Model created in COMSOL Multiphysics 6.4

Heterogeneous Electrode Geometry Generation

Introduction

This example demonstrates how to create a representative 3D geometry of a Nickel-Manganese-Cobalt (NMC) electrode, based on X-ray tomography data. The generated geometry may be used for subsequent heterogeneous electrode modeling.

The X-ray data differentiates between the active NMC particles, and a surrounding mix of electron-conductive carbon additives, binder, and ion-conducting electrolyte.

A model method is used to loop through tabulated data on particle volumes and center coordinates.

The geometry generated is used in the Heterogeneous NMC Electrode and Homogenizing a Heterogeneous Electrode Model tutorials in the Battery Design Module Application Library.

Model Definition

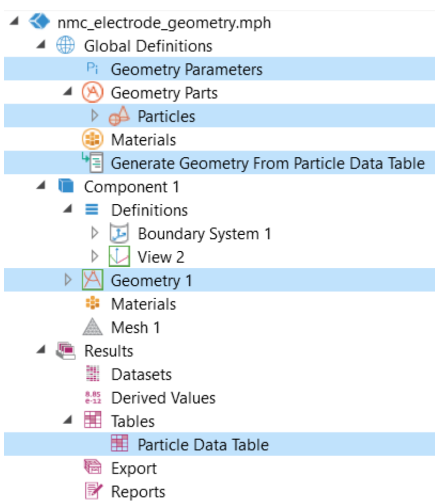


Figure 1: Model tree setup. All nodes involved in the geometry generation are highlighted in blue.

Figure 1 indicates the nodes in the model tree used for creating the geometry.

Global Definitions > Geometry Parameters

This node contains parameters related to the generation of the geometry, such as tolerance factors and bounding box.

Results > Tables > Particle Data Table

This table contains the particle center coordinates and the particle volumes.

The data, available as open source, was downloaded from dx.doi.org/10.5905/ethz-iis-1. See Ref. 1 for additional information about the data.

Global Definitions > Geometry Parts > Particles

This geometry part contains the individual particle geometric objects (spheres and cylinders) generated from **Particle Data Table**.

Global Definitions > Generate Geometry From Particle Data Table

This node calls the corresponding model method for generating the **Geometry Parts** > **Particles** geometric objects, based on the **Particle Data Table**.

Each entry in the **Particle Data Table** generates a **Sphere** object in **Particles**, given that the particle is located within the bounding box defined in **Geometry Parameters**.

Cylinder objects are also added in **Geometry Parts** > **Particles** in order to avoid sharp angles between overlapping spheres, or to join spheres together when the mutual distance is lower than the tolerance factor.

The model method also calculates and updates the electrode thickness parameter in **Geometry Parameters**.

The model method is written in Java, and maybe edited by switching to the **Application Builder** desktop. Note however that the model method editor is only available in the COMSOL desktop when using Windows. The model method node created in the model is however available and may be executed on all operating systems.

Component 1 > Geometry

The final geometry sequence imports the **Geometry Parts** > **Particles**, and also includes block geometry objects to define the separator and porous conductive binder domains, based on the settings in **Geometry Parameters**. Geometry selections are also included in order to facility physics setup.

Results and Discussion

Figure 2 shows the generated model geometry.

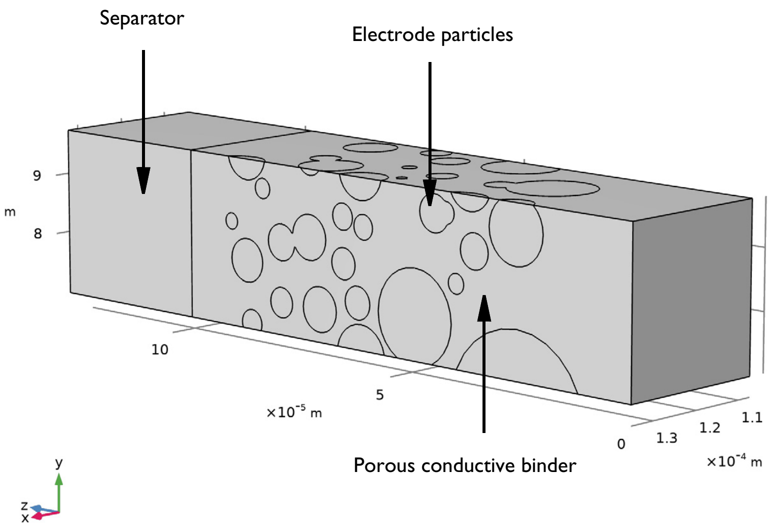


Figure 2: Generated model geometry.

