Particle Trajectories in a Laminar Static Mixer

Introduction

In static mixers, also called motionless or in-line mixers, a fluid is pumped through a pipe containing stationary blades. This mixing technique is particularly well suited for laminar flow mixing because it generates only small pressure losses in this flow regime. This example studies the flow in a twisted-blade static mixer. It evaluates the mixing performance by calculating the trajectory of suspended particles through the mixer.

Model Definition

This model studies the mixing of one species dissolved in water at room temperature. The geometry consists of a tube with three twisted blades of alternating rotations (Figure 1).

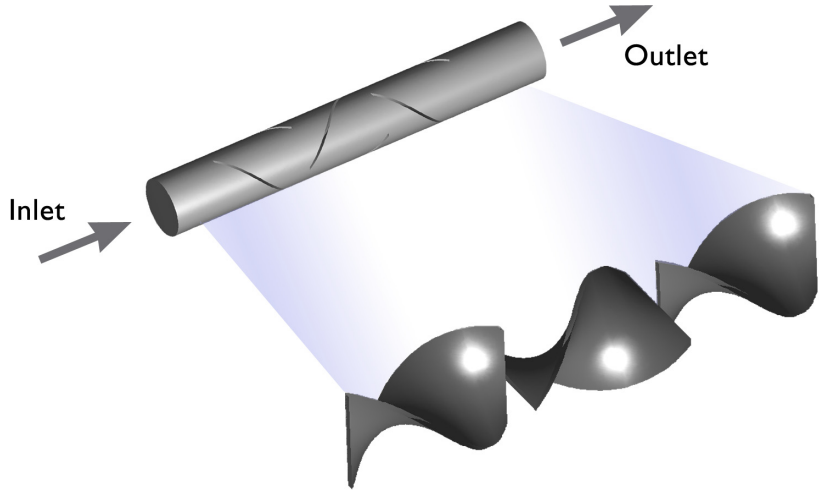

Figure 1: Depiction of a laminar static mixer containing three blades with alternating rotations.

The tube's radius, R, is 6 mm; the length is $14R$, and the length of each blade is $3R$. The inlet flow is laminar and fully developed with an average velocity of 1 cm/s. At the

outlet, the model specifies a constant reference pressure of 0 Pa. The equations for the momentum transport are the stationary Navier-Stokes equations in 3D:

$$\begin{aligned} \rho(\mathbf{u}\cdot\nabla)\mathbf{u} &= \nabla\cdot[-p\mathbf{I}+\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T})] \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned} \quad (1)$$

Here η denotes the dynamic viscosity (kg/(m·s)), $\mathbf{u}$ is the velocity (m/s), ρ represents the fluid density (kg/m^3), and p denotes the pressure (Pa).

The particle trajectories are computed using a Newtonian formulation

$$\frac{d}{dt}(m_p\mathbf{v}) = m_p F_d(\mathbf{u}-\mathbf{v}) \quad (2)$$

where F_d is the drag force per unit mass:

$$F_d = \frac{18\eta}{\rho_p d_p^2}. \quad (3)$$

The particle velocity is $\mathbf{v}$, ρ_p is the density of the particles, and d_p is the particle diameter. There are 3000 particles released. The density of the particles released is normalized to the magnitude of the fluid velocity at the inlet. This means that there are more particles released where the inlet velocity is highest and fewer particles released where the velocity field is low.

Results and Discussion

The particle trajectories are plotted in Figure 1. Because the particles have mass, they do not necessarily all reach the outlet; some of the particles will get stuck to the mixer walls. The transmission probability is defined as the ratio of the number of particles that reach the outlet divided by the number of particles released. For this specific configuration the transmission probability is 0.82. This means that 18 % of the particles will remain trapped in the mixer.

