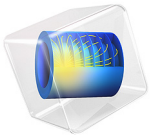

Model created in COMSOL Multiphysics 6.4

Precipitation of Barium Sulfate

Introduction

Crystallization is an important separation process in the chemical industry. It is used for the production of pharmaceuticals and industrial chemicals. It can also be used in resource recovery as a way of separating valuable materials from waste. An example of this is the recovery of metals from batteries.

The driving force for crystallization is the amount of solute in excess of its solubility. This is referred to as the supersaturation. Different methods of generating supersaturation are typically used to categorize crystallization processes. These include cooling, evaporation, addition of a secondary solvent (antisolvent), and by chemical reaction (precipitation).

The two main mechanisms that occur during crystallization is nucleation and growth. Nucleation is the formation of new crystal particles in the form of nuclei from solute molecules. Crystal growth is the incorporation of solute molecules into an already existing crystal lattice.

The model is based on the work by Ölander (Ref. 1), Schwarzer and Peukert (Ref. 2), and Tang and others (Ref. 3). The model aims to simulate the evolution of a crystal particle population by solving the population balance equation. The system is modeled both as a perfectly mixed 0D batch reactor and a 3D T-mixer.

Model Definition

The precipitation in 0D is modeled as a time-dependent system where barium chloride and sulphuric acid are assumed perfectly mixed at initial concentrations of 500 and 330 mol/m^3. The 3D barium sulfate precipitation takes place in a tubular T-mixer consisting of a 10 mm long mixing pipe with a diameter of 1 mm. Two oppositely placed inlets each with a diameter of 0.5 mm are located at the top of the mixing pipe. The inlets are placed offset from each other. An overview of the geometry can be seen in Figure 1. In 3D, barium chloride and sulphuric acid enter from the oppositely placed inlets at concentrations of 500 and 330 mol/m^3. The inlet velocity is adjusted to achieve a Reynolds number of 250 based on the diameter of the mixing pipe. The flow field used for species and particle transport is solved for by the Laminar Flow interface. The T-mixer is modeled at steady state.

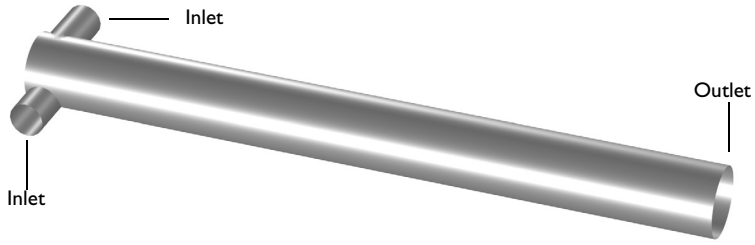

Figure 1: T-mixer geometry consisting of two inlet pipes and one main mixing pipe.

In both scenarios, the dissociation of barium chloride and the first step dissociation of sulphuric acid are assumed complete. The second step dissociation of sulphuric acid and formation of aqueous barium sulfate take place according to

$$HSO_4^- \leftrightarrow SO_4^{2-} + H^+$$

$$Ba^{2+} + SO_4^{2-} \leftrightarrow BaSO_4(aq)$$

while the formation of solid barium sulfate takes place according to

$$Ba^{2+} + SO_4^{2-} \leftrightarrow BaSO_4(s)$$

The reactions are set up with the Reaction Engineering interface in 0D and Chemistry interface coupled with the Transport of Diluted Species interface in 3D. The supersaturation is defined as

$$S = \frac{c_e}{c^*} \tag{1}$$

where the effective concentration c_e and equilibrium concentration c^* are calculated from the reactant concentrations using the mean activity coefficient, γ, and the solubility product K_{SP} (mol^2/m^6) according to

$$c_e = \gamma_\pm \sqrt{c_{Ba^{2+}} c_{SO_4^{2-}}} \tag{2}$$

$$c^* = \sqrt{K_{SP}} \tag{3}$$

Multiple models are available to describe the activity coefficient. Here, the extended Debye–Hückel model presented by Bromley (Ref. 4) is used. The activity coefficient is calculated as

$$\gamma_{\pm} = \frac{-A\left|Z_{Ba^{2+}} Z_{SO_4^{2-}}\right|\sqrt{I_m}}{1+\sqrt{I_m}} + \frac{\left|Z_{Ba^{2+}} Z_{SO_4^{2-}}\right|}{\left|Z_{Ba^{2+}}\right|+\left|Z_{SO_4^{2-}}\right|}\left(\frac{F_{Ba^{2+}}}{\left|Z_{Ba^{2+}}\right|}+\frac{F_{SO_4^{2-}}}{\left|Z_{SO_4^{2-}}\right|}\right) \tag{4}$$

and

$$F_{Ba^{2+}} = \sum_a \left(\frac{(0.06+0.6B_{Ba^{2+},a})\left|Z_{Ba^{2+}} Z_a\right|}{\left(1+\frac{1.5}{\left|Z_{Ba^{2+}} Z_a\right|}I_m\right)^2}\left(\frac{\left|Z_{Ba^{2+}}\right|+\left|Z_a\right|}{2}\right)^2 m_a \right) \tag{5}$$

$$F_{SO_4^{2-}} = \sum_c \left(\frac{(0.06+0.6B_{SO_4^{2-},c})\left|Z_{SO_4^{2-}} Z_c\right|}{\left(1+\frac{1.5}{\left|Z_{SO_4^{2-}} Z_c\right|}I_m\right)^2}\left(\frac{\left|Z_{SO_4^{2-}}\right|+\left|Z_c\right|}{2}\right)^2 m_c \right) \tag{6}$$

where a and c are the anions and cations in the solution. The constants $B_{a,c}$ are calculated from tabulated values from Bromley (Ref. 4) according to

$$B_{a,c} = B_a + B_c + \delta_a\delta_c \tag{7}$$

For interactions with hydrogen sulfate ions the values are instead taken from and calculations done according to Ref. 3.

THE POPULATION BALANCE EQUATION

The change in particle number density, n ($1/\mathrm{m}^4$), with respect to time in a crystal particle population can be described using the population balance equation

$$\frac{\partial n}{\partial t} + \nabla\cdot(\mathbf{u}n) + \frac{\partial(G(S,L)n(L))}{\partial L} = \frac{\nu}{S_c}\nabla^2 n + B_0\delta(L-L_{c0}) \tag{8}$$

where

- L is the particle diameter (m)
- G is the crystal growth rate (m/s)
- ν is the kinematic viscosity (m^2/s)
- S_c is the Schmidt number

- B_0 the nucleation rate as a source of number density ($1/m^4/s$)
- L_{c0} the smallest stable crystal size (m)

The terms on the left-hand side represent the change of population density with respect to time, the convective crystal transport, and crystal growth, respectively. The terms on the right-hand side represent the diffusive crystal transport according to Fick's second law and the birth rate from crystal nucleation. The size distribution is modeled with the population balance equation using the Size-Based Population Balance interface which solves a discretized formulation with discrete size intervals. The number density n_i of a discrete size interval spanning the range $L_{i\text{-}1/2}$ to $L_{i+1/2}$ is defined as

$$n_i = \frac{\int_{L_{i-1/2}}^{L_{i+1/2}} n(L)dL}{L_{i+1/2} - L_{i-1/2}} \tag{9}$$

