



Model created in COMSOL Multiphysics 6.4

Multiobjective Optimization of Paracetamol Cooling Crystallization

Introduction

Cooling crystallization is a common separation process in many fields where crystal properties such as crystal size and crystal shape are important. To get the desired end product, the cooling curve can be programmatically predefined.

This example model shows the multiobjective optimization of a cooling curve used for the unseeded batch crystallization of paracetamol in ethanol. The model uses Efficient Global Optimization (EGO) to maximize yield within a specified size range and minimize the number of small crystals.

Model Definition

The crystallization is assumed to occur in a perfectly mixed reactor and is thus modeled in 0D. The crystallization process is modeled with the Size-Based Population Balance interface across a size range of 1 nm to 1000 μm . The size range is discretized logarithmically using 100 intervals. A logarithmic distribution is suitable when nucleation is included. For the crystals, a volume shape factor, k_v , of 0.797 is used (Ref. 1).

Crystal nucleation is modeled according to (Ref. 1)

$$B_{\text{primary}} = K_{b,1} \exp\left(-\frac{16\pi v_{\text{mol}}^2 \sigma^3}{3k_B^3 T^3 (\ln S)^2}\right), S > 1 \quad (1)$$

and

$$B_{\text{secondary}} = K_{b,2} (S - 1)^\alpha m_s^\beta, S > 1 \quad (2)$$

where $K_{b,1}$ and $K_{b,2}$ are the primary and secondary nucleation rate constants ($1/\text{m}^3/\text{s}$), v_{mol} is the solute molecule volume (m^3), m_s is the mass fraction of solid particles (kg/kg), σ is the interfacial energy (J/m^2), while α and β are dimensionless constants. The solute molecule volume is estimated from its solid form density and molar mass. The growth and dissolution rates are modeled according to (Ref. 1)

$$G = K_g \exp\left(\frac{-E_{\text{ag}}}{RT}\right) \Delta C^{\gamma_g}, S > 1 \quad (3)$$

and

$$D = -K_d \exp\left(\frac{-E_{\text{ad}}}{RT}\right) (-\Delta C)^{\gamma_d}, S < 1 \quad (4)$$

where K_g and K_d are the growth and dissolution rate constants (m/s) and E_{ag} and E_{ad} are the growth and dissolution rate activation energies (J/mol). The dissolution rate is defined such that it assumes a negative value. The Size-Based Population Balance interface expects a negative dissolution rate. In the above equations, S (-) and ΔC (g/g) are measures of the supersaturation defined as

$$S = \frac{C}{C^*} \quad (5)$$

$$\Delta C = C - C^* \quad (6)$$

where C is the paracetamol concentration (g/g) and C^* is the paracetamol solubility as a function of temperature (g/g). The parameter values in equations 1-4 are taken from [Ref. 1](#).

The temperature, T , follows a parameterized cooling curve consisting of a constant temperature region followed by a temperature cycling region, similar to what was done in [Ref. 1](#). The constant temperature region is typically where most of the crystal mass is formed while the temperature cycling region typically provides an opportunity to dissolve small crystals. Cooling takes place across 350 minutes starting at 50°C and ending at 20°C. The curve shape depends on five parameter values. The p parameter controls the height of the initial plateau temperature while the parameters a , b , c , and d control the height of subsequent peaks in the temperature cycling region. The constant plateau temperature can vary between 20 and 45°C while each individual peak height can vary between 0 and 10°C.

