Created in COMSOL Multiphysics 5.6

Turbulent Mixing of a Trace Species

Introduction

This tutorial demonstrates how mixing can be simulated in a stirred vessel by seeding a trace species from a point. The flow is modeled using the Rotating Machinery, Fluid Flow interface, which solves the Navier-Stokes equations on geometries with rotating parts such as impellers. The transport of the trace species is modeled using the Transport of Diluted Species interface.

Model Definition

MODEL GEOMETRY

Figure 1 shows the model geometry, which is a schematic cross section of a tank with a four-blade impeller. The tank has four baffles attached to the wall to enhance mixing. The mixer blades and the impellers are approximated to be infinitely thin. The seeding of the trace species is done at the marked point.

The circle between the impeller and the tank wall is the assembly boundary where the mesh is allowed to slide when the impeller rotates.

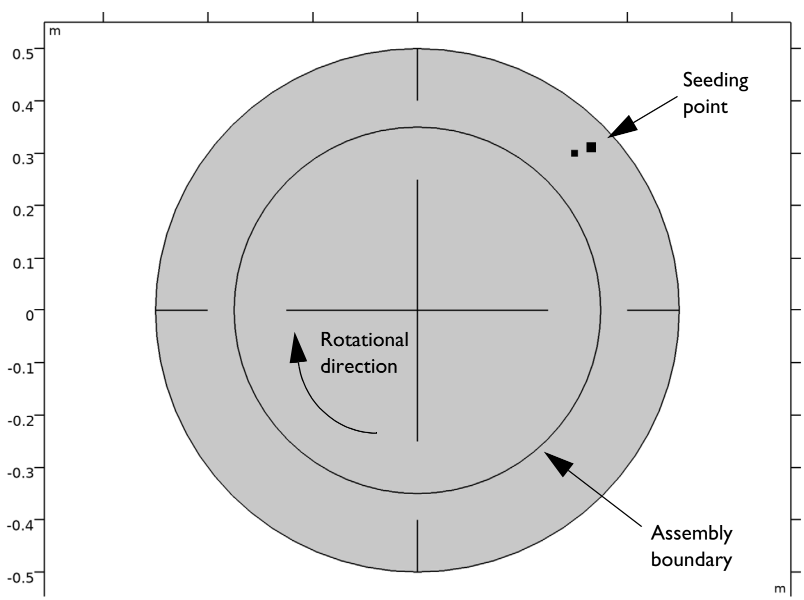

Figure 1: Model geometry.

DOMAIN EQUATION AND BOUNDARY CONDITIONS

The mixer fluid is water, and a rotational speed of 20 rpm is prescribed for the impeller. This rotation is achieved by prescribing the inner domain to be a rotating domain. The boundary between the inner and the outer domain is prescribed to be a continuity boundary that transfers momentum to the fluid in the outer domain.

The Reynolds number based on the impeller radius and the impeller tip speed is approximately 1.9×10^6, which means that the flow is turbulent. The k–ε turbulence model is applied in this example.

There are two methods to reach operating conditions. One is to accelerate the impeller up to full speed and wait for the flow to reach a quasi steady-state. This approach is simple but can be time consuming. A computationally more efficient method is to first simulate the flow using the frozen rotor approach. Frozen rotor means that the impeller, or rotor, is frozen in position. The flow in the rotating domain is assumed to be stationary in terms of a rotating coordinate system. The effect of the rotation is then accounted for by Coriolis and centrifugal forces. This solution couples to the nonrotating parts where the flow is also assumed to be stationary, but in a nonrotating coordinate system. See the *CFD Module User's Guide* for more information about frozen rotor.

The result of a frozen rotor simulation is an approximation to the flow at operating conditions. The result depends on the angular position of the impeller and cannot represent transient effects. It is still a very good starting condition to reach operating conditions. Quasi-steady state from a frozen rotor simulation is typically reached within a few revolutions, while starting from zero velocity requires tens of revolutions to reach operating conditions.