Reference

1. M.Ebner, F. Geldmacher, F. Marone, M. Stampanoni, and V. Wood, "X-Ray Tomography of Porous, Transition Metal Oxide Based Lithium Ion Battery Electrodes," *Adv. Energy Mater.*, vol. 3, pp. 845–850, 2013. See also supporting information at doi.org/10.1002/aenm.201200932.

Application Library path: `Battery_Design_Module/Heterogeneous_Models/nmc_electrode_geometry`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Blank Model**.

GLOBAL DEFINITIONS

Geometry Parameters

Load some geometry parameters from a text file.

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `Geometry Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `nmc_electrode_geometry_parameters.txt`.

PARTICLES

The particle data is placed in **Geometry Parts**, which is then imported into the model geometry.

1 In the **Model Builder** window, right-click **Global Definitions** and choose **Geometry Parts** > **3D Part**.

2 In the **Settings** window for **Part**, type `Particles` in the **Label** text field.

Create a dummy sphere in the part. This will later be replaced by a collection of objects, generated from a model method.

Sphere 1 (sph1)

1 In the **Geometry** toolbar, click **Sphere**.

2 In the **Settings** window for **Sphere**, locate the **Size** section.

3 In the **Radius** text field, type `2e-6`.

4 Locate the **Position** section. In the **x** text field, type `11e-5`.

5 In the **y** text field, type `7e-5`.

6 In the **z** text field, type `4e-6`.

7 Click **Build Selected**.

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **3D**.

GEOMETRY 1

Now set up the model geometry sequence, making use of the **Particles** geometry part.

Particles Part

1 In the **Geometry** toolbar, click **Part Instance** and choose **Particles**.

2 In the **Settings** window for **Part Instance**, type `Particles Part` in the **Label** text field.

3 Click **Build Selected**.

Particles

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Union**.

2 In the **Settings** window for **Union**, type `Particles` in the **Label** text field.

3 Select the object **pi1** only.

4 Locate the **Union** section. Clear the **Keep interior boundaries** checkbox.

5 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

Block 1 (blk1)

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type `xmax-xmin`.

4 In the **Depth** text field, type `ymax-ymin`.

5 In the **Height** text field, type `L_elec+L_sep`.

6 Locate the **Position** section. In the **x** text field, type `xmin`.

7 In the **y** text field, type `ymin`.

8 Click **Build Selected**.

Partition Objects 1 (par1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Partition Objects**.

2 Select the object **uni1** only.

3 In the **Settings** window for **Partition Objects**, locate the **Partition Objects** section.

4 Click to select the **Activate Selection** toggle button for **Tool objects**.

5 Select the object **blk1** only.

Box Selection 1 (boxsel1)

1 In the **Geometry** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, locate the **Box Limits** section.

3 In the **x minimum** text field, type xmin+geom_tol.

4 In the **x maximum** text field, type xmax-geom_tol.

5 In the **y minimum** text field, type ymin+geom_tol.

6 In the **y maximum** text field, type ymax-geom_tol.

7 Locate the **Resulting Selection** section. From the **Show in physics** list, choose **Off**.

8 Click **Build Selected**.

Complement Selection 1 (comsel1)

1 In the **Geometry** toolbar, click **Selections** and choose **Complement Selection**.

2 In the **Settings** window for **Complement Selection**, locate the **Input Entities** section.

3 Click **Add**.

4 In the **Add** dialog, select **Box Selection 1** in the **Selections to invert** list.

5 Click **OK**.

6 In the **Settings** window for **Complement Selection**, locate the **Resulting Selection** section.

7 From the **Show in physics** list, choose **Off**.

8 Click **Build Selected**.

Delete Entities 1 (del1)

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Delete Entities**.

