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EDEM Tutorial

Mixing in a Tablet Coater

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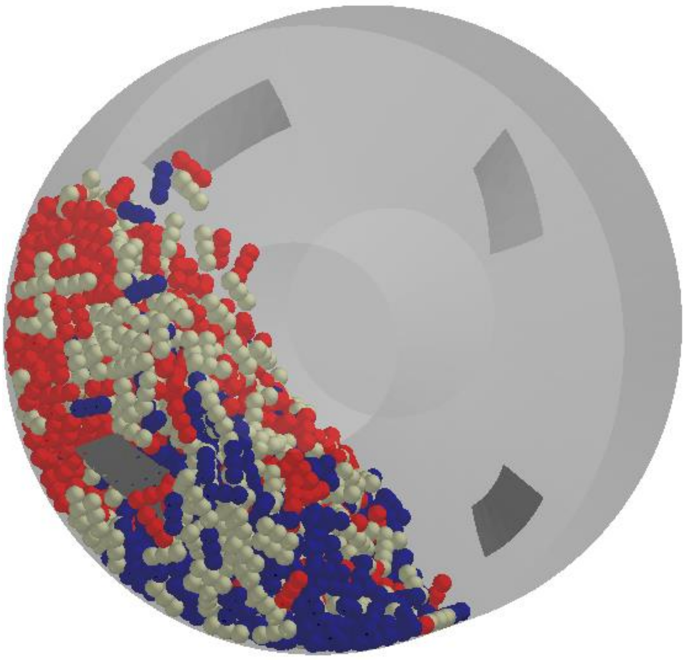
Introduction

This is an advanced tutorial suitable for users with a significant level of experience with EDEM. In case of any uncertainties or problems, refer to previous tutorials or the EDEM Help section.

The model used here is a generic tablet coater of small dimensions (200mm in diameter). Since the particles need to be mixed properly first before they are coated, the mixing efficiency is investigated here.

The Creator and Simulator parts of the simulation are not explained in detail as the focus is on the EDEM Analyst capabilities, such as:

- Visualizing mixing efficiency through particle representation
- Analyzing particles in Grid Bin Groups
- Analyzing the contacts between different types of particles through Graphs and Grid Bin Groups
- Creating Manual Selections
- Visualizing the Particle flow profile
- Exporting .jpg images



1. Start EDEM and save your project as **Mixer.dem** in your desired location.
2. Remember Save often when setting up the simulation.

EDEM Creator: Setting up the model

Step 1: Define the Project and Settings

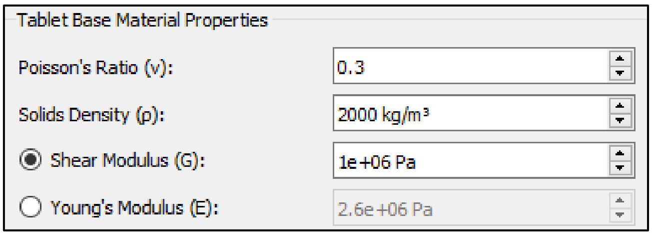
Choose the units and name the model

1. Set the measurement units as follows:
    - Angle: **deg**
    - Angular Velocity: **rpm**
    - Length: **mm**
2. Click on Project in the Creator Tree and set the simulation Title to **Tablet Coater**.

Step2: Define the Bulk Material

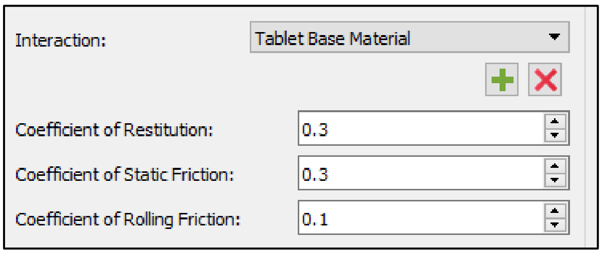
Add a new Bulk Material and define its properties

1. Create a Bulk Material called **Tablet Base Material** with the following properties:



Define the bulk material interaction

1. Add the interaction between elements made of **Tablet Base Material** with the following coefficients:

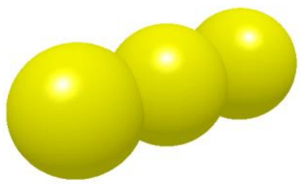


Create a new Multi Sphere particle type and define the surfaces and properties

Three types of particles will be created for the mixing analysis. They are all made of three aligned spheres and are essentially the same. However, it is necessary to have different types for the purposes of post-processing and analysis.

1. Create a new Multi Sphere particle of the material **Tablet Base Material**.
2. Rename the particle to **Tablet Base**.
3. Change the Radii of the 3 spheres of the particle to **3mm**.
4. Set the coordinates as follows:

	Name	Position X (mm)	Position Y (mm)	Position Z (mm)	**Physical Radius (mm)**
1	sphere 0	-4.5	0	0	3
2	sphere 1	0	0	0	3
3	sphere 2	4.5	0	0	3

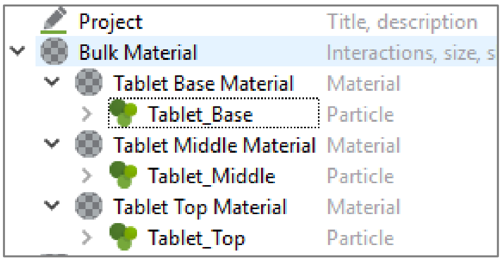


5. Go to Tablet Base > Properties and click on Calculate Properties button.

Duplicate the Bulk Material

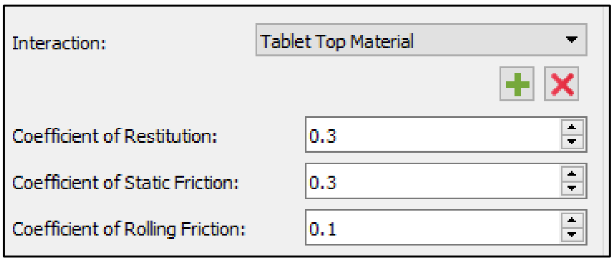
1. Right click **Tablet Base Material** in the Creator Tree and select **Copy Material**. Do this twice to create two identical copies of the material and particle.
2. Rename the two new materials **Tablet Middle Material** and **Tablet Top Material**.
3. Rename the corresponding particles **Tablet Middle** and **Tablet Top**.