A trace species is a species introduced in very small quantities. It is often of a sharp color to be clearly visible even in small amounts. A trace species is not supposed to affect the flow, and hence, the flow can be solved for first and then the trace species transport solved for subsequently. Because it is the mixing at operating condition that is interesting, the trace species is introduced only once the flow is closed to fully developed, which it is after approximately six seconds starting from the frozen rotor simulation.

The seeding is modeled as a point source with normal distribution around the release time, $t = 7.0$ seconds. The absolute value of the pulse is arbitrary since the trace species does not affect the flow.

Results and Discussion

Figure 2 shows the frozen rotor velocity field. As expected, the highest velocity magnitude is found at the tip of the mixer blades. There are also clearly visible recirculation zones both before and behind the baffles.

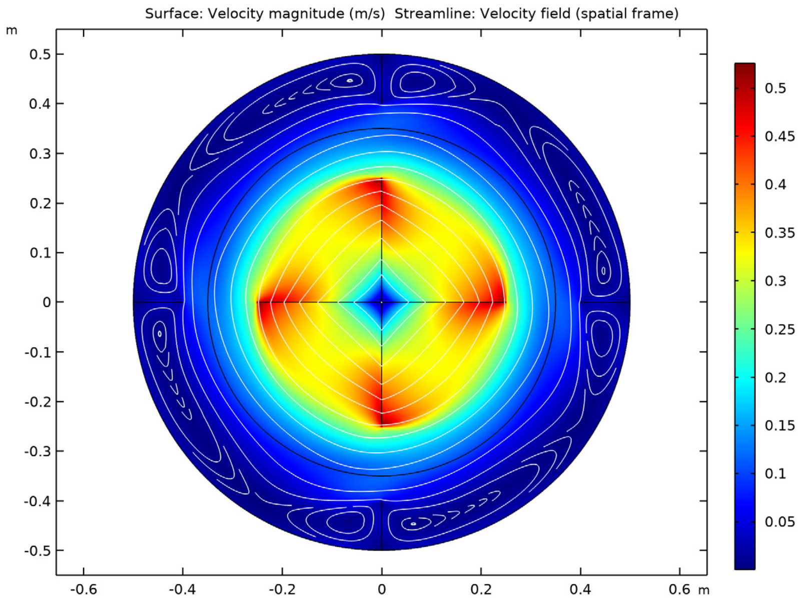

Figure 2: The velocity field obtained from the frozen rotor simulation.

Figure 3 shows the velocity field at t = 30 s. The rotor position is the same as in Figure 2, and the results in the figures are similar. There are however differences. The most notably difference is the recirculation zones before the baffles that are smaller in Figure 3 than in Figure 2. The size and shape of the recirculation zones for the time-dependent simulation also vary with the position of the impeller.