The nucleation rate as a source of number density, B_0, correlates to the nucleation rate as a source of particle number, B ($1/m^3/s$), as $B_0 = B/\Delta L_0$, where ΔL_0 is the width of the interval containing newly formed particles. The rate B is defined according to classical nucleation theory as (Ref. 1, Ref. 3)

$$B = \frac{3}{2} D_{AB} (c_e N_A)^{7/3} \sqrt{\frac{\gamma_S}{k_B T}} V_m \exp\left(\frac{-16\pi}{3} \frac{\gamma_S^3}{T^3 k_B^3} \frac{V_m^2}{(\ln S)^2}\right) \tag{10}$$

where

- D_{AB} is the apparent diffusion coefficient (m^2/s)
- N_A is the Avogadro number ($1/mol$)
- γ_S is the interfacial energy (J/m^2)
- k_B is the Boltzmann constant (J/K)
- V_m is the molecular volume (m^3)
- T is the temperature (K)

Nucleation occurs at the smallest stable crystal size L_{c0} defined as

$$L_{c0} = \frac{4\gamma_S V_m}{\nu_d k_B T \ln S} \tag{11}$$

with the dissociation number ν_d. In this model the smallest crystal size at which nucleation occurs is taken as constant. The transport controlled growth rate can be described as (Ref. 3)

$$G = \frac{k_a}{3k_v}\frac{\mathrm{Sh}D_{AB}M_p(c_e - c^*)}{\rho_p L} \tag{12}$$

Here k_a and k_v are the area and volume shape factors relating the particle area and volume to the size, while Sh is the Sherwood number, M_p is the crystal molar mass (kg/mol) and ρ_p the density of the precipitate (kg/m^3).

REACTION RATE

The reaction rate, R_{BaSO4}, resulting from the formation of solid barium sulfate, in units of mol/m^3/s, is calculated from the summed growth and nucleation source terms of each discrete size interval j according to

$$R_{BaSO4} = \frac{\rho_p \sum (V_{av,j}\Delta L_j S_{T,j})}{M_p} \tag{13}$$

and

$$S_{T,j} = B_0\delta(L_j - L_0) - \frac{\partial(Gn_j)}{\partial L_j} \tag{14}$$

where $V_{av,j}$ is the average volume of particles and ΔL_j is the width of interval j.

When the formation of aqueous barium sulfate is modeled as an equilibrium reaction, where the equilibrium condition is upheld at each point in space and time, the reaction rate can be added either to the aqueous barium sulfate or the barium and sulfate ions. Here, the reaction rate is applied to the aqueous barium sulfate. The reaction rate is added by using the **Precipitation in Fluid Flow** coupling feature.

MESH

The mesh is constructed as a tradeoff between computation time and accuracy. The resolution is the highest between the oppositely placed inlets to resolve the mixing of streams. The mesh along the length of the mixing pipe is focused on resolving gradients in the cross-flow direction. Using meshes finer than what this model implements will give more accurate flow fields and crystal growth but require longer times to find a solution.

Results and Discussion

The crystal size distribution for both the perfectly mixed batch reactor and T-mixer scenarios are presented along with complementing data.

PERFECTLY MIXED BATCH REACTOR

The supersaturation simultaneously acts as the driving force for the precipitation and represents the amount of available reactant in the solution. The change in supersaturation with time in a perfectly mixed batch reactor is seen in Figure 2. The initial supersaturation is consumed as barium sulfate precipitates until reaching an equilibrium where the ion concentrations are equal to the solubility.

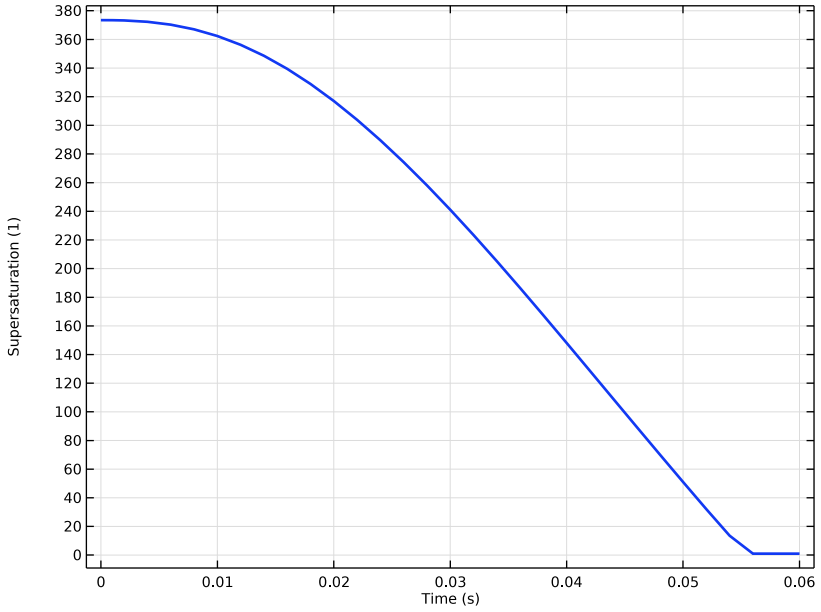

Figure 2: Supersaturation as a function of time in a perfectly mixed batch reactor.

The size distribution of crystals formed from the supersaturation is shown at various times in Figure 3.

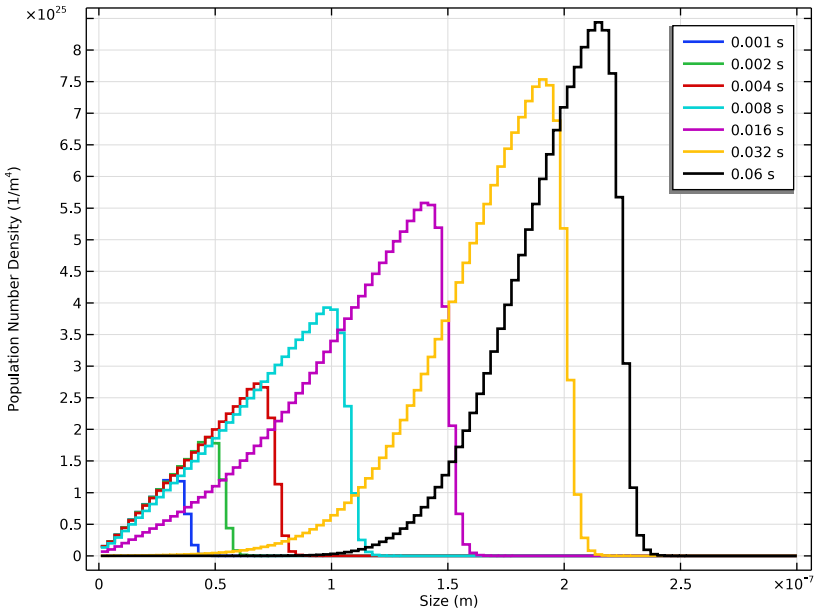

Figure 3: Size distribution at various times in a perfectly mixed batch reactor.