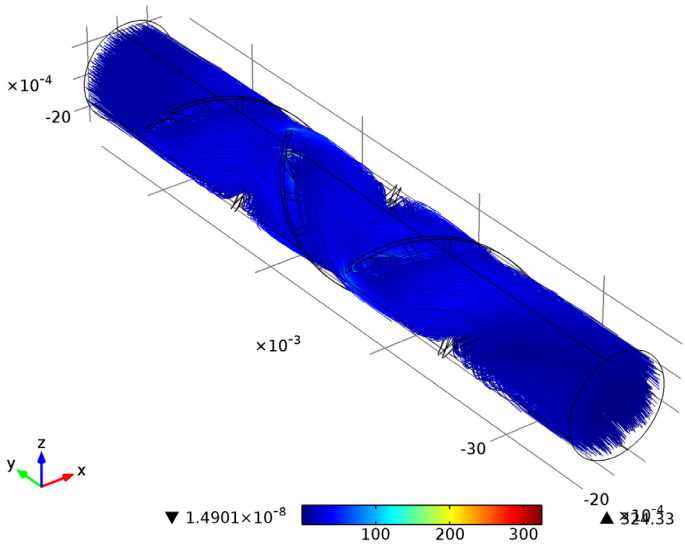

Figure 2: Plot of the particle trajectories inside the laminar mixer. The color is the shear rate.

One useful way of visualizing how to particles mix is to use a Poincaré plot. The Poincaré plot places a colored dot for each particles at the location at which the particle passes through a cut plane (known as a Poincaré section). In Figure 3, the location of the particles at 6 Poincaré sections are shown. The color represents the location of the particle at its initial position. So, particles marked as red had an initial position of $x < 0$ and particles marked as blue had an initial position of $x > 0$. The `at()` operator is used to mark the particles with the color of their initial position. The first Poincaré section (the one furthest to the left in Figure 3) clearly indicates which particles start with coordinates of $x < 0$. As the particles begin to follow the flow field, they begin to mix together. By the end of the mixer, the particles have not mixed completely—there are still significant pockets of only red and only blue particles.

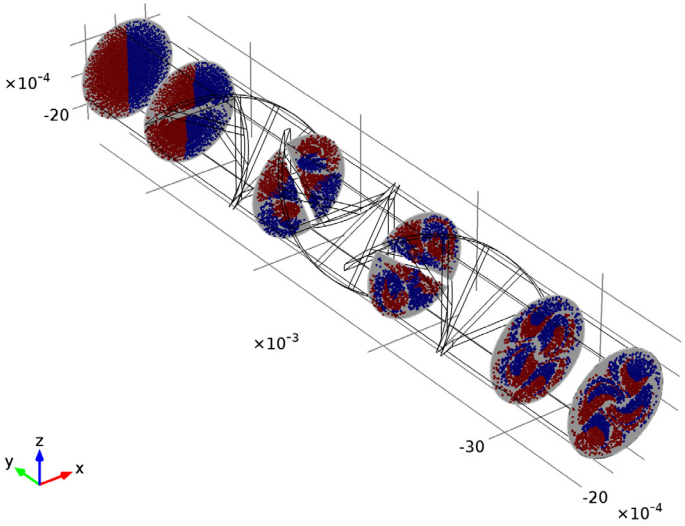

Figure 3: Poincaré maps of the particle trajectories at different Poincaré sections. The color is a logical expression indicating which particles had an initial position at $x < 0$.

A phase portrait can also be used to visualize the effect of particle mixing, but it is not as useful as the Poincaré map because it applies to all particles at a given snapshot in time rather than a plane in space. A standard phase portrait plots the particle position versus velocity (or momentum), but in COMSOL the default expressions can be overridden. In Figure 4 the x-axis represents the y-location of the particles, and the y-axis represents the z-location of the particles at different snapshots in time. At $t = 5$ s there are still pockets where only blue and only red particles exist, indicating that if 2 distinct streams were introduced at the inlet, they would not be completely mixed.