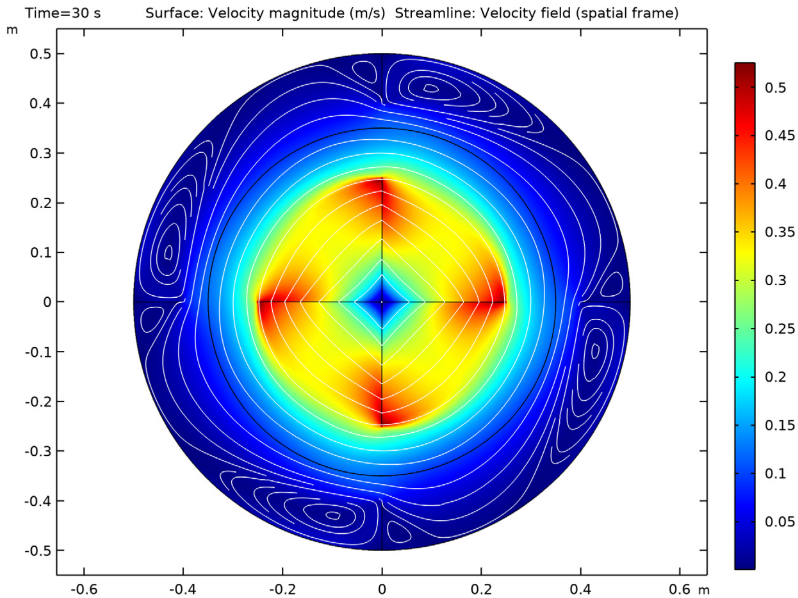

Figure 3: A snapshot of the time-dependent velocity field at t=30 s.

Figure 4 shows four snapshots of the mixing process, time running from top left to lower-right picture. Since the velocity is rather slow at the seeding point (see also Figure 3), the initial transport is almost isotropic from the seeding point ($t = 9$ s). Some trace species is however entrained in the faster velocity field in the center of the mixer and becomes thereby spread in the azimuthal direction ($t = 14.7$ s). It only takes a few seconds more for the trace species to be almost homogeneous distributed in the mixer. The slowest spreading is to the regions in between the impeller blades. This is a well known phenomenon and is the reason to why chemical substances are commonly added as close to the impeller axis as possible.

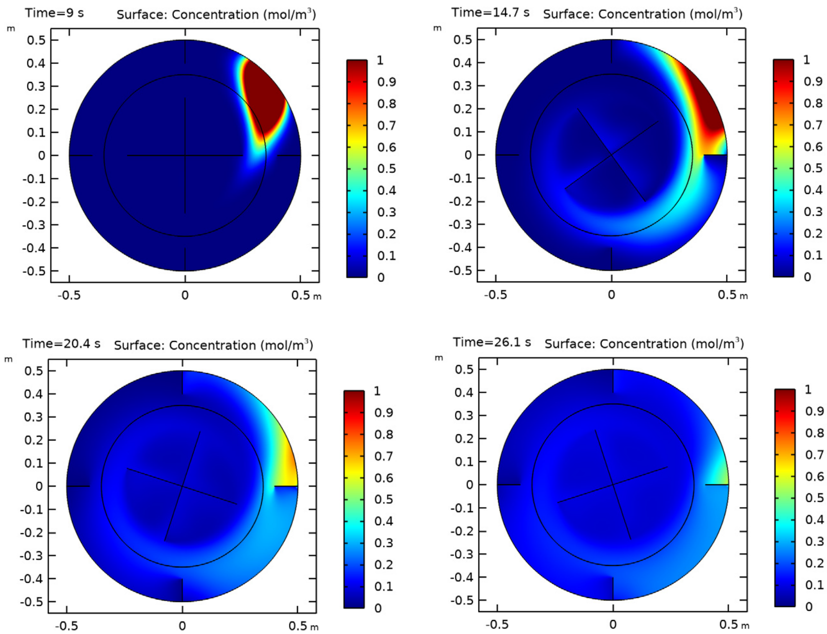

Figure 4: The mixing process. Surface plots of the trace species at t = 9, 14.7, 20.4 and 26.1 seconds.

Application Library path: `CFD_Module/Single-Phase_Flow/turbulent_mixing`

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 **Fluid Flow>Single-Phase Flow>Rotating Machinery, Fluid Flow>Turbulent Flow>Turbulent Flow, k-ε**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces>Frozen Rotor**.

6 Click **Done**.

GEOMETRY 1

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 `0.5`.

Circle 2 (c2)

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 `0.35`.

4 Click **Build Selected**.

Difference 1 (dif1)

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

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

3 Select the **Keep input objects** check box.

4 Select the object **c1** only.

5 Find the **Objects to subtract** subsection. Select the **Activate Selection** toggle button.

6 Select the object **c2** only.

Delete Entities 1 (del1)

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

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

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

4 Select the object **c1** only.

5 Click **Build Selected**.

Line Segment 1 (ls1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 Locate the **Starting Point** section. In the **x** text field, type `-0.5`.

