



Model created in COMSOL Multiphysics 6.4

Turbulent Aggregation of Nanoparticles

Introduction

Nanoparticles have become widely used in a range of applications. For example, in pharmaceuticals, particles on the nanoscale, such as nanocrystals, are often used as an effective means of drug delivery. Meanwhile in material sciences, nanoparticle coating is an increasingly common way to improve or change the properties of materials. Understanding the factors affecting the size of these particles is an important step to develop production processes that optimize the desired particle properties.

Model Definition

The term nanoparticle is used to describe particles on the nanoscale. This example models the turbulence-induced aggregation of nanoparticles in the size range of a few hundred nanometers in a beaker fitted with a square blade impeller to predict the size distribution of volume-equivalent spherical particle diameters. The model is set up with a 2D geometry describing the aggregation and movement of particles in a turbulent flow in the mixing plane (Figure 1). The entire domain is modeled as a rotating domain and the impeller is set to a rotational speed of 350 rpm.

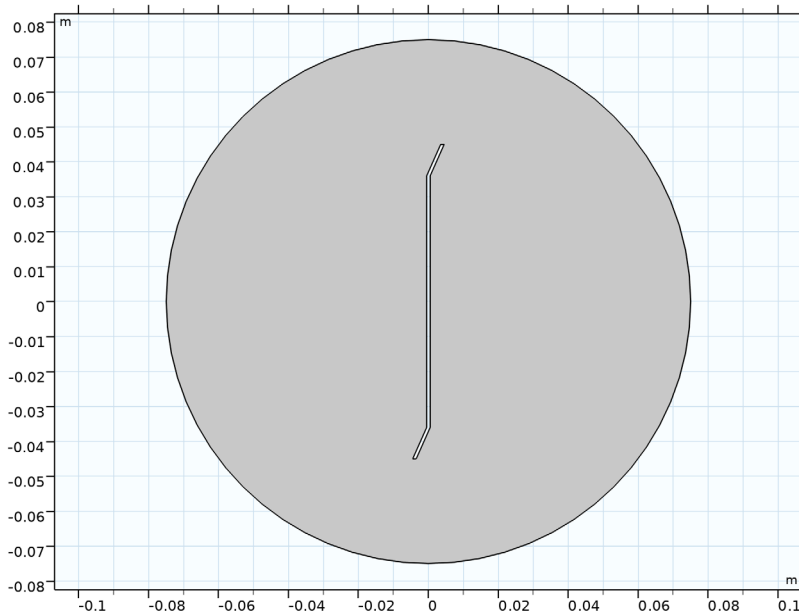


Figure 1: Model geometry consisting of beaker with impeller.

The aggregation and flow is modeled with the Precipitation in Fluid Flow interface which couples a Size-Based Population Balance interface with a Single-Phase Fluid Flow interface. A k-ε model is used to account for the turbulent flow resulting from the mixing. In this example we exclude nucleation, growth and dissolution. Furthermore, the particles are also assumed small enough that breakage is negligible. The size distribution is modeled using a discretization of 20 size intervals, or bins, and a logarithmic interval distribution. For aggregation, logarithmic distributions are recommended. The aggregation contribution is modeled as (Ref. 1)

$$\frac{\partial n(L)}{\partial t} = \frac{L^2}{2} \int_0^L \frac{1}{(L^3 - \lambda^3)^{2/3}} K(\sqrt[3]{L^3 - \lambda^3}, L) n(\sqrt[3]{L^3 - \lambda^3}) n(\lambda) d\lambda \quad (1)$$

$$- n(L) \int_0^\infty K(L, \lambda) n(\lambda) d\lambda$$

where L is the characteristic length and K is the aggregation kernel. This model assumes spherical particles in which case the characteristic length, L , is the diameter. The aggregation kernel is written with both a perikinetic and orthokinetic contribution. They describe the collisions due to Brownian motion and convective transport by the fluid respectively. They are given by (Ref. 2 and Ref. 3)

$$K_{\text{peri}} = \frac{2k_b T}{3\nu\rho} (L_j + L_k) \left(\frac{1}{L_k} + \frac{1}{L_j} \right) \quad (2)$$

and

$$K_{\text{ortho}} = \sqrt{\frac{\pi}{8 \times 15}} (L_j + L_k)^3 \sqrt{\frac{\varepsilon}{\nu}} \quad (3)$$

where L_j and L_k are the sizes of the two colliding particles. Furthermore, ν is the kinematic viscosity (m^2/s), ε is the turbulent dissipation rate (m^2/s^3), ρ is the fluid density (kg/m^3), k_b is the Boltzmann constant ($\text{m}^2 \cdot \text{kg}/\text{s}^2/\text{K}$) and T is the temperature (K). The turbulent dissipation rate are solved for by the fluid flow interface. All particles are modeled as spherical where the size, L , is the diameter such that the system, in absence of nucleation, growth and dissolution, conserves the total particle volume. Assuming that the collision contributions (Equation 2 and Equation 3) are independent of each other and that the contributions are additive we can write

$$K = \frac{1}{W} (K_{\text{ortho}} + K_{\text{peri}}) \quad (4)$$

Here, W is the stability ratio. In this model a joint stability ratio is applied to both collision contributions. The stability ratio can range from 1 (no stabilization) to infinity (complete stabilization) and the specific value will depend on the system. Experiments are often required to find a suitable stability ratio. For example, if ions are adsorbed on the particle surface, the stability ratio will increase due to repelling electrostatic forces. Or, if the solution is supersaturated, it is possible for the crystal particles to form strong bonds using the solute, in the form of agglomerates, which gives a lower stability ratio. As was done by Schwarzer and Peukert in their model of barium sulfate nanoparticle aggregation (Ref. 2), we therefore test multiple stabilization ratios. Three weak stabilization scenarios are tested; $W = 1$, $W = 10$, and $W = 100$. A stabilization of $W = 1$ is equal to having no stabilization and is a common approximation for systems with negligible electrostatic forces.