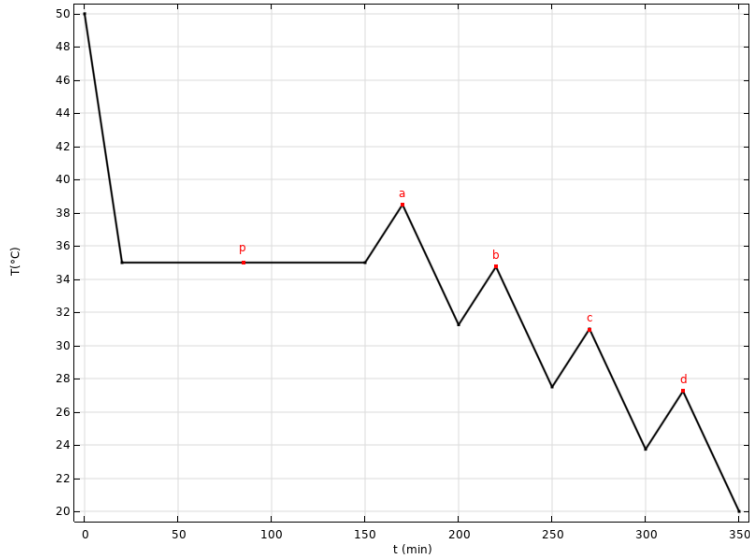


Figure 1: Cooling curve with optimization parameters.

The optimization objective for the model was based on maximizing yield within a specified size range (145–330 μm) and minimize the number of small crystals (< 145 μm). The objective function to be maximized can be written as the sum of three separate objective functions

$$F_{\text{obj}} = \frac{F_{\text{obj},1}}{4} + \frac{F_{\text{obj},2}}{4} + \frac{F_{\text{obj},3}}{2} \quad (7)$$

The objective function assumes a value between 0 and 1. The separate objective functions describe the normalized volume concentration of target particles

$$F_{\text{obj},1} = \frac{\int_{L_1}^{L_2} k_v L^3 n(L) dL}{\int_0^{\infty} k_v L^3 n(L) dL}, \quad (8)$$

the mass of target particles normalized by the theoretical maximum mass

$$F_{\text{obj},2} = \frac{\rho_p}{(C_0 - C^*(20^\circ\text{C}))\rho_{\text{sol}}} \int_{L_1}^{L_2} k_v L^3 n(L) dL, \quad (9)$$

and the number fraction of particles smaller than the target particles

$$F_{\text{obj, 3}} = 1 - \frac{\int_0^{L_1} n(L)dL}{\int_0^{\infty} n(L)dL} \quad (10)$$

In the above objective functions, n is the continuous number density distribution ($1/\text{m}^4$), L is the particle size (m), ρ_p is the solid crystal particle density (kg/m^3), ρ_{sol} is the solvent density (kg/m^3), and C_0 is the initial concentration (g/g). The sizes L_1 and L_2 equal 145 and 330 μm respectively.

Results and Discussion

Figure 2 shows the cooling curve for five different cases from the optimization process. The color legend shows the total objective score for each case and the solid line is the optimized case. The objective score of the optimal solution (solid line) was 0.68 and the cooling curve had a plateau at 30.5°C followed by one large and two smaller peaks in the temperature cycling region.

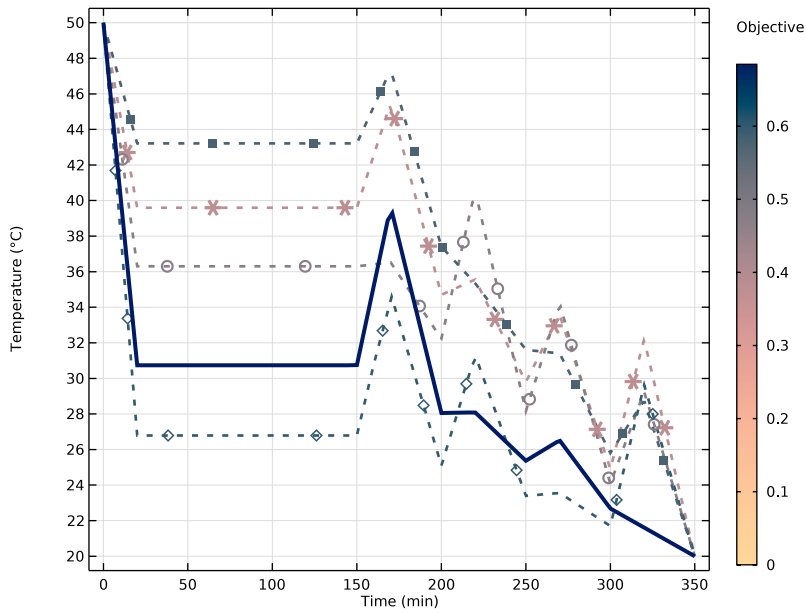


Figure 2: Cooling curves for different cases. The optimized case is shown with a solid line.