6 Locate the **Endpoint** section. In the **x** text field, type `-0.4`.

Rotate 1 (rot1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Rotate**.

2 Select the object **ls1** only.

3 In the **Settings** window for **Rotate**, locate the **Rotation** section.

4 Click **Range**.

5 In the **Range** dialog box, type `90` in the **Start** text field.

6 In the **Step** text field, type `90`.

7 In the **Stop** text field, type `270`.

8 Click **Replace**.

9 In the **Settings** window for **Rotate**, locate the **Input** section.

10 Select the **Keep input objects** check box.

Point 1 (pt1)

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

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

3 In the **x** text field, type `0.3`.

4 In the **y** text field, type `0.3`.

Union 1 (uni1)

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

The final operation will later be set to **Form an assembly**. Union operations are therefore necessary to merge the domains and the lines.

2 Select the objects **dif1**, **ls1**, **pt1**, **rot1(1)**, **rot1(2)**, and **rot1(3)** only.

Line Segment 2 (ls2)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 Locate the **Starting Point** section. In the **x** text field, type `-0.25`.

6 Locate the **Endpoint** section. In the **x** text field, type `0.25`.

Line Segment 3 (ls3)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Line Segment**.

2 In the **Settings** window for **Line Segment**, locate the **Starting Point** section.

3 From the **Specify** list, choose **Coordinates**.

4 Locate the **Endpoint** section. From the **Specify** list, choose **Coordinates**.

5 Locate the **Starting Point** section. In the **y** text field, type `-0.25`.

6 Locate the **Endpoint** section. In the **y** text field, type `0.25`.

Union 2 (uni2)

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

2 Select the objects **c2**, **ls2**, and **ls3** only.

Form Union (fin)

The boundary between the rotating and nonrotating domain must be an assembly boundary so that the parts can move relative to each other.

1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, locate the **Form Union/Assembly** section.

3 From the **Action** list, choose **Form an assembly**.

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

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

ADD MATERIAL

1 In the **Home** 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 **Add to Component** in the window toolbar.

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

DEFINITIONS

Rotating Domain 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions>Moving Mesh** click **Rotating Domain 1**.
2 Select Domain 2 only.
3 In the **Settings** window for **Rotating Domain**, locate the **Rotation** section.
4 In the f text field, type `-20[1/min]`.

TURBULENT FLOW, K-ε (SPF)

Flow Continuity 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Turbulent Flow, k-ε (spf)** and choose **Pairs>Flow Continuity**.
2 In the **Settings** window for **Flow Continuity**, locate the **Pair Selection** section.
3 Under **Pairs**, click **Add**.
4 In the **Add** dialog box, select **Identity Boundary Pair 1 (ap1)** in the **Pairs** list.
5 Click **OK**.

Interior Wall 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Interior Wall**.
2 Select Boundaries 1–4 and 13–16 only.

Pressure Point Constraint 1

1 In the **Physics** toolbar, click **Points** and choose **Pressure Point Constraint**.
2 Select Point 10 only.

The pressure level must be specified to obtain a unique solution since water is an incompressible liquid.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.
3 From the **Element size** list, choose **Fine**.

STUDY 1

Step 1: Frozen Rotor

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

RESULTS

Velocity (spf)

Create Figure 2 using the following steps.

Streamline 1

1 Right-click **Velocity (spf)** and choose **Streamline**.

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

3 From the **Positioning** list, choose **Uniform density**.

4 In the **Separating distance** text field, type `0.02`.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **White**.

6 In the **Velocity (spf)** toolbar, click **Plot**.

Add a **Time Dependent** study.

ADD STUDY

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

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

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

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

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

STUDY 2

Step 1: Time Dependent

It is important to specify frequent enough output times for the flow field. The subsequent species simulation might otherwise be affected by interpolation errors.

