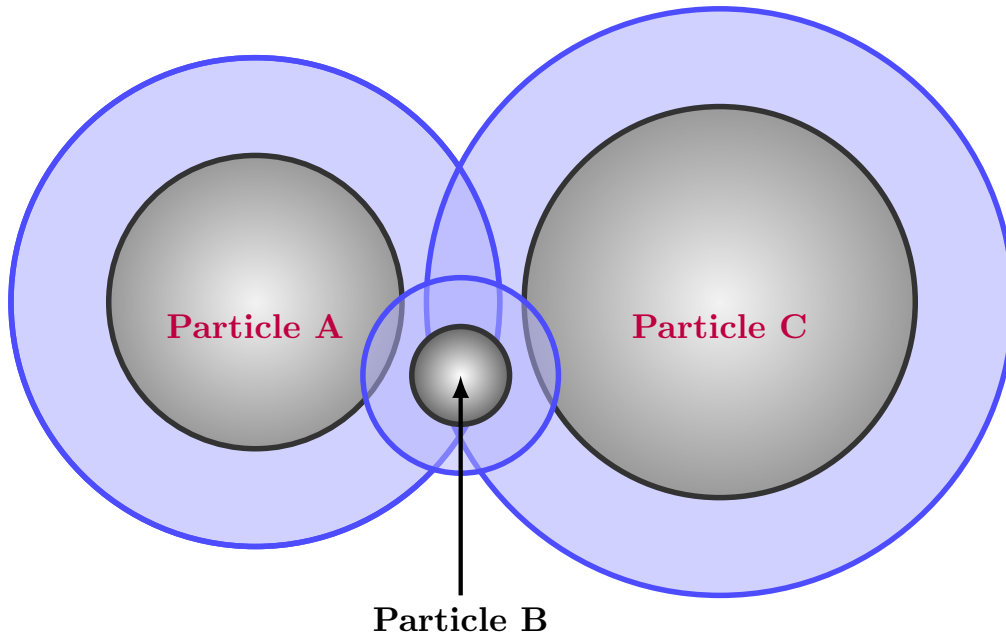


FIGURE 3.3: Schematic of Neighbour Bonding - Particles A and C can be bonded through particle B

The influence of contact radius multiplier on the number of bonds in the specimen is significant, as can be seen in Figure 3.4. As the contact radius multiplier increases, the number of particles that an individual particle can bond to increase significantly, leading to an increase in the average number of bonds formed per particle and the total number of bonds in the simulation. Increasing the contact radius multiplier, and thus the number of bonds, will normally lead to an increasing the failure strength of the assembly. The increased number of bond will also affect the total required computation time for a simulation.

If using EDEM versions prior to 2.7 for particle generation, and using particles with a higher contact radius to physical radius, it is important to ensure that a bonded contact model (either the TBBM or the in-built Hertz-Mindlin with bonding model) is loaded as both the particle-particle and the particle-geometry contact model, especially for simulations requiring particle packing. If a non-bonded contact model were used (i.e. Hertz-Mindlin) then the contact model would activate when the contact radii of two particles came into contact rather than their physical radii. Loading a non-bonded contact model into EDEM for particle generation with contact radii set higher than physical radii may lead to a lower than desired solid fraction. By exporting the simulation deck to an .xml format it is possible to modify the contact radius after the particles have been generated. This new simulation deck can then be re-imported to EDEM with the modified contact radii.

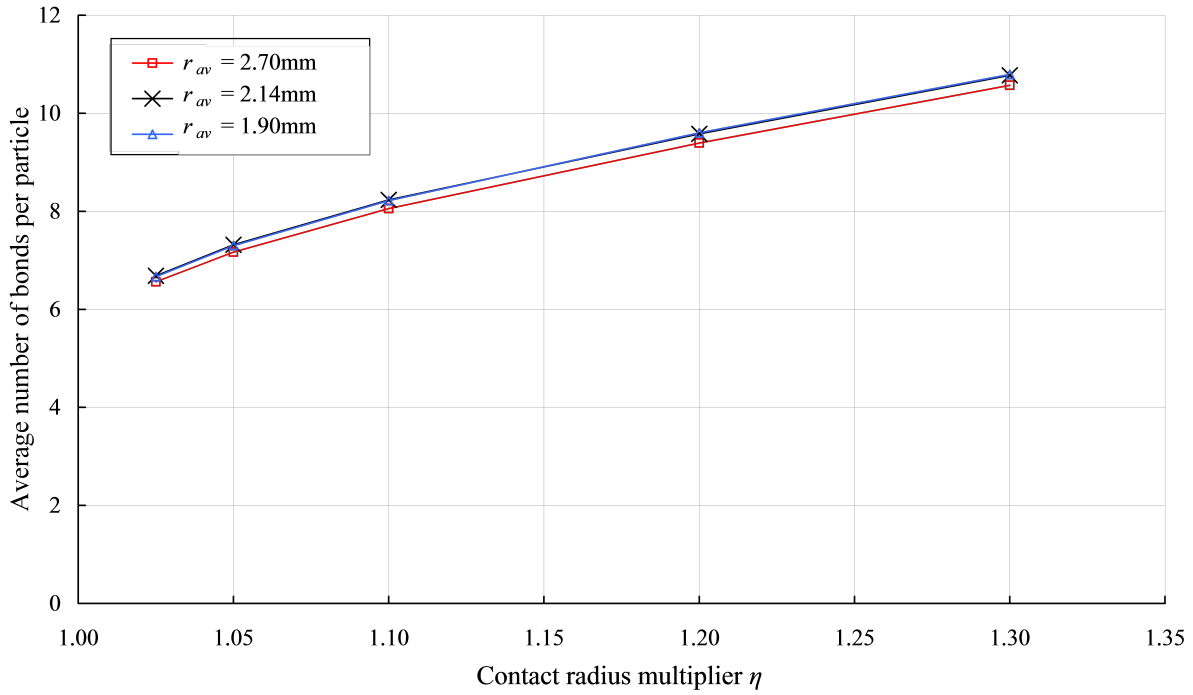


FIGURE 3.4: Average number of bonds per particle for varying contact radius multiplier

3.2 BOND MODEL INPUT PARAMETERS

It is recommended, but not required, that the generated particle assembly be introduced as a new deck into EDEM with the simulation time can set to $t = 0$. This is also the point to ensure the TBBM is loaded into EDEM in three locations:

1. As a custom particle-particle model
2. As a custom particle-geometry model
3. As a custom body force model

The user defined input parameters for the Hertz-Mindlin (no slip) contact model are specified in EDEM through the user interface as normal. However, the additional parameters required for the TBBM are loaded into EDEM via an external preference file titled “BondedParameters.txt” which should be saved in the same folder as the contact model library file. An example preference file is shown in Figure 3.5. The preference files consist of two sections – the simulation properties and the interaction properties. The first parameter in the simulation properties is the global damping coefficient, while the second line defines the bond initialisation time. The format of the interaction properties in the preference file are discussed further in mapped out in Table 3.1. As can be seen from Table 3.1 is it possible to put numbers in any form, e.g. 500e6 could have been written as 5e8, likewise both 0 and 0.0 are acceptable.