The corresponding supersaturation curves can be seen in Figure 3. The supersaturation curve for the optimized case ends near the saturation line ($S=1$) giving a high product yield.

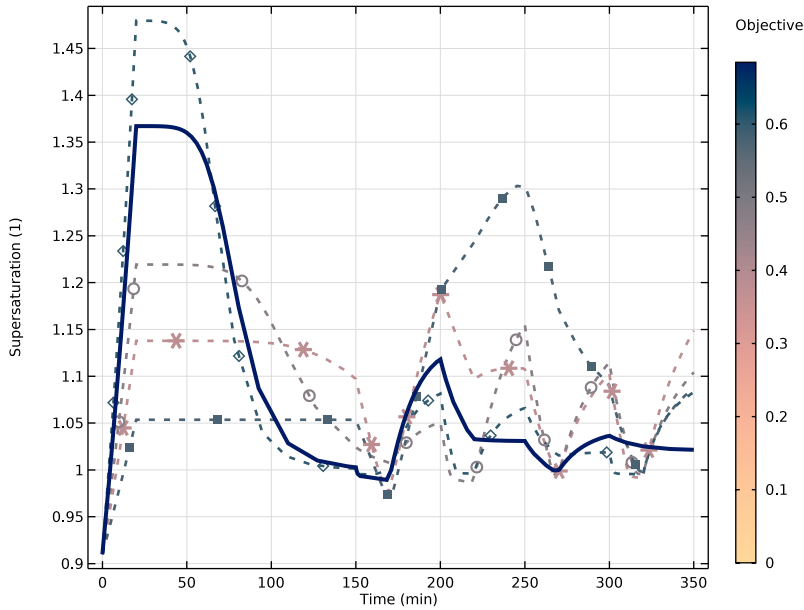


Figure 3: Supersaturation curves for different cases. The optimized case is shown with a solid line.

The volume density distribution for the same cases as in the two previous figures can be seen in Figure 4. It shows that cooling curves that have a higher initial plateau, leading to an overall slower cooling rate, result in wider distributions. For the cases marked with asterisks, two distinct bumps can be seen in the distribution. This is caused by undersaturation at 170 minutes prompting dissolution and creating a divide in the distribution. When investigating the cooling curves, it can be seen that this corresponds to the first peak in the cycling region. As there is a high temperature plateau, the solution is close to the saturation point before the first temperature cycle, causing undersaturation.

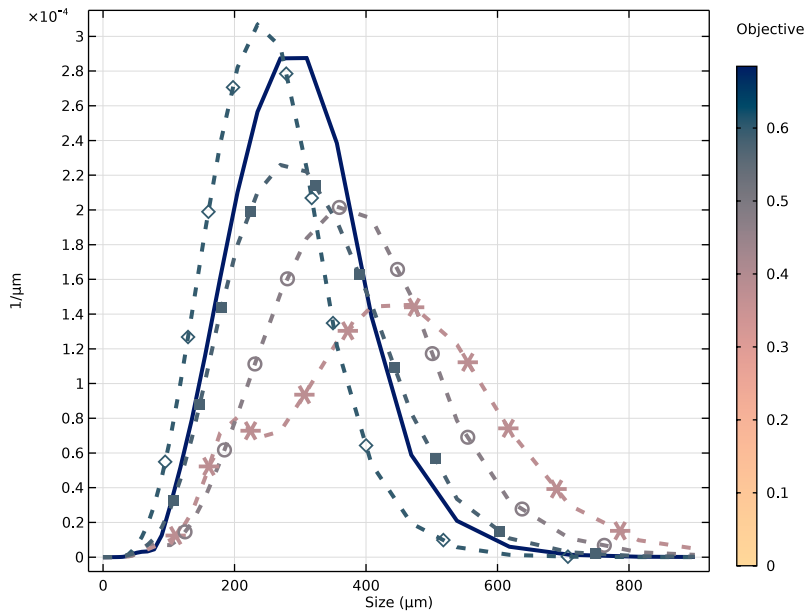


Figure 4: Volume density distributions for different cases. The optimized case is shown with a solid line.