Note how in duplicating the material with a particle already created, we were able to duplicate that particle as well.



We could have created the three types of particle from the same material, however when defining the **particle factory** later, it will become clear why we have taken this approach.

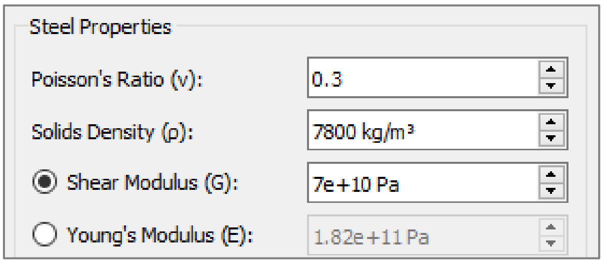
The three Bulk Material types have the same coefficients as for **Tablet Base Material**:



Step 3: Define the Equipment Material

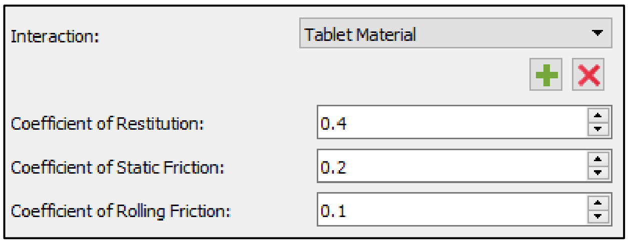
Add and define a new equipment material

1. Create an Equipment Material called **Steel** with the following properties:



Define the bulk material - equipment material interaction

1. Add three interactions, between elements made of the three Bulk Materials and elements made of **Steel** with the following coefficients:

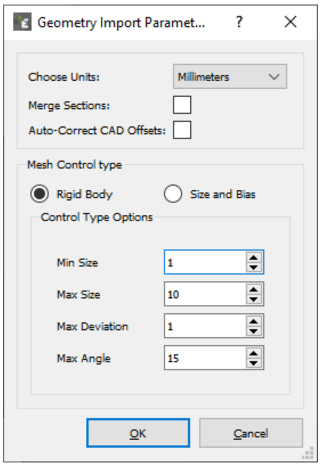


Step 4: Define the Geometry

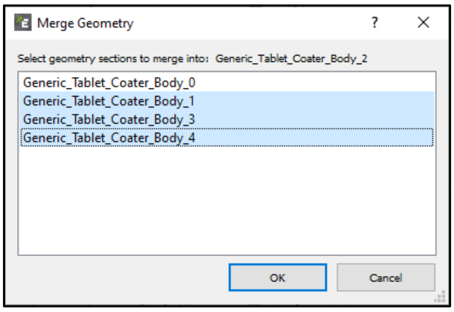
Import the mill geometry

The pan coater geometry has been created in a CAD package and is ready to be imported into EDEM.

1. Right click on Geometries and import **Generic_Tablet_Coater.igs** from the tutorial folder.
2. When prompted to, set the Units of measurement to **Millimeters,** set the **min size** to **1** and **max size** to **10**. Leave all other settings at the default values.



3. Right click on one of the blades of the mill in the Creator Tree and select **Merge Geometry**.
4. Select the other thee blades to merge with and click OK.

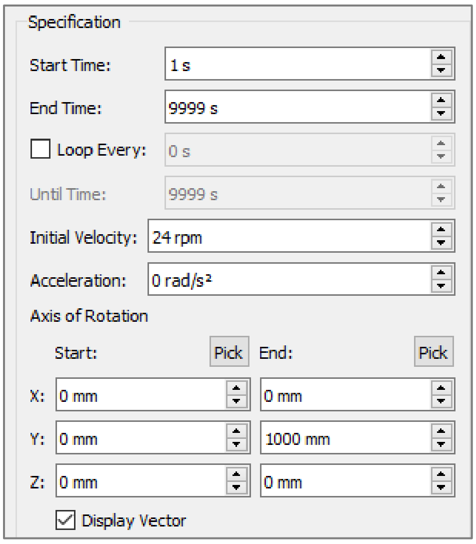


5. Rename this newly merged geometry to **Blades,** and rename the main body of the geometry to **Drum.**

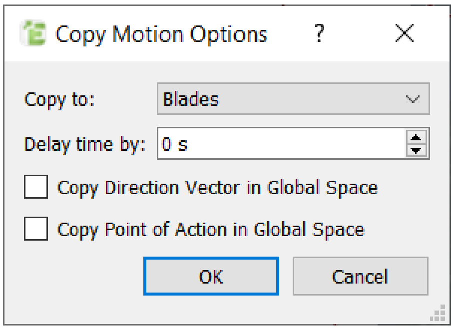
Specify the geometry dynamics

In this model, the coater rotates so that all the tablets mix properly and can remain in the spray zone.