2 In the **Settings** window for **Delete Entities**, locate the **Entities or Objects to Delete** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Complement Selection 1**.

5 Click **Build Selected**.

Electrode

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, type Electrode in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type xmax-xmin.

4 In the **Depth** text field, type ymax-ymin.

5 In the **Height** text field, type L_elec.

6 Locate the **Position** section. In the **x** text field, type xmin.

7 In the **y** text field, type ymin.

8 Click **Build Selected**.

Difference 1 (dif1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Difference**.

2 Select the object **blk2** only.

3 In the **Settings** window for **Difference**, locate the **Difference** section.

4 Click to select the **Activate Selection** toggle button for **Objects to subtract**.

5 Select the object **del1** only.

6 Select the **Keep objects to add** checkbox.

7 Select the **Keep objects to subtract** checkbox.

8 Click **Build Selected**.

Delete Entities 2 (del2)

1 Right-click **Geometry 1** and choose **Delete Entities**.

2 In the **Settings** window for **Delete Entities**, locate the **Entities or Objects to Delete** section.

3 From the **Geometric entity level** list, choose **Object**.

4 Select the object **dif1** only.

5 Click the **Clear Selection** button for **Selection**.

6 Select the object **blk2** only.

Separator

1 In the **Geometry** toolbar, click **Block**.

2 In the **Settings** window for **Block**, type `Separator` in the **Label** text field.

3 Locate the **Size and Shape** section. In the **Width** text field, type `xmax-xmin`.

4 In the **Depth** text field, type `ymax-ymin`.

5 In the **Height** text field, type `L_sep`.

6 Locate the **Position** section. In the **x** text field, type `xmin`.

7 In the **y** text field, type `ymin`.

8 In the **z** text field, type `L_elec`.

9 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** checkbox.

10 Click **Build Selected**.

11 Click the **Zoom Extents** button in the **Graphics** toolbar.

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

Porous Conductive Binder

1 In the **Geometry** toolbar, click **Selections** and choose **Complement Selection**.

2 In the **Settings** window for **Complement Selection**, type `Porous Conductive Binder` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, in the **Selections to invert** list, choose **Particles** and **Separator**.

5 Click **OK**.

Lithium Foil

1 In the **Geometry** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, type `Lithium Foil` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Box Limits** section. In the **z minimum** text field, type `L_elec+L_sep/2`.

5 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.

NMC Current Collector

1 In the **Geometry** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, type `NMC Current Collector` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Box Limits** section. In the **z maximum** text field, type `0`.

5 Locate the **Output Entities** section. From the **Include entity if** list, choose **Entity inside box**.

Particle Boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Adjacent Selection**.

2 In the **Settings** window for **Adjacent Selection**, type `Particle Boundaries` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, select **Particles** in the **Input selections** list.

5 Click **OK**.

6 In the **Settings** window for **Adjacent Selection**, locate the **Resulting Selection** section.

7 From the **Show in physics** list, choose **Off**.

Binder Boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Adjacent Selection**.

2 In the **Settings** window for **Adjacent Selection**, type `Binder Boundaries` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, select **Porous Conductive Binder** in the **Input selections** list.

5 Click **OK**.

6 In the **Settings** window for **Adjacent Selection**, locate the **Resulting Selection** section.

7 From the **Show in physics** list, choose **Off**.

Particle Surfaces

1 In the **Geometry** toolbar, click **Selections** and choose **Intersection Selection**.

2 In the **Settings** window for **Intersection Selection**, type `Particle Surfaces` in the **Label** text field.

3 Locate the **Geometric Entity Level** section. From the **Level** list, choose **Boundary**.

4 Locate the **Input Entities** section. Click **Add**.

5 In the **Add** dialog, in the **Selections to intersect** list, choose **Particle Boundaries** and **Binder Boundaries**.