At time $t = 0$, there is an arbitrary initial distribution of particles according to (modified from Ref. 4)

$$n(0, L) = 3(L - L_{\text{offset}})^2 \frac{N_0}{(L_{\text{mean}} - L_{\text{offset}})^3} n \exp\left(-\frac{(L - L_{\text{offset}})^3}{(L_{\text{mean}} - L_{\text{offset}})^3}\right) \quad (5)$$

if $L > L_{\text{offset}}$ and 0 otherwise. The constants N_0 , L_{mean} , and L_{offset} control the initial particle concentration, mean size, and starting point, respectively. The distribution can be seen in Figure 2.

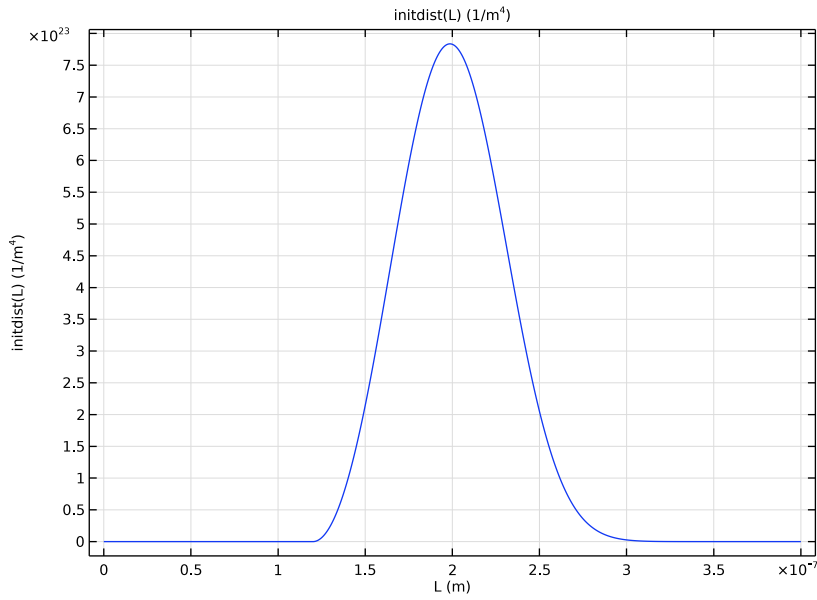


Figure 2: Initial size distribution.

Results and Discussion

The velocity field can be seen in [Figure 3](#). The largest velocity magnitude is located at the tips of the impeller. This is also where we will see the most orthokinetic aggregation.

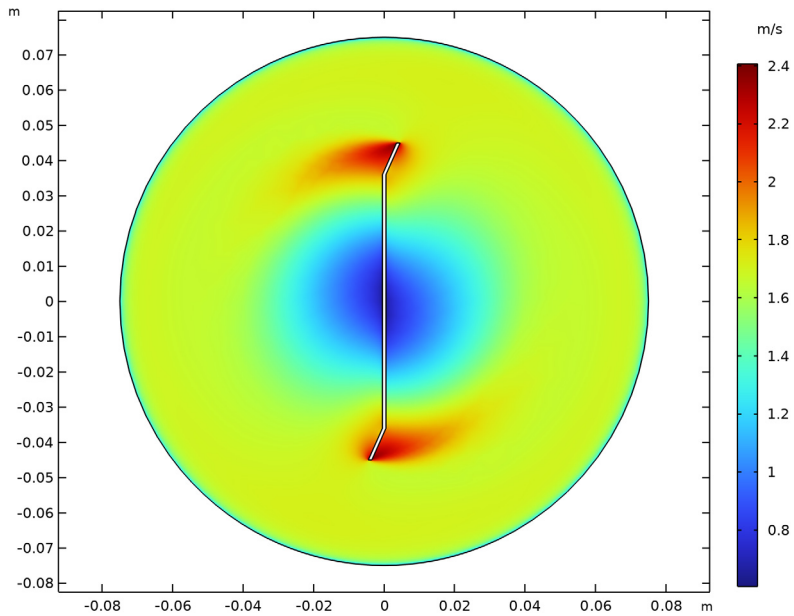


Figure 3: Velocity field in the mixing plane.

Figure 4 shows the concentration of particles at 0.2, 0.4, 0.8, and 1.2 seconds after mixing has begun with $w = 1$. A more pronounced decrease in particle concentration is seen near the impeller where the turbulent dissipation rate is higher and the orthokinetic aggregation contribution is larger.

