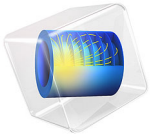

Precipitation of Barium Sulfate

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 $\mathrm{mol/m^3}$. 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. 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 $\mathrm{mol/m^3}$. The inlet velocity is adjusted to achieve a Reynolds number of 255 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.

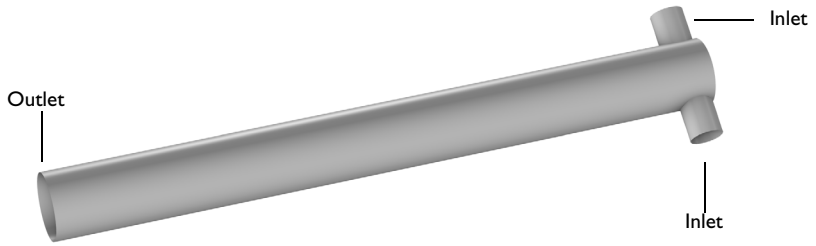

Figure 1: T-mixer geometry consisting of two inlet pipes and one main mixing pipe.

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

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

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

while the formation of crystalline barium sulfate takes place according to

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

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 from the reactant concentrations using the mean activity coefficient, γ, and the solubility product K_{SP} ($\mathrm{mol^2/m^6}$) according to

$$S = \gamma_{\pm} \sqrt{\frac{c_{\mathrm{Ba^{2+}}}\, c_{SO_4^{2-}}}{K_{\mathrm{SP}}}} \tag{1}$$

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

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

and

$$F_{Ba^{2+}} = \sum_a \left(\frac{(0.06 + 0.6B_{Ba^{2+},a})\left|Z_{Ba^{2+}} Z_a\right| \left(\frac{\left|Z_{Ba^{2+}}\right| + \left|Z_a\right|}{2} \right)^2 m_a}{\left(1 + \frac{1.5}{\left|Z_{Ba^{2+}} Z_a\right|} I_m\right)^2} \right) \tag{3}$$

$$F_{SO_4^{2-}} = \sum_c \left(\frac{(0.06 + 0.6B_{SO_4^{2-},c})\left|Z_{SO_4^{2-}} Z_c\right| \left(\frac{\left|Z_{SO_4^{2-}}\right| + \left|Z_c\right|}{2} \right)^2 m_c}{\left(1 + \frac{1.5}{\left|Z_{SO_4^{2-}} Z_c\right|} I_m\right)^2} \right) \tag{4}$$

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

$$B_{a,c} = B_a + B_c + \delta_a \delta_c \tag{5}$$

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

THE POPULATION BALANCE EQUATION

To model the population distribution as a function of particle size, the particle number density, n ($1/\mathrm{m}^4$), is defined as:

$$n = \frac{N}{L} \tag{6}$$

Where L describes the particle size expressed as particle diameter (m) and N is the number of particles per unit volume ($1/\mathrm{m}^3$). The change in particle number density with respect to time in a crystal particle population can be described using the population balance equation

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{u}n) + \frac{\partial (G(S,L)n(L))}{\partial L} = \frac{\nu}{S_c} \nabla^2 n + B_0 \delta(L - L_{c0}) \tag{7}$$

where

- 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 ($1/\mathrm{m}^4/\mathrm{s}$)
- 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. Here, the nucleation rate as a source of number density, B_0, correlates to the nucleation rate as a source of particle number, B_N ($1/m^3/s$), as $B_0 = B_N/L$, where B_N is defined according to classical nucleation theory as (Ref. 1, Ref. 3).

$$B_N = \frac{3}{2} D_{AB} \left(\sqrt{K_{SP} S N_A}\right)^{7/3} \sqrt{\frac{\gamma_{CL}}{k_B T}} V_m \exp\left(\frac{-16\pi}{3} \frac{\gamma_{CL}^3}{T^3 k_B^3} \frac{V_m^2}{(\ln S)^2}\right) \tag{8}$$

where

- D_{AB} is the apparent diffusion coefficient (m^2/s)
- N_A is the Avogadro number ($1/mol$)
- γ_{CL} 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

$$L_{c0} = \frac{4\gamma_{CL} V_m}{\nu_d k_B T \ln S} \tag{9}$$

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)

$$G = \frac{k_a}{3k_v} \frac{\mathrm{Sh} D_{AB} \sqrt{K_{SP}} M_{W,C} (S-1)}{\rho_C L} \tag{10}$$

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, $M_{W,C}$ is the crystal molar mass (kg/mol) and ρ_C the crystal density (kg/m^3).

CRYSTAL SIZE DISCRETIZATION

The continuous population balance equation (Equation 7) is discretized using a number of intervals (bins). Each interval, $i = 1, 2, 3, \ldots, I$, corresponds to a crystal-size interval

spanning from size L_{i-1} to L_i with an interval length ΔL_i. The smallest crystal size, L_0, is taken as the smallest stable crystal size, L_{c0}. Thus, the nucleation source term becomes the particle flux at the left-hand side face of the interval $i = 1$. The size points, L_i, are defined geometrically such that the interval length increases with the interval index according to (Ref. 1)

$$L_i = \frac{L_0 - 2^{(-I/q)} L_I}{1 - 2^{(-I/q)}} + 2^{(i-I)/q}\left(L_I - \frac{L_0 - 2^{(-I/q)} L_I}{1 - 2^{(-I/q)}}\right) \tag{11}$$

The model implements 100 size intervals in the perfectly mixed reactor and 30 for the T-mixer scenario covering crystal sizes from 0.82 to 500 nm. The discretized population balance equations for each crystal size interval is modeled with a Global ODEs and DAEs interface in 0D and separate Stabilized Convection-Diffusion Equation interfaces in 3D with nucleation and growth added as source terms.