The transition from solute reactants to solid particles can be seen from Figure 4, which shows the mass concentrations of the reacting species and the solid product over time. The total concentration remains constant, verifying the conservation of mass in the system.

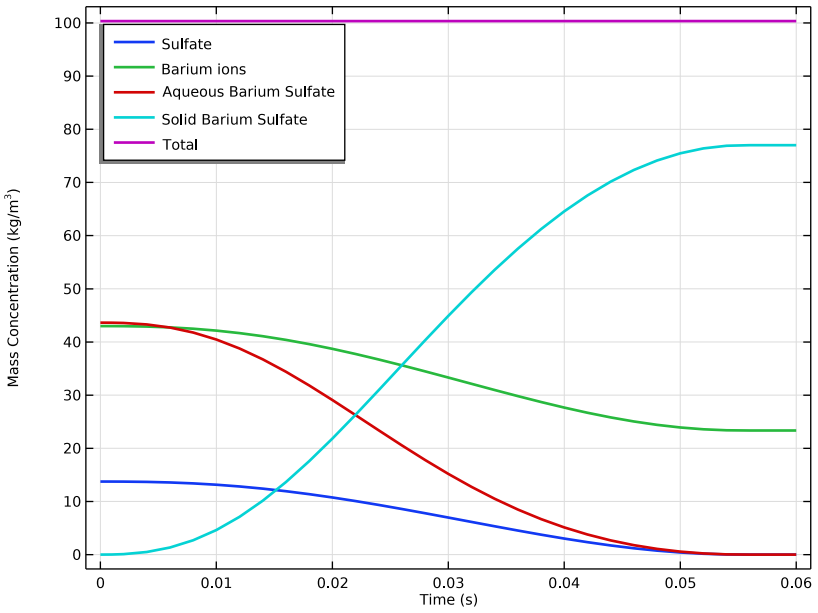

Figure 4: Mass concentrations of reacting species and solid product over time.

T-MIXER

The total particle concentration, particle flux, and supersaturation in the T-mixer at steady state is shown in Figure 5. The two separate inlet flows mix at the top of the mixing pipe. Along the length of the mixing pipe the combined flow becomes increasingly uniform. The supersaturated state occurs in areas where barium and sulfate ions interact. This is initially at the top part of the mixing pipe. The supersaturated decreases throughout the mixing pipe, indicating nucleation and crystal growth.

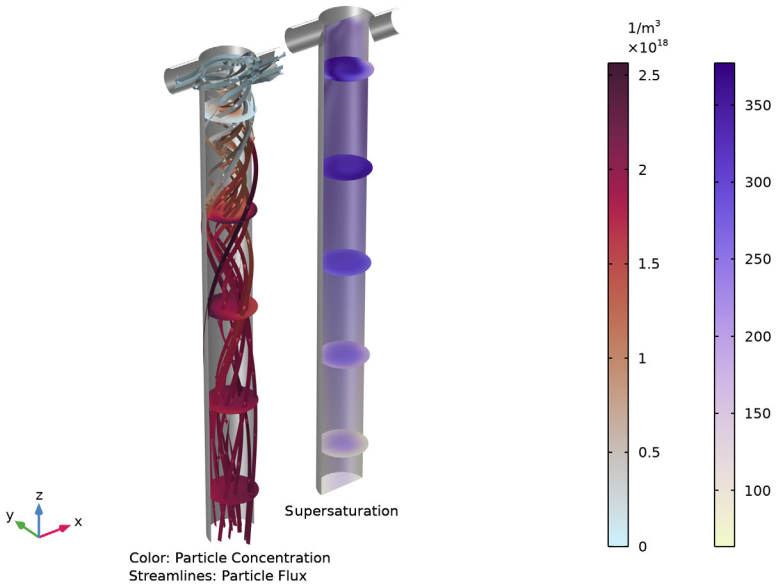

Figure 5: Particle Concentration and supersaturation in the T-mixer.

The density distribution at different points along the main mixing channel is shown in Figure 6. The distribution moves toward larger sizes and the total amount of particles increases with retention time.

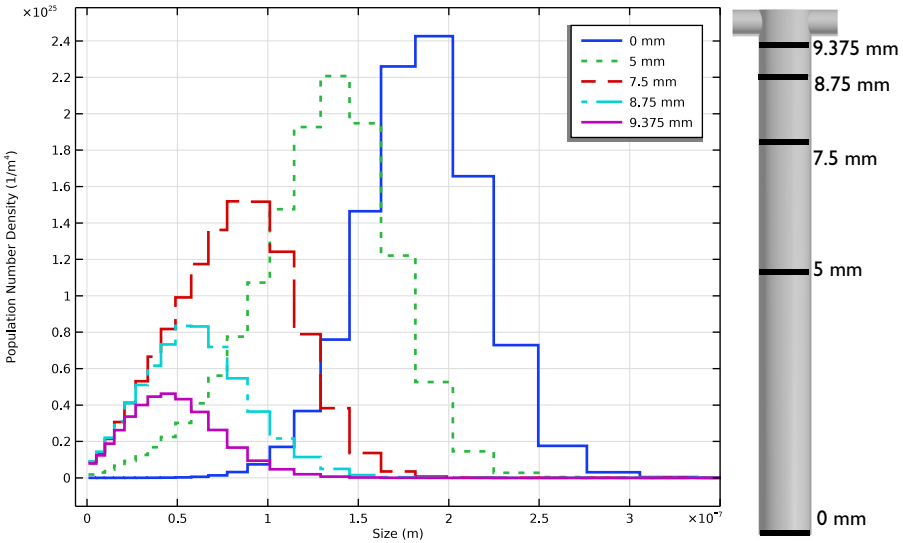

Figure 6: Number density distribution at various points along the T-mixer main mixing channel.

References

1. M. Ölander, *Numerical Simulations for Battery Recycling*, master's thesis, KTH, Royal Institute of Technology, 2023.

2. H.C. Schwarzer and W. Peukert, "Combined experimental/numerical study on the precipitation of nanoparticles," *AICHE J.*, vol. 50, no. 12, pp. 3234–3247, 2004.

3. H.Y. Tang, S. Rigopoulos, and G. Papadakis, "On the interaction of turbulence with nucleation and growth in reaction crystallisation," *J. Fluid Mech*, vol. 944, p. A48, 2022.

4. L.A. Bromley, "Thermodynamic properties of strong electrolytes in aqueous solution," *AICHE J.*, vol. 19, no. 2, pp. 313–320, 1973.

Application Library path: `Chemical_Reaction_Engineering_Module/Mixing_and_Separation/barium_sulfate_precipitation`

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

NEW

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

MODEL WIZARD

1. In the **Model Wizard** window, click **0D**.
2. In the **Select Physics** tree, select **Chemical Species Transport** > **Precipitation and Crystallization** > **Precipitation and Crystallization in Fluid Flow**.
3. Click **Add**.
4. In the **Added physics interfaces** tree, select **Size-Based Population Balance (pbsb)**.
5. Click **Study**.
6. In the **Select Study** tree, select **General Studies** > **Time Dependent**.
7. Click **Done**.