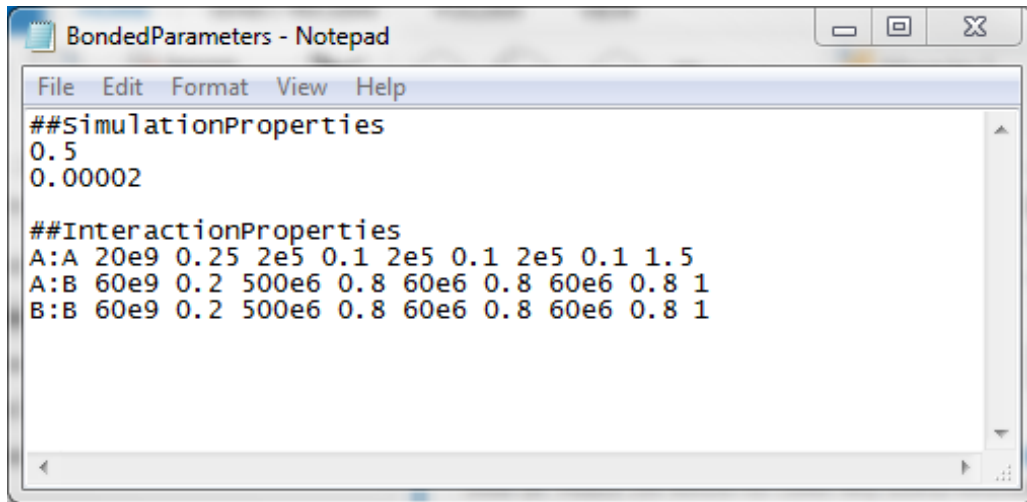


FIGURE 3.5: Example preference file

TABLE 3.1: Layout of example preference file

	A	B	C	D	E	F	G	H	I	J
1	##SimulationProperties									
2	0.5									
3	0.00002									
4										
5	##InteractionProperties									
6	A:A	20E+09	0.25	2.0E+05	0.1	2.0E+05	0.1	2.0E+05	0.1	1.5
7	A:B	6.0E+10	0.2	5.0E+08	0.8	6.0E+07	0.8	6.0E+07	0.8	1
8	B:B	60E+09	0.2	500E+06	0.8	6.0E+07	0.8	6.0E+07	0.8	1

To clarify, the position of each input parameter in the preference file the values shown in Figure 3.5 have been mapped out into columns (A-J) and rows (1-8) in Table 3.1, these relate to the statement in square brackets in the descriptors that follow.

NOTE 3: LOADING PREFERENCE FILE

The parameters in the preference file are transferred to EDEM when the contact model is loaded so any changes made to the preference file after the initial loading will not be automatically registered and the contact model should be reloaded.

3.2.1 SIMULATION PROPERTIES IN PREFERENCE FILE

The simulation properties are defined in lines two and three of the preference file.

3.2.1.1 Global damping coefficient

[Cell A2] The first simulation property refers to the dimensionless constant global damping coefficient ι_d . When required, for example if frictional sliding does not represent the full damping effect seen in the real material, artificial damping can be introduced to reduce the kinetic energy.

By inserting a non-zero value, non-viscous damping is applied to the particles through the equations of motion. Energy is dissipated in every particle in the system (both bonded and non-bonded). As only the acceleration term is dampened stable motion is not affected and particles with a fixed velocity will maintain that velocity. This makes it's usage suitable for static and quasi-static problems. Careful consideration is required by the user when applying global damping to dynamic problems.

The range of values for this coefficient are zero to one, with zero providing no damping and one meaning the damping is equal in magnitude to the total forces. The full equations for damping are included in Appendix A.

3.2.1.2 Bond time

[Cell A3] The second line in the preference file identifies the bond time t_{bond} (s). When the simulation exceeds the bond time for the first time the bond initialisation procedure is triggered i.e. the time at which, among other things, bonds will form between particles. At the bond time, bonds are initialised before any interactions between particles are resolved. The bond initialisation procedure is explained in Section 3.4.

3.2.2 BOND INTERACTION PROPERTIES IN PREFERENCE FILE

Bond interaction properties are defined pair-wise from line six onwards.

3.2.2.1 Particle interaction indicator

[Column A] In EDEM each particle has a defined type; in many simulations only particles of one type are generated. However, by including an indicator multiple particle types with different bond properties can be used in a single simulation. Using the preference file shown in Figure 3.5 if a bond is between two particles, both of type A, then the properties in row 6 will be used; if the bond is between one particle of type A and one of type B then the properties in row 7 will be used for the bond between them. Particle types can consist of a string of any characters, but should avoid spaces as this may not be properly read on some systems.

3.2.2.2 Bond Young's Modulus

[Column B] The value for bond Young's Modulus E_b (N/m^2) modifies the stiffness of the bond. In the preference file shown in Figure 3.5 bonds between particles A and B will be three times as stiff as bonds between particles A and A, assuming all other factors (e.g. bond length) are the same.

3.2.2.3 Bond Poisson's Ratio

[Column C] The value for Bond Poisson's ratio, ν_b , allows the ratio of the shear modulus to Young's modulus of the bond to change. In the example shown in Figure 3.5 the value of ν_b for bonds between particles of type B will be 0.2.

3.2.2.4 Mean bond compressive strength

[Column D] The compressive strengths for all bonds of one interaction type follow a Gaussian distribution. The factor S_C (N/m^2) modifies the mean for this distribution. See Section 4.4 for more details on how this distribution is determined.

3.2.2.5 Coefficient of variation of compressive strength

[Column E] The compressive strengths for all bonds of one interaction type follow a Gaussian distribution. The factor ζ_C modifies the coefficient of variation for this distribution. See Section 4.4 for more details on how this distribution is determined.

3.2.2.6 Mean bond tensile strength

[Column F] The tensile strengths for all bonds of one interaction type follow a Gaussian distribution. The factor S_T (N/m^2) modifies the mean for this distribution. See Section 4.4 for more details on how this distribution is determined.

3.2.2.7 Coefficient of variation of tensile strength

[Column G] The tensile strengths for all bonds of one interaction type follow a Gaussian distribution. The factor ζ_T modifies the coefficient of variation for this distribution. See Section 4.4 for more details on how this distribution is determined.

3.2.2.8 Mean bond shear strength

[Column H] The shear strengths for all bonds of one interaction type follow a Gaussian distribution. The factor S_S (N/m^2) modifies the mean for this distribution. See Section 4.4 for more details on how this distribution is determined.

3.2.2.9 Coefficient of variation of shear strength

[Column I] The shear strengths for all bonds of one interaction type follow a Gaussian distribution. The factor ζ_S modifies the coefficient of variation for this distribution. See Section 4.4 for more details on how this distribution is determined.

3.2.2.10 Bond radius multiplier

[Column J] The bond radius multiplier λ modifies the radius of each bond, influencing the bonds stiffness and strength. See Section 4.1 for more details on how the bond radius multiplier is used.

NOTE 4: CHANGING PREFERENCE FILE PARAMETERS

Changing the parameters in the preference file only has an effect before the bonds are created - the bond strengths are stored in the simulation when the bond is created at the bond time (Section 3.2.1.2).

However, the bond radius multiplier, λ (Section 3.2.2.10), is not stored, so care needs to be taken not to change this value in the preference file after the bond time, as it will affect the evaluation of the current strength of the bond.

3.2.3 BOND INTERACTION PROPERTIES IN EDEM**3.2.3.1 Contact Radius multiplier**

In order for bonds to be formed between particles that are not in physical contact EDEM® requires the contact radius of those particles to be greater than their physical radius. This property has been defined as the contact radius multiplier η and can be modified in the particle creator section of EDEM®, as shown in Figure 3.2.

3.3 TIMESTEP SELECTION

The parameters discussed in Section 3.2 are those that cannot be modified in EDEM through the user interface and are specific to this model. However, due to the generally high stiffness of bonds, the DEM time step needs to be selected with consideration of the stiffness of the system to ensure a stable explicit integration. As both bonded and non-bonded contacts are considered, the critical

computational time step should be determined for both with the lower of these two values being used.