1. Assign a **Linear Rotation** kinematics to the **Drum** geometry.
2. Set the Start Time to **1s** to allow the particles in the mill to settle before the rotation starts.
3. Specify the Initial Velocity to be **24 rpm**.
4. Specify the Axis of Rotation as follows:



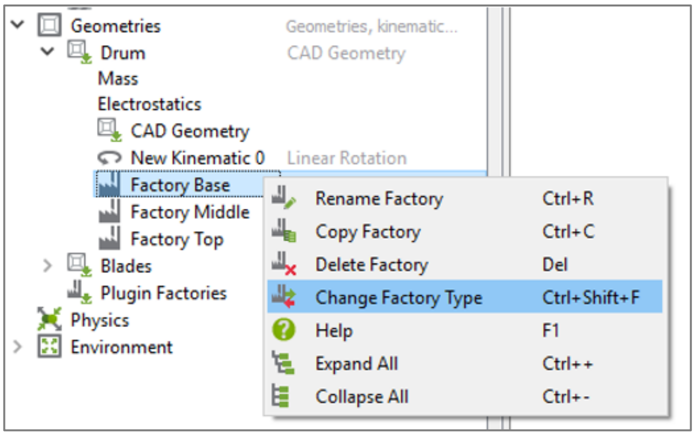
5. Right click on the kinematic (New Motion 1) and choose Copy Motion and select Blades. Leave the Delay Time option as 0 s.



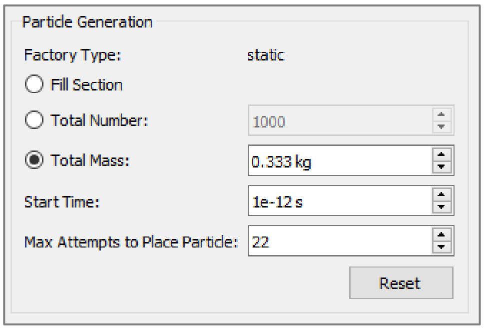
Create the particle factory and set its properties

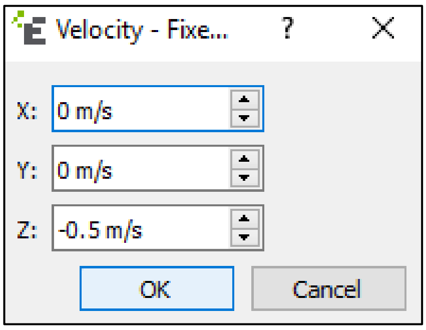
In this model 1 kg of tablets are produced using three static factories.

1. Add a factory to the Drum geometry and rename it **Factory_Base**.
2. Right click on the factory and change the Factory Type to **static**.



3. Select **Total Mass** and set the value to **0.333 kg**.
4. Set the Material to **Tablet Base Material**.
5. Set the Velocity to **fixed** with the following parameters:





Duplicate the factory

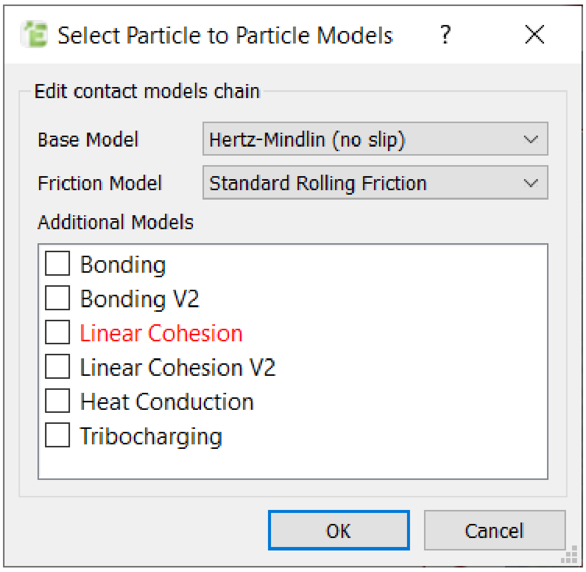
1. Right click on **Factory Base** and select **Copy Factory**. Make a second copy of Factory Base so there are three factories in total.

2. Rename the two copies to **Factory Middle** and **Factory Top**.
3. For the **Factory Middle**, set the Start Time to **0.25 s** and Material to **Tablet Middle Material**.
4. For the **Factory Top**, set the Start Time to **0.5 s** and Material to **Tablet Top Material**.
5. Leave the other specifications unmodified.

Step 5: Define the Physics

Set the contact models

1. For the **Particle to Particle** and **Particle to Geometry** Interactions, check that the **Hertz-Mindlin (no slip)** contact model is being used and the **Standard Rolling Friction** selected.



Step 6: Define the Environment

Set the acceleration due to gravity

1. Check that Gravity is set to **-9.81 m/s^2** in the Z direction.
2. Ensure that the Auto Update from Geometry checkbox is selected.
3. Select File > Save, to save the final setup of the simulation.