Import the parameters for the model from a separate file.

GLOBAL DEFINITIONS

Parameters 1

1. In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
2. In the **Settings** window for **Parameters**, locate the **Parameters** section.
3. Click **Load from File**.
4. Browse to the model's Application Libraries folder and double-click the file `barium_sulfate_precipitation_parameters.txt`.

Import the constants for the Debye-Hückel model.

Debye Huckel Constants

1. In the **Home** toolbar, click **Parameters** and choose **Add** > **Parameters**.
2. In the **Settings** window for **Parameters**, type `Debye Huckel Constants` 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 `barium_sulfate_precipitation_debye_huckel_constants.txt`.

Ion Interaction

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global** > **Analytic**.

Define a function to be used for the Debye-Hückel model.

2 In the **Settings** window for **Analytic**, type `Ion Interaction` in the **Label** text field.

3 In the **Function name** text field, type `B_dot`.

4 Locate the **Definition** section. In the **Expression** text field, type `((0.06+0.6*B)*(Z1*Z2))/((1+I*1.5/(Z1*Z2))^2)+B`.

5 In the **Arguments** text field, type `B, Z1, Z2, I`.

6 Locate the **Units** section. In the **Function** text field, type `kg/mol`.

7 In the table, enter the following settings:

Argument	Unit
B	kg/mol
Z1	1
Z2	1
I	mol/kg

DEFINITIONS

Variables 1

1 In the **Definitions** toolbar, click a= **Local Variables**.

Import the required variable expressions for the effective concentration.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `barium_sulfate_precipitation_variables1.txt`.

REACTION ENGINEERING (RE)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.

2 In the **Settings** window for **Reaction Engineering**, locate the **Energy Balance** section.

3 In the T text field, type `T`.

Reaction 1

1 In the **Reaction Engineering** toolbar, click **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `HSO4(-) = H(+) + SO4(2-)`.

4 Click **Apply**.

5 Locate the **Equilibrium Settings** section. In the K_{eq0j} text field, type `k1`.

Reaction 2

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `Ba(++) + SO4(2-) = BaSO4`.

4 Click **Apply**.

5 Locate the **Equilibrium Settings** section. In the K_{eq0j} text field, type `k2`.

Species 1

1 In the **Reaction Engineering** toolbar, click  **Species**.

2 In the **Settings** window for **Species**, locate the **Name** section.

3 In the text field, type `Cl-`.

4 In the **Reaction Engineering** toolbar, click  **Species**.

1 In the **Settings** window for **Species**, locate the **Name** section.

2 In the text field, type `H2O`.

3 Locate the **Type** section. From the list, choose **Solvent**.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Volumetric Species Initial Values** section.

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
Ba(++)	`cBa_2p_0`
Cl-	`cCl_1m_0`
H(+)	`cH_1p_0`
HSO4(-)	`cHSO4_1m_0`
SO4(2-)	`cSO4_2m_0`

SIZE-BASED POPULATION BALANCE (PBSB)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Size-Based Population Balance (pbsb)**.

2 In the **Settings** window for **Size-Based Population Balance**, locate the **Particle Properties** section.

3 In the ρ_p text field, type `rho_BaSO4`.

4 Locate the **Size Intervals** section. In the I text field, type `100`.

5 In the L_0 text field, type `0.82[nm]`.

6 In the L_I text field, type `300[nm]`.

7 Locate the **Nucleation** section. From the **Nucleation rate** list, choose **Homogeneous nucleation**.

8 In the γ_s text field, type `gamma_CL`.

9 In the ν text field, type `2`.

10 In the T text field, type `T`.

11 Locate the **Growth** section. From the **Growth rate** list, choose **Transport controlled**.

12 In the Sh text field, type `Sh`.

MULTIPHYSICS

Precipitation in Fluid Flow 1 (pffg1)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Multiphysics** click **Precipitation in Fluid Flow 1 (pffg1)**.

2 In the **Settings** window for **Precipitation in Fluid Flow**, locate the **Precipitant** section.

3 From the list, choose **BaSO4**.

4 From the c list, choose **User defined**.

5 In the text field, type `c_effective`.

6 In the c^* text field, type `c_eq`.

7 In the D_s text field, type `D_AB`.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `0 0.001 range(0.002,2.0e-3,0.06)`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

When the variables solved for have different orders of magnitude, you can modify the scaling of the variables to help the solver converge. In this case, expect the population number density of each bin to be over 1e20 while the concentration values will be significantly lower.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Dependent Variables 1**.

3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.

4 From the **Method** list, choose **Manual**.

5 In the **Scale** text field, type `1e20`.

6 In the **Model Builder** window, expand the **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Dependent Variables 1** node, then click **Concentration (comp1.ODE1)**.

7 In the **Settings** window for **State**, locate the **Scaling** section.

8 From the **Method** list, choose **Initial-value based**.

Repeat steps **7** and **8** for the remaining concentration variables: **Concentration (comp1.ODE2)**, **Concentration (comp1.ODE3)**, **Concentration (comp1.ODE4)**, **Concentration (comp1.ODE5)**, and **Concentration (comp1.ODE6)**.

9 In the **Model Builder** window, under **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** click **Time-Dependent Solver 1**.

10 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.

11 From the **Times to store** list, choose **Output times by interpolation**.

12 Click **Run**.

RESULTS

Average Size Distribution (pbsb)

1 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

2 From the **Time selection** list, choose **From list**.

3 In the **Times (s)** list, choose **0.001**, **0.002**, **0.004**, **0.008**, **0.016**, **0.032**, and **0.06**.

Line Segments 1

1 In the **Model Builder** window, expand the **Average Size Distribution (pbsb)** node, then click **Line Segments 1**.

2 In the **Settings** window for **Line Segments**, click to expand the **Coloring and Style** section.

3 From the **Width** list, choose **2**.

4 Click to expand the **Legends** section. Select the **Show legends** checkbox.

5 In the **Average Size Distribution (pbsb)** toolbar, click **Plot**.

Supersaturation

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Supersaturation` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** checkbox. In the associated text field, type `Supersaturation (1)`.

6 Locate the **Legend** section. Clear the **Show legends** checkbox.

Global 1

1 In the **Supersaturation** toolbar, click **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 Click **Clear Table**.

4 In the table, enter the following settings:

Expression	Unit	Description
`pbsb.c/pbsb.cstar`	1	

5 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

6 In the **Supersaturation** toolbar, click **Plot**.

Mass Balance

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Mass Balance` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **None**.

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** checkbox. In the associated text field, type `Mass Concentration (kg/m<SUP>3</SUP>)`.

6 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 In the **Mass Balance** toolbar, click **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 Click **Clear Table**.