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

2 In the **Output times** text field, type `0 range(6,0.15,30)`.

Start from the frozen rotor solution.

3 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**.

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

5 From the **Study** list, choose **Study 1, Frozen Rotor**.

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

RESULTS

Velocity (spf) 1

Re-create Figure 3 using the following steps.

Streamline 1

1 Right-click **Velocity (spf) 1** and choose **Streamline**.

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

3 From the **Positioning** list, choose **Uniform density**.

4 In the **Separating distance** text field, type `0.02`.

5 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Color** list, choose **White**.

6 In the **Velocity (spf) 1** toolbar, click **Plot**.

DEFINITIONS

Gaussian Pulse 1 (gp1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Local>Gaussian Pulse**.

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

3 In the **Location** text field, type `7`.

4 In the **Standard deviation** text field, type `0.25`.

ADD PHYSICS

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

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

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

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check boxes for **Study 1** and **Study 2**.

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

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

ADD STUDY

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

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

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

4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Turbulent Flow, k-ε (spf)**.

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

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

TRANSPORT OF DILUTED SPECIES (TDS)

Transport Properties 1

In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species (tds)** click **Transport Properties 1**.

Turbulent Mixing 1

1 In the **Physics** toolbar, click **Attributes** and choose **Turbulent Mixing**.

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

3 From the ν_T list, choose **Turbulent kinematic viscosity (spf/fp1)**.

4 In the Sc_T text field, type 1.

Transport Properties 1

1 In the **Model Builder** window, click **Transport Properties 1**.

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

3 From the $\mathbf{u}$ list, choose **Velocity field (spf)**.

Continuity 1

1 In the **Physics** toolbar, click **Pairs** and choose **Continuity**.

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

3 Under **Pairs**, click **Add**.

4 In the **Add** dialog box, select **Identity Boundary Pair 1 (ap1)** in the **Pairs** list.

5 Click **OK**.

Thin Impermeable Barrier 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Thin Impermeable Barrier**.

2 Select Boundaries 1–4 and 13–16 only.

Line Mass Source 1

1 In the **Physics** toolbar, click **Points** and choose **Line Mass Source**.

2 Select Point 10 only.

3 In the **Species Source** edit field, enter `gp1(t[1/s])/10`.

STUDY 3

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 3** 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(6,0.15,30)`.

4 Locate the **Values of Dependent Variables** section. Find the **Values of variables not solved for** subsection. From the **Settings** list, choose **User controlled**.

5 From the **Method** list, choose **Solution**.

6 From the **Study** list, choose **Study 2, Time Dependent**.

The **Automatic Time** setting would only use the last solution from **Study 2**. Change to **All**.

7 From the **Time (s)** list, choose **All**.

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

RESULTS

Concentration (tds)

The following steps create an animation that contains the plots in Figure 4.

Plot the dataset edges on the spatial frame to make them follow the rotation.

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

2 From the **Frame** list, choose **Spatial (x, y, z)**.

Surface 1

1 In the **Model Builder** window, expand the **Concentration (tds)** node, then click **Surface 1**.

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

3 Select the **Manual color range** check box.

4 In the **Minimum** text field, type `0`.

5 In the **Maximum** text field, type `1`.

Streamline 1

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

Animation 1

1 In the **Results** toolbar, click **Animation** and choose **File**.

2 In the **Settings** window for **Animation**, locate the **Target** section.

3 From the **Target** list, choose **Player**.

4 Locate the **Scene** section. From the **Subject** list, choose **Concentration (tds)**.

Set the frames to be displayed for as long as the time between the saved solutions.

5 Locate the **Playing** section. In the **Display each frame for** text field, type `0.15`.

6 Locate the **Frames** section. From the **Frame selection** list, choose **All**.

7 Right-click **Animation 1** and choose **Play**.