The concentration and solubility for the optimized case can be seen in [Figure 5](#).

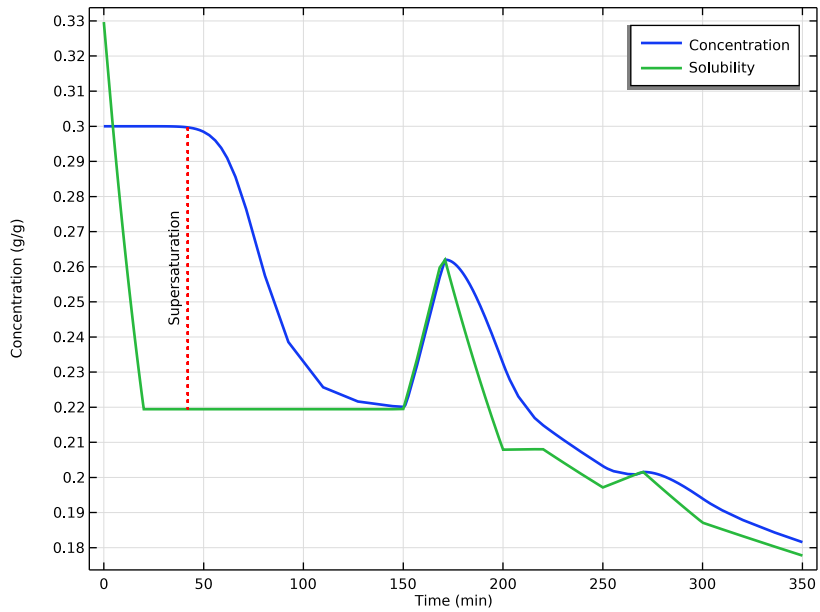


Figure 5: Concentration and solubility for the optimized case.

Figure 6 shows the growth/dissolution rate of crystals for the optimized case. The time interval where crystals are dissolving aligns with where the concentration is below the solubility in Figure 5.

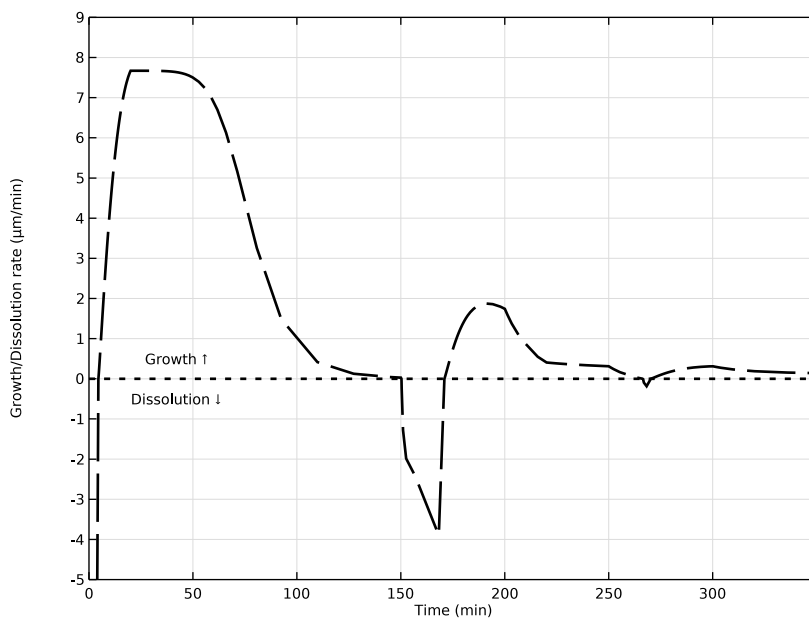


Figure 6: Growth/dissolution rate for the optimized case.