4 In the table, enter the following settings:

Expression	Unit	Description
(re.c_SO4_2m+re.c_HSO4_1m)*M_SO4_2m	kg/m^3	
re.c_Ba_2p*M_Ba_2p	kg/m^3	
re.c_BaSO4*M_BaSO4	kg/m^3	
pbsb.Vtot*rho_BaSO4	kg/m^3	
(re.c_SO4_2m+re.c_HSO4_1m)*M_SO4_2m + re.c_Ba_2p*M_Ba_2p + re.c_BaSO4*M_BaSO4 + pbsb.Vtot*rho_BaSO4	kg/m^3	

5 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

6 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
Sulfate
Barium ions
Aqueous Barium Sulfate
Solid Barium Sulfate
Total

8 In the **Mass Balance** toolbar, click **Plot**.

REACTION ENGINEERING (RE)

Generate Space-Dependent Model 1

1 In the **Reaction Engineering** toolbar, click **Generate Space-Dependent Model**.

2 In the **Settings** window for **Generate Space-Dependent Model**, locate the **Physics Interfaces** section.

3 Find the **Fluid flow** subsection. From the list, choose **Laminar Flow: New**.

4 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

COMPONENT 2 (COMP2)

In the **Model Builder** window, click **Component 2 (comp2)**.

ADD PHYSICS

1 In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.

2 Go to the **Add Physics** window.

3 In the tree, select **Chemical Species Transport** > **Precipitation and Crystallization** > **Size-Based Population Balance (pbsb)**.

4 Click the **Add to Component 2** button in the window toolbar.

5 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

MULTIPHYSICS

Reacting Flow, Diluted Species 1 (rfd1)

1 In the **Model Builder** window, expand the **Component 2 (comp2)** > **Multiphysics** node.

2 Right-click **Component 2 (comp2)** > **Multiphysics** > **Reacting Flow, Diluted Species 1 (rfd1)** and choose **Delete**.

Precipitation in Fluid Flow 1a (pff1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain** > **Precipitation in Fluid Flow**.

DEFINITIONS (COMP2)

Effective Concentration

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, type `Effective Concentration` in the **Label** text field.

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

4 Browse to the model's Application Libraries folder and double-click the file `barium_sulfate_precipitation_variables2.txt`.

GEOMETRY 1 (3D)

Cylinder 1 (cyl1)

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

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

3 In the **Radius** text field, type `D/2`.

4 In the **Height** text field, type `Lc`.

Cylinder 2 (cyl2)

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

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

3 In the **Radius** text field, type `D/4`.

4 In the **Height** text field, type `D`.

5 Locate the **Position** section. In the **x** text field, type `-D`.

6 In the **y** text field, type `D/4`.

7 In the **z** text field, type `Lc-D/4`.

8 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Cylinder 3 (cyl3)

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

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

3 In the **Radius** text field, type `D/4`.

4 In the **Height** text field, type `D`.

5 Locate the **Position** section. In the **y** text field, type `-D/4`.

6 In the **z** text field, type `Lc-D/4`.

7 Locate the **Axis** section. From the **Axis type** list, choose **x-axis**.

Work Plane 1 (wp1)

1 In the **Geometry** toolbar, click **Work Plane**.

2 In the **Settings** window for **Work Plane**, locate the **Plane Definition** section.

3 In the **z-coordinate** text field, type `9[mm]`.

Work Plane 1 (wp1) > Plane Geometry

In the **Model Builder** window, click **Plane Geometry**.

Work Plane 1 (wp1) > Circle 1 (c1)

1 In the **Work Plane** toolbar, click **Circle**.

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

3 In the **Radius** text field, type `D/2`.

Ignore Faces 1 (igf1)

1 In the **Model Builder** window, right-click **Geometry 1(3D)** and choose **Virtual Operations** > **Ignore Faces**.

2 On the object **fin**, select Boundaries 13–15, 17, 18, 23–26, and 29–31 only.

3 In the **Geometry** toolbar, click **Build All**.

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

4 In the **Model Builder** window, click **Geometry 1(3D)**.

5 In the **Settings** window for **Geometry**, locate the **Cleanup** section.

6 Clear the **Automatic detection of small details** checkbox.

CHEMISTRY (CHEM)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Chemistry (chem)**.

2 In the **Settings** window for **Chemistry**, locate the **Mixture Properties** section.

3 From the **Phase** list, choose **Liquid**.

4 Locate the **Species Matching** section. Find the **Bulk species** subsection. In the table, enter the following settings:

Species	Type	Molar concentration	Value (mol/m^3)
Ba(++)	Variable	cBa_2p	Solved for
BaSO4	Variable	cBaSO4	Solved for
Cl-	Variable	cCl_1m	Solved for
H(+)	Variable	cH_1p	Solved for
H2O	Solvent	User defined	`c_sol`
HSO4(-)	Variable	cHSO4_1m	Solved for
SO4(2-)	Variable	cSO4_2m	Solved for

To ensure that the species transport equations converge, change the **Reaction type** from **Equilibrium** to **Reversible** with a high forward rate constant.

1: HSO4(-) = H(+) + SO4(2-)

1 In the **Model Builder** window, expand the **Chemistry (chem)** node, then click **1: HSO4(-) = H(+) + SO4(2-)**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 From the **Reaction type** list, choose **Reversible**.

4 Locate the **Rate Constants** section. Select the **Specify equilibrium constant** checkbox.

5 In the k^{f} text field, type `1e5`.

2: Ba(++) + SO4(2-) = BaSO4

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Chemistry (chem)** click **2: Ba(++) + SO4(2-) = BaSO4**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 From the **Reaction type** list, choose **Reversible**.

4 Locate the **Rate Constants** section. Select the **Specify equilibrium constant** checkbox.

5 In the k^f text field, type `1e5`.

Species: H2O (Solvent)

1 In the **Model Builder** window, click **Species: H2O (Solvent)**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the ρ text field, type `rho_sol`.

TRANSPORT OF DILUTED SPECIES (TDS)

In the **Model Builder** window, expand the **Component 2 (comp2)** > **Transport of Diluted Species (tds)** node.

Equilibrium Reaction 1, Equilibrium Reaction 2

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Transport of Diluted Species (tds)**, Ctrl-click to select **Equilibrium Reaction 1** and **Equilibrium Reaction 2**.

2 Right-click and choose **Delete**.

Fluid 1

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Transport of Diluted Species (tds)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.

3 From the **Source** list, choose **Material**.

4 Locate the **Model Input** section. From the T list, choose **User defined**. In the associated text field, type `T`.

5 Locate the **Diffusion** section. In the D_{cBa2p} text field, type `D_species`.

6 In the D_{cSO42m} text field, type `D_species`.

7 In the D_{cHSO41m} text field, type `D_species`.

8 In the D_{cH1p} text field, type `D_species`.

9 In the D_{cCl1m} text field, type `D_species`.

10 In the D_{cBaSO4} text field, type `D_species`.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Inflow**, locate the **Concentration** section.

4 In the $c_{0,\mathrm{cBa2p}}$ text field, type `cBa_2p_0`.

5 In the $c_{0,cCl1m}$ text field, type `cCl_1m_0`.

Inflow 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 25 only.