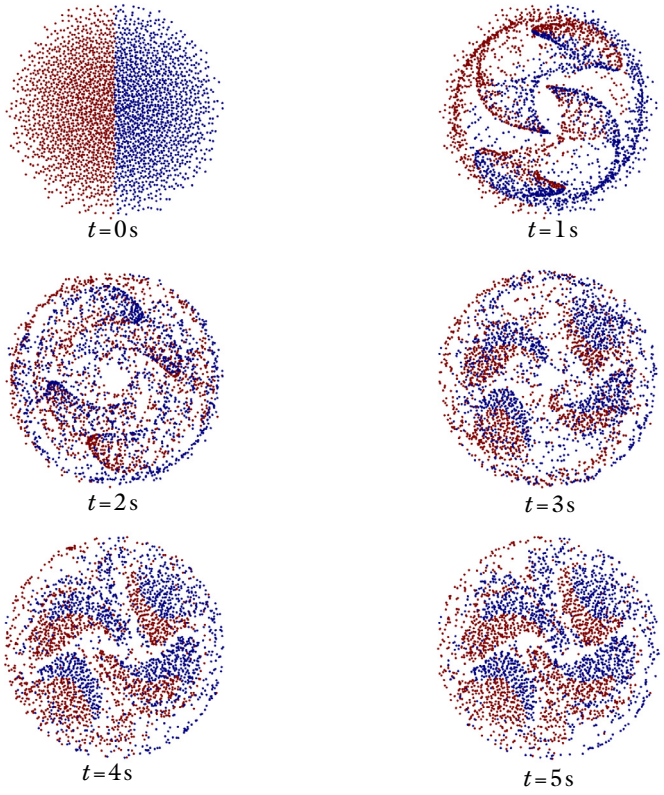

Figure 4: Plot of the particle position in the xz-plane at different points in time. The red colored particles had an initial position of $x < 0$ and the blue colored particles had an initial position of $x > 0$.

Notes About the COMSOL Implementation

The model is solved in two stages: first the fluid velocity and pressure are computed, then, using a separate study, the particle trajectories are computed.

Reference

1. R. Perry and D. Green, *Perry's Chemical Engineering Handbook*, 7th ed., McGraw-Hill, 1997.

Model Library path: `Particle_Tracing_Module/Fluid_Flow/laminar_mixer_particle`

Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click **Next**.

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

4 Click **Add Selected**.

5 Click **Next**.

6 Find the **Studies** subsection. In the tree, select **Preset Studies>Stationary**.

7 Click **Finish**.

GEOMETRY 1

The mixer geometry is quite complicated so start by importing it from a file.

Import 1

1 In the **Model Builder** window, under **Model 1** right-click **Geometry 1** and choose **Import**.

2 In the **Import** settings window, locate the **Import** section.

3 Click the **Browse** button.

4 Browse to the model's Model Library folder and double-click the file `laminar_mixer_particle.mphbin`.

5 Click the **Import** button.

GLOBAL DEFINITIONS

Parameters

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

2 In the **Parameters** settings window, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression
ra	3[mm]
u_mean	10[mm/s]

MATERIALS

Material 1

1 In the **Model Builder** window, under **Model 1** right-click **Materials** and choose **Material**.

2 In the **Material** settings window, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Name	Value
Density	rho	1000
Dynamic viscosity	mu	1e-3

LAMINAR FLOW

Now add an expression for the inflow velocity which is parabolic.

1 In the **Model Builder** window, expand the **Model 1>Laminar Flow** node.

Inlet 1

1 Right-click **Laminar Flow** and choose **Inlet**.

2 Select Boundary 23 only.

3 In the **Inlet** settings window, locate the **Velocity** section.

4 In the U_0 edit field, type `2*(1-(x^2+z^2)/ra^2)*u_mean`.

The boundary condition which was just added was rather complicated but necessary to get a fully developed flow profile. The CFD, Microfluidics and Plasma modules all have a special **Laminar Inflow** boundary condition which ensures laminar flow. It is not neccesary to enter a complicated expression for the velocity profile, just the average velocity of flowrate.

Outlet 1

1 Right-click **Laminar Flow** and choose **Outlet**.

2 Select Boundary 20 only.

MESH 1

The mesh needs to be quite fine to ensure that the particle motion is accurate through the modeling domain. In this case, take care to ensure that the mesh is fine on the mixing blades.

Free Triangular 1

1 In the **Model Builder** window, under **Model 1** right-click **Mesh 1** and choose **More Operations>Free Triangular**.

2 Click the **Wireframe Rendering** button on the Graphics toolbar.

3 Select Boundaries 5, 16–18, and 53–55 only.

Size 1

1 Right-click **Model 1>Mesh 1>Free Triangular 1** and choose **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Extremely fine**.

Size

1 In the **Model Builder** window, under **Model 1>Mesh 1** click **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extremely fine**.