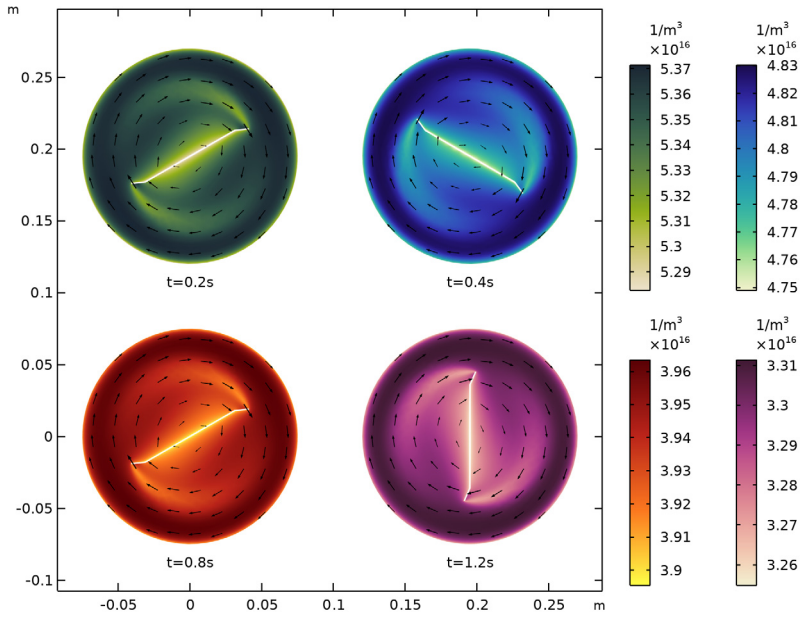


Figure 4: Particle concentration at different times for $W = 1$.

Figure 5 shows the average particle concentration and average size across the beaker. The average size can be seen to increase from 200 to 388, 229, and 203 nm while the particle concentration decreases from 6×10^{16} to 3.1×10^{15} , 3.6×10^{16} , and 5.7×10^{16} $1/\text{m}^3$ for $W = 1, 50,$ and $100,$ respectively.

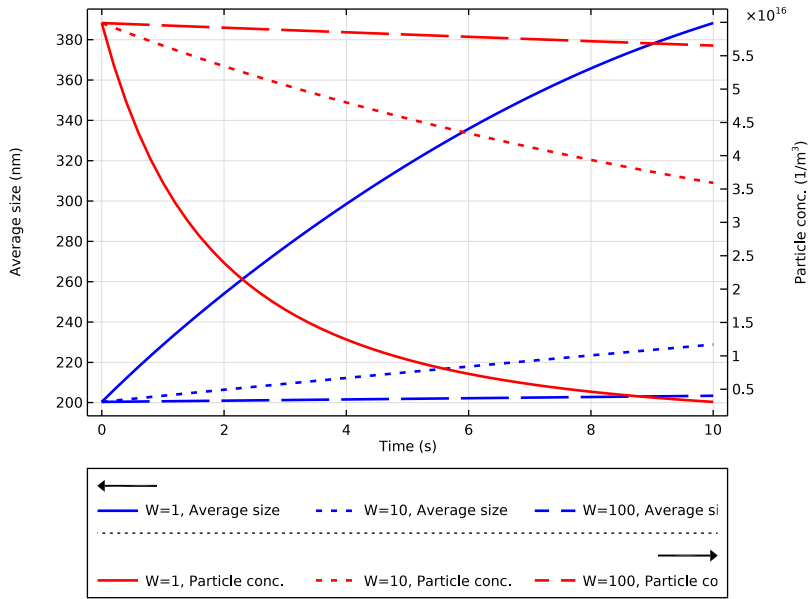


Figure 5: Average particle size and number of particles.

Finally, Figure 6 shows the average size distribution at different times and stability ratios. The distribution is given at $t = 0, 3, 6,$ and 10 seconds. For no stabilization, $W = 1$, the distribution almost immediately collapses into a smaller number of larger particles. This is also what was seen in Figure 5. The distribution for $W = 10$ flattens out at a slower rate. At this stability ratio the change in distribution profile is still pronounced. The combinations of sizes that can form a particles are fewer at smaller sizes, so for small particles we see that the death term (sink term) dominates. At the highest modeled stability ratio, $W = 100$, aggregation still takes place but the overall distribution profile does not change much over the modeled time span.