Reference


I. Y. Kim, Y. Kawajiri, R.W. Rousseau, and M.A. Grover, “Modeling of Nucleation, Growth, and Dissolution of Paracetamol in Ethanol Solution for Unseeded Batch Cooling Crystallization with Temperature-Cycling Strategy,” *Ind. Eng. Chem. Res.*, vol. 62, no. 6, pp. 2866-2881, 2017; Copyright 2023 The Authors. Published by American Chemical Society. This publication is licensed under [CC-BY 4.0](https://creativecommons.org/licenses/by/4.0/).

Application Library path: Chemical_Reaction_Engineering_Module/
Mixing_and_Separation/cooling_crystallization_optimization




Modeling Instructions

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

NEW


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

MODEL WIZARD

- 1 In the **Model Wizard** window, click  **OD**.
- 2 In the **Select Physics** tree, select **Chemical Species Transport** > **Precipitation and Crystallization** > **Precipitation and Crystallization**.
- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **General Studies** > **Time Dependent**.
- 6 Click  **Done**.



GLOBAL DEFINITIONS

Parameters I


- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 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 `cooling_crystallization_optimization_parameters.txt`.

DEFINITIONS

Variables I

- 1 In the **Definitions** toolbar, click  **Local Variables**.
- 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 `cooling_crystallization_optimization_variables.txt`.

Solubility Curve

- 1 In the **Home** toolbar, click  **Functions** and choose **Local** > **Analytic**.
- 2 In the **Settings** window for **Analytic**, type Solubility Curve in the **Label** text field.
- 3 In the **Function name** text field, type `sol`.
- 4 Locate the **Definition** section. In the **Expression** text field, type $-8.707+9.669*1e-2*T-3.610*1e-4*T^2+4.590*1e-7*T^3$.
- 5 In the **Arguments** text field, type `T`.

6 Locate the **Units** section. In the **Function** text field, type g/g .

7 In the table, enter the following settings:

Argument	Unit
T	K

Cooling Curve

1 In the **Home** toolbar, click  **Functions** and choose **Local > Interpolation**.

2 In the **Settings** window for **Interpolation**, type *Cooling Curve* in the **Label** text field.

3 Locate the **Definition** section. In the **Function name** text field, type *temp*.

4 Click  **Load from File**.

5 Browse to the model's Application Libraries folder and double-click the file *cooling_crystallization_optimization_cooling_curve.txt*.

6 Locate the **Interpolation and Extrapolation** section. From the **Extrapolation** list, choose **Linear**.

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

Function	Unit
<i>temp</i>	degC

8 In the **Argument** table, enter the following settings:

Argument	Unit
<i>t</i>	min

The imported cooling curve depends on five parameters, a , b , c , d , and p . The first four control the temperature cycling in the second half of the process, while the fifth controls the plateau temperature in the first half.

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 $\text{temp}(t)$.

4 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

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 C8H9NO2.

Initial Values I

- 1 In the **Model Builder** window, click **Initial Values I**.
- 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)
C8H9NO2	Cini

SIZE-BASED POPULATION BALANCE (PBSB)