The growth-rate term in the PBE (Equation 7) is approximated with a total variation diminishing scheme blending central and backward differences according to (Ref. 5)

$$\frac{\partial (Gn)_i}{\partial L} = \frac{(Gn)_i - (Gn)_{i-1}}{\Delta L_i} \tag{12}$$

where

$$(Gn)_i = G_i\left(n_i + \frac{1}{2}\Phi\left(\frac{n_{i+1} - n_i + \varepsilon}{n_i - n_{i-1} + \varepsilon}\right)(n_i - n_{i-1})\right), \tag{13}$$

Here, Φ is a limiting function to reduce numerical fluctuations and ε is a built-in nonzero constant to avoid division by zero. The limiting function, initially introduced by Koren in Ref. 6, is implemented according to

$$\Phi(r) = \max\left(0, \min\left(2r, \min\left(\frac{\frac{1-\kappa}{4}}{\frac{1-\kappa}{4} + \frac{1+\kappa}{4}} + \frac{\frac{1+\kappa}{4}}{\frac{1-\kappa}{4} + \frac{1+\kappa}{4}} r, 2\right)\right)\right) \tag{14}$$

where $\kappa \in [-1, 1]$ is the blending constant. At $\kappa = -1$, the approximation takes on the form of a second-order backward finite-element scheme and at $\kappa = 1$ a first-order central scheme. The number density of all intervals smaller than the smallest defined interval is assumed to be zero while the number density of intervals at crystal sizes greater than the largest defined size is assumed to be equal to the largest defined interval. Here, Equation 13 represents the growth-induced particle flux at the right-hand side interval

face. The left-hand side particle flux, $(Gn)_{i-1}$, is similarly written by reducing the interval index by 1.

REACTION RATE

The reaction rate, r, resulting from the formation of crystalline barium sulfate, in units of $mol/m^3/s$, is expressed using the nucleation and growth rates according to

$$r = \frac{\rho_c}{M_{W,C}}\left(B_{nuc}L_0{}^3 k_v \Delta L_1 + \sum_i^I \left(\frac{L_i + L_{i-1}}{2}\right)^3 k_v \frac{\partial (Gn)_i}{\partial L}\Delta L_i\right) \quad (15)$$

The reaction rate is added as a consumption term to the barium and sulfate species in the Chemistry interface. Assuming that aqueous barium sulfate is in equilibrium with barium and sulfate ions, the consumption term can instead be added to aqueous barium sulfate. The discretized equations along with the required sum expressions are generated with the Crystal PBE Discretization add-in, available in the Chemical Reaction Engineering Module Add-in Library.

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.

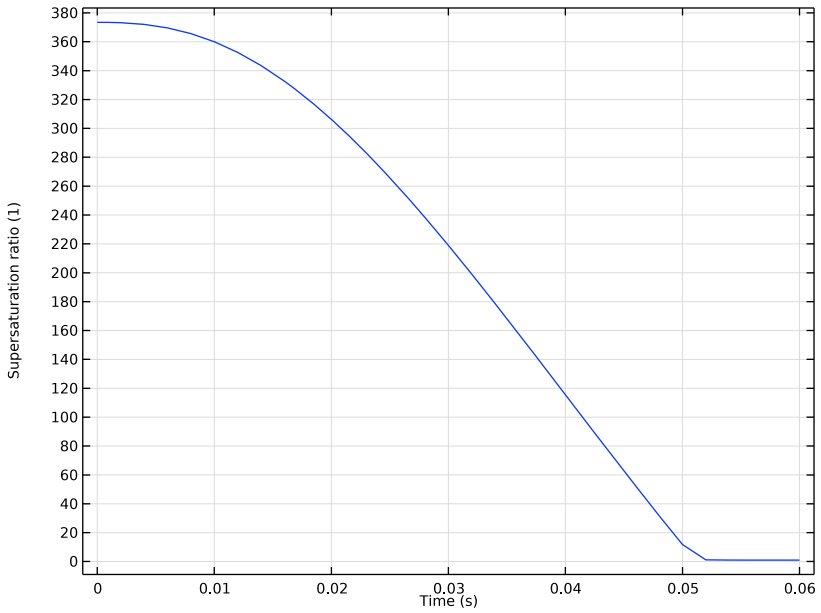

Figure 2: Supersaturation as a function of time in a perfectly mixed batch reactor.

The size distribution of crystals formed from the supersaturation over time is shown in Figure 3. The density distribution is normalized by the total amount of crystal particles per unit volume at each time.

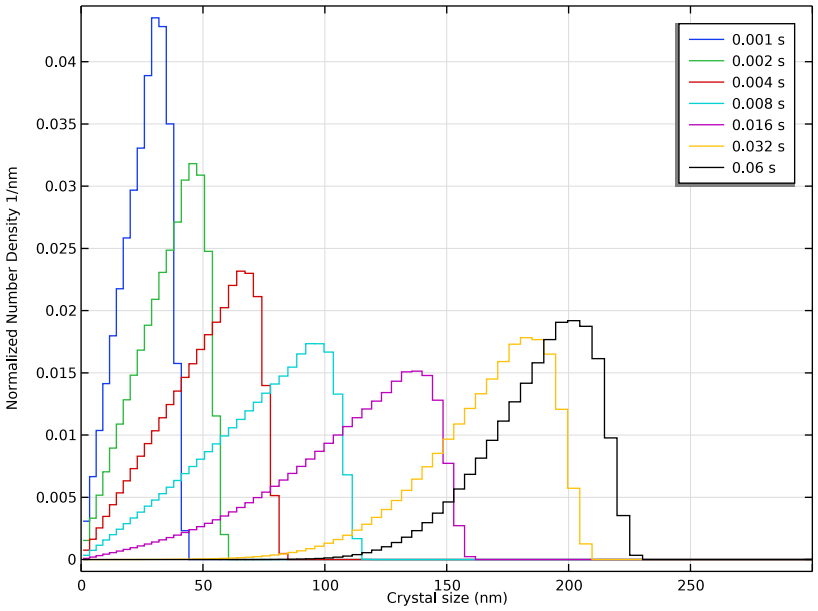

Figure 3: Normalized density distribution at various times in a perfectly mixed batch reactor.

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

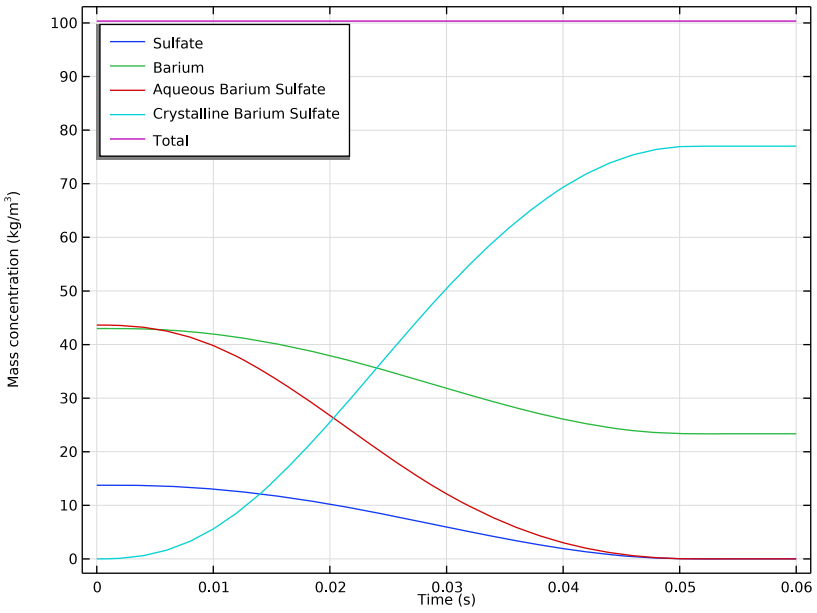

Figure 4: Mass concentrations of reacting species and crystalline product over time.