3 In the **Settings** window for **Inflow**, locate the **Concentration** section.

4 In the $c_{0,cH1p}$ text field, type `cH_1p_0`.

5 In the $c_{0,cHSO41m}$ text field, type `cHSO4_1m_0`.

6 In the $c_{0,cSO42m}$ text field, type `cSO4_2m_0`.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 8 only.

SIZE-BASED POPULATION BALANCE 2 (PBSB2)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Size-Based Population Balance 2 (pbsb2)**.

2 In the **Settings** window for **Size-Based Population Balance**, locate the **Particle Properties** section.

3 In the ρ_p text field, type `rho_BaSO4`.

4 Locate the **Size Intervals** section. From the **Discretization** list, choose **Geometric**.

5 In the I text field, type `30`.

6 In the L_0 text field, type `0.82[nm]`.

7 In the L_I text field, type `600[nm]`.

8 In the q text field, type `8`.

9 Locate the **Nucleation** section. From the **Nucleation rate** list, choose **Homogeneous nucleation**.

10 In the γ_s text field, type `gamma_CL`.

11 In the ν text field, type `2`.

12 Locate the **Growth** section. From the **Growth rate** list, choose **Transport controlled**.

13 In the Sh text field, type `Sh`.

LAMINAR FLOW (SPF)

1 Click the **Show More Options** button in the **Model Builder** toolbar.

2 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

3 Click **OK**.

4 In the **Model Builder** window, under **Component 2 (comp2)** click **Laminar Flow (spf)**.

5 In the **Settings** window for **Laminar Flow**, click to expand the **Advanced Settings** section.

6 Find the **Pseudo time stepping** subsection. From the **Use pseudo time stepping for stationary equation form** list, choose **On**.

SIZE-BASED POPULATION BALANCE 2 (PBSB2)

Fluid 1

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Size-Based Population Balance 2 (pbsb2)** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Model Input** section.

3 From the T list, choose **User defined**. In the associated text field, type `T`.

4 Locate the **Particle Diffusion** section. In the D text field, type `D_particles`.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundaries 1 and 25 only.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 8 only.

LAMINAR FLOW (SPF)

1 In the **Model Builder** window, expand the **Component 2 (comp2)** > **Laminar Flow (spf)** node, then click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

3 In the T_{ref} text field, type `T`.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 In the **Settings** window for **Inlet**, locate the **Boundary Condition** section.

3 From the list, choose **Fully developed flow**.

4 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `u_in`.

5 Select Boundaries 1 and 25 only.

Outlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.

2 Select Boundary 8 only.

MULTIPHYSICS

Precipitation in Fluid Flow 1a (pff1)

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Multiphysics** click **Precipitation in Fluid Flow 1a (pff1)**.

2 In the **Settings** window for **Precipitation in Fluid Flow**, locate the **Precipitant** section.

3 From the list, choose **cBaSO4**.

4 From the *c* list, choose **User defined**.

5 In the text field, type `c_effective`.

6 From the D_s list, choose **User defined**.

7 In the text field, type `D_AB`.

8 In the c^* text field, type `c_eq`.

9 Locate the **Precipitate** section. In the M_p text field, type `M_BaSO4`.

MESH 1

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size

1 In the **Model Builder** window, under **Component 2 (comp2)** > **Mesh 1** click **Size**.

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

3 From the **Predefined** list, choose **Normal**.

Size 1

In the **Model Builder** window, right-click **Size 1** and choose **Disable**.

Corner Refinement 1

1 In the **Model Builder** window, click **Corner Refinement 1**.

2 In the **Settings** window for **Corner Refinement**, locate the **Refinement** section.

3 In the **Element size scaling factor** text field, type `0.5`.

Free Tetrahedral 1

1 In the **Model Builder** window, click **Free Tetrahedral 1**.

2 In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.

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

4 Select Domain 1 only.

Swept 1

1 In the **Model Builder** window, expand the **Boundary Layers 1** node.

2 Right-click **Mesh 1** and choose **Swept**.

3 In the **Settings** window for **Swept**, locate the **Domain Selection** section.

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

5 Click **Paste Selection**.

6 In the **Paste Selection** dialog, type `2 3` in the **Selection** text field.

7 Click **OK**.

Distribution 1

1 Right-click **Swept 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 From the **Distribution type** list, choose **Predefined**.

4 In the **Number of elements** text field, type `30`.

5 In the **Element ratio** text field, type `8`.

Swept 1

1 In the **Model Builder** window, click **Swept 1**.

2 Drag and drop below **Free Tetrahedral 1**.

3 In the **Settings** window for **Swept**, click **Build All**.

STUDY 2

In the **Model Builder** window, right-click **Study 2** and choose **Delete**.

ADD STUDY

1 In the **Study** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkboxes for **Reaction Engineering (re)** and **Size-Based Population Balance (pbsb)**.

4 Find the **Multiphysics couplings in study** subsection. In the table, clear the **Solve** checkbox for **Precipitation in Fluid Flow 1 (pffg1)**.

5 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Multiphysics** > **Stationary Precipitation in Fluid Flow**.

6 Click the **Add Study** button in the window toolbar.

7 In the **Study** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Stationary

In the **Study** toolbar, click **Compute**.

RESULTS

Number of Particles and Supersaturation

Follow these steps to create Figure 5.

1 In the **Settings** window for **3D Plot Group**, type `Number of Particles and Supersaturation` in the **Label** text field.

2 Click to expand the **Title** section. From the **Title type** list, choose **None**.

3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

4 Locate the **Color Legend** section. Select the **Show units** checkbox.

5 Click to expand the **Plot Array** section. Select the **Enable** checkbox.

Reactor Walls

1 In the **Number of Particles and Supersaturation** toolbar, click **Surface**.

2 In the **Settings** window for **Surface**, type `Reactor Walls` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `1`.

4 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Selection 1

1 In the **Number of Particles and Supersaturation** toolbar, click **Selection**.

2 Select Boundaries 4, 5, 7, 10, 12, 14, and 20–24 only.

Reactor Walls

In the **Model Builder** window, click **Reactor Walls**.

Material Appearance 1

1 In the **Number of Particles and Supersaturation** toolbar, click **Material Appearance**.

2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.

3 From the **Appearance** list, choose **Custom**.

4 From the **Material type** list, choose **Steel (anodized)**.

Number of Particles and Supersaturation

In the **Number of Particles and Supersaturation** toolbar, click  **Slice**.

Slice 1

1 In the **Settings** window for **Slice**, locate the **Expression** section.

2 In the **Expression** text field, type `pbsb2.N`.

3 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Streamline 1**.

5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Reactor Walls, Slice 1

1 In the **Model Builder** window, under **Results** > **Number of Particles and Supersaturation**, Ctrl-click to select **Reactor Walls** and **Slice 1**.

2 Right-click and choose **Duplicate**.

Reactor Walls 1

1 In the **Settings** window for **Surface**, locate the **Plot Array** section.

2 In the **Index** text field, type `1`.

Slice 2

1 In the **Model Builder** window, click **Slice 2**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 In the **Expression** text field, type `pbsb2.c/pbsb2.cstar`.