For non-bonded contacts, since the Hertz-Mindlin (no slip) model is implemented, the critical time step is determined using the Rayleigh time step (calculated by EDEM). The critical time step for bonded contacts is estimated from an approximate solution based on a single degree of freedom in a mass spring system [11].

$$t_{b,crit} = 2\sqrt{\frac{m_{p,min}}{K_{b,max}}} \quad (3.1)$$

The critical time step is determined for each bonded contact using the smallest particle mass $m_{p,min}$ and the largest bond stiffness component $K_{b,max}$ for that contact. These values can be obtained for every bond by exporting data from the analyst and the smallest time step determined accordingly. A walk through of this procedure is included in the accompanying example problem guide.

3.4 BOND INITIALISATION

Part of the material model preparation process is the bond initialisation procedure; this is conducted when the simulation time t exceeds the bond time t_{bond} for the first time. During the bond initialisation procedure bonds will be inserted between particles if the two particles contact radii overlap and they are allowed to bond i.e. that there is a bond definition for that interaction in the interaction properties section of the preference file. An example particle configuration for the preference file in Figure 3.5 is shown in Figure 3.6 below. In the example preference file shown in Figure 3.5, when the simulation time exceeds 0.01 s for the first time bonds will be formed between particles 1 and 2, particles 2 and 3 and also particles 3 and 4.

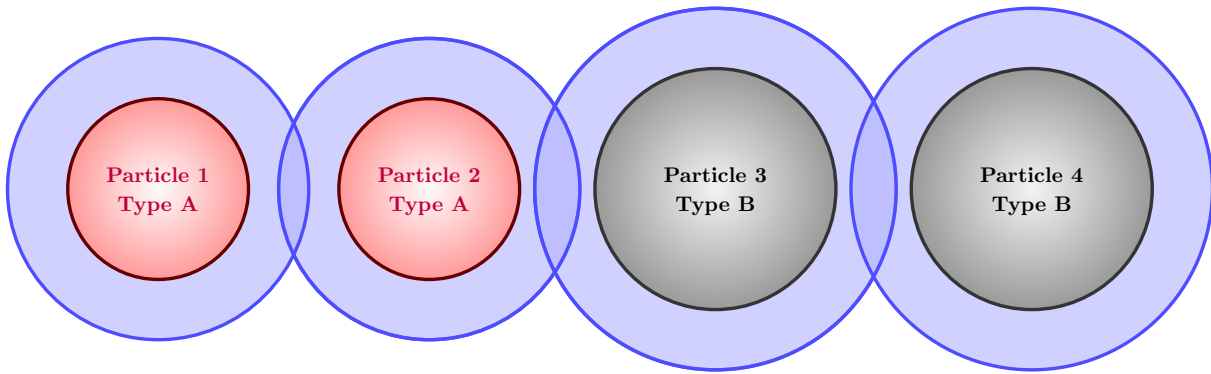


FIGURE 3.6: Example particle layout

However, if the preference file given in Figure 3.7 was used, then bonds would only form between particles 1 & 2 and particles 3 & 4, but not between particle 2 & 3. This is because although the contact radii of particles 2 and 3 overlap, there is no bond characteristic defined for a bond between type A and type B particles.

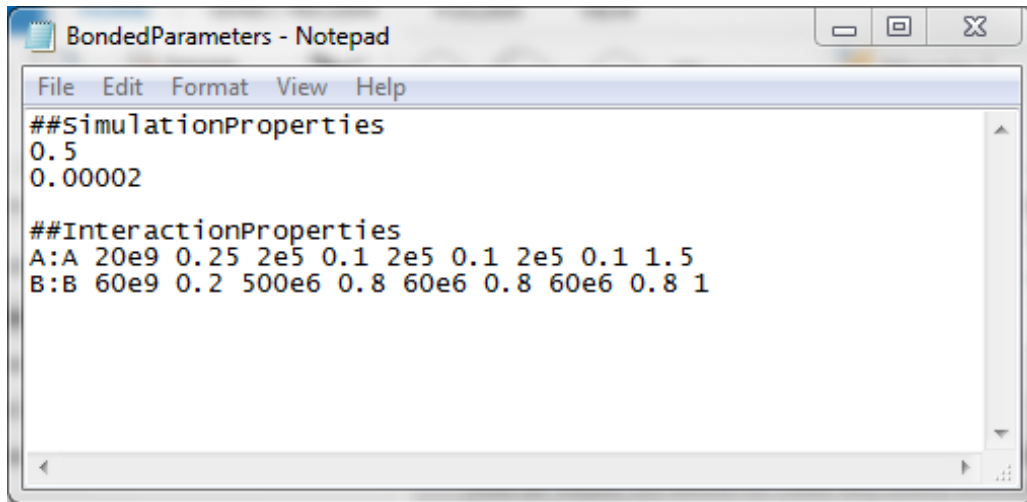


FIGURE 3.7: Alternative preference file

If a third party software was used for particle generation or a particle-particle contact model other than the Hertz-Mindlin (no slip) contact model was used for particle generation in EDEM then the particles may behave erratically on the first computation using the TBBM as the contact model between particles will have changed. To combat this simply limit the particle velocities and angular velocities to zero. This essentially locks the particles in place until after they have been bonded.

At the end of the computational time step where bonds have been initialised an initial stress-free state is achieved by resetting all physical overlaps to zero. This results in a static assembly of bonded particles with zero overlap and no contact force at the start of each loading simulation. This means that as long as all particles in the simulation have been bonded there is no need for the particles linear or angular velocity to be restricted, an equilibrium will have been reached. It also means that if two particles are in contact after the bond between them fails then the new overlap will not be exaggerated.

3.5 RESULTS IN EDEM ANALYST

The TBBM is integrated into EDEM as a custom contact model. As such when using the EDEM Analyst the user should ensure to look at the properties of interest under the “contacts” category rather than the “bond” category. This will remain the case whilst the model is an external contact model.

There are a number of custom properties that can be viewed in the analyst. As they are all external properties the names for each option are not given rather they are supplied as element of that property. The following tables (Tables 3.2 to 3.4) can be used to determine the meaning of each property element.

The properties shown in Table 3.2 are simulation properties, hence only a single value is available for export for each timestep for each of the three elements.

The properties shown in Table 3.3 are custom contact properties, specifically custom bonded contact properties. Values for each property are available at each timestep. However, values will all be zero if examined before the bond time. After a bonded contact has broken the last value for that property will be recorded for the remainder of the simulation i.e. if the compressive bond stress was 40 MPa at

TABLE 3.2: List of additional custom simulation properties available in EDEM analyst

Property	Element	Definition
Failure Mode	0	The number of bonds in the simulation that failed because the compressive strength was exceeded
	1	The number of bonds in the simulation that failed because the tensile strength was exceeded
	2	The number of bonds in the simulation that failed because the shear strength was exceeded

the point at which the bond failed a value of 40 will be recorded for compressive bond stress for the remainder of the simulation.

The properties shown in Table 3.4 are custom particle properties. Values for each option will be available for each particle at each timestep.