T-MIXER

The computed velocity field 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.

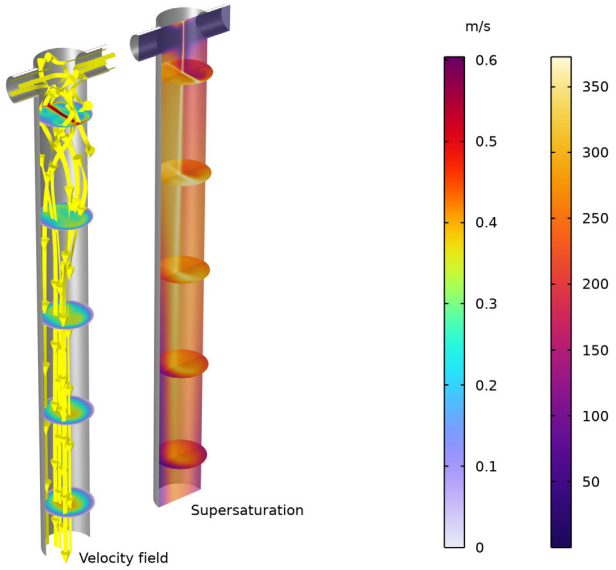

Figure 5: Velocity field and supersaturation in the T-mixer.

The density distribution at different points along the main mixing channel is shown in Figure 6. The distribution at $z = 9.375$ mm and $z = 8.75$ mm represent a very small number of crystals. At these crystal sizes the distribution is highly dependent on the mesh. To a lesser degree this is also true for distributions at larger crystal sizes.

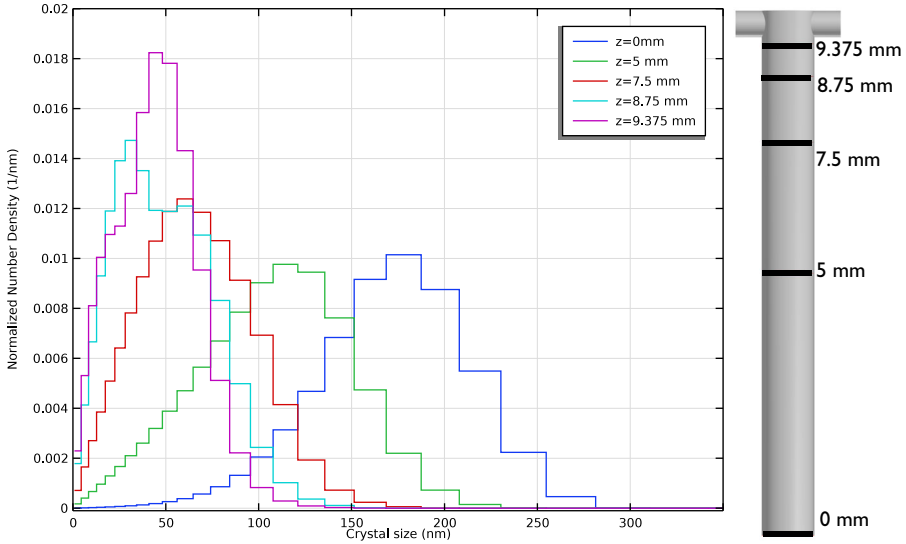

Figure 6: Number density distribution at various points along the T-mixer main mixing channel.

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.

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6. B. Koren, "A robust upwind discretization method for advection, diffusion and source terms," *Notes Numer. Fluid Mech.*, vol. 45, pp. 117–138, 1993.

Application Library path: `Chemical_Reaction_Engineering_Module/Mixing_and_Separation/barium_sulfate_precipitation`

Modeling Instructions

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

NEW

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

2 In the **Home** toolbar, click **Windows** and choose **Add-in Libraries**.

ADD-IN LIBRARIES

1 In the **Add-in Libraries** window, select **Chemical Reaction Engineering Module> population_balance_equation_discretization** in the tree.

2 In the tree, clear the check box for the node **Chemical Reaction Engineering Module> population_balance_equation_discretization**.

3 In the tree, select the check box for the node **Chemical Reaction Engineering Module> population_balance_equation_discretization**.

4 Click **Done**.

5 In the **Developer** toolbar, click **Add-ins** and choose **Population Balance Equation Discretization>Population Balance Equation Discretization**.

Import the parameters for the model from a separate file.

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, 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 Hückel constants

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Debye Hückel 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`.

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

Ion interaction

1 In the **Home** toolbar, click **Functions** and choose **Global>Analytic**.

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
I	mol/kg

ADD COMPONENT

In the **Home** toolbar, click **Add Component** and choose **0D**.

Import the required variable expressions for the Debye-Hückel model and the nucleation rate from separate files.

DEFINITIONS

Activity coefficient (Debye Hückel model)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Activity coefficient (Debye Hückel model)` 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_debye_huckel_model1.txt`.

Nucleation rate

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Nucleation rate` 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_nucleation_rate.txt`.

ADD PHYSICS

1 In the **Home** toolbar, click **Windows** and choose **Add Physics**.

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

3 In the tree, select **Chemical Species Transport>Reaction Engineering (re)**.

4 Click **Add to Component 1** in the window toolbar.

REACTION ENGINEERING (RE)

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

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

Reaction 1

1 Right-click **Component 1 (comp1)>Reaction Engineering (re)** and choose **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_j text field, type `K_dis`.

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 `BaSO4 = Ba(++) + SO4(2-)`.

4 Click **Apply**.

5 Locate the **Equilibrium Settings** section. In the K_j text field, type `K_ip`.

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(-)`.