4 Locate the **Inherit Style** section. From the **Plot** list, choose **None**.

5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Baptisia**.

6 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Slice 3

1 Right-click **Results** > **Number of Particles and Supersaturation** > **Slice 2** and choose **Duplicate**.

2 In the **Settings** window for **Slice**, locate the **Plane Data** section.

3 From the **Plane** list, choose **zx-planes**.

4 In the **Planes** text field, type `1`.

5 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 2**.

Transparency 1

In the **Number of Particles and Supersaturation** toolbar, click **Transparency**.

Number of Particles and Supersaturation

In the **Number of Particles and Supersaturation** toolbar, click **Annotation**.

Annotation 1

1 In the **Settings** window for **Annotation**, locate the **Annotation** section.

2 In the **Text** text field, type `Color: Particle Concentration \\ Streamlines: Particle Flux`.

3 Select the **LaTeX markup** checkbox.

4 Locate the **Position** section. In the **z** text field, type `-0.3[mm]`.

5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

6 From the **Anchor point** list, choose **Upper middle**.

7 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Number of Particles and Supersaturation

In the **Number of Particles and Supersaturation** toolbar, click **Annotation**.

Annotation 2

1 In the **Settings** window for **Annotation**, locate the **Annotation** section.

2 In the **Text** text field, type `Supersaturation`.

3 Locate the **Position** section. In the **z** text field, type `-0.3[mm]`.

4 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

5 From the **Anchor point** list, choose **Upper middle**.

6 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

7 In the **Index** text field, type `1`.

8 In the **Number of Particles and Supersaturation** toolbar, click **Plot**.

Follow these steps to create Figure 6.

Cut Plane 1

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

2 Right-click **Results** > **Datasets** and choose **Cut Plane**.

3 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

4 From the **Plane type** list, choose **General**.

5 From the **Plane entry method** list, choose **Point and normal vector**.

6 Find the **Point** subsection. In the **z** text field, type `5e-3`.

Cut Plane 2

1 Right-click **Cut Plane 1** and choose **Duplicate**.

2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

3 Find the **Point** subsection. In the **z** text field, type `7.5e-3`.

Cut Plane 3

1 Right-click **Cut Plane 2** and choose **Duplicate**.

2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

3 Find the **Point** subsection. In the **z** text field, type `8.75e-3`.

Cut Plane 4

1 Right-click **Cut Plane 3** and choose **Duplicate**.

2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

3 Find the **Point** subsection. In the **z** text field, type `9.375e-3`.

Average 3

In the **Results** toolbar, click  **More Datasets** and choose **Evaluation** > **Average**.

Cut Plane Average 5e-3

1 In the **Model Builder** window, expand the **Results** > **Population Number Density, n121, Streamline (pbsb2)** node, then click **Results** > **Datasets** > **Average 3**.

2 In the **Settings** window for **Average**, type `Cut Plane Average 5e-3` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Plane 1**.

Cut Plane Average 7.5e-3

1 Right-click **Cut Plane Average 5e-3** and choose **Duplicate**.

2 In the **Settings** window for **Average**, type `Cut Plane Average 7.5e-3` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Plane 2**.

Cut Plane Average 8.75e-3

1 Right-click **Cut Plane Average 7.5e-3** and choose **Duplicate**.

2 In the **Settings** window for **Average**, type `Cut Plane Average 8.75e-3` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Plane 3**.

Cut Plane Average 9.375e-3

1 Right-click **Cut Plane Average 8.75e-3** and choose **Duplicate**.

2 In the **Settings** window for **Average**, type `Cut Plane Average 9.375e-3` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Cut Plane 4**.

Average Size Distribution at Specified z-Coordinates

1 In the **Model Builder** window, under **Results** click **Average Size Distribution at Outlet (pbsb2)**.

2 In the **Settings** window for **1D Plot Group**, type `Average Size Distribution at Specified z-Coordinates` in the **Label** text field.

3 Locate the **Axis** section. Select the **Manual axis limits** checkbox.

4 In the **x maximum** text field, type `3.5E-7`.

Line Segments 1

1 In the **Model Builder** window, expand the **Average Size Distribution at Specified z-Coordinates** node, then click **Line Segments 1**.

2 In the **Settings** window for **Line Segments**, click to expand the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

4 From the **Width** list, choose **2**.

5 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

6 Select the **Show legends** checkbox.

7 In the table, enter the following settings:

Legends
0 mm

Line Segments 2

1 Right-click **Results** > **Average Size Distribution at Specified z-Coordinates** > **Line Segments 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Segments**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane Average 5e-3**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
5 mm

Line Segments 3

1 Right-click **Line Segments 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Segments**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane Average 7.5e-3**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
7.5 mm

Line Segments 4

1 Right-click **Line Segments 3** and choose **Duplicate**.

2 In the **Settings** window for **Line Segments**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane Average 8.75e-3**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
8.75 mm

Line Segments 5

1 Right-click **Line Segments 4** and choose **Duplicate**.

2 In the **Settings** window for **Line Segments**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane Average 9.375e-3**.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
9.375 mm

5 In the **Average Size Distribution at Specified z-Coordinates** toolbar, click **Plot**.

Follow these steps to create the **Concentration of Particles at Different Sizes** plot found in the model file.

Concentration of Particles at Different Sizes

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Concentration of Particles at Different Sizes` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Concentration of Particles at Different Sizes`.

5 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

6 Locate the **Color Legend** section. Select the **Show units** checkbox.

7 Locate the **Plot Array** section. Select the **Enable** checkbox.

Slice 1

1 In the **Concentration of Particles at Different Sizes** toolbar, click  **Slice**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 In the **Expression** text field, type `n105`.

4 Locate the **Plane Data** section. From the **Plane** list, choose **xy-planes**.

5 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

Concentration of Particles at Different Sizes

In the **Concentration of Particles at Different Sizes** toolbar, click  **Slice**.

Slice 2

1 In the **Settings** window for **Slice**, locate the **Expression** section.

2 In the **Expression** text field, type `n105`.

3 Locate the **Plane Data** section. From the **Plane** list, choose **zx-planes**.

4 In the **Planes** text field, type `1`.

5 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

6 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.

Transparency 1

In the **Concentration of Particles at Different Sizes** toolbar, click  **Transparency**.

Concentration of Particles at Different Sizes

In the **Concentration of Particles at Different Sizes** toolbar, click  **Annotation**.

Annotation 1

1 In the **Settings** window for **Annotation**, locate the **Annotation** section.

2 In the **Text** text field, type `20.7 - 26.9 nm`.

3 Locate the **Position** section. In the **y** text field, type `D/2`.

4 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.

5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

Reactor Walls

In the **Model Builder** window, under **Results** > **Number of Particles and Supersaturation** right-click **Reactor Walls** and choose **Copy**.

Reactor Walls

In the **Model Builder** window, right-click **Concentration of Particles at Different Sizes** and choose **Paste Surface**.