TABLE 3.3: List of custom contact (bond) properties available in EDEM analyst

Property		Symbol	Definition
Bonded	0	-	The contact is a non-bonded contact
	1	-	The contact is a bonded contact
BOND LENGTH	0	-	The length of the bond between the two particles
BOND STIFFNESS ^a	0	k_1	The 1st unique component of the stiffness matrix
	1	k_2	The 2nd unique component of the stiffness matrix
	2	k_3	The 3rd unique component of the stiffness matrix
	3	k_4	The 4th unique component of the stiffness matrix
	4	k_5	The 5th unique component of the stiffness matrix
	5	k_6	The 6th unique component of the stiffness matrix
TRANSFORMATION MATRIX ^b	0	-	The 1st unique component of the stiffness matrix
	1	-	The 2nd unique component of the stiffness matrix
	2	-	The 3rd unique component of the stiffness matrix
	3	-	The 4th unique component of the stiffness matrix
	4	-	The 5th unique component of the stiffness matrix
	5	-	The 6th unique component of the stiffness matrix
	6	-	The 7th unique component of the stiffness matrix
	7	-	The 8th unique component of the stiffness matrix
	8	-	The 9th unique component of the stiffness matrix
BOND STRESS ^c	0	$\sigma_{c,max}$	The current maximum compressive stress in the bond
	1	$\sigma_{t,max}$	The current maximum tensile stress in the bond
	2	τ_{max}	The current maximum shear stress in the bond
BONDSTRENGTH ^d	0	σ_c	The compressive strength of the bond
	1	σ_t	The tensile strength of the bond
	2	τ	The shear strength of the bond
PHYSICAL OVERLAP	0	-	The physical overlap in the contact at the bond time
	1	-	The physical overlap in the contact at the current time
BOND FORCE	0	-	The force in the x direction of the bond *
	1	-	The force in the y direction of the bond *
	2	-	The force in the z direction of the bond *
	3	-	The torque in the x axis of the bond *
	4	-	The torque in the y axis of the bond at the 1 st end
	5	-	The torque in the z axis of the bond at the 1 st end
	6	-	The torque in the y axis of the bond at the 2 nd end
	7	-	The torque in the z axis of the bond at the 2 nd end

^a The six components of the stiffness matrix are shown in Appendix B

^b The nine components of the transformation matrix are shown in Section 4.2

^c The bond stress calculations are shown in Section 4.3

^d The bond strength calculations are shown in Section 4.4

* equal and opposite at each end

TABLE 3.4: List of additional custom particle properties available in EDEM analyst

Property	Symbol	Definition
BondForce	0 -	Resultant bonded contact force acting on the particle in the global X axis
	1 -	Resultant bonded contact force acting on the particle in the global Y axis
	2 -	Resultant bonded contact force acting on the particle in the global Z axis
BondTorque	0 -	Resultant bonded contact torque acting on the particle in the global X axis
	1 -	Resultant bonded contact torque acting on the particle in the global Y axis
	2 -	Resultant bonded contact torque acting on the particle in the global Z axis
HMForce	0 -	Resultant non-bonded contact force acting on the particle in the global X axis
	1 -	Resultant non-bonded contact force acting on the particle in the global Y axis
	2 -	Resultant non-bonded contact force acting on the particle in the global Z axis
HMTorque	0 -	Resultant non-bonded contact torque acting on the particle in the global X axis
	1 -	Resultant non-bonded contact torque acting on the particle in the global Y axis
	2 -	Resultant non-bonded contact torque acting on the particle in the global Z axis
Damage	0 B_0	Number of bonds connected to the particle at the bond time
	1 D	Particles damage factor

The custom particle property ‘Damage’ refers to the proportion of bonded contacts that have failed for a given particle, as described in Equation (3.2). This is equivalent to continuum damage theory.

$$D = 1 - \frac{B}{B_0} \quad (3.2)$$

where D is the particle damage parameter, B is the number of bonds connected to that particle at the current time step and B_0 denotes the number of bonds that were connected to that particle at the bond time. As D increases to 1 the particle becomes less bonded to its neighbours.

NOTE 5: DAMAGE

Note that the ‘Damage’ parameter will be zero before the bond time and/or if the particle is not bonded to any other particle.

4 BONDED CONTACT MODEL DESCRIPTION

At each bonded contact a Timoshenko beam element is assumed to rigidly connect the two particles in contact. The behaviour of this bond is assumed to follow the Timoshenko beam theory [13]. For simplicity, it is assumed that the beam element connects to the centres of the two particles, Figure 4.1, so that each end of the bond shares the same six degrees of freedom as the particle.

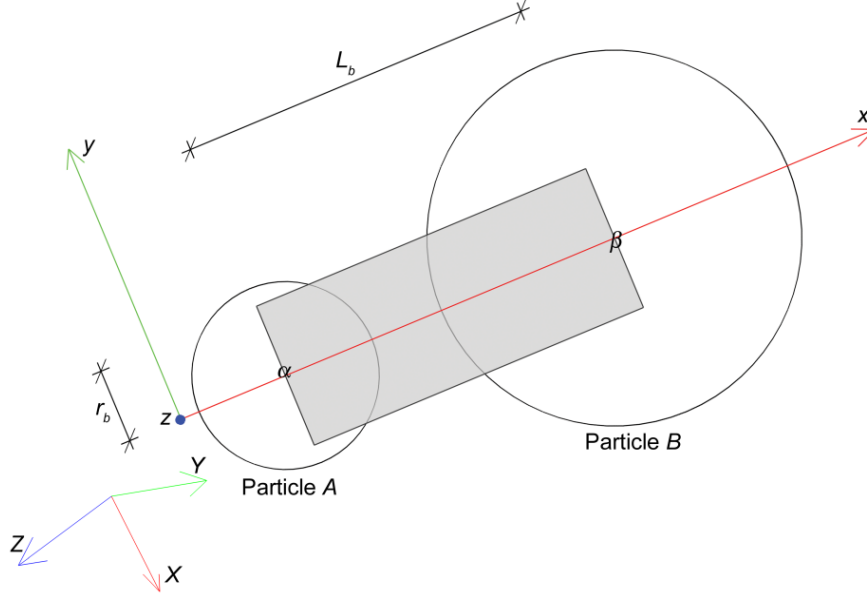


FIGURE 4.1: Projected view through the central axis of a bond connecting particles A and B

NOTE 6: BEAM END NODES

There are no significant difficulties to implement, if it is desirable, the assumption that the bond element connects the two particles away from their respective centres.

In Figure 4.1 the two ends of a single bond, marked as points α and β , are shown to connect to the centres of particles A and B respectively; the bond has a length L_b and a radius r_b . Vectors $\{P_A\}$ and $\{P_B\}$ define the positions of the two particles in the global Cartesian co-ordinate system (X, Y, Z) .

$$\{P_i\} = \{X_i Y_i Z_i\} i = A, B \quad (4.1)$$

In addition to the single global co-ordinate system each bond has its own unique local co-ordinate system (x, y, z) , as shown in Figure 4.1, with the x axis originating at α and passing through β . The length of this bond is therefore:

$$L_b = \|P_B - P_A\| = \chi_\beta - \chi_\alpha \quad (4.2)$$

where χ_α and χ_β are the x-coordinates of the two ends of the beam in the local coordinate system.

The bonds are assumed to have no mass in the DEM model – all mass is appropriately assigned to the particles. They are subjected to internal forces caused by relative displacements and rotations of the particles they connect.