6 Click **OK**.

Separator + Binder

1 In the **Geometry** toolbar, click **Selections** and choose **Union Selection**.

2 In the **Settings** window for **Union Selection**, type `Separator + Binder` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, in the **Selections to add** list, choose **Separator** and **Porous Conductive Binder**.

5 Click **OK**.

All Domains

1 In the **Geometry** toolbar, click **Selections** and choose **Box Selection**.

2 In the **Settings** window for **Box Selection**, type `All Domains` in the **Label** text field.

3 Locate the **Box Limits** section. In the **x minimum** text field, type `xmin`.

4 In the **x maximum** text field, type `xmax`.

5 In the **y minimum** text field, type `ymin`.

6 In the **y maximum** text field, type `ymax`.

7 Locate the **Output Entities** section. From the **Include entity if** list, choose **All vertices inside box**.

8 Locate the **Resulting Selection** section. From the **Show in physics** list, choose **Off**.

All External Boundaries

1 In the **Geometry** toolbar, click **Selections** and choose **Adjacent Selection**.

2 In the **Settings** window for **Adjacent Selection**, type `All External Boundaries` in the **Label** text field.

3 Locate the **Input Entities** section. Click **Add**.

4 In the **Add** dialog, select **All Domains** in the **Input selections** list.

5 Click **OK**.

RESULTS

Import particle data in the form of a table.

Particle Data Table

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results** > **Tables** and choose **Table**.

3 In the **Settings** window for **Table**, type `Particle Data Table` in the **Label** text field.

Download the data from the entry `Particle Statistics (NMC_94wt_0bar)` from http://dx.doi.org/10.5905/ethz-iis-1 and import it as a text file to the table.

4 Locate the **Data** section. Click **Import**.

For generating the **Particles** geometry part based on the table data, we will use a model method. Note that the method editor is only available in the Windows® version of the COMSOL Desktop.

APPLICATION BUILDER

In the **Home** toolbar, click **Application Builder**.