Selection 1

1 In the **Model Builder** window, expand the **Reactor Walls** node, then click **Selection 1**.

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

3 Click to select the  **Activate Selection** toggle button.

4 Select Boundaries 4, 5, 7, 10, 12–14, and 20–24 only.

Annotation 1, Reactor Walls, Slice 1, Slice 2

1 In the **Model Builder** window, under **Results** > **Concentration of Particles at Different Sizes**, Ctrl-click to select **Slice 1**, **Slice 2**, **Annotation 1**, and **Reactor Walls**.

2 Right-click and choose **Duplicate**.

Slice 3

1 In the **Settings** window for **Slice**, locate the **Inherit Style** section.

2 From the **Plot** list, choose **Slice 1**.

3 Locate the **Expression** section. In the **Expression** text field, type `n110`.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Slice 4

1 In the **Model Builder** window, click **Slice 4**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 In the **Expression** text field, type `n110`.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Annotation 2

1 In the **Model Builder** window, click **Annotation 2**.

2 In the **Settings** window for **Annotation**, locate the **Annotation** section.

3 In the **Text** text field, type `57.6 - 67.1 nm`.

4 Locate the **Plot Array** section. In the **Index** text field, type `1`.

Reactor Walls 1

1 In the **Model Builder** window, click **Reactor Walls 1**.

2 In the **Settings** window for **Surface**, locate the **Plot Array** section.

3 In the **Index** text field, type `1`.

Annotation 2, Reactor Walls 1, Slice 3, Slice 4

1 In the **Model Builder** window, under **Results** > **Concentration of Particles at Different Sizes**, Ctrl-click to select **Slice 3**, **Slice 4**, **Annotation 2**, and **Reactor Walls 1**.

2 Right-click and choose **Duplicate**.

Slice 5

1 In the **Settings** window for **Slice**, locate the **Expression** section.

2 In the **Expression** text field, type `n115`.

3 Locate the **Plot Array** section. In the **Index** text field, type `2`.

Slice 6

1 In the **Model Builder** window, click **Slice 6**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 In the **Expression** text field, type `n115`.

4 Locate the **Plot Array** section. In the **Index** text field, type `2`.

Annotation 3

1 In the **Model Builder** window, click **Annotation 3**.

2 In the **Settings** window for **Annotation**, locate the **Annotation** section.

3 In the **Text** text field, type `115 - 129 nm`.

4 Locate the **Plot Array** section. In the **Index** text field, type `2`.

Reactor Walls 1.1

1 In the **Model Builder** window, click **Reactor Walls 1.1**.

2 In the **Settings** window for **Surface**, locate the **Plot Array** section.

3 In the **Index** text field, type `2`.

Annotation 3, Reactor Walls 1.1, Slice 5, Slice 6

1 In the **Model Builder** window, under **Results** > **Concentration of Particles at Different Sizes**, Ctrl-click to select **Slice 5**, **Slice 6**, **Annotation 3**, and **Reactor Walls 1.1**.

2 Right-click and choose **Duplicate**.

Slice 7

1 In the **Settings** window for **Slice**, locate the **Expression** section.

2 In the **Expression** text field, type `n120`.

3 Locate the **Plot Array** section. In the **Index** text field, type `3`.

Slice 8

1 In the **Model Builder** window, click **Slice 8**.

2 In the **Settings** window for **Slice**, locate the **Expression** section.

3 In the **Expression** text field, type `n120`.

4 Locate the **Plot Array** section. In the **Index** text field, type `3`.

Annotation 4

1 In the **Model Builder** window, click **Annotation 4**.

2 In the **Settings** window for **Annotation**, locate the **Annotation** section.

3 In the **Text** text field, type `202 - 225 nm`.

4 Locate the **Plot Array** section. In the **Index** text field, type `3`.

Reactor Walls 1.1.1

1 In the **Model Builder** window, click **Reactor Walls 1.1.1**.

2 In the **Settings** window for **Surface**, locate the **Plot Array** section.

3 In the **Index** text field, type `3`.

Delete some superfluous plot groups.

Concentration, BaSO4, Surface (tds), Concentration, Ba_2p, Surface (tds), Concentration, Cl_1m, Surface (tds), Concentration, HSO4_1m, Surface (tds), Concentration, H_1p, Surface (tds), Population Number Density, n101, Streamline (pbsb2), Population Number Density, n101, Surface (pbsb2), Population Number Density, n111, Streamline (pbsb2), Population Number Density, n111, Surface (pbsb2), Population Number Density, n121, Streamline (pbsb2), Population Number Density, n121, Surface (pbsb2)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Concentration, Ba_2p, Surface (tds)**, **Concentration, BaSO4, Surface (tds)**, **Concentration, Cl_1m, Surface (tds)**, **Concentration, H_1p, Surface (tds)**, **Concentration, HSO4_1m, Surface (tds)**, **Population Number Density, n101, Streamline (pbsb2)**, **Population Number Density, n101, Surface (pbsb2)**, **Population Number Density, n111, Streamline (pbsb2)**, **Population Number Density, n111, Surface (pbsb2)**, **Population Number Density, n121, Streamline (pbsb2)**, and **Population Number Density, n121, Surface (pbsb2)**.

2 Right-click and choose **Delete**.

Lastly, use **Group** nodes to organize the result plots.

Average Size Distribution (pbsb), Concentration (re), Mass Balance, Size Intervals (pbsb), Supersaturation

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Concentration (re)**, **Average Size Distribution (pbsb)**, **Size Intervals (pbsb)**, **Supersaturation**, and **Mass Balance**.

2 Right-click and choose **Group**.

Perfectly Mixed Batch Reactor

In the **Settings** window for **Group**, type `Perfectly Mixed Batch Reactor` in the **Label** text field.

Average Size Distribution (pbsb2), Average Size Distribution at Specified z-Coordinates, Concentration of Particles at Different Sizes, Concentration, BaSO4, Streamline (tds), Concentration, Ba_2p, Streamline (tds), Concentration, Cl_1m, Streamline (tds), Concentration, HSO4_1m, Streamline (tds), Concentration, H_1p, Streamline (tds), Number of Particles and Supersaturation, Number of Particles, Surface (pbsb2), Pressure (spf), Size Intervals (pbsb2), Velocity (spf)

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Concentration, Ba_2p, Streamline (tds)**, **Concentration, BaSO4, Streamline (tds)**, **Concentration, Cl_1m, Streamline (tds)**, **Concentration, H_1p, Streamline (tds)**, **Concentration, HSO4_1m, Streamline (tds)**, **Velocity (spf)**, **Pressure (spf)**, **Number of Particles and Supersaturation**, **Number of Particles, Surface (pbsb2)**, **Size Intervals (pbsb2)**, **Average Size Distribution (pbsb2)**, **Average Size Distribution at Specified z-Coordinates**, and **Concentration of Particles at Different Sizes**.

2 Right-click and choose **Group**.

T-Mixer

In the **Settings** window for **Group**, type `T-Mixer` in the **Label** text field.