The Timoshenko beam theory, which is suited for stocky beams where the shear deformation is important, can be used to relate the internal forces and moments to the particle displacements and rotations. In this study, the internal forces are calculated in an incremental manner. In each time step, the increment of the internal forces (and moments) are determined from the incremental displacements (and rotations) at the bond ends (particles) using the Timoshenko beam theory:

$$\{\Delta F\} = [K] \cdot \{\Delta \mu\} \quad (4.3)$$

where the incremental force vector $\{\Delta F\}$ and displacement (rotation) vector $\{\Delta \mu\}$ are

$$\{\Delta F\} = \{\Delta F_{\alpha x} \Delta F_{\alpha y} \Delta F_{\alpha z} \Delta M_{\alpha x} \Delta M_{\alpha y} \Delta M_{\alpha z} \Delta F_{\beta x} \Delta F_{\beta y} \Delta F_{\beta z} \Delta M_{\beta x} \Delta M_{\beta y} \Delta M_{\beta z}\} \quad (4.4)$$

$$\{\Delta \mu\} = \{\Delta d_{\alpha x} \Delta d_{\alpha y} \Delta d_{\alpha z} \Delta \theta_{\alpha x} \Delta \theta_{\alpha y} \Delta \theta_{\alpha z} \Delta d_{\beta x} \Delta d_{\beta y} \Delta d_{\beta z} \Delta \theta_{\beta x} \Delta \theta_{\beta y} \Delta \theta_{\beta z}\} \quad (4.5)$$

in which $\{\Delta F\}$ contains 12 force (F) and moment (M) increments at the two ends of the bond, $\{\Delta \mu\}$ contains 12 displacement (d) and rotation (θ) increments at the two ends of the bond, and $[K]$ is a 12x12 tangential stiffness matrix. The location and positive direction of both the rotations and moments follow the right hand rule. The internal total forces (F) and moments (M) are shown in Figure 4.2. Each force (moment) and displacement (rotation) has two subscripts: α or β denoting the two ends of the bond, and x, y or z denoting the direction of the force in the local coordinate system of the bond (e.g. $\Delta F_{\alpha x}$ is the force increment in x direction at the α end).

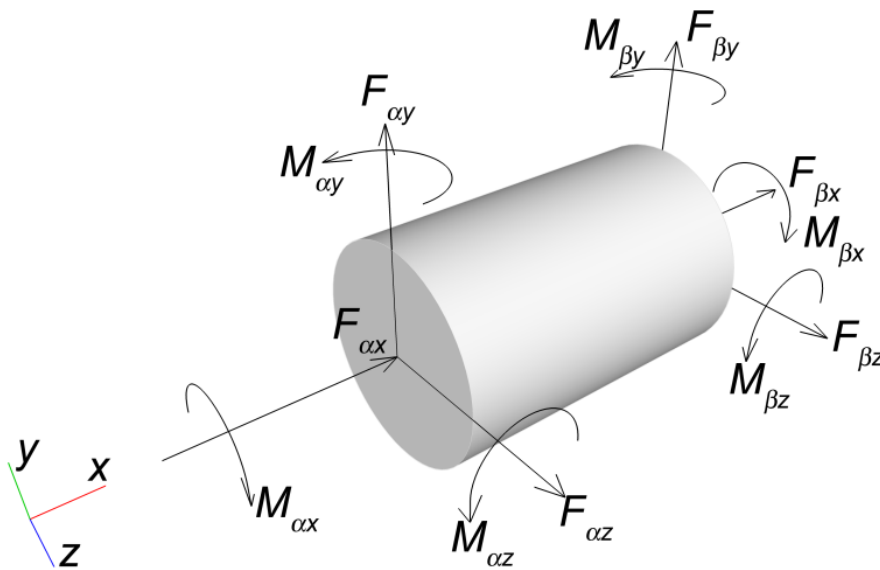


FIGURE 4.2: Forces and moments acting at the ends of a bond in the local co-ordinate system

4.1 STIFFNESS MATRIX

For small deformation linear elastic bonds, the tangential stiffness matrix $[K]$ remains constant before failure, and its general form can be derived from the differential equations for beam deformation using the unit displacement theory for a Timoshenko beam, as presented by Przemieniecki [13]:

$$[K] = \begin{bmatrix} k_1 & \cdot & \cdot & \cdot & \cdot & \cdot & -k_1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & k_2 & \cdot & \cdot & \cdot & k_3 & \cdot & -k_2 & \cdot & \cdot & \cdot & k_3 \\ \cdot & \cdot & k_2 & \cdot & -k_3 & \cdot & \cdot & \cdot & -k_2 & \cdot & -k_3 & \cdot \\ \cdot & \cdot & \cdot & k_4 & \cdot & \cdot & \cdot & \cdot & \cdot & -k_4 & \cdot & \cdot \\ \cdot & \cdot & -k_3 & \cdot & k_5 & \cdot & \cdot & \cdot & k_3 & \cdot & k_6 & \cdot \\ \cdot & k_3 & \cdot & \cdot & \cdot & k_5 & \cdot & -k_3 & \cdot & \cdot & \cdot & k_6 \\ -k_1 & \cdot & \cdot & \cdot & \cdot & \cdot & k_1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -k_2 & \cdot & \cdot & \cdot & k_3 & \cdot & k_2 & \cdot & \cdot & \cdot & -k_3 \\ \cdot & \cdot & -k_2 & \cdot & k_3 & \cdot & \cdot & \cdot & k_2 & \cdot & k_3 & \cdot \\ \cdot & \cdot & \cdot & -k_4 & \cdot & \cdot & \cdot & \cdot & \cdot & k_4 & \cdot & \cdot \\ \cdot & \cdot & -k_3 & \cdot & k_6 & \cdot & \cdot & \cdot & k_3 & \cdot & k_5 & \cdot \\ \cdot & k_3 & \cdot & \cdot & \cdot & k_6 & \cdot & -k_3 & \cdot & \cdot & \cdot & k_5 \end{bmatrix} \quad (4.6)$$

Where:

$$k_1 = \frac{E_b A_b}{L_b} \quad (4.7)$$

$$k_2 = \frac{12E_b I_b}{L_b^3(1 + \phi)} \quad (4.8)$$

$$k_3 = \frac{6E_b I_b}{L_b^2(1 + \phi)} \quad (4.9)$$

$$k_4 = \frac{E_b I_b}{L_b(1 + \nu_b)} \quad (4.10)$$

$$k_5 = \frac{E_b I_b(4 + \phi)}{L_b(1 + \phi)} \quad (4.11)$$

$$k_6 = \frac{E_b I_b(2 - \phi)}{L_b(1 + \phi)} \quad (4.12)$$

where E_b is the Young's modulus, ν_b the Poisson's ratio. The cross-sectional area, A_b , and the second moment of area of the bond, I_b , are given by equations (4.13) and (4.14) respectively, while the Timoshenko shear coefficient, ϕ , is given by equation (4.15):

$$A_b = r_b^2 \pi \quad (4.13)$$

$$I_b = \frac{r_b^4 \pi}{4} \quad (4.14)$$

$$\phi = \frac{f_s 12 E_b I_b}{G_b A_b L_b^2} = \frac{20 r_b^2 (1 + \nu_b)}{3 L_b^2} \quad (4.15)$$

where G_b is the bond's shear modulus, f_s is the form factor for shear (which for a circular cross-section can be estimated to be 10/9) and r_b is the bond radius:

$$r_b = \lambda \min(r_A, r_B) \quad (4.16)$$

with r_A and r_B as the radii of particles A and B respectively. The numerical parameter λ is the bond radius multiplier; this parameter introduces flexibility into the way the bond radius is determined.