EDEM Simulator: Running a Simulation

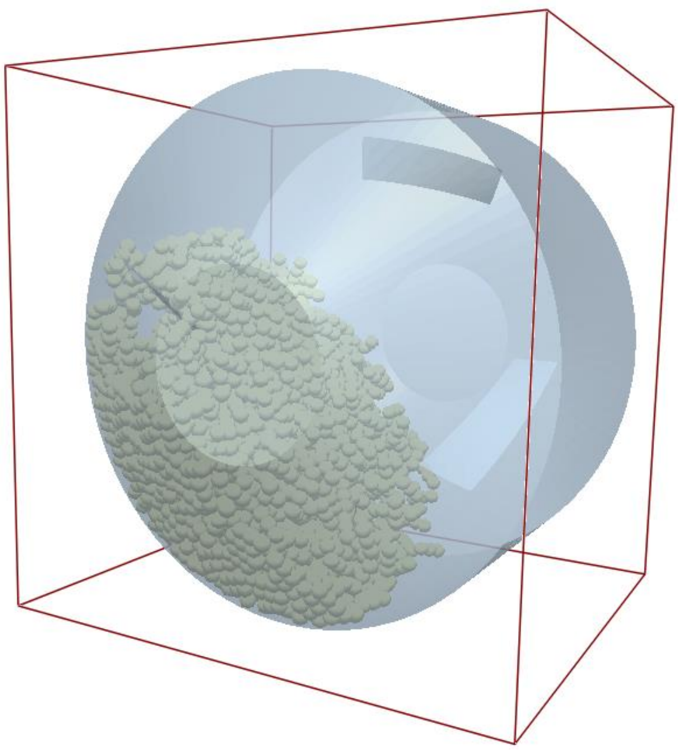
1. Click on the Simulator button on the toolbar.

Step 1: Set the Time and Grid Options

1. **Uncheck** the Auto Time Step checkbox.
2. Set the Fixed Time Step upper box to **20%** of Rayleigh time-step (corresponding to ~9e-05s).
3. In the Simulation Time section, set the Total Time to **6s**.
4. Set the Target Save Interval to **0.01s** to specify write-out frequency.
5. Set the Cell Size to **3 Rmin**.

Step 2: Run the Simulation

1. Click the start Progress button at the bottom of the Viewer window.
2. In Viewer Controls, click the **Refresh Viewer** button or enable **Auto Update** to see how the simulation is progressing.
3. In Viewer Controls, reduce the opacity of the geometry to see how the particles are created and mixed inside the drum.



EDEM Analyst: Analyzing the Results

Step 1: Configure the Display

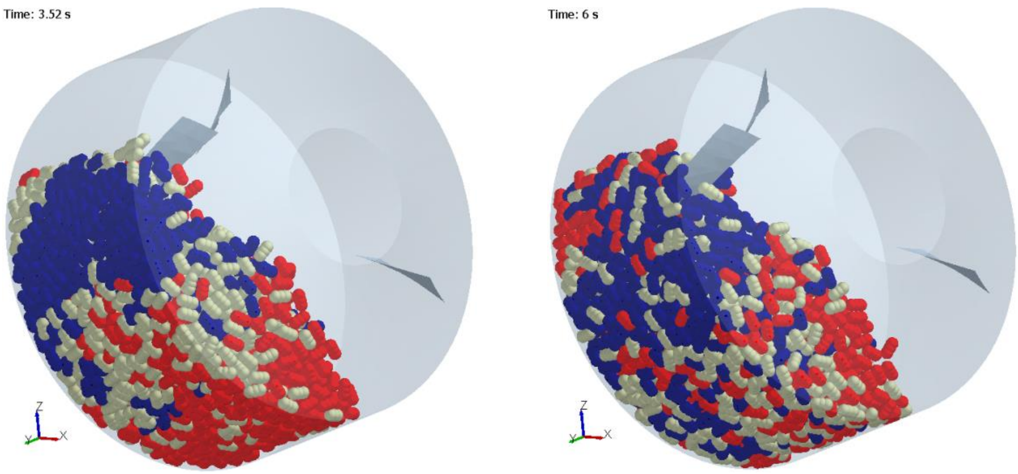
Mixing efficiency is very important in pharmaceutical applications. To ensure that the spray does not always coat the same tablets, the first thing to check is whether the particles were properly mixed.

1. Switch to the Analyst by selecting the  button on the toolbar.

Visualize the mixing

1. Reduce the opacity of the **Drum** to **0.5**.
2. Set the Current Time to **1 s** and View to **+Y**.
3. Color the different particle types separately to be able to distinguish between them. Recommended colors are: **Red, Particle Default** and **Dark Blue**.

Replay the simulation and observe the mixing quality at **3.5 s** (1 rotation) and **6s** (2 rotations).



After one rotation, the three groups of particles are still easily distinguishable but after two rotations the mixing efficiency increases significantly.

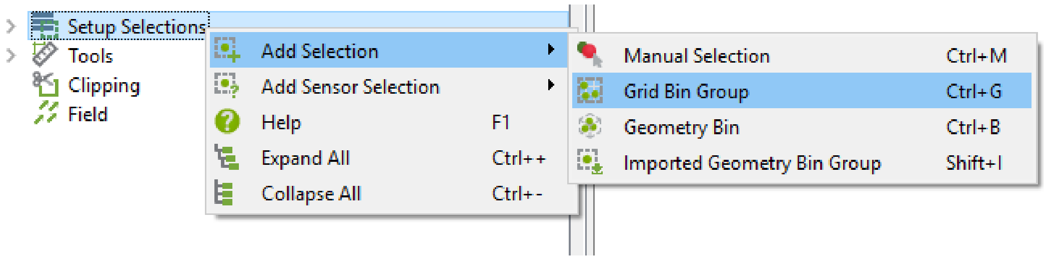
Step 2: Analyze the mixing using Bin Groups

Bin groups can be used to analyze the number of particles of each type in a specific area. The mixing efficiency can be further concluded from this data.

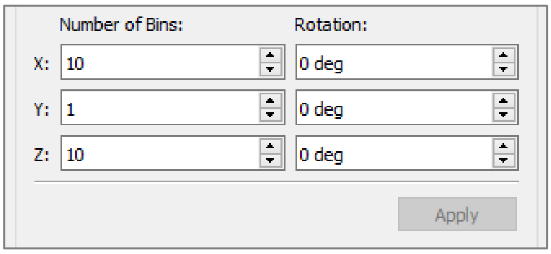
Create grid bin groups

1. Set the Current Time to the last time-step.
2. Make sure that the particles are no longer displayed in the Viewer Window.