4 Click the **Custom** button.

5 Locate the **Element Size Parameters** section. In the **Resolution of curvature** edit field, type `0.15`.

Free Triangular 2

1 In the **Model Builder** window, right-click **Mesh 1** and choose **More Operations>Free Triangular**.

2 Select Boundary 23 only.

Size 1

1 Right-click **Model 1>Mesh 1>Free Triangular 2** and choose **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Calibrate for** list, choose **Fluid dynamics**.

4 From the **Predefined** list, choose **Extra fine**.

Free Tetrahedral 1

1 In the **Model Builder** window, right-click **Mesh 1** and choose **Free Tetrahedral**.

2 In the **Settings** window, click **Build All**.

STUDY 1

In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

RESULTS

Velocity (spf)

Now that the flow field has been computed, add the interface to compute the particle trajectories.

MODEL 1

In the **Model Builder** window, right-click **Model 1** and choose **Add Physics**.

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 In the **Add physics** tree, select **Fluid Flow>Particle Tracing for Fluid Flow (fpt)**.

3 Click **Add Selected**.

4 Click **Next**.

5 Find the **Studies** subsection. In the tree, select **Preset Studies for Selected Physics>Time Dependent**.

6 Click **Finish**.

PARTICLE TRACING FOR FLUID FLOW

The drag force feature should get the fluid velocity field and viscosity from the **Single Phase, Laminar flow** interface.

1 In the **Model Builder** window, expand the **Particle Tracing for Fluid Flow** node.

Drag Force 1

1 Right-click **Model 1>Particle Tracing for Fluid Flow** and choose **Drag Force**.

2 Select Domain 1 only.

3 In the **Drag Force** settings window, locate the **Drag Force** section.

4 From the $\mathbf{u}$ list, choose **Velocity field (spf/fp1)**.

5 From the μ list, choose **Dynamic viscosity (spf/fp1)**.

The goal is to release particles in a way where they are more dense where the velocity field is higher.

Inlet 1

1 In the **Model Builder** window, right-click **Particle Tracing for Fluid Flow** and choose **Inlet**.

2 Select Boundary 23 only.

3 In the **Inlet** settings window, locate the **Initial Position** section.

4 From the **Initial position** list, choose **Density**.

5 In the N edit field, type `3000`.

6 In the ρ edit field, type `spf.U`.

7 Locate the **Initial Velocity** section. From the $\mathbf{u}$ list, choose **Velocity field (spf/fp1)**.

Outlet 1

1 Right-click **Particle Tracing for Fluid Flow** and choose **Outlet**.

2 Select Boundary 20 only.

Particle Properties 1

1 In the **Model Builder** window, under **Model 1>Particle Tracing for Fluid Flow** click **Particle Properties 1**.

2 In the **Particle Properties** settings window, locate the **Particle Properties** section.

3 From the **Particle property specification** list, choose **Specify particle density and diameter**.

4 In the d_p edit field, type `5E-7[m]`.

STUDY 2

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 2** node, then click **Step 1: Time Dependent**.

2 In the **Time Dependent** settings window, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics	Solve for
Laminar Flow (spf)	×

4 Click to expand the **Values of Dependent Variables** section. Select the **Values of variables not solved for** check box.

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

6 From the **Study** list, choose **Study 1, Stationary**.

7 Locate the **Study Settings** section. Click the **Range** button.

8 Go to the **Range** dialog box.

9 In the **Step** edit field, type `0.2`.

10 In the **Stop** edit field, type `5`.

11 Click the **Replace** button.

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

RESULTS

Particle Trajectories (fpt)

1 In the **3D Plot Group** settings window, click to expand the **Color Legend** section.

2 From the **Position** list, choose **Bottom**.

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

4 In the **Model Builder** window, expand the **Particle Trajectories (fpt)** node, then click **Particle Trajectories 1**.

5 In the **Particle Trajectories** settings window, locate the **Coloring and Style** section.

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

7 Find the **Point style** subsection. From the **Type** list, choose **None**.

8 In the **Model Builder** window, expand the **Results>Particle Trajectories (fpt)>Particle Trajectories 1** node, then click **Color Expression 1**.

9 In the **Color Expression** settings window, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Laminar Flow>Shear rate (spf.sr)**.

10 Click the **Plot** button.

Now create a new Particle dataset with a selection at the outlet so the transmission probability can be evaluated.