4.2 TRANSFORMATION MATRIX

The displacement increment of a particle between two consecutive iterations can be determined from the standard DEM calculation cycle [6]. For each bonded contact the displacement increment of the two particles in the global coordinate system is stored as a vector $\{u_g\}$. The displacement increment of the bond ends in the local co-ordinate system is determined by multiplying the global displacement increment vector by the transformation matrix $[\gamma]$, so that:

$$\{\mu\} = \begin{bmatrix} \gamma & \cdot & \cdot & \cdot \\ \cdot & \gamma & \cdot & \cdot \\ \cdot & \cdot & \gamma & \cdot \\ \cdot & \cdot & \cdot & \gamma \end{bmatrix} \{\mu_g\} \quad (4.17)$$

The transformation matrix $[\gamma]$ contains nine directional cosines, which represent the nine angles between the three vectors defining the axes of the global co-ordinate system ($\{X\} \{Y\} \{Z\}$) and the three vectors defining the axes of the local co-ordinate system ($\{x\} \{y\} \{z\}$).

$$[\gamma] = \begin{bmatrix} x_x & x_y & x_z \\ y_x & y_y & y_z \\ z_x & z_y & z_z \end{bmatrix} \quad (4.18)$$

Each element in the transformation matrix contains a letter which represents the local coordinate axis and a subscript which represents the global coordinate axis. For example the directional cosine x_y defines the cosine of the angle between the vectors defining the local x axis and the global Y axis. The transformation matrix thus consists of three vectors that define the local co-ordinate system:

$$\{\hat{x}\} = \{x_x x_y x_z\}^T \quad (4.19)$$

$$\{\hat{y}\} = \{y_x y_y y_z\}^T \quad (4.20)$$

$$\{\hat{z}\} = \{z_x z_y z_z\}^T \quad (4.21)$$

As shown in Figure 4.1 the local x axis follows the longitudinal axis of the beam bond, so that:

$$\{\hat{x}\} = \frac{P_B - P_A}{L_b} \quad (4.22)$$

The y axis is calculated first using the cross product of the local x axis vector, and the global Z axis vector $\hat{Z}$. The angle between x and y axes is 90. The normalised y axis can be determined as:

$$\{\hat{y}\} = \frac{\hat{Z} \hat{x}}{|\hat{Z}| |\hat{x}|} \quad (4.23)$$

This shall always produce a local y axis, unless the vectors Z and x are collinear in which case:

$$\{\hat{y}\} = \{0 \ 1 \ 0\}^T \quad (4.24)$$

The local z axis can then be determined as the cross product of the local x axis vector and the local y axis vector, such that:

$$\{\hat{z}\} = \frac{\hat{x} \hat{y}}{|\hat{x}| |\hat{y}|} \quad (4.25)$$

4.3 BOND STRESS CALCULATIONS

Assuming small deformation, the total internal forces and moments at the bond ends at any time can be determined by summing increments from the start of the simulation:

$$\{F\} = \sum \Delta F \quad (4.26)$$

where $\{F\}$ contains 12 total forces and moments.

$$\{F\} = \{F_{\alpha x} \ F_{\alpha y} \ F_{\alpha z} \ M_{\alpha x} \ M_{\alpha y} \ M_{\alpha z} \ F_{\beta x} \ F_{\beta y} \ F_{\beta z} \ M_{\beta x} \ M_{\beta y} \ M_{\beta z}\}^T \quad (4.27)$$

Bonds are assumed to behave in a linear elastic and brittle manner; a bond fails if one of the maximum stresses exceeds the corresponding strength. Three strength criteria are considered: compressive σ_C , tensile σ_T and shear τ . In the TBBM each strength component is considered independent of the others, i.e. the shear stress has no influence on the tensile failure criterion.

$$\sigma_C < \{\sigma_{C_{max}}\} \quad (4.28)$$

$$\sigma_T < \sigma_{T_{max}} \quad (4.29)$$

$$\tau < \tau_{max} \quad (4.30)$$

The maximum compressive stress $\sigma_{C_{max}}$, tensile stress $\sigma_{T_{max}}$ and shear stress τ_{max} in each bond are determined from beam theory such that:

$$\sigma_{C_i} = \left(\frac{F_{\beta x}}{A_b} - \frac{r_b \sqrt{M_{iy}^2 + M_{iz}^2}}{I_b} \right) \quad i = \alpha, \beta \quad (4.31)$$

$$\sigma_{C_{max}} = -\min(\sigma_{c\alpha}, \sigma_{c\beta}) \quad (4.32)$$

$$\sigma_{T_i} = \left(\frac{F_{\beta x}}{A_b} - \frac{r_b \sqrt{M_{iy}^2 + M_{iz}^2}}{I_b} \right) \quad i = \alpha, \beta \quad (4.33)$$

$$\sigma_{T_{max}} = \max(\sigma_{T\alpha}, \sigma_{T\beta}) \quad (4.34)$$

$$\tau_{max} = \frac{|M_{\alpha x}|r_b}{2I_b} + \frac{4\sqrt{F_{\alpha y}^2 + F_{\alpha z}^2}}{3A_b} \quad (4.35)$$

If at any iteration a bond does not fail then a set of forces equal but opposite to the total bond end forces (moments) $\{F\}$ are applied to the respective particles. If a bond fails the bonded contact is removed and cannot be reintroduced.

4.4 BOND STRENGTH DISTRIBUTIONS

In the TBBM, each bond is assigned a compressive stress limit σ_C , a tensile stress limit σ_T and a shear stress limit τ ; these limits define the maximum stresses that the bond can withstand before failing. The stress limits are calculated for each bond, such that:

$$\sigma_C = S_C((\zeta_C N) + 1) \quad (4.36)$$

$$\sigma_T = S_T((\zeta_T N) + 1) \quad (4.37)$$

$$\tau = S_S((\zeta_S N) + 1) \quad (4.38)$$

where S_C is the mean bond compressive strength, S_T is the mean bond tensile strength, S_S is the mean bond shear strength, ζ_C is the coefficient of variation of compressive strength, ζ_T is the coefficient of variation of tensile strength, ζ_S is the coefficient of variation of shear strength and N is a random number. Apart from the random number, which is generated internally, all of the other parameters are custom parameters which are defined by the user in the preference file (see Section 3.2).

Whilst other statistical distributions are possible, the value for N is drawn from a normal distribution with a mean of zero and a standard deviation of one. The value of N is constant in the calculation of all three stress limits for a bond but varies between bonds in a simulation. The value of the bond strengths are capped so that they must fall in a range of between zero and twice the mean strength.

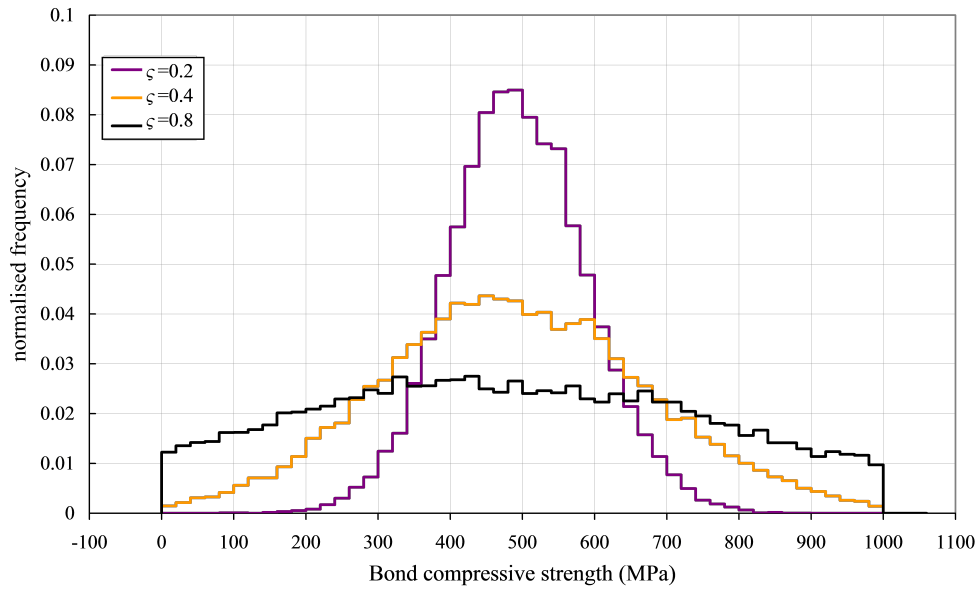


FIGURE 4.3: Comparing three values for coefficient of variation of strength

In Figure 4.3, three histograms describe the distribution of compressive stress limits for three values of coefficient of variation for compressive strength: the purple histogram has a mean strength of 500 MPa and a coefficient of variation of 0.2, the yellow histogram has a mean strength of 500 MPa and a coefficient of variation of 0.4, and the black histogram also has a mean strength of 500 MPa but a coefficient of variation of 0.8. As can be seen, the higher the coefficient of variation the more evenly distributed the bond strengths in the simulation.