NEW METHOD

1 In the **Application Builder** window, right-click **Methods** and choose **New Method**.

2 In the **New Method** dialog, type `GenerateGeometryFromTable` in the **Name** text field.

3 Click **OK**.

GenerateGeometryFromTable

1 In the **Application Builder** window, under **Methods** click **GenerateGeometryFromTable**.

2 Copy the following code into the **GenerateGeometryFromTable** window:

```
// Read data from Results > Table in model builder tree
String tableData[][] = model.result().table().get("tbl1").getTableData(false);

// Read some geometry parameter values from Parameters
Double voxel_size = model.param().evaluate("vox_size");
Double geom_tol = model.param().evaluate("geom_tol");
Double xmin = model.param().evaluate("xmin")+geom_tol;
Double xmax = model.param().evaluate("xmax")+geom_tol;
Double ymin = model.param().evaluate("ymin")+geom_tol;
Double ymax = model.param().evaluate("ymax")+geom_tol;

// Clear geometry part
model.geom("part1").feature().clear();

// Create matrix for added spheres
Double sphereData[][] = new Double[tableData.length][4];
int i = 0; // Row counter for matrix

// Variable for electrode thickness calculation
Double maxz = new Double(0.0);

// Variables for calculating mass-averaged sphere radius
Double Vsum = new Double(0.0);
Double rVsum = new Double(0.0);

// Loop for all rows in the table
for (String[] row : tableData) {
  Double xminData = Double.parseDouble(row[2])*voxel_size;
  Double yminData = Double.parseDouble(row[3])*voxel_size;
  Double xmaxData = Double.parseDouble(row[5])*voxel_size;
  Double ymaxData = Double.parseDouble(row[6])*voxel_size;

  // Check if within bounding box, and add sphere if radius larger than tolerance
  if (((xminData < xmax && xminData > xmin) || (xmaxData < xmax && xmaxData > 
xmin)) &&
      ((yminData < ymax && yminData > ymin) || (ymaxData < ymax && ymaxData > 
ymin))) {
    Double volume = Double.parseDouble(row[1])*Math.pow(voxel_size, 3.0);
    Double radius = Math.pow(0.75*volume/Math.PI, 0.333333);

    if (radius > geom_tol) {
      Double xpos = Double.parseDouble(row[8])*voxel_size;
      Double ypos = Double.parseDouble(row[9])*voxel_size;
      Double zpos = Double.parseDouble(row[10])*voxel_size;

      // Add data to sphere data matrix
      sphereData[i][0] = xpos;
      sphereData[i][1] = ypos;
      sphereData[i][2] = zpos;
      sphereData[i][3] = radius;
      i++;

      // Update electrode thickness variable
      maxz = maxz < (zpos+radius) ? zpos+radius : maxz;
```

```
      // Update mass-averaged radius variables if center of sphere inside
bounding box
      if (((xpos < xmax && xpos > xmin) && (ypos < ymax && ypos > ymin))) {
        Vsum = Vsum+volume;
        rVsum = rVsum+radius*volume;
      }

      // Add sphere to part geometry
      GeomFeature sph = model.geom("part1").create("sph"+i, "Sphere");
      sph.set("pos", new String[]{Double.toString(xpos)+"[m]",
Double.toString(ypos)+"[m]", Double.toString(zpos)+"[m]"});
      sph.label("Particle "+(int) Math.round(Double.parseDouble(row[0])));
      sph.set("r", radius+"[m]");
    }
  }
}

// Add cylinders to eliminate narrow regions or sharp angles between spheres
double hmin = model.param().evaluate("hmin"); // Minimum mesh element size
int cyl = 1;

// Check distances and gaps between all binary combinations of spheres
for (int j = 0; j < i; j++) {
  for (int k = j+1; k < i; k++) {
    Double x = sphereData[k][0]-sphereData[j][0];
    Double y = sphereData[k][1]-sphereData[j][1];
    Double z = sphereData[k][2]-sphereData[j][2];

    Double dist = Math.sqrt(x*x+y*y+z*z);

    Double gap = dist-(sphereData[k][3]+sphereData[j][3]);
    int index1 = sphereData[k][3] < sphereData[j][3] ? k : j;
    int index2 = sphereData[k][3] > sphereData[j][3] ? k : j;
    Double r_sphere = sphereData[index1][3];

    // Add cylinder if spheres are too close or overlapping
    if (gap < hmin && gap > -0.667*r_sphere) {

      Double x_sphere = sphereData[index1][0];
      Double y_sphere = sphereData[index1][1];
      Double z_sphere = sphereData[index1][2];

      Double direction = sphereData[k][3] < sphereData[j][3] ? -1.0 : 1.0;

      Double r_help = r_sphere+gap-hmin;
      Double r_cyl = Math.max(Math.sqrt(r_sphere*r_sphere-r_help*r_help), hmin*
2);

      // Solve root to nonlinear equation for cylinder radius (so that sphere-
to-sphere distance = hmin along cylinder surface).
      Double r1 = r_sphere;
      Double r2 = sphereData[index2][3];
      double ta = 2*r2;
      double tb = 2*r1;
```

```
      double tc = Math.sqrt(-((gap-hmin+tb+ta)*(gap-hmin+tb)*(gap-hmin+ta)*
(gap-hmin)));
      r_cyl = ((1/(gap-hmin+r1+r2))*tc)/2;

      Double dist_corr = Math.sqrt(r_sphere*r_sphere-r_cyl*r_cyl)-2*hmin;
      Double posx = x_sphere+x/dist*dist_corr*direction;
      Double posy = y_sphere+y/dist*dist_corr*direction;
      Double posz = z_sphere+z/dist*dist_corr*direction;

      // Create cylinder
      GeomFeature cylinder = model.geom("part1").create("cyl"+cyl++,
"Cylinder");
      with(cylinder);
        set("pos", new String[]{Double.toString(posx)+"[m]",
Double.toString(posy)+"[m]", Double.toString(posz)+"[m]"});
        set("axistype", "cartesian");
        set("ax3", new String[]{Double.toString(x*direction)+"[m]",
Double.toString(y*direction)+"[m]", Double.toString(z*direction)+"[m]"});
        set("r", r_cyl+"[m]");
        set("h", hmin*5+"[m]");
      endwith();
    }
  }
}

// Set electrode length in model
model.param().set("L_elec", maxz+geom_tol+"[m]");

// Build geometry in model
model.geom("part1").run();
model.component("comp1").geom("geom1").run();

// Measure and update volume parameter
model.component("comp1").geom("geom1").measure().selection().init(3);
model.component("comp1").geom("geom1").measure().selection().named("uni1");
model.param().set("Vp", model.geom("geom1").measure().getVolume()+"[m^3]");

// Measure and update area parameter
model.component("comp1").geom("geom1").measure().selection().init(2);
model.component("comp1").geom("geom1").measure().selection().named("intsel1");
model.param().set("Ap", model.geom("geom1").measure().getVolume()+"[m^2]");

// Update mass-averaged radius parameter
model.param().set("rp_avg_spheres", rVsum/Vsum+"[m]");
```