   Create a new **Grid Bin Group** and Notice that the bin group is automatically positioned in the centre of the domain.

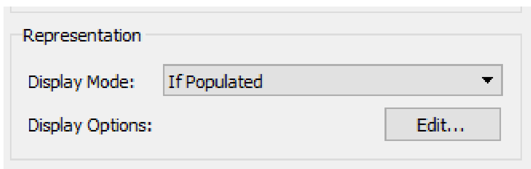


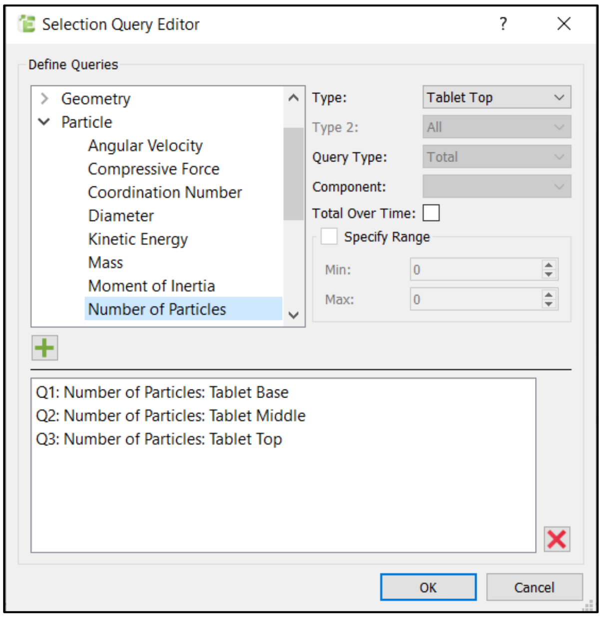
3. Set the Number of Bins as follows and click Apply:

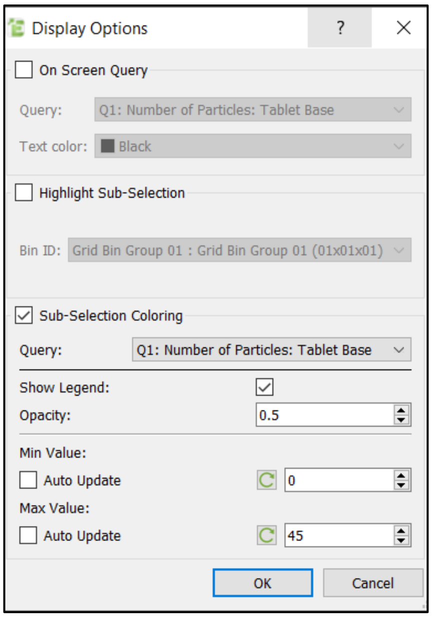


   Define Queries for **Number of Particles** for each particle type as shown below.

4. In the Representation section, set a Display Mode to **If Populated** and select the Edit… button to color the bin groups as shown:

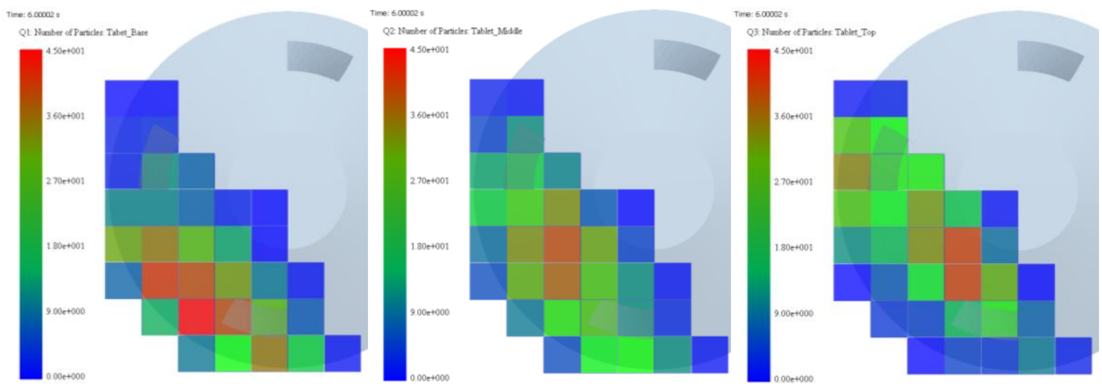






5. If you check the **On Screen Query** box, you will see exactly how many particles are present in each bin group in this time-step.
6. Modify the Display Options to see the query for different particle types and export the images as **.jpg** files (File > Export > Image).

The images should be similar to the ones below. The bin analysis shows that the particles are not completely mixed yet. There are more Tablet_Base particles in the base of the drum, whereas most of the Tablet_Top particles reside on top.



7. Before continuing, set the bin group Display Mode to **Never**.

Step 3: Examine Contact Forces between layers

To evaluate the mixing, it is also possible to plot the number of contacts between the different types of particles. If the number of contacts reaches a steady value, it would indicate that the material is fully mixed.

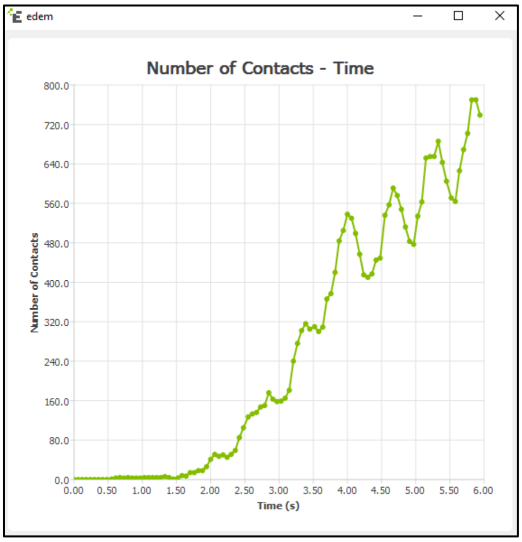
With the current setting conditions, the number of particles of each type should be 520. You can verify this by checking the Data Browser window.