NOTE 7: USING BOND STRENGTH VARIATIONS

To achieve a bond strength that is equal for all bonds of a particular interaction type, then the coefficient of variation for that property should be set to 0. A coefficient of variation of 1 will provide an assembly of uniformly distributed strengths.

5 VERIFICATION

Verifying the implementation of a numerical model is an important step to ensure that the mathematical descriptions in the programmed code match the theory underpinning the model. The TBBM has been verified across a wide range of benchmark tests.

In the first set of benchmark tests, a single bond was placed under a number of different loading actions (tensile, compression, shear, twisting and multiple bending configurations) by applying external forces to the particles connecting the bond. The bond breakage stresses were found to match the bond's failure criteria and by varying the orientation of the bond for each loading action the transformation matrix calculations were verified. The results of these tests can be found in Appendix A of Brown [2].

As an extension of this process further tests involved the construction of simple structural elements which are subjected to different loading actions. In the second set of verification tests the response of a bond under more complex loading actions was examined. Tests for the static and dynamic loading of a simply-supported beam are described in Sections 5.1 and 5.2 respectively. A further verification example, the loading of thin rectangular plates, is shown in ??.

5.1 STATIC LOADING OF A SIMPLY SUPPORTED BEAM

A simply supported beam can be formed by bonding particles in a line; an example with 5 particles is shown in Figure 5.1. In the EDEM simulation the extreme left-hand particle is fixed so that no translational displacements can occur, but the particle can rotate freely; the extreme right hand particle is fixed against translational displacements, apart from in the axial direction, and can also rotate freely.

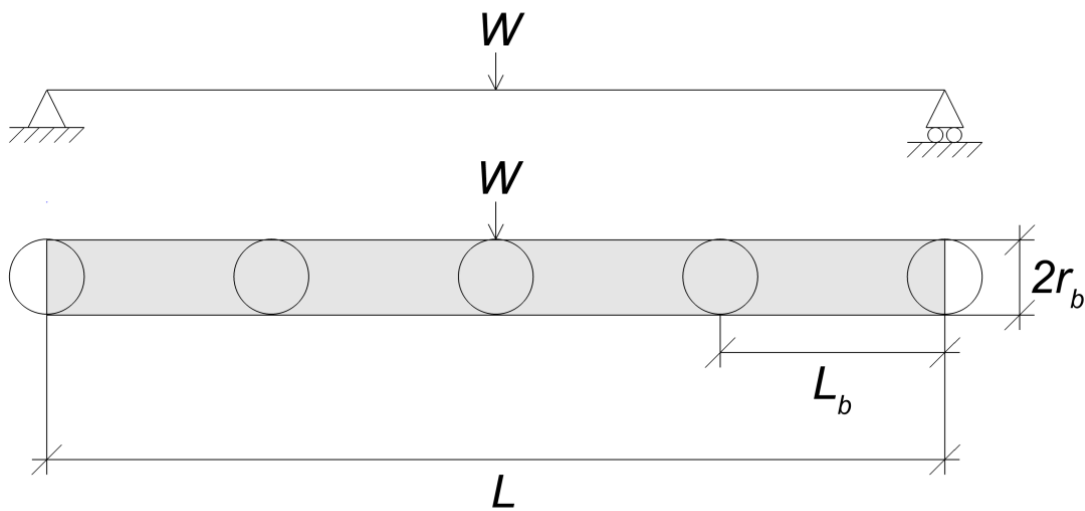


FIGURE 5.1: A simply supported beam of length L made from connecting 5 particles with 4 bonds of length L_b

For a circular beam under a mid-span point load W , the theoretical mid-span deflection δ can be calculated using Equation (5.1), where L is the beams length, EI is the flexural rigidity and GA/f_s is

the shear rigidity of the beam.

$$\delta = \frac{WL^3}{48EI} + \frac{WLf_s}{4GA} \quad (5.1)$$

In the DEM simulation of the simply supported beam the bonds representing the sections of the beam are given material properties for steel so that $E_b = 200$ GPa and $\nu_b = 0.3$. The radius of the bond (and therefore the radius of the circular beam being modelled) is $r_b = 0.1$ m and the form factor for shear f_s for a circular cross-section is 10/9. Bonds are initialised so that a beam of total length $L = 6$ m is formed.

All of the bonds forming the beam have the same material and geometrical properties throughout, so the spacing or the number of particles should not affect its response to load. In the verification example presented here beams made of between three and 31 particles are used. In the DEM simulations of these beams a central load of 100 kN is applied to the particle at the centre and the predicted transverse deflection recorded.

Using Equation (5.1) the theoretical mid-span deflection was determined to be 28.7169 mm. The predicted mid span deflections using the DEM simulations of the various particle configurations are shown in Table 5.1. As can be seen in Table 5.1 there is a very good agreement between theory and DEM simulation irrespective of the number of bonds used to form the simply supported beam.

TABLE 5.1: Predicted central deflection compared with theoretical solution

Number of Particles	DEM Predicted Central Deflection [mm]	Error [%]
3	28.7151	-0.0061
5	28.7144	-0.0086
17	28.7142	-0.0093
31	28.7142	-0.0093

5.2 FREE VIBRATION OF A SIMPLY SUPPORTED BEAM

The three particle version of the representation of the simply supported beam as described in Section 5.1 is used to verify the TBBM for dynamic motion. This verification test places the simply supported beam in free vibration. As the bonds are massless, the only mass affecting the beam vibration is from the concentrated mass of the central particle, from Case *et al.* [5] the fundamental natural frequency $f_{natural}$ for the beam can be determined using Equation (5.2).

$$f_{natural} = \frac{1}{2\pi} \sqrt{\frac{K_{beam}}{m}} \quad (5.2)$$

where m is the mid-span mass and K_{beam} is the beam's stiffness given by:

$$K_{beam} = \frac{192EIGA}{4L^3GA + 48f_sEIL} \quad (5.3)$$

If the central particle has a mass of 1000 kg, and the beam has the same properties as described in Sec-

tion 5.1 then the theoretical fundamental natural frequency for this beam is found from Equation (5.2) to be 9.392 Hz.