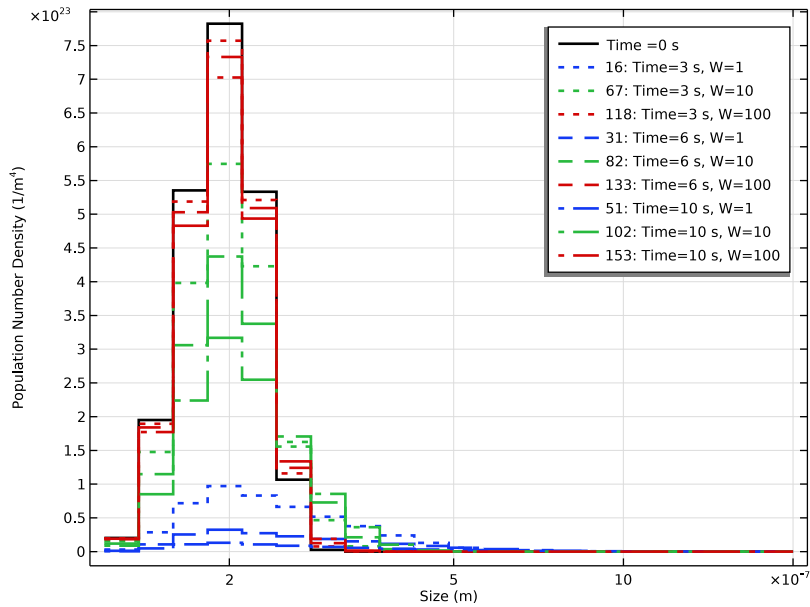


Figure 6: Size distribution at different times.

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. A. Raponi, S. Romano, G. Battaglia, A. Buffo, M. Vannie, A. Cipollina, and D. Marchisio, "Computational Modeling of Magnesium Hydroxide Precipitation and Kinetics Parameters Identification," *Cryst. Growth Des.*, vol. 23, no. 12, pp. 4748–4759, 2023.
4. W. Zhang, T. Przybycien, J.M. Breuer, and E. von Lieres, "Solving crystallization/precipitation population balance models in CADET, Part II: Size-based Smoluchowski coagulation and fragmentation equations in batch and continuous modes," *Comput. Chem. Eng.*, vol. 192, 2025.

Application Library path: Chemical_Reaction_Engineering_Module/
Mixing_and_Separation/turbulent_aggregation



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  **2D**.
- 2 In the **Select Physics** tree, select **Chemical Species Transport > Precipitation and Crystallization > Precipitation and Crystallization in Fluid Flow**.
- 3 Click **Add**.
- 4 In the **Added physics interfaces** tree, select **Transport of Diluted Species (tds)**.
- 5 Click **Remove**.
- 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 `turbulent_aggregation_parameters.txt`.

DEFINITIONS

Initial distribution

- 1 In the **Definitions** toolbar, click  **Analytic**.
- 2 In the **Settings** window for **Analytic**, type Initial distribution in the **Label** text field.
- 3 In the **Function name** text field, type `initdist`.

4 Locate the **Definition** section. In the **Expression** text field, type $(L > L_{\text{offset}}) * 3 * (L - L_{\text{offset}})^2 * (NO) / ((L_{\text{mean}} - L_{\text{offset}})^3) * \exp(-(L - L_{\text{offset}})^3 / (L_{\text{mean}} - L_{\text{offset}})^3)$.

5 In the **Arguments** text field, type L.

6 Locate the **Units** section. In the **Function** text field, type $1/m^4$.

7 In the table, enter the following settings:

Argument	Unit
L	m

8 Locate the **Plot Parameters** section. In the table, enter the following settings:

Plot	Argument	Lower limit	Upper limit	Fixed value	Unit
√	L	0	400 [nm]	0	m

9 Click  **Plot**.

GEOMETRY I


Circle 1 (c1)

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

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

3 In the **Radius** text field, type $D_{\text{beaker}}/2$.

Polygon 1 (pol1)

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

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 Click  **Load from File**.

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

Difference 1 (dif1)

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


2 Select the object **c1** only.

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


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

5 Select the object **pol1** only.

6 Click  **Build All Objects**.


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

ADD MATERIAL

- 1 In the **Materials** toolbar, click  **Add Material** to open the **Add Material** window.
- 2 Go to the **Add Material** window.
- 3 In the tree, select **Built-in > Water, liquid**.
- 4 Click the **Add to Component** button in the window toolbar.

COMPONENT 1 (COMP1)

Rotating Domain 1

- 1 In the **Physics** toolbar, click  **Moving Mesh** and choose **Rotating Domain**.
- 2 In the **Settings** window for **Rotating Domain**, locate the **Rotation** section.
- 3 From the **Rotation type** list, choose **Specified rotational velocity**.
- 4 From the **Rotational velocity expression** list, choose **General revolutions per time**.
- 5 In the f text field, type rpm_impeller.


LAMINAR FLOW (SPF)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.
- 2 In the **Settings** window for **Laminar Flow**, locate the **Turbulence** section.
- 3 From the **Turbulence model type** list, choose **RANS-EVM**.


Wall 1

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Turbulent Flow, k-ε (spf)** click **Wall 1**.
- 2 In the **Settings** window for **Wall**, click to expand the **Wall Movement** section.
- 3 From the **Translational velocity** list, choose **Zero (Fixed wall)**.

Wall 2

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Wall**.
- 2 Select Boundaries 1–8 only.

Pressure Point Constraint 1

- 1 In the **Physics** toolbar, click  **Points** and choose **Pressure Point Constraint**.
- 2 Select Point 6 only.