Species: SO4(2-)

1 In the **Model Builder** window, click **Species: SO4(2-)**.

2 In the **Settings** window for **Species**, click to expand the **Reaction Rate** section.

3 From the list, choose **User defined**.

4 In the R_i text field, type `re.r_1+re.r_2-r_c_sum`.

Species: Ba(++)

1 In the **Model Builder** window, click **Species: Ba(++)**.

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

3 From the list, choose **User defined**.

4 In the R_i text field, type `re.r_2-r_c_sum`.

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`

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component>3D**.

Import variable expressions for the Debye-Hückel model and nucleation rate from separate files.

DEFINITIONS (COMP2)

Activity coefficient (Debye Hückel model)

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Activity coefficient (Debye Hückel model)` 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_debye_huckel_model2.txt`.

Nucleation rate

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Nucleation rate` 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_nucleation_rate.txt`.

GEOMETRY 1

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 `2*D`.

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

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`.

Work Plane 2 (wp2)

1 In the **Model Builder** window, right-click **Geometry 1** and choose **Work Plane**.

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

3 From the **Plane** list, choose **yz-plane**.

Work Plane 2 (wp2)>Plane Geometry

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

Work Plane 2 (wp2)>Rectangle 1 (r1)

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

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

3 In the **Width** text field, type `D`.

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

5 Locate the **Position** section. In the **xw** text field, type `-D/2`.

Ignore Faces 1 (igf1)

1 In the **Model Builder** window, under **Component 2 (comp2)>Geometry 1** right-click **Work Plane 2 (wp2)** and choose **Virtual Operations>Ignore Faces**.

2 On the object **fin**, select Boundaries 12–17, 28–31, 35, and 38 only.

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

ADD MATERIAL FROM LIBRARY

In the **Home** toolbar, click **Windows** and choose **Add Material from Library**.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-in>Water, liquid**.

3 Click **Add to Component** in the window toolbar.

ADD PHYSICS

1 In the **Home** toolbar, click **Windows** and choose **Add Physics**.

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

3 In the tree, select **Chemical Species Transport>Chemistry (chem)**.

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

CHEMISTRY (CHEM)

Reaction 1

1 Right-click **Component 2 (comp2)>Chemistry (chem)** and choose **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 **Rate Constants** section. In the k^{f} text field, type `1e5`.

6 Select the **Specify equilibrium constant** check box.

7 Locate the **Equilibrium Settings** section. From the **Equilibrium constant** list, choose **User defined**.

8 In the K_j text field, type `K_dis`.

Reaction 2

1 In the **Physics** toolbar, click **Domains** and choose **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 **Rate Constants** section. In the k^{f} text field, type `1e5`.

6 Select the **Specify equilibrium constant** check box.

7 Locate the **Equilibrium Settings** section. From the **Equilibrium constant** list, choose **User defined**.

8 In the K_j text field, type `1/K_ip`.

Species 1

1 In the **Physics** toolbar, click **Domains** and choose **Species**.

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

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

4 In the **Physics** toolbar, click **Domains** and choose **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**.

Species: SO4(2-)

1 In the **Model Builder** window, click **Species: SO4(2-)**.

2 In the **Settings** window for **Species**, click to expand the **Reaction Rate** section.

3 From the list, choose **User defined**.

4 In the R_i text field, type `chem.r_1-chem.r_2-r_c_sum`.

Species: Ba(++)

1 In the **Model Builder** window, click **Species: Ba(++)**.

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

3 From the list, choose **User defined**.

4 In the R_i text field, type `-chem.r_2-r_c_sum`.

5 In the **Model Builder** window, click **Chemistry (chem)**.

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

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

ADD PHYSICS

1 In the **Home** toolbar, click **Windows** and choose **Add Physics**.

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

3 In the tree, select **Fluid Flow>Single-Phase Flow>Laminar Flow (spf)**.

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

LAMINAR FLOW (SPF)

Inlet 1

1 Right-click **Component 2 (comp2)>Laminar Flow (spf)** 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 Boundary 1 only.

Inlet 2

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 Boundary 26 only.

Outlet 1

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

2 Select Boundaries 8 and 15 only.

3 In the **Model Builder** window, click **Laminar Flow (spf)**.

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

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

GLOBAL DEFINITIONS

Default Model Inputs

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

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General>Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T`.

ADD PHYSICS

1 In the **Home** toolbar, click **Windows** and choose **Add Physics**.

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

3 In the tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

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

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Settings** window for **Transport of Diluted Species**, click to expand the **Dependent Variables** section.

2 In the **Number of species** text field, type `6`.

3 In the **Concentrations (mol/m³)** table, enter the following settings:

`cBa_2p`
`cSO4_2m`
`cHSO4_1m`
`cH_1p`
`cCl_1m`
`cBaSO4`

Transport Properties 1

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

2 In the **Settings** window for **Transport Properties**, locate the **Convection** section.

3 From the **u** list, choose **Velocity field (spf)**.

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

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

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

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

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

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

Initial Values 1

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

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

3 In the $cBa_{2\mathrm{p}}$ text field, type `cBa_2p_0`.

4 In the $cSO4_{2\mathrm{m}}$ text field, type `cSO4_2m_0`.

5 In the $cHSO4_{1\mathrm{m}}$ text field, type `cHSO4_1m_0`.

6 In the $cH_{1\mathrm{p}}$ text field, type `cH_1p_0`.

7 In the $cCl_{1\mathrm{m}}$ text field, type `cCl_1m_0`.

Inflow 1

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

2 Select Boundary 26 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 $c_{0,\mathrm{cCl1m}}$ text field, type `cCl_1m_0`.

Inflow 2

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 $c_{0,\mathrm{cSO42m}}$ text field, type `cSO4_2m_0`.

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

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

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

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

3 From the R_{cBa2p} list, choose **Reaction rate for species Ba_2p (chem)**.

4 From the R_{cSO42m} list, choose **Reaction rate for species SO4_2m (chem)**.

5 From the $R_{cHSO41m}$ list, choose **Reaction rate for species HSO4_1m (chem)**.

6 From the R_{cH1p} list, choose **Reaction rate for species H_1p (chem)**.

7 From the R_{cCl1m} list, choose **Reaction rate for species Cl_1m (chem)**.

8 From the R_{cBaSO4} list, choose **Reaction rate for species BaSO4 (chem)**.

9 Click to expand the **Equation** section. Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

Outflow 1

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

2 Select Boundaries 8 and 15 only.

CHEMISTRY (CHEM)

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

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

3 From the **Species solved for** list, choose **Transport of Diluted Species**.

4 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(-)	Free species	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

MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Normal**.