Each particle is composed of three spheres and each sphere can have several contacts. Hence a number of contacts would be much higher than 520.

Plot the graphs

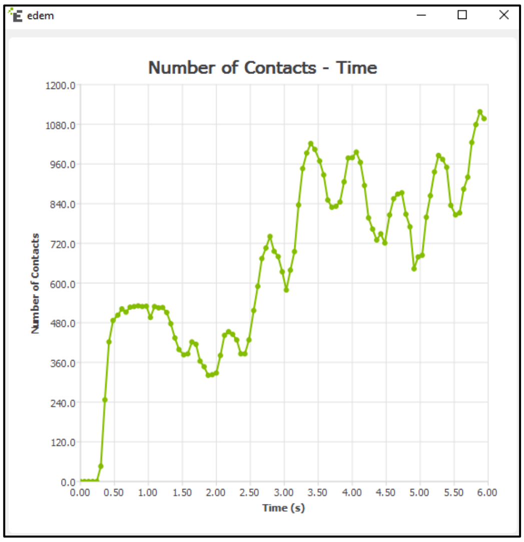
1. To plot the number of contacts, click on the Create Graph  button.
2. In the Line Graph tab, set the Element as follow:

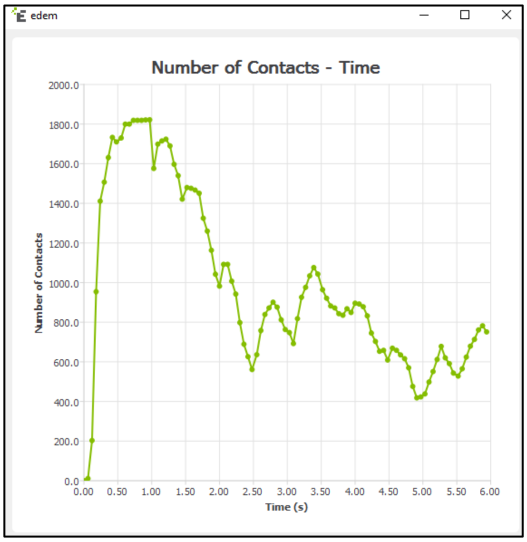
3. In the X-axis tab, ensure that the graph would be created over entire simulation time and set Number of Intervals to **12**.
4. Click on the Y-axis tab and set the Primary Attribute to **Number of Contacts** and the Component to **Total**.
5. In the Settings Tab, check **User Defined** box for Y-axis range and set Min and Max Values to **0** and **800** respectively.
6. Click **Create Graph**.



As expected, there are no contacts at the beginning of the simulation. As the Tablet_Top particles appear and start to mix, the number of contacts increase. It can be seen in the graph that a steady state has not been achieved after two rotations of the drum. That indicates that the particles are not yet homogeneously mixed.

7. Create two more graphs changing Type 2 to **Tablet_Middle** and **Tablet_Base**. Update the Y-axis scale if necessary.





Note that the number of contacts between the Base and Middle tablets is relatively stable at the beginning of the simulation when they are in two separate layers. Once the mixing starts, the number of contact increases.

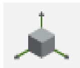
The Tablet_Base – Tablet_Base number of contacts is high at the beginning of the simulation since all the particles are close to each other. Once the mixing takes places it rapidly decreases and the particles become in contact with other types of material.

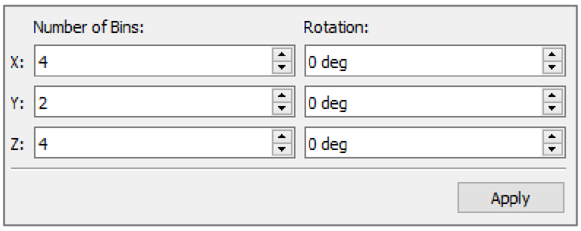
Step 4: Examine the Forces on the Particles

In tablet coating applications, tablets should not be subjected to large forces as this increases the risk of breakage. Therefore, it is important to study the maximum contact forces sustained by the particles and to establish where in the geometry high force collisions occur.

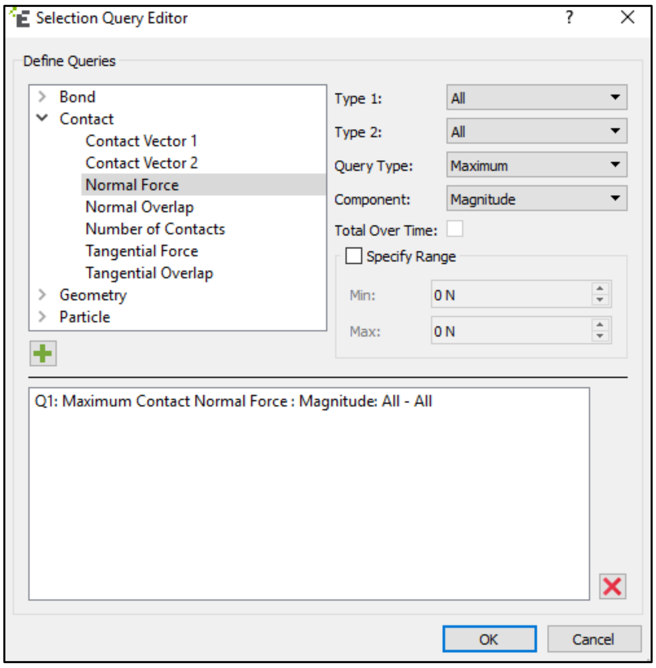
Create grid bin groups

To study the forces on the particles, we will create a set of bins that are colored by the maximum force sustained by one particle inside that bin.