SIZE-BASED POPULATION BALANCE (PBSB)

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Size-Based Population Balance (pbsb)**.
- 2 In the **Settings** window for **Size-Based Population Balance**, locate the **Particle Properties** section.
- 3 In the ρ_p text field, type rho_p.
- 4 Locate the **Size Intervals** section. From the **Discretization** list, choose **Logarithmic**.
- 5 In the I text field, type 20.
- 6 In the L_0 text field, type L_offset.
- 7 In the L_1 text field, type 2000[nm].
- 8 Locate the **Aggregation** section. Select the **Include** checkbox.
- 9 In the K text field, type $1/W*(\text{sqrt}(\text{pi}/(15*8))*(\text{pop.Lj}+\text{pop.Lk})^3*\text{sqrt}(\text{max}(\text{ep},\text{eps})/\text{spf.nu})+2*k_B_const*T/(3*\text{spf.nu}*\text{spf.rho})*(\text{pop.Lj}+\text{pop.Lk})*(1/\text{pop.Lj}+1/\text{pop.Lk}))$.

Initial Values 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Size-Based Population Balance (pbsb)** click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Population Number Density** section.
- 3 In the n_0 text field, type $\text{initdist}(\text{pop.L})$.


MESH 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.
- 3 From the list, choose **User-controlled mesh**.

Size 1


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size 1**.
- 2 Select Boundaries 1–8 only.

Size 2


- 1 In the **Mesh** toolbar, click  **Sizing** and choose **Size**.
- 2 Drag and drop below **Size 1**.
- 3 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 4 From the **Geometric entity level** list, choose **Boundary**.
- 5 Select Boundaries 1 and 8 only.

- 6 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.
- 7 Click the **Custom** button.
- 8 Locate the **Element Size Parameters** section.
- 9 Select the **Maximum element size** checkbox. In the associated text field, type 0.00125.

Boundary Layers I

- 1 In the **Model Builder** window, click **Boundary Layers I**.
- 2 In the **Settings** window for **Boundary Layers**, click to expand the **Corner Settings** section.
- 3 From the **Handling of sharp corners** list, choose **Splitting**.
- 4 Click  **Build All**.


ADD STUDY

- 1 In the **Study** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Multiphysics couplings in study** subsection. In the table, clear the **Solve** checkbox for **Precipitation in Fluid Flow I (pffl)**.
- 4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** checkbox for **Size-Based Population Balance (pbsb)**.
- 5 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces > Frozen Rotor**.
- 6 Click the **Add Study** button in the window toolbar.

FLUID FLOW INITIALIZATION

- 1 In the **Settings** window for **Study**, type Fluid flow initialization in the **Label** text field.
- 2 Locate the **Study Settings** section. Clear the **Generate default plots** checkbox.

Step 1: Frozen Rotor

- 1 In the **Model Builder** window, under **Fluid flow initialization** click **Step 1: Frozen Rotor**.
- 2 In the **Settings** window for **Frozen Rotor**, locate the **Physics and Variables Selection** section.
- 3 Select the **Modify model configuration for study step** checkbox.
- 4 In the tree, select **Component 1 (comp1) > Size-Based Population Balance (pbsb)**.
- 5 Click  **Disable in Model**.
- 6 In the tree, select **Component 1 (comp1) > Multiphysics > Precipitation in Fluid Flow I (pffl)**.

7 Click  **Disable in Model**.



ADD STUDY

- 1 Go to the **Add Study** window.
- 2 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies > Time Dependent**.
- 3 Click the **Add Study** button in the window toolbar.

FLUID FLOW

In the **Settings** window for **Study**, type Fluid flow in the **Label** text field.

Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Fluid flow** 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, rev_t/20, frev_tEnd)`.
- 4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** checkbox.
- 5 In the tree, select **Component 1 (comp1) > Size-Based Population Balance (pbsb)**.
- 6 Click  **Disable in Model**.
- 7 In the tree, select **Component 1 (comp1) > Multiphysics > Precipitation in Fluid Flow 1 (pff1)**.
- 8 Click  **Disable in Model**.
- 9 Click to expand the **Values of Dependent Variables** section. Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.
- 10 From the **Method** list, choose **Solution**.
- 11 From the **Study** list, choose **Fluid flow initialization, Frozen Rotor**.

ADD STUDY

- 1 Go to the **Add Study** window.
- 2 Click the **Add Study** button in the window toolbar.

POPULATION BALANCE



In the **Settings** window for **Study**, type Population balance in the **Label** text field.

- 1 In the **Model Builder** window, under **Population balance** 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 (0,0.2,10).
- 4 Locate the **Physics and Variables Selection** section. In the **Solve for** column of the table, under **Component 1 (comp1)**, clear the checkbox for **Turbulent Flow, k-ε (spf)**.
- 5 Locate the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.
- 6 From the **Method** list, choose **Solution**.
- 7 From the **Study** list, choose **Fluid flow, Time Dependent**.
- 8 From the **Selection** list, choose **Automatic (all solutions)**.
- 9 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.
- 10 Click **+ Add**.
- 11 In the table, enter the following settings:


Parameter name	Parameter value list	Parameter unit
W (Stability ratio)	1, 10, 100	

No Study

- 1 In the **Study** toolbar, click  **More Study Extensions** and choose **Study Reference**.
- 2 In the **Settings** window for **Study Reference**, locate the **Study Reference** section.
- 3 From the **Study reference** list, choose **Fluid flow initialization**.
- 4 In the **Study** toolbar, click  **More Study Extensions** and choose **Study Reference**.
- 1 In the **Settings** window for **Study Reference**, locate the **Study Reference** section.
- 2 From the **Study reference** list, choose **Fluid flow**.