Information 1

In the **Model Builder** window, right-click **Mesh 1** and choose **Build All**.

MESH 2

1 In the **Mesh** toolbar, click **Add Mesh** and choose **Add Mesh**.

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)>Meshes>Mesh 2** click **Size**.

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

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `5E-5`.

5 In the **Minimum element size** text field, type `2E-5`.

6 In the **Curvature factor** text field, type `0.6`.

7 In the **Resolution of narrow regions** text field, type `0.5`.

Size 1

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

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

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section.

5 Select the **Maximum element size** check box. In the associated text field, type `4E-5`.

6 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 Domains 1 and 4 only.

Swept 1

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

2 Right-click **Mesh 2** 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 box, 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 `50`.

5 In the **Element ratio** text field, type `10`.

Boundary Layers 2

In the **Mesh** toolbar, click  **Boundary Layers**.

Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 Select Boundaries 13 and 16 only.

3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.

4 In the **Number of layers** text field, type `10`.

5 In the **Stretching factor** text field, type `1`.

6 From the **Thickness specification** list, choose **First layer**.

7 In the **Thickness** text field, type `0.8E-5`.

Boundary Layers 2

1 In the **Model Builder** window, click **Boundary Layers 2**.

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

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**.

The discretized population balance equation will be described using the imported add-in.

GLOBAL DEFINITIONS

Population Balance Equation Discretization 1

1 In the **Model Builder** window, under **Global Definitions** click **Population Balance Equation Discretization 1.**

2 In the **Smallest particle size** text field, type 0.82.

3 In the **Largest particle size** text field, type 500.

4 In the **Settings** window for **Population Balance Equation Discretization**, select the **0D component** check box.

5 Choose **0D Component (comp1)** from the **0D component** list.

6 Select the **3D component** check box.

7 Choose **3D Component (comp2)** from the **3D component** list.

8 Locate the **0D Component** section. In the text field **Number of intervals**, type 100.

9 Click the **Geometric** button.

10 In the **Geometric constant** text field, type 60.

11 Locate the **3D Component** section. In the text field **Number of intervals**, type 30.

12 Click the **Geometric** button.

13 In the **Geometric constant** text field, type 8.

14 Locate the **Growth Rate Approximation** section.

15 Click the **Total variation diminishing** button.

16 In the text field **Blending constant**, type 1/3.

17 Locate the **Generate Default Plots** section.

18 Select the **Generate default plots** check box.

19 At the top of the settings window, click **Create/Refresh**.

After running the add-in, a growth rate function, crystal parameters and supersaturation and nucleation expressions need to be added.

GLOBAL DEFINITIONS

Growth Rate (GL)

1 In the **Model Builder** window, under **Global Definitions** click **Growth Rate (GL)**.

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

3 In the **Expression** text field, type `k_a/(3*k_v)*Sh*D_AB*sqrt(K_sp)*M_C*(S-1)/rho_C/L`.

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

Argument	Unit
L	m
S	(mol/m^3)*(mol/m^3)/(mol^2/m^6)

Crystal properties

1 In the **Model Builder** window, click **Crystal properties**.

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

3 In the table, enter the following settings:

Name	Expression	Value	Description
k_v	pi/6	0.5236	Crystal volume shape factor
rho_C	rho_BaSO4	4480 kg/m³	Crystal density
M_C	M_BaSO4	0.23338 kg/mol	Crystal molecular weight
nstart	1e10	1E10	Initial number density

DEFINITIONS (COMP1)

Crystallization variables

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions** click **Crystallization variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
S	gamma*sqrt(max(eps,re.c_Ba_2p*re.c_SO4_2m/K_sp))		Supersaturation ratio
B0	B_0	1/(m^4·s)	Nucleation rate as source of number density

DEFINITIONS (COMP2)

1 In the **Model Builder** window, under **Component 2 (comp2)>Definitions** click **Crystallization variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
S	`gamma* sqrt(max(eps, cBa_2p* cSO4_2m/ K_sp))`		`Supersaturation ratio`
B0	`B_0`	$1/(m^4 \cdot s)$	`Nucleation rate as source of number density`

Select the inlet of the T-mixer.

Inlet selection

1 In the **Model Builder** window, expand the **Component 2 (comp2)>Definitions>Selections** node, then click **Inlet selection**.

2 Select Boundaries 1 and 26 only.

ADD STUDY

1 In the **Home** toolbar, click **Windows** and choose **Add Study**.

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

3 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for all interfaces apart from **Reaction Engineering (RE)** and **Global ODEs and DAEs (ge)**.

4 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

5 Click **Add Study** in the window toolbar.

STUDY 1

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

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

3 Clear the **Generate default plots** check box.

Solution 1 (sol1)

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

COMPONENT 1 (COMP1)

In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

STUDY 1

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

Solver Configurations

In the **Model Builder** window, expand the **Study 1>Solver Configurations** node.

Solution 1 (sol1)

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

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

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

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)`.

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

RESULTS

Particle Number Density Distribution 1

1 In the **Model Builder** window, expand the **Results** node, then click **Particle Number Density Distribution 1**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

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

6 In the **Particle Number Density Distribution 1** toolbar, click **Plot**.

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

8 Locate the **Plot Settings** section.

9 Select the **x-axis label** check box. In the associated text field, type `Crystal size (nm)`.

10 Select the **y-axis label** check box. In the associated text field, type `Normalized Number Density 1/nm`.

11 Locate the **Axis** section. Select the **Manual axis limits** check box.

12 In the **x minimum** text field, type 0.

13 In the **x maximum** text field, type 300.

14 In the **Model Builder** window, expand the **Particle Number Density Distribution 1** node.

Line Segments 1

1 In the **Model Builder** window, expand the **Particle Number Density Distribution 1** node, then click **Line Segments 1**.

2 In the **Settings** window for **Line Segments**, click to expand the **Legends** section.

3 Select the **Show legends** check box.

4 In the **Particle Number Density Distribution 1** toolbar, click **Plot**.

Discretized points 1

1 In the **Model Builder** window, under **Results** click **Discretized points 1**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

4 From the **Time selection** list, choose **Last**.

5 In the **Discretized points 1** 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**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

5 In the **Label** text field, type `Supersaturation`.

Global 1

1 Right-click **Supersaturation** and choose **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
`comp1.S`	1	`Supersaturation ratio`

5 Click to expand the **Legends** section. Clear the **Show legends** check box.

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 **Data** section. From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

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

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** check box. In the associated text field, type `Time (s)`.