- 1 In the **Model Builder** window, under **Component I (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_p.
- 4 From the **Particle shape** list, choose **User defined**. In the k_a text field, type 1.
- 5 In the k_v text field, type 0.797.
- 6 Locate the **Size Intervals** section. From the **Discretization** list, choose **Logarithmic**.
- 7 In the I text field, type 100.
- 8 In the L_0 text field, type 1[nm].
- 9 In the L_I text field, type 1000[μ m].
- 10 Locate the **Nucleation** section. In the B_{nuc} text field, type $\text{if}(S>1, kb2*(S-1+\text{eps})^\alpha * m^{\text{beta}}, 0) + \text{if}(S>1, kb * \exp(-(16 * \pi * v_{mol}^2 * \text{sig}^3) / (3 * k_B * \text{const}^3 * T^3 * (\log(S))^2)), 0)$.
- 11 Locate the **Growth and Dissolution** section. In the G_L text field, type $\text{if}(\Delta C > 0, kg * \exp(-E_{ag} / (R_{const} * T)) * \Delta C^{\text{gamma}_g}, 0)$.
- 12 In the D_L text field, type $\text{if}(\Delta C < 0, -kd * \exp(-E_{ad} / (R_{const} * T)) * (-\Delta C)^{\text{gamma}_d}, 0)$.
- 1 In the **Model Builder** window, under **Component I (comp1)** > **Size-Based Population Balance (pbsb)** click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Population Number Density** section.
- 3 In the n_0 text field, type 1.

STUDY 1


Parameter Optimization

- 1 In the **Study** toolbar, click  **Optimization** and choose **Parameter Optimization**.
- 2 In the **Settings** window for **Parameter Optimization**, locate the **Optimization Solver** section.
- 3 From the **Method** list, choose **EGO**.
- 4 Locate the **Objective Function** section. In the table, enter the following settings:


Expression	Description	Evaluate for
comp1.TVf/4	Volume fraction of particles in target area	Time Dependent
comp1.Vf/4	Mass concentration of particles in target area normalized by theoretical max	Time Dependent
(1-comp1.N_small)/2	Normalized number of particles larger than 145 μm	Time Dependent

- 5 From the **Type** list, choose **Maximization**.
- 6 From the **Solution** list, choose **Use last**.
- 7 Locate the **Control Parameters** section. Click  **Add**.
- 8 In the table, enter the following settings:

Parameter	Lower bound	Upper bound	Unit
p (Plateau height parameter)	20	45	

- 9 Click  **Add**.
- 10 In the table, enter the following settings:

Parameter	Lower bound	Upper bound	Unit
a (Cycling parameter)	0	1	


- 11 Click  **Add**.
- 12 In the table, enter the following settings:

Parameter	Lower bound	Upper bound	Unit
b (Cycling parameter)	0	1	

- 13 Click  **Add**.

14 In the table, enter the following settings:

Parameter	Lower bound	Upper bound	Unit
c (Cycling parameter)	0	1	

15 Click  **Add**.

16 In the table, enter the following settings:



Parameter	Lower bound	Upper bound	Unit
d (Cycling parameter)	0	1	

17 Click to expand the **Output** section. From the **Keep solutions** list, choose **All**.

Step 1: Time Dependent

- 1 In the **Model Builder** window, 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 range (0,0.5[min],tf).



Solution 1 (sol1)

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.
- 3 In the **Settings** window for **Time-Dependent Solver**, locate the **General** section.
- 4 In the **Store every Nth step** text field, type 50.
- 5 In the **Study** toolbar, click  **Compute**.

RESULTS

- 1 In the **Model Builder** window, click **Results**.
- 2 In the **Settings** window for **Results**, locate the **Update of Results** section.
- 3 Select the **Only plot when requested** checkbox.

Preferred Units 1

- 1 In the **Results** toolbar, click  **Configurations** and choose **Preferred Units**.
- 2 In the **Settings** window for **Preferred Units**, locate the **Units** section.
- 3 Click  **Add Physical Quantity**.
- 4 In the **Physical Quantity** dialog, type 1en in the text field.
- 5 In the tree, select **General > Length (m)**.
- 6 Click **OK**.

7 In the **Settings** window for **Preferred Units**, locate the **Units** section.

8 In the table, enter the following settings:

Quantity	Unit	Preferred unit
Length	m	μm

Concentration and Solubility

1 In the **Model Builder** window, under **Results** click **Concentration (re)**.

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

3 From the **Parameter selection (p, a, b, c, d)** list, choose **Last**.

4 In the **Label** text field, type Concentration and Solubility.

5 Locate the **Plot Settings** section.

6 Select the **y-axis label** checkbox. In the associated text field, type Concentration (g/g).

Global I

1 In the **Model Builder** window, expand the **Concentration and Solubility** node, then click **Global I**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
C	1	Concentration
sol(T)	1	Solubility

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **min**.