1. Go back to the 3D Viewer by clicking the  button on the toolbar.
2. Set the geometry to its Default Color and reduce the opacity of all geometry elements to **0.3**.
3. Create a new **Grid Bin Group**. Notice that the bins are placed about the centre of the domain.
4. Set the number of bins as follows:

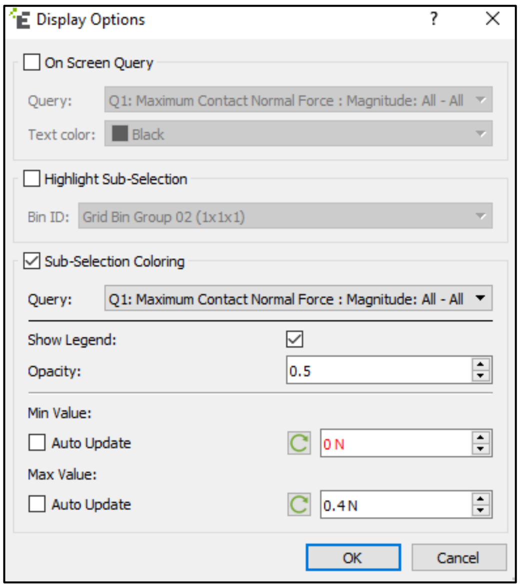


5. Add a new query by clicking on Edit button and define it as follows:



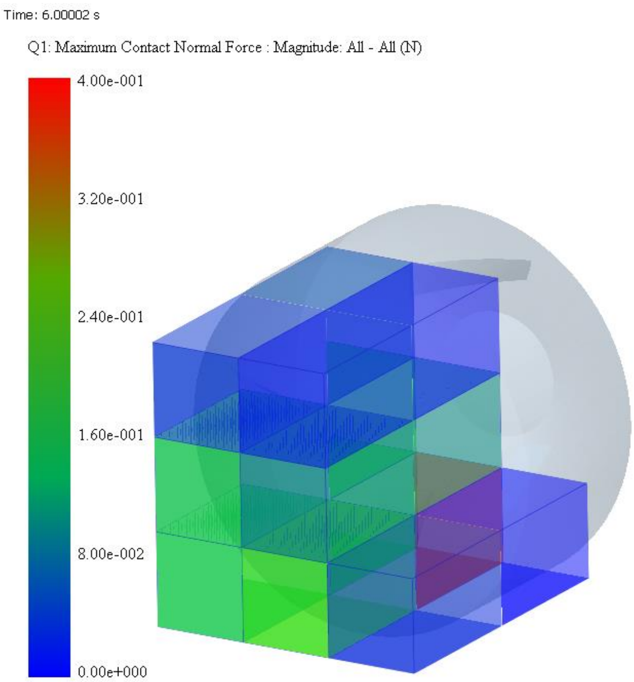
6. In the Type Filter section, select **No Particle <> Geometry Contacts** and **All Particle <> Sphere Contacts** options. In this way, only the contacts between particles are taken into account to determine the value of the previously defined query.

7. Set Display Mode to **If Populated** and edit the Display Options as follows:



8. Review the simulation.

Throughout the simulation the highest forces sustained by the particles are recorded at the base of the particle bed when the blades are impacting the particles.

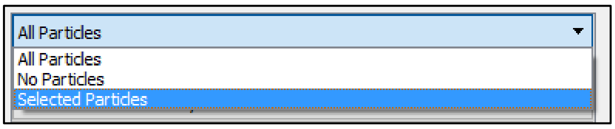


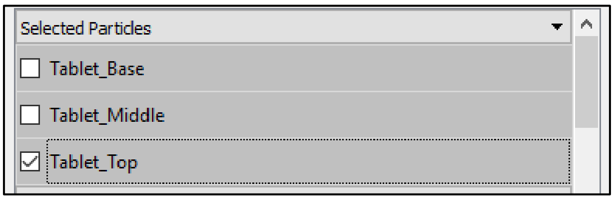
Step 5: Particle Flow Profile

To evaluate the mixing it is also interesting to study the trajectory of individual particles.

Create multiple manual selections

1. Set the Current Time to **1s**.
2. Create a Manual Selection and rename it ***Top***.
3. Set the Type Filter to **Tablet_Top**, chosen from Selected Particles dropdown list.

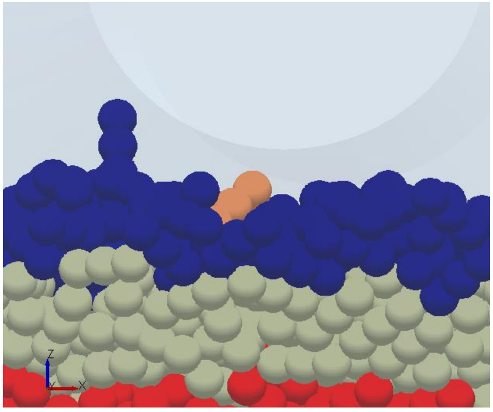




4. Check the **Enable Manual Selection** box.

Once this option is checked it is not possible to change the view of the camera.

5. Using Left Mouse Click or holding CTRL and left mouse to create a box select a single particle from Tablet_Top type of top layer as shown below:



Note particles are selected on their center point and anything in the box/under the mouse cursor is selected.