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 **Dependent Variables 1**.
- 3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
- 4 From the **Method** list, choose **Manual**.
- 5 In the **Scale** text field, type $1.0e24$.
- 6 In the **Model Builder** window, under **Population balance > Solver Configurations > Solution 1 (sol1)** click **Time-Dependent Solver 1**.

- 7 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.
- 8 Select the **Initial step** checkbox. In the associated text field, type $\text{rev_t}/1000$.
- 9 Click in the **Graphics** window and then press Ctrl+A to select all domains.
- 10 From the **Maximum step constraint** list, choose **Constant**.
- 11 In the **Maximum step** text field, type 0.05.
- 12 Click in the **Graphics** window and then press Ctrl+A to select all domains.
- 13 From the **Maximum BDF order** list, choose **2**.
- 14 Click to expand the **Advanced** section. Select the **Periodic values of variables not solved for** checkbox.
- 15 In the **Start time** text field, type $f\text{rev_tEnd} - \text{rev_t}$.
- 16 In the **Interval length** text field, type rev_t .
- 17 Click in the **Graphics** window and then press Ctrl+A to select all domains.
- 18 In the **Study** toolbar, click  **Compute**.

RESULTS

Number of Particles and Velocity

- 1 Right-click **Number of Particles (pbsb)** and choose **Duplicate**.
- 2 In the **Settings** window for **2D Plot Group**, type **Number of Particles and Velocity** in the **Label** text field.
- 3 Locate the **Data** section. From the **Parameter value (W)** list, choose **1**.
- 4 From the **Time (s)** list, choose **5**.
- 5 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 6 Locate the **Plot Settings** section. From the **Frame** list, choose **Spatial (x, y, z)**.
- 7 Locate the **Color Legend** section. Select the **Show maximum and minimum values** checkbox.
- 8 Select the **Show units** checkbox.

Surface I

- 1 In the **Model Builder** window, expand the **Number of Particles and Velocity** node, then click **Surface I**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type $\text{pbsb} \cdot N$.


Number of Particles and Velocity

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

Surface 2

- 1 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 2 From the **Color table** list, choose **RanaArvalis**.

Filter 1

- 1 In the **Number of Particles and Velocity** toolbar, click  **Filter**.
- 2 In the **Settings** window for **Filter**, locate the **Element Selection** section.
- 3 In the **Logical expression for inclusion** text field, type $x-y>0$.

Number of Particles and Velocity

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


Annotation 1

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type `Particle\\concentration`.
- 3 Select the **LaTeX markup** checkbox.
- 4 Locate the **Position** section. In the **x** text field, type -0.04 .
- 5 In the **y** text field, type 0.07 .
- 6 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 7 From the **Anchor point** list, choose **Middle right**.

Number of Particles and Velocity

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

Annotation 2

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type `Velocity`.
- 3 Locate the **Position** section. In the **x** text field, type 0.05 .
- 4 In the **y** text field, type -0.06 .
- 5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 6 From the **Anchor point** list, choose **Middle left**.
- 7 In the **Number of Particles and Velocity** toolbar, click  **Plot**.

Velocity (spf)

- 1 In the **Model Builder** window, under **Results** click **Velocity (spf)**.

- 2 In the **Settings** window for **2D Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **None**.
- 4 Locate the **Color Legend** section. Select the **Show units** checkbox.

Pressure (spf), Velocity (spf), Wall Resolution (spf)

- 1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Velocity (spf)**, **Pressure (spf)**, and **Wall Resolution (spf)**.
- 2 Right-click and choose **Group**.

Fluid Flow

In the **Settings** window for **Group**, type Fluid Flow in the **Label** text field.

Number of Particles at Different Times

- 1 In the **Model Builder** window, under **Results** click **Population Number Density, n1 (pbsb)**.
- 2 In the **Settings** window for **2D Plot Group**, type Number of Particles at Different Times in the **Label** text field.
- 3 Locate the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 5 Locate the **Color Legend** section. Select the **Show units** checkbox.
- 6 From the **Position** list, choose **Right double**.
- 7 Click to expand the **Plot Array** section. From the **Array type** list, choose **Square**.

Surface 1

- 1 In the **Model Builder** window, expand the **Number of Particles at Different Times** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Population balance/Solution 1 (sol1)**.
- 4 From the **Parameter value (W)** list, choose **1**.
- 5 From the **Time (s)** list, choose **0.2**.
- 6 Locate the **Expression** section. In the **Expression** text field, type pbsb.N.
- 7 Locate the **Coloring and Style** section. From the **Color table** list, choose **Algae**.
- 8 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.
- 9 In the **Row index** text field, type 1.

Arrow Surface 1

- 1 In the **Model Builder** window, click **Arrow Surface 1**.

- 2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Population balance/Solution 1 (sol1)**.
- 4 From the **Time (s)** list, choose **0.2**.
- 5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.
- 6 In the **Row index** text field, type 1.

Number of Particles at Different Times

In the **Number of Particles at Different Times** toolbar, click  **Annotation**.