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

6 Click to expand the **Legends** section. Find the **Include** subsection. Clear the **Solution** checkbox.

7 Clear the **Expression** checkbox.

8 Select the **Description** checkbox.

Concentration and Solubility

In the **Concentration and Solubility** toolbar, click  **Line Segments**.

Line Segments I

1 In the **Settings** window for **Line Segments**, locate the **x-Coordinates** section.

2 In the table, enter the following settings:

Expression	Unit	Description
42	1	
42	1	

3 Locate the **y-Coordinates** section. In the table, enter the following settings:

Expression	Unit	Description
at(42[<i>min</i>],C)	1	
at(42[<i>min</i>],sol(T))	1	

4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.

5 From the **Color** list, choose **Red**.

Concentration and Solubility

In the **Concentration and Solubility** toolbar, click  **Annotation**.

Annotation 1

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 **x** text field, type 42.

4 In the **y** text field, type $(\text{at}(42[\text{min}], C) + \text{at}(42[\text{min}], \text{sol}(T))) / 2$.

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

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

7 From the **Orientation** list, choose **Vertical**.

8 In the **Concentration and Solubility** toolbar, click  **Plot**.

Average Size Distribution (pbsb)

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

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


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

4 From the **Parameter selection (p, a, b, c, d)** list, choose **Last**.

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

RESULT TEMPLATES

1 In the **Results** toolbar, click  **Result Templates** to open the **Result Templates** window.

- 2 Go to the **Result Templates** window.
- 3 In the tree, select **Study I/Parametric Solutions I (sol2) > Size-Based Population Balance > Volume Density Distribution (pbsb)**.
- 4 Click the **Add Result Template** button in the window toolbar.
- 5 In the **Results** toolbar, click  **Result Templates** to close the **Result Templates** window.

RESULTS

Volume Density Distribution (pbsb)

- 1 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 2 From the **Parameter selection (p, a, b, c, d)** list, choose **Last**.
- 3 From the **Time selection** list, choose **Last**.
- 4 Locate the **Plot Settings** section. In the **x-axis label** text field, type **Size (μm)**.

Line Segments 1

- 1 In the **Model Builder** window, expand the **Volume Density Distribution (pbsb)** node, then click **Line Segments 1**.
- 2 In the **Settings** window for **Line Segments**, locate the **Coloring and Style** section.
- 3 From the **Color** list, choose **Black**.
- 4 From the **Width** list, choose **2**.

Volume Density Distribution (pbsb)

In the **Volume Density Distribution (pbsb)** toolbar, click  **Line Segments**.

Line Segments 2

- 1 In the **Settings** window for **Line Segments**, locate the **x-Coordinates** section.
- 2 In the table, enter the following settings:


Expression	Unit	Description
380	1	
380	1	

- 3 Locate the **y-Coordinates** section. In the table, enter the following settings:

Expression	Unit	Description
0	1	
300	1	

- 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 Growth/Dissolution rate ($\mu\text{m}/\text{min}$).
- 6 Locate the **Axis** section. Select the **Manual axis limits** checkbox.
- 7 In the **x minimum** text field, type 0.
- 8 In the **x maximum** text field, type $t_f/60$.
- 9 In the **y minimum** text field, type -5.
- 10 In the **y maximum** text field, type 9.
- 11 Locate the **Legend** section. Clear the **Show legends** checkbox.

Global 1

- 1 In the **Growth and Dissolution** toolbar, click  **Global**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
pbsb.GL_n2-pbsb.DL_n2	$\mu\text{m}/\text{min}$	

- 4 Locate the **x-Axis Data** section. From the **Unit** list, choose **min**.
- 5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.
- 6 From the **Color** list, choose **Black**.
- 7 From the **Width** list, choose **2**.