METHODS

In the **Home** toolbar, click **Model Builder**.

GLOBAL DEFINITIONS

Make the model method available in the model tree, and run it as follows:

Click **Method Call** and choose **GenerateGeometryFromTable**.

Generate Geometry From Particle Data Table

1 In the **Model Builder** window, under **Global Definitions** click **GenerateGeometryFromTable 1**.
2 In the **Settings** window for **Method Call**, type `Generate Geometry From Particle Data Table` in the **Label** text field.
3 Click **Run**.

PARTICLES

In the **Model Builder** window, collapse the **Global Definitions** > **Geometry Parts** > **Particles** node.

DEFINITIONS

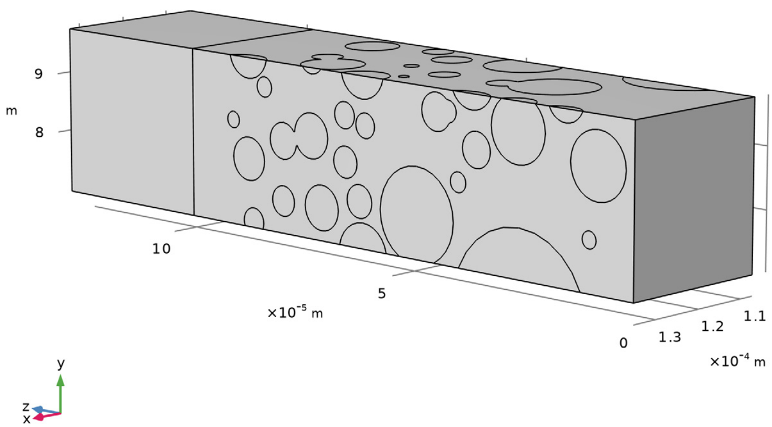
Finally, update the view so that the *y*-axis points upward, and the *z*-axis to the left, and the *x*-axis toward you.

1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** node.

Camera

1 Click the **Zoom Extents** button in the **Graphics** toolbar.
2 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Definitions** > **View 2** node, then click **Camera**.
3 In the **Settings** window for **Camera**, locate the **Position** section.
4 In the **x** text field, type `6.1e-4`.
5 In the **y** text field, type `2.1e-4`.
6 In the **z** text field, type `-4.1e-4`.
7 Locate the **Up Vector** section. In the **x** text field, type `0`.
8 In the **y** text field, type `1`.
9 In the **z** text field, type `0`.
10 Click **Update**.

11 Click the **Zoom Extents** button in the **Graphics** toolbar.



View 2

In the **Model Builder** window, collapse the **Component 1 (comp1)** > **Definitions** > **View 2** node.

ROOT

Disable the analysis of the geometry as the remaining small geometric details can be kept.

GEOMETRY 1

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.
2. In the **Settings** window for **Geometry**, locate the **Cleanup** section.
3. Clear the **Automatic detection of small details** checkbox.
4. In the **Geometry** toolbar, click **Build All**.