7 Select the **y-axis label** check box. In the associated text field, type `Mass concentration (kg/m<SUP>3</SUP>)`.

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

Global 1

1 Right-click **Mass Balance** and choose **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
`(comp1.re.c_HSO4_1m+ comp1.re.c_SO4_2m)* M_SO4_2m`	`kg/m^3`	`Sulfate mass concentration`
`M_Ba_2p*comp1.re.c_Ba_2p`	`kg/m^3`	`Barium mass concentration`
`M_C*comp1.re.c_BaSO4`	`kg/m^3`	`Barium sulfate mass concentration`
`comp1.M_c_sum`	`kg/m^3`	`Total crystal mass concentration`
`M_SO4_2m* (comp1.re.c_SO4_2m+ comp1.re.c_HSO4_1m)+ M_Ba_2p*comp1.re.c_Ba_2p+ M_C*comp1.re.c_BaSO4+ comp1.M_c_sum`	`kg/m^3`	`Total mass concentration`

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

6 In the table, enter the following settings:

Legends
`Sulfate`
`Barium`

Legends
Aqueous Barium Sulfate
Crystalline Barium Sulfate
Total

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

Discretized points 1, Mass Balance, Particle Number Density Distribution 1, Supersaturation

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Particle Number Density Distribution 1**, **Discretized points 1**, **Supersaturation**, and **Mass Balance**.

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

RESULTS

Perfectly Mixed Batch Reactor

1 In the **Model Builder** window, under **Results** click **Group 1**.

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

ADD STUDY

The study used to solve for crystallization in the T-mixer is generated by a model method added to the **Application Builder**. Note that the method editor is only available in the Windows® version of the COMSOL desktop. To see the method, please refer to the method **generateStudy** under **methods** in the existing model file **barium_sulfate_precipitation**.

STUDY 2

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

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

3 Clear the **Generate default plots** check box.

4 In the **Home** toolbar, click **Compute**.

RESULTS

Create Evaluation Groups

To evaluate the crystal number density distribution at various points along the T-mixer, additional evaluation groups with a set normal (in z-direction) are required. This is done with a model method, similar to how **Study 2** was set up.

NEW METHOD

1 In the **Developer** toolbar, click  **New Method**.

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

3 Click **OK**.

APPLICATION BUILDER

generateEvaluationGroups

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

2 Copy the following code into the **generateEvaluationGroups** method editor window:

```
int N = 30;
for (int i3 = 1; i3 <= 4; i3++) {
 model.result().evaluationGroup().create("eg_densdistr"+toString(i3),
"EvaluationGroup");
 model.result().evaluationGroup("eg_densdistr"+toString(i3)).create("gev1",
"EvalGlobal");
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").set("data", "dset2");
 model.result().evaluationGroup("eg_densdistr"+toString(i3)).create("int1",
"IntSurface");
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int1").set("intvolume", true);
 model.result().evaluationGroup("eg_densdistr"+toString(i3)).create("int2",
"IntSurface");
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int2").set("intvolume", true);
 model.result().evaluationGroup("eg_densdistr"+toString(i3)).create("int3",
"IntSurface");
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int3").set("intvolume", true);
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").set("expr", new String[]{});
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").set("descr", new String[]{});
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").setIndex("expr", "comp2.LO", 0);
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int1").setIndex("expr", "comp2.n1"+"*w+(scdeq"+
".dfluxz)", 0);
 model.result().evaluationGroup("eg_densdistr"+
```

```
toString(i3)).feature("int1").setIndex("expr", "comp2.n1"+"*w+(scdeq"+
".dfluxz)", 1);

 int i2 = 1;
 for (int i = 1; i <= N; i++) {
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").setIndex("expr", "comp2.L"+toString(i), i2);
 if (i > 1) {
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int1").setIndex("expr", "comp2.n"+toString(i)+"*w+
(scdeq"+toString(i)+".dfluxz)", i2-1);
 }
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int2").setIndex("expr", "w", i2-1);
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int3").setIndex("expr", "comp2.N_c*w", i2-1);
 i2 = i2+1;
 if (i > 1) {
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int1").setIndex("expr", "comp2.n"+toString(i)+"*w+
(scdeq"+toString(i)+".dfluxz)", i2-1);
 }
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int2").setIndex("expr", "w", i2-1);
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("int3").setIndex("expr", "comp2.N_c*w", i2-1);
 if (i < N) {
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").setIndex("expr", "comp2.L"+toString(i), i2);
 }
 i2 = i2+1;
 }
 for (int i = 0; i <= i2-2; i++) {
 model.result().evaluationGroup("eg_densdistr"+
toString(i3)).feature("gev1").setIndex("unit", "nm", i);
 }
 with(model.result().evaluationGroup("eg_densdistr"+toString(i3)));
 set("type", "general");
 set("generalexpr", "(int1/int2)/(int3/int2)*1e-9");
 set("keepchildnodes", true);
 set("includeparameters", false);
 set("concatenation", "vertical");
 endwith();
}
```

METHODS

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

GLOBAL DEFINITIONS

Click **Method Call** and choose **generateEvaluationGroups**.

GenerateEvaluationGroups 1

In the **Model Builder** window, under **Global Definitions** right-click **GenerateEvaluationGroups 1** and choose **Run**.

RESULTS

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

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 **Data** section.
4. From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.
5. Locate the **Plane Data** section. From the **Plane type** list, choose **General**.
6. From the **Plane entry method** list, choose **Point and normal vector**.
7. Find the **Point** subsection. In the **z** text field, type `5e-3`.
8. Right-click **Cut Plane 1** and choose **Duplicate**.

Cut Plane 2

1. In the **Model Builder** window, click **Cut Plane 2**.
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`.
4. Right-click **Cut Plane 2** and choose **Duplicate**.

Cut Plane 3

1. In the **Model Builder** window, click **Cut Plane 3**.
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`.
4. Right-click **Cut Plane 3** and choose **Duplicate**.

Cut Plane 4

1. In the **Model Builder** window, click **Cut Plane 4**.
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`.

Density Distribution Evaluation Group

1. In the **Model Builder** window, under **Results** click **Density Distribution Evaluation Group**.
2. In the **Settings** window for **Evaluation Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

Surface Integration 1

1 In the **Model Builder** window, expand the **Density Distribution Evaluation Group** node, then click **Surface Integration 1**.