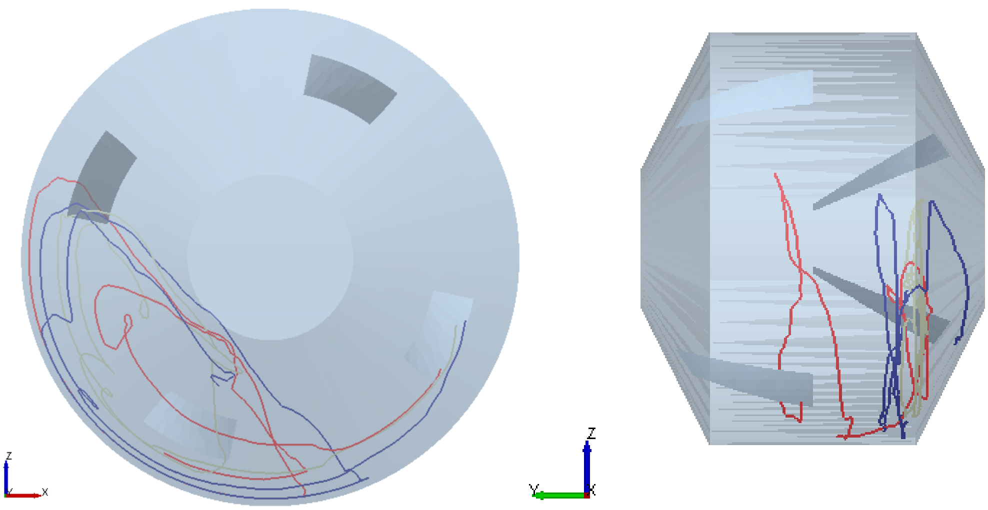
6. In similar way, create two more Manual Selections for **Tablet Middle** (select particle from middle layer) and **Tablet Base** (select particle from the bottom) particles. Rename these **Middle** and **Base**, respectively.

When picking the particles, it might help to display only one layer of the material. Then it would be easier to pick one particle at the time.

Display selections as streams

1. In the Particles section uncheck the **Display All Particles** box. Click Apply All.

2. Expand the Selections section in the Display tab in the Analyst Tree, then expand Particle Selections.
3. Select Base.
4. Make sure both the Properties by Selection Group and Display Particle Selection Base checkboxes are **selected**.
5. Change Representation to **Stream**.
6. Click the Options button and check **Stream All Steps** box.
7. Click OK.
8. **Select** the Color by selection group checkbox and set the color to the same color you applied to the Tablet_Base particles (red, if you followed the coloring in this tutorial).
9. Repeat instruction 3-7 for Manual Selections **Middle** and **Top**.
10. Play through the simulation from 1s to 6s.



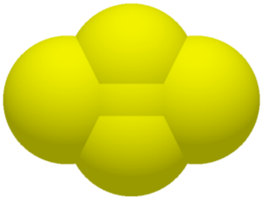
The trajectory of each particle shows that, independent of the initial position, a particle will travel to different locations in the drum. None of the material types stay stuck in one location but move around the drum evenly.

Each particle first travels to the top then the base of the particle pile, which is an important mixing criteria.

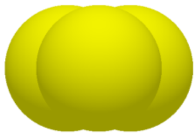
Suggested further work

This tutorial has shown some of the possibilities offered by the Analyst in EDEM, however it does not investigate the different parameters related to tablet coating. For the application of mixing or tablet coating in a drum, it is interesting to study the influence of the particle shapes on the quality of mixing. You can try to investigate this with one of the tablet shape shown below:

Rhombus shape

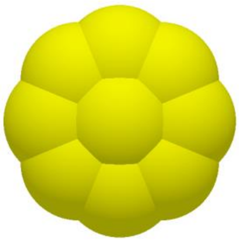


View +Z

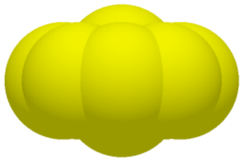


View +X

Ellipsoid shape



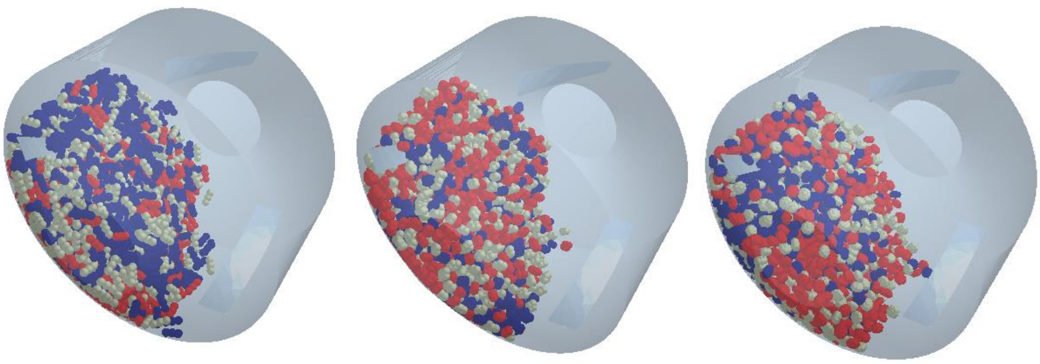
View +Z



View +X

Follow the analysis described in this tutorial to compare the results for various shapes. The images below show the same time step (~6s) for different particle shapes (three-spheres, rhombus, ellipsoid). As you can see, the level of mixing varies.

Notice also how the increased number of spheres per particle influences the computational effort and thus simulation time in EDEM.



It is also interesting to look at the effect of the rotation speed. Higher rotation speed usually means faster mixing, however, it also increases the forces exerted on the particles which can lead to breakage of the tablets.