Growth and Dissolution

In the **Growth and Dissolution** toolbar, click  **Global**.

Global 2


- 1 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 2 In the table, enter the following settings:

Expression	Unit	Description
0	1	

- 3 Locate the **x-Axis Data** section. From the **Unit** list, choose **min**.

- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
- 5 From the **Color** list, choose **Black**.
- 6 From the **Width** list, choose **2**.


Growth and Dissolution

In the **Growth and Dissolution** toolbar, click  **Annotation**.


Annotation 1

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type Growth ?.
- 3 Locate the **Position** section. In the **x** text field, type 42.
- 4 In the **y** text field, type 0.5.
- 5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 6 From the **Anchor point** list, choose **Center**.


Annotation 2

- 1 Right-click **Results > Growth and Dissolution > Annotation 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Dissolution ?.
- 4 Locate the **Position** section. In the **y** text field, type -0.5.
- 5 In the **Growth and Dissolution** toolbar, click  **Plot**.

Cooling Curve

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Cooling Curve in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/ Parametric Solutions 1 (sol2)**.
- 4 From the **Parameter selection (p, a, b, c, d)** list, choose **Manual**.
- 5 In the **Parameter indices (1-62)** text field, type 1, 19, 27, 46.
- 6 Locate the **Title** section. From the **Title type** list, choose **None**.
- 7 Locate the **Plot Settings** section.
- 8 Select the **y-axis label** checkbox. In the associated text field, type Temperature (°C).

Global 1

- 1 In the **Cooling Curve** toolbar, click  **Global**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
T	degC	Temperature

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **min**.

5 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.

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


7 Find the **Line markers** subsection. From the **Marker** list, choose **Cycle**.

8 From the **Positioning** list, choose **Interpolated**.

9 In the **Number** text field, type 10.

10 Locate the **Legends** section. Clear the **Show legends** checkbox.

Color Expression I

1 In the **Cooling Curve** toolbar, click  **Color Expression**.

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

3 In the **Expression** text field, type $at(tf, (1-comp1.N_small)/2+comp1.TVf/4+comp1.Vf/4)$.

4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Agama**.

5 Click to expand the **Range** section. Select the **Manual color range** checkbox.

6 In the **Maximum** text field, type 0.68465.

7 Locate the **Coloring and Style** section. From the **Color table transformation** list, choose **Nonlinear**.

8 In the **Color calibration parameter** text field, type 1.

Cooling Curve

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

2 In the **Settings** window for **ID Plot Group**, locate the **Color Legend** section.

3 Select the **Show titles** checkbox.

Color Expression I

1 In the **Model Builder** window, under **Results > Cooling Curve > Global I** click **Color Expression I**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 In the **Color legend title** text field, type **Objective**.

Cooling Curve

In the **Cooling Curve** toolbar, click  **Global**.

Global 2

1 In the **Settings** window for **Global**, locate the **Data** section.

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

3 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
T	degC	Temperature

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **min**.

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

6 From the **Color table** list, choose **Agama**.


7 Select the **Reverse color table** checkbox.

8 From the **Length of cycle** list, choose **Manual**.

9 In the **Number of colors** text field, type 2.

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

11 Locate the **Legends** section. Clear the **Show legends** checkbox.

12 In the **Cooling Curve** toolbar, click  **Plot**.

Supersaturation

1 In the **Model Builder** window, right-click **Cooling Curve** and choose **Duplicate**.

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

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type **Supersaturation (1)**.

Global 1

1 In the **Model Builder** window, expand the **Supersaturation** node, then click **Global 1**.

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


3 In the table, enter the following settings:

Expression	Unit	Description
S	1	Supersaturation ratio

Global 2

- 1 In the **Model Builder** window, click **Global 2**.
- 2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
S	1	Supersaturation ratio

- 4 In the **Supersaturation** toolbar, click  **Plot**.