2 Select Boundaries 8 and 15 only.

Surface Integration 2

1 In the **Model Builder** window, click **Surface Integration 2**.

2 Select Boundaries 8 and 15 only.

Surface Integration 3

1 In the **Model Builder** window, click **Surface Integration 3**.

2 Select Boundaries 8 and 15 only.

Density Distribution Evaluation Group

1 In the **Model Builder** window, click **Density Distribution Evaluation Group**.

2 In the **Density Distribution Evaluation Group** toolbar, click **Evaluate**.

Evaluation Group 1

1 In the **Model Builder** window, click **Evaluation Group 1**.

2 In the **Settings** window for **Evaluation Group**, locate the **Data** section.

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

4 In the **Evaluation Group 1** toolbar, click **Evaluate**.

Evaluation Group 2

1 In the **Model Builder** window, click **Evaluation Group 2**.

2 In the **Settings** window for **Evaluation Group**, locate the **Data** section.

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

4 In the **Evaluation Group 2** toolbar, click **Evaluate**.

Evaluation Group 3

1 In the **Model Builder** window, click **Evaluation Group 3**.

2 In the **Settings** window for **Evaluation Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane 3**.

4 In the **Evaluation Group 3** toolbar, click **Evaluate**.

Evaluation Group 4

1 In the **Model Builder** window, click **Evaluation Group 4**.

2 In the **Settings** window for **Evaluation Group**, locate the **Data** section.

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

4 In the **Evaluation Group 4** toolbar, click **Evaluate**.

Particle Number Density Distribution 2

1 In the **Model Builder** window, click **Particle Number Density Distribution 2**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

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

4 Locate the **Plot Settings** section. Select the **x-axis label** check box.

5 Select the **y-axis label** check box.

6 In the **x-axis label** text field, type `Crystal size (nm)`.

7 In the **y-axis label** text field, type `Normalized Number Density (1/nm)`.

Table Graph 1

1 In the **Model Builder** window, expand the **Particle Number Density Distribution 2** node, then click **Table Graph 1**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 Select the **Row-based** check box.

4 From the **x-axis data** list, choose **Row 2**.

5 From the **Plot rows** list, choose **Manual**.

6 In the **Rows** list, select **Row 1**.

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

8 Select the **Show legends** check box.

9 In the table, enter the following settings:

Legends
z=0mm

10 Right-click **Table Graph 1** and choose **Duplicate**.

Table Graph 2

1 In the **Model Builder** window, click **Table Graph 2**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Evaluation group** list, choose **Evaluation Group 1**.

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

Legends
z=5 mm

5 Right-click **Table Graph 2** and choose **Duplicate**.

Table Graph 3

1 In the **Model Builder** window, click **Table Graph 3**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Evaluation group** list, choose **Evaluation Group 2**.

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

Legends
z=7.5 mm

5 Right-click **Table Graph 3** and choose **Duplicate**.

Table Graph 4

1 In the **Model Builder** window, click **Table Graph 4**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Evaluation group** list, choose **Evaluation Group 3**.

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

Legends
z=8.75 mm

5 Right-click **Table Graph 4** and choose **Duplicate**.

Table Graph 5

1 In the **Model Builder** window, click **Table Graph 5**.

2 In the **Settings** window for **Table Graph**, locate the **Legends** section.

3 In the table, enter the following settings:

Legends
z=9.375 mm

4 Locate the **Data** section. From the **Evaluation group** list, choose **Evaluation Group 4**.

Particle Number Density Distribution 2

1 In the **Model Builder** window, click **Particle Number Density Distribution 2**.

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

3 Select the **Manual axis limits** check box.

4 In the **x minimum** text field, type `0`.

5 In the **x maximum** text field, type `350`.

6 In the **y minimum** text field, type `-1e-4`.

7 In the **y maximum** text field, type `0.02`.

8 In the **Particle Number Density Distribution 2** toolbar, click **Plot**.

Velocity Field, Supersaturation and Concentrations

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

4 In the **Label** text field, type `Velocity Field, Supersaturation and Concentrations`.

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

6 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

7 Locate the **Color Legend** section. Select the **Show units** check box.

8 From the **Position** list, choose **Right double**.

9 Click to expand the **Plot Array** section. Select the **Enable** check box.

Slice 1

1 Right-click **Velocity Field, Supersaturation and Concentrations** and choose **Slice**.

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

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

4 Click to expand the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Slice**, click to expand the **Plot Array** section.

8 Select the **Manual indexing** check box.

Surface 1

1 In the **Model Builder** window, right-click **Velocity Field, Supersaturation and Concentrations** and choose **Surface**.

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

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

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

Selection 1

1 Right-click **Surface 1** and choose **Selection**.

2 Select Boundaries 4, 5, 7, 10, 20, 21, 24, and 25 only.

Material Appearance 1

1 In the **Model Builder** window, right-click **Surface 1** and choose **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)**.

Streamline 1

1 In the **Model Builder** window, right-click **Velocity Field, Supersaturation and Concentrations** and choose **Streamline**.

2 Select Boundary 1 only.

3 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

4 In the **Number** text field, type `3`.

5 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Ribbon**.

6 Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

7 Select the **Scale factor** check box. In the associated text field, type `0.0016`.

8 From the **Color** list, choose **Yellow**.

9 Click to expand the **Plot Array** section. Select the **Manual indexing** check box.

10 Right-click **Streamline 1** and choose **Duplicate**.

Streamline 2

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

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

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

4 Select Boundary 26 only.

Slice 2

1 In the **Model Builder** window, right-click **Velocity Field, Supersaturation and Concentrations** and choose **Slice**.

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

3 In the **Expression** text field, type S.

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

5 In the **Planes** text field, type 1.

6 Click to expand the **Coloring and Style** section. Click  **Change Color Table**.

7 In the **Color Table** dialog box, select **Thermal>HeatCamera** in the tree.

8 Click **OK**.

9 In the **Settings** window for **Slice**, locate the **Plot Array** section.

10 Select the **Manual indexing** check box.

11 In the **Index** text field, type 1.

Slice 1, Surface 1

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 1** and **Surface 1**.

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

Transparency 1

1 In the **Model Builder** window, right-click **Slice 2** and choose **Transparency**.

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

3 Set the **Transparency** value to **0.4**.

Slice 3

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations** click **Slice 3**.

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

3 In the **Expression** text field, type S.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice 2**.

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

Surface 2

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

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

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

Slice 2, Slice 3, Surface 2

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 2**, **Slice 3**, and **Surface 2**.