Data Sets

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

2 Right-click **Particle 1** and choose **Duplicate**.

3 Right-click **Results>Data Sets>Particle 2** and choose **Add Selection**.

4 In the **Selection** settings window, locate the **Geometric Entity Selection** section.

5 From the **Geometric entity level** list, choose **Boundary**.

6 Select Boundary 20 only.

Derived Values

1 In the **Model Builder** window, under **Results** right-click **Derived Values** and choose **Global Evaluation**.

2 In the **Global Evaluation** settings window, locate the **Data** section.

3 From the **Data set** list, choose **Particle 2**.

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

5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Particle Tracing for Fluid Flow>Particle statistics>Transmission probability (fpt.alpha)**.

6 Click the **Evaluate** button.

Data Sets

1 In the **Model Builder** window, under **Results** right-click **Data Sets** and choose **Cut Plane**.

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

3 From the **Data set** list, choose **Particle 1**.

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

5 In the **y-coordinates** edit field, type `0.006`.

6 Select the **Additional parallel planes** check box.

7 In the **Distances** edit field, type `0.006 0.016 0.026 0.036 0.042`.

8 Click the **Plot** button.

3D Plot Group 4

1 In the **Model Builder** window, right-click **Results** and choose **3D Plot Group**.

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

3 From the **Data set** list, choose **Particle 1**.

4 Click to expand the **Color Legend** section. From the **Position** list, choose **Bottom**.

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

6 Right-click **Results>3D Plot Group 4** and choose **Poincaré Map**.

7 In the **Poincaré Map** settings window, locate the **Data** section.

8 From the **Cut plane** list, choose **Cut Plane 1**.

9 Locate the **Coloring and Style** section. Select the **Radius scale factor** check box.

10 In the associated edit field, type `6E-5`.

11 Click the **Plot** button.

12 Right-click **Results>3D Plot Group 4>Poincaré Map 1** and choose **Color Expression**.

13 In the **Color Expression** settings window, locate the **Expression** section.

14 In the **Expression** edit field, type `at(0,qx<0)`.

15 Locate the **Coloring and Style** section. Clear the **Color legend** check box.

16 In the **Model Builder** window, right-click **3D Plot Group 4** and choose **Surface**.

17 In the **Surface** settings window, locate the **Data** section.

18 From the **Data set** list, choose **Cut Plane 1**.

19 Locate the **Expression** section. In the **Expression** edit field, type `1`.

20 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.

21 From the **Color** list, choose **Gray**.

22 Click the **Go to Default 3D View** button on the Graphics toolbar.

23 Click the **Plot** button.

2D Plot Group 5

1 In the **Model Builder** window, right-click **Results** and choose **2D Plot Group**.

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

3 Clear the **Plot data set edges** check box.

4 Locate the **Data** section. From the **Data set** list, choose **Particle 1**.

5 Right-click **Results>2D Plot Group 5** and choose **Phase Portrait**.

6 In the **Phase Portrait** settings window, locate the **Expression** section.

7 From the **x-axis** list, choose **Manual**.

8 In the **Expression** edit field, type `mod1.qx`.

9 From the **y-axis** list, choose **Manual**.

10 In the **Expression** edit field, type `mod1.qz`.

11 Click the **Plot** button.

12 Click the **Zoom Extents** button on the Graphics toolbar.

13 Locate the **Coloring and Style** section. Select the **Radius scale factor** check box.

14 In the associated edit field, type `3E-5`.

15 Right-click **Results>2D Plot Group 5>Phase Portrait 1** and choose **Color Expression**.

16 In the **Color Expression** settings window, locate the **Coloring and Style** section.

17 Clear the **Color legend** check box.

18 Locate the **Expression** section. In the **Expression** edit field, type `at(0,qx<0)`.

19 Click the **Plot** button.

20 In the **Model Builder** window, click **2D Plot Group 5**.

To generate each of the plots in Figure 4, simply do the following:

21 In the **2D Plot Group** settings window, locate the **Data** section.

22 From the **Time** list, choose **0**.

23 Click the **Plot** button.

24 From the **Time** list, choose **1**.

25 Click the **Plot** button.

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

27 Click the **Plot** button.

28 From the **Time** list, choose **3**.

29 Click the **Plot** button.

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

31 Click the **Plot** button.

32 From the **Time** list, choose **5**.

33 Click the **Plot** button.