Annotation 1

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type $t=0.2s$.
- 3 Locate the **Position** section. In the **y** text field, type -0.08 .
- 4 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 5 From the **Anchor point** list, choose **Upper middle**.
- 6 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.
- 7 In the **Row index** text field, type 1.

Annotation 1, Arrow Surface 1, Surface 1

- 1 In the **Model Builder** window, under **Results > Number of Particles at Different Times**, Ctrl-click to select **Surface 1**, **Arrow Surface 1**, and **Annotation 1**.
- 2 Right-click and choose **Duplicate**.

Surface 2

- 1 In the **Settings** window for **Surface**, locate the **Data** section.
- 2 From the **Time (s)** list, choose **0.4**.
- 3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Cynanthus**.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Arrow Surface 2

- 1 In the **Model Builder** window, click **Arrow Surface 2**.
- 2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.
- 3 From the **Time (s)** list, choose **0.4**.
- 4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Arrow Surface 1**.
- 5 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Annotation 2

- 1 In the **Model Builder** window, click **Annotation 2**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type $t=0.4s$.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Annotation 2, Arrow Surface 2, Surface 2

- 1 In the **Model Builder** window, under **Results > Number of Particles at Different Times**, Ctrl-click to select **Surface 2**, **Arrow Surface 2**, and **Annotation 2**.
- 2 Right-click and choose **Duplicate**.

Surface 3

- 1 In the **Settings** window for **Surface**, locate the **Data** section.
- 2 From the **Time (s)** list, choose **0.8**.
- 3 Locate the **Coloring and Style** section. From the **Color table** list, choose **RanaDraytonii**.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 5 In the **Column index** text field, type 0.

Arrow Surface 3

- 1 In the **Model Builder** window, click **Arrow Surface 3**.
- 2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.
- 3 From the **Time (s)** list, choose **0.8**.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 5 In the **Column index** text field, type 0.

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 $t=0.8s$.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 5 In the **Column index** text field, type 0.

Annotation 3, Arrow Surface 3, Surface 3

- 1 In the **Model Builder** window, under **Results > Number of Particles at Different Times**, Ctrl-click to select **Surface 3**, **Arrow Surface 3**, and **Annotation 3**.
- 2 Right-click and choose **Duplicate**.

Annotation 4, Arrow Surface 4, Surface 4

- 1 In the **Settings** window for **Surface**, locate the **Data** section.
- 2 From the **Time (s)** list, choose **1.2**.
- 3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Arctium**.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Arrow Surface 4

- 1 In the **Model Builder** window, click **Arrow Surface 4**.
- 2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.
- 3 From the **Time (s)** list, choose **1.2**.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.


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 $t=1.2s$.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Annotation 3, Arrow Surface 3, Surface 3

In the **Model Builder** window, under **Results** > **Number of Particles at Different Times**, Ctrl-click to select **Surface 3**, **Arrow Surface 3**, and **Annotation 3**.

Surface 3

- 1 Drag and drop below **Annotation 1**.
- 2 In the **Number of Particles at Different Times** toolbar, click  **Plot**.

Particle Concentrations of Different Sizes

- 1 In the **Model Builder** window, under **Results** click **Population Number Density, n7 (pbsb)**.
- 2 In the **Settings** window for **2D Plot Group**, type Particle Concentrations of Different Sizes in the **Label** text field.
- 3 Locate the **Data** section. From the **Parameter value (W)** list, choose **1**.
- 4 Locate the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section. From the **Frame** list, choose **Spatial (x, y, z)**.
- 6 Locate the **Color Legend** section. Select the **Show units** checkbox.
- 7 From the **Position** list, choose **Right double**.
- 8 Locate the **Plot Array** section. From the **Array type** list, choose **Square**.

Surface 1

- 1 In the **Model Builder** window, expand the **Particle Concentrations of Different Sizes** node, then click **Surface 1**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.
- 3 In the **Expression** text field, type $n2 * pbsb.dL_n2$.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Algae**.
- 5 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.
- 6 In the **Row index** text field, type 1.

Arrow Surface 1

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

Particle Concentrations of Different Sizes

In the **Particle Concentrations of Different Sizes** toolbar, click  **Annotation**.

Annotation 1

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type 138-159 nm.
- 3 Locate the **Position** section. In the **y** text field, type -0.08.
- 4 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 5 From the **Anchor point** list, choose **Upper middle**.
- 6 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.
- 7 In the **Row index** text field, type 1.

Annotation 1, Surface 1

- 1 In the **Model Builder** window, under **Results > Particle Concentrations of Different Sizes**, Ctrl-click to select **Surface 1** and **Annotation 1**.
- 2 Right-click and choose **Duplicate**.

Surface 2

- 1 In the **Settings** window for **Surface**, locate the **Expression** section.
- 2 In the **Expression** text field, type $n4 * pbsb.dL_n4$.
- 3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Cynanthus**.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Annotation 2

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

- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type 183-211 nm.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Annotation 2, Surface 2

- 1 In the **Model Builder** window, under **Results > Particle Concentrations of Different Sizes**, Ctrl-click to select **Surface 2** and **Annotation 2**.
- 2 Right-click and choose **Duplicate**.