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

Slice 4, Slice 5, Surface 3

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 4**, **Slice 5**, and **Surface 3**.

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

3 In the **Expression** text field, type `cBaSO4`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Slice**, locate the **Plot Array** section.

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

Slice 5

1 In the **Model Builder** window, click **Slice 5**.

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

3 In the **Expression** text field, type `cBaSO4`.

4 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 4**.

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

Surface 3

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

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

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

Slice 4, Slice 5, Surface 3

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 4**, **Slice 5**, and **Surface 3**.

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

Slice 6, Slice 7, Surface 4

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 6**, **Slice 7**, and **Surface 4**.

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

3 In the **Expression** text field, type `cSO4_2m`.

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

Slice 7

1 In the **Model Builder** window, click **Slice 7**.

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

3 In the **Expression** text field, type `cSO4_2m`.

4 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 6**.

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

Surface 4

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

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

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

Slice 6, Slice 7, Surface 4

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 6**, **Slice 7**, and **Surface 4**.

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

Slice 8, Slice 9, Surface 5

1 In the **Model Builder** window, under **Results>Velocity Field, Supersaturation and Concentrations**, Ctrl-click to select **Slice 8**, **Slice 9**, and **Surface 5**.

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

3 In the **Expression** text field, type `cBa_2p`.

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

Slice 9

1 In the **Model Builder** window, click **Slice 9**.

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

3 In the **Expression** text field, type `cBa_2p`.

4 Locate the **Inherit Style** section. From the **Plot** list, choose **Slice 8**.

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

Surface 5

1 In the **Model Builder** window, click **Surface 5**.

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

3 In the **Index** text field, type `4`.

Annotation 1

1 In the **Model Builder** window, right-click **Velocity Field, Supersaturation and Concentrations** and choose **Annotation**.

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

3 In the **Text** text field, type `Velocity field`.

4 Click to expand the **Coloring and Style** section. Clear the **Show point** check box.

5 Right-click **Annotation 1** and choose **Duplicate**.

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 `Supersaturation`.

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

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 `Aqueous barium sulfate`.

4 Right-click **Annotation 3** and choose **Duplicate**.

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 `Sulfate`.

4 Right-click **Annotation 4** and choose **Duplicate**.

Annotation 5

1 In the **Model Builder** window, click **Annotation 5**.

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

3 In the **Text** text field, type `Barium`.

4 In the **Velocity Field, Supersaturation and Concentrations** toolbar, click **Plot**.

Size bins

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 (sol2)**.

4 In the **Label** text field, type `Size bins`.

5 Locate the **Color Legend** section. From the **Position** list, choose **Right double**.

6 Locate the **Plot Array** section. Select the **Enable** check box.

7 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Slice 1

1 Right-click **Size bins** and choose **Slice**.

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

3 In the **Expression** text field, type `n5`.

4 Click to expand the **Coloring and Style** section. Click  **Change Color Table**.

5 In the **Color Table** dialog box, select **Rainbow>Prism** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Slice**, click to expand the **Title** section.

8 From the **Title type** list, choose **Manual**.

9 In the **Title** text area, type `n5 (1/m<SUP>4</SUP>)`.

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

11 Locate the **Plot Array** section. Select the **Manual indexing** check box.

Slice 2

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

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

3 In the **Expression** text field, type `n5`.

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

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

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

7 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Slice 1**.

8 Locate the **Plot Array** section. Select the **Manual indexing** check box.

Transparency 1

1 Right-click **Slice 2** and choose **Transparency**.

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

3 Set the **Transparency** value to **0.4**.

Surface 1

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

2 In the **Settings** window for **Surface**, click to expand the **Title** section.

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

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

5 Locate the **Plot Array** section. Select the **Manual indexing** check box.

Selection 1

1 Right-click **Surface 1** and choose **Selection**.

2 Select Boundaries 4, 5, 7, 10, 20, 21, 24, and 25 only.

Material Appearance 1

1 In the **Model Builder** window, right-click **Surface 1** and choose **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)**.

Slice 1, Slice 2, Surface 1

1 In the **Model Builder** window, under **Results>Size bins**, Ctrl-click to select **Slice 1**, **Slice 2**, and **Surface 1**.

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

Slice 3, Slice 4, Surface 2

1 In the **Model Builder** window, under **Results>Size bins**, Ctrl-click to select **Slice 3**, **Slice 4**, and **Surface 2**.

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

3 In the **Expression** text field, type `n10`.

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

5 Locate the **Title** section. In the **Title** text area, type `n10 (1/m<SUP>4</SUP>)`.

6 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 `n10`.

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

Surface 2

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

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

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

Slice 3, Slice 4, Surface 2

1 In the **Model Builder** window, under **Results>Size bins**, Ctrl-click to select **Slice 3**, **Slice 4**, and **Surface 2**.

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

Slice 5

1 In the **Model Builder** window, click **Slice 5**.

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

3 In the **Expression** text field, type `n15`.

4 Locate the **Title** section. In the **Title** text area, type `n15 (1/m<SUP>4</SUP>)`.

5 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 `n15`.

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

Surface 3

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

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

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

Slice 5, Slice 6, Surface 3

1 In the **Model Builder** window, under **Results>Size bins**, Ctrl-click to select **Slice 5**, **Slice 6**, and **Surface 3**.

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

Slice 7, Slice 8, Surface 4

1 In the **Model Builder** window, under **Results>Size bins**, Ctrl-click to select **Slice 7**, **Slice 8**, and **Surface 4**.

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

3 In the **Expression** text field, type `n20`.

4 Locate the **Title** section. In the **Title** text area, type `n20 (1/m<SUP>4</SUP>)`.

5 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 `n20`.

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

Surface 4

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

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

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

Annotation 1

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

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

3 In the **Text** text field, type `Interval 5`.

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

5 Right-click **Annotation 1** and choose **Duplicate**.

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 `Interval 10`.

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

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 `Interval 15`.

4 Right-click **Annotation 3** and choose **Duplicate**.

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 `Interval 20`.

Discretized points 2

1 In the **Model Builder** window, under **Results** click **Discretized points 2**.

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

3 From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.

4 In the **Discretized points 2** toolbar, click **Plot**.

Discretized points 2, Particle Number Density Distribution 2, Size bins, Velocity Field, Supersaturation and Concentrations

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Particle Number Density Distribution 2**, **Discretized points 2**, **Velocity Field, Supersaturation and Concentrations**, and **Size bins**.

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

T-mixer

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