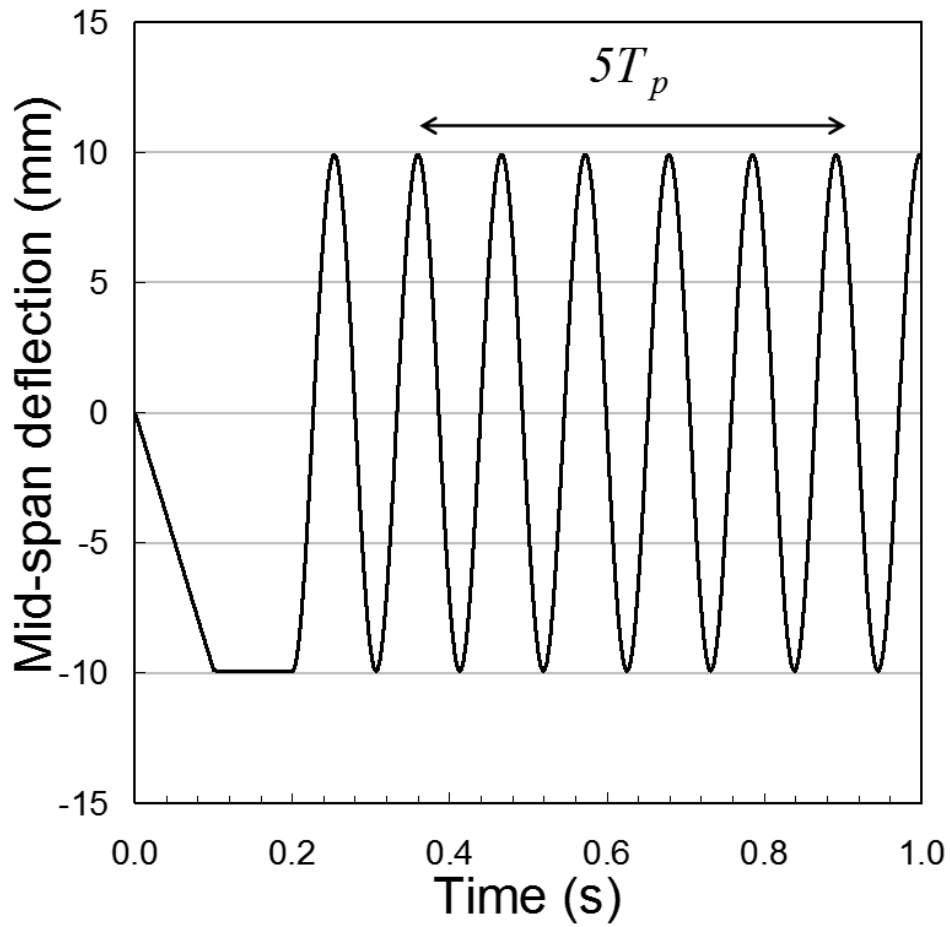


FIGURE 5.2: Transverse deflection of the free particle over time

In the DEM simulation, the central particle is displaced 10 mm vertically and then set free to vibrate, as shown in Figure 5.2. The DEM predicted fundamental natural frequency is 9.407 Hz which is only 0.16% greater than the theoretical solution.

6 FUTURE DEVELOPMENT

Although the TBBM is fully verified and validated there are always features that can be added and development continues. Any comments, queries or feedback can be passed back to DEM Solutions Ltd. or:

NOTE 8: CONTACT DETAILS

Prof. Jin Ooi.

Institute for Infrastructure and Environment,
School of Engineering,
The University of Edinburgh,
William Rankine Building,
Thomas Bayes Road, King's Buildings,
Edinburgh, EH9 3FG
Scotland, U.K.

email: J.Ooi@ed.ac.uk

The following suggestions are under consideration for integration into future versions of the TBBM model:

- Option to track total bond end displacements and rotations.
- Include a factor to modify the stiffness matrix over the course of the simulation; the aim would be to add plasticity. This may be linked to another factor e.g. damage or local highest stress values.
- Incorporation of a failure envelope principal to relate the normal strength to the shear strength.
- Currently bonds are assumed to behave in a linear elastic brittle manner, more sophisticated models will be considered after future research.

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A GLOBAL DAMPING

In real materials, kinetic energy is dissipated through microscopic actions such as internal friction and wave scattering [12]. When required, for example if frictional sliding does not represent the full damping effect seen in the real material, additional artificial damping can be introduced to reduce the kinetic energy and bring the simulation to a quasi-static state.

In the TBBM, non-viscous damping is applied through the equations of motion so that energy is dissipated in every particle in the system. In essence this modifies the final forces acting on each particle so that the resulting particles acceleration is changed. As only the acceleration term is dampened stable motion is not affected, and elements with a fixed velocity will maintain that velocity. The damping used in the TBBM is based on the damping provided in the bonded particle model proposed by Potyondy and Cundall [12]. The damping forces and moments F_d and M_d are applied to each of the six degrees of freedom for each particle so that:

$$F_{di} = \frac{-t_d |F_i| V_i}{|V_i|} \quad i = X, Y, Z \quad (\text{A.1})$$

$$M_{di} = \frac{-t_d |M_i| \omega_i}{|\omega_i|} \quad i = X, Y, Z \quad (\text{A.2})$$

where F and M are the sum of the forces and moments acting on the particles, V and ω are the translational and angular velocity, X , Y and Z represent each degree of freedom and t_d is a dimensionless constant which defines the magnitude of the damping. The global damping coefficient is set by the user in the preference file (Section 3.2.1.1). The range of values for this constant are zero to one, with zero providing no damping and one meaning the damping is equal in magnitude to the total forces.

B STIFFNESS MATRIX VALUES

The values for the stiffness matrix can be determined using the relations below:

$$m_BondStiffness[0] = k_1 = [K1,1] , [K7,7] , -[K1,7] , -[K7,1]$$

$$k_1 = \frac{E_b A_b}{L_b} \quad (B.1)$$

$$m_BondStiffness[1] = k_2 = [K2,2] , -[K2,8] , [K3,3] , -[K3,9] , -[K8,2] , [K8,8] , -[K9,3] , [K9,9]$$

$$k_2 = \frac{12E_b I_b}{L_b^3(1 + \phi)} \quad (B.2)$$

$$m_BondStiffness[2] = k_3 = [K2,6] , [K2,12] , -[K3,5] , -[K3,11] , -[K5,3] , [K5,9] , [K6,2] , -[K6,8] , [K8,6] , -[K8,12] , [K9,5] , [K9,11] , -[K11,3] , [K11,9] , [K12,2] , -[K12,8]$$

$$k_3 = \frac{6E_b I_b}{L_b^2(1 + \phi)} \quad (B.3)$$

$$m_BondStiffness[3] = k_4 = [K4,4] , -[K4,10] , -[K10,4] , [K10,10]$$

$$k_4 = \frac{E_b I_b}{L_b(1 + \nu_b)} \quad (B.4)$$

$$m_BondStiffness[4] = k_5 = [K5,5] , [K6,6] , [K11,11] , [K12,12]$$

$$k_5 = \frac{E_b I_b(4 + \phi)}{L_b(1 + \phi)} \quad (B.5)$$

$$m_BondStiffness[5] = k_6 = [K5,11] , [K6,12] , [K11,5] , [K12,6]$$

$$k_6 = \frac{E_b I_b(2 - \phi)}{L_b(1 + \phi)} \quad (B.6)$$

C THIN PLATE BOND PROPERTIES

In order for the TBBM to mimic the response of a plate the beams have to represent the properties of a portion of the plate. The flexural rigidity of the bonds can be determined so that for a single element of width Δ_b :

$$E_b I_b = \frac{E_b \pi r_b^4}{4} = \frac{E_{plate} t^3}{12(1 - \nu_{plate}^2)} \Delta b \quad (C.1)$$

Where E_b , I_b and r_b are the bond's Young's modulus, second moment of area and radius respectively and E_{plate} , ν_{plate} and t are the plate's Young's modulus, Poisson's ratio and thickness respectively. The axial stiffness of the bond is also matched to that of the plate such that:

$$\frac{E_b \pi r_b^2}{L_b} = \frac{E_{plate} t \Delta b}{\Delta a} \quad (C.2)$$

Knowing that the bond length $L_b = \Delta_b = \Delta_a$ Equation (C.2) can be simplified and rearranged in terms of E_b and then substituted into Equation (C.1) to determine r_b , such that:

$$r_b = \sqrt{\frac{t^2}{3(1 - \nu_{plate}^2)}} \quad (C.3)$$

By substituting Equation (C.3) into Equation (C.2) E_b can be determined:

$$E_b = \frac{3E_{plate} \Delta b (1 - \nu_{plate}^2)}{\pi t} \quad (C.4)$$

It can be seen from Equations (C.3) and (C.4) that, unlike the bond's Young's modulus E_b , the bond radius r_b is independent of the number of grid elements used.