Surface 3

- 1 In the **Settings** window for **Surface**, locate the **Expression** section.
- 2 In the **Expression** text field, type $n8 * pbsb.dL_n8$.
- 3 Locate the **Coloring and Style** section. From the **Color table** list, choose **RanaDraytonii**.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 5 In the **Column index** text field, type 0.

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 321-370 nm.
- 4 Locate the **Plot Array** section. In the **Row index** text field, type 0.
- 5 In the **Column index** text field, type 0.

Annotation 3, Surface 3

- 1 In the **Model Builder** window, under **Results > Particle Concentrations of Different Sizes**, Ctrl-click to select **Surface 3** and **Annotation 3**.
- 2 Right-click and choose **Duplicate**.

Surface 4

- 1 In the **Settings** window for **Surface**, locate the **Expression** section.
- 2 In the **Expression** text field, type $n12 * pbsb.dL_n12$.
- 3 Locate the **Coloring and Style** section. From the **Color table** list, choose **Arctium**.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

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 564 - 649 nm.
- 4 Locate the **Plot Array** section. In the **Column index** text field, type 1.

Annotation 3, Surface 3

In the **Model Builder** window, under **Results > Particle Concentrations of Different Sizes**, Ctrl-click to select **Surface 3** and **Annotation 3**.

Surface 3

- 1 Drag and drop below **Annotation 1**.
- 2 In the **Particle Concentrations of Different Sizes** toolbar, click  **Plot**.

Population Number Density, n13 (pbsb)

In the **Model Builder** window, under **Results** right-click **Population Number Density, n13 (pbsb)** and choose **Delete**.

Line Segments 1

- 1 In the **Model Builder** window, expand the **Average Size Distribution (pbsb)** node, then click **Line Segments 1**.
- 2 In the **Settings** window for **Line Segments**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Average 1**.
- 4 From the **Parameter selection (W)** list, choose **First**.
- 5 From the **Time selection** list, choose **First**.
- 6 Click to expand the **Coloring and Style** section. From the **Color** list, choose **Black**.
- 7 From the **Width** list, choose **2**.
- 8 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 9 From the **Legends** list, choose **Manual**.
- 10 In the table, enter the following settings:

Legends
Time =0 s

Line Segments 2



- 1 Right-click **Results > Average Size Distribution (pbsb) > Line Segments 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Segments**, locate the **Data** section.
- 3 From the **Parameter selection (W)** list, choose **All**.
- 4 From the **Time selection** list, choose **From list**.

- 5 In the **Times (s)** list box, select **3**.
- 6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
- 7 From the **Color** list, choose **Cycle (reset)**.
- 8 Locate the **Legends** section. From the **Legends** list, choose **Automatic**.


Line Segments 3

- 1 Right-click **Line Segments 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Segments**, locate the **Data** section.
- 3 In the **Times (s)** list box, select **6**.
- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.


Line Segments 4

- 1 Right-click **Line Segments 3** and choose **Duplicate**.
- 2 In the **Settings** window for **Line Segments**, locate the **Data** section.
- 3 From the **Time selection** list, choose **Last**.
- 4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dash-dot**.
- 5 In the **Average Size Distribution (pbsb)** toolbar, click  **Plot**.
- 6 Click the  **x-Axis Log Scale** button in the **Graphics** toolbar.

Average Size and Number of Particles

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, type Average Size and Number of Particles in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Average I**.
- 4 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section. Select the **Two y-axes** checkbox.
- 6 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.
- 7 From the **Position** list, choose **Bottom**.

Global 1

- 1 In the **Average Size and Number of Particles** 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.Lav	nm	Average size

4 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle (reset)**.

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

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

Average Size and Number of Particles

In the **Average Size and Number of Particles** 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
pbsb.N	1/m ³	Particle conc.

3 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** checkbox.


4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle (reset)**.

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

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

7 In the **Average Size and Number of Particles** toolbar, click  **Plot**.

Volume Conservation

1 In the **Results** toolbar, click  **Evaluation Group**.

2 In the **Settings** window for **Evaluation Group**, type Volume Conservation in the **Label** text field.

3 Locate the **Transformation** section. From the **Transformation type** list, choose **General**.


4 Select the **Keep child nodes** checkbox.

5 In the **Expression** text field, type `abs(int1-int2)/int1`.

6 In the **Column header** text field, type Relative volume change.

7 Click to expand the **Format** section. From the **Include parameters** list, choose **Off**.

Surface Integration 1

- 1 In the **Volume Conservation** toolbar, click  **Integration** and choose **Surface Integration**.
- 2 In the **Settings** window for **Surface Integration**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Population balance/Solution 1 (sol1)**.
- 4 From the **Time selection** list, choose **First**.
- 5 Select Domain 1 only.
- 6 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
pbsb.Vtot	m ²	Total volume t=0

Volume Conservation

In the **Volume Conservation** toolbar, click  **Integration** and choose **Surface Integration**.

Surface Integration 2

- 1 In the **Settings** window for **Surface Integration**, locate the **Data** section.
- 2 From the **Dataset** list, choose **Population balance/Solution 1 (sol1)**.
- 3 From the **Time selection** list, choose **Last**.
- 4 Select Domain 1 only.
- 5 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
pbsb.Vtot	m ²	Total volume t=60

- 6 In the **Volume Conservation** toolbar, click  **Evaluate**.