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.](image)

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:
Here \( \eta \) denotes the dynamic viscosity (\( \text{kg}/(\text{m} \cdot \text{s}) \)), \( u \) is the velocity (\( \text{m}/\text{s} \)), \( \rho \) represents the fluid density (\( \text{kg}/\text{m}^3 \)), and \( p \) denotes the pressure (\( \text{Pa} \)).

The particle trajectories are computed using a Newtonian formulation

\[
\frac{d}{dt}(m_p \mathbf{v}) = m_p F_d (\mathbf{u} - \mathbf{v})
\]

where \( F_d \) is the drag force per unit mass:

\[
F_d = \frac{18 \eta}{\rho_p d_p^2}.
\]

The particle velocity is \( \mathbf{v} \), \( \rho_p \) 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. Since the particles have mass, they don’t 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 which reach the outlet divided by the number of particles released. For this specific configuration the transmission probability is 0.81. This means that 19\% 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 Poincare plot. The Poincare plot places a colored dot for each particles at the location at which the particle passes through a cut plane (known as a Poincare section). In Figure 3, the location of the particles at 6 Poincare 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 $\text{at()}$ operator is used to mark the particles with the color of their initial position. The first Poincare 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: Poincare maps of the particle trajectories at different Poincare sections. The color is a logical expression indicating which particles had an initial position at $x < 0$.

The phase portrait can also be used to visualize the effect of particle mixing but is not as useful as the Poincare map since 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 v.s. 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 wouldn’t be completely mixed.
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

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.
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, right-click Model 1>Geometry 1 and choose Import.
2. Go to the Settings window for Import.
3. Locate the Import section. 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. Go to the Settings window for Parameters.
3 Locate the **Parameters** section. In the **Parameters** table, enter the following settings:

<table>
<thead>
<tr>
<th>NAME</th>
<th>EXPRESSION</th>
</tr>
</thead>
<tbody>
<tr>
<td>ra</td>
<td>3[mm]</td>
</tr>
<tr>
<td>u_mean</td>
<td>10[mm/s]</td>
</tr>
</tbody>
</table>

**MATERIALS**

*Material 1*

1 In the **Model Builder** window, right-click **Model 1>Materials** and choose **Material**.
2 Go to the **Settings** window for Material.
3 Locate the **Material Contents** section. In the **Material contents** table, enter the following settings:

<table>
<thead>
<tr>
<th>PROPERTY</th>
<th>NAME</th>
<th>VALUE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>rho</td>
<td>1000</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>mu</td>
<td>1e-3</td>
</tr>
</tbody>
</table>

**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 Go to the **Settings** window for Inlet.
4 Locate the **Velocity** section. 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 necessary to enter a complicated expression for the velocity profile, just the average velocity of flowrate.

*Outlet 1*

1 In the **Model Builder** window, 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, right-click Model 1>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 Free Triangular 1 and choose Size.
2 Go to the Settings window for Size.
3 Locate the Element Size section. From the Calibrate for list, choose Fluid dynamics.
4 From the Predefined list, choose Extremely fine.

Size
1 In the Model Builder window, click Size.
2 Go to the Settings window for Size.
3 Locate the Element Size section. 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 Free Triangular 2 and choose Size.
2 Go to the Settings window for Size.
3 Locate the Element Size section. 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 WIZARD
1 In the Model Builder window, right-click Model 1 and choose Add Physics.
2 Go to the Model Wizard window.
3 In the Add physics tree, select Fluid Flow>Particle Tracing for Fluid Flow (fpt).
4 Click Add Selected.
5 Click Next.
6 Find the Studies subsection. In the tree, select Preset Studies for Selected Physics>Time Dependent.
7 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 Go to the Settings window for Drag Force.
4 Locate the Drag Force section. From the 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. Go to the **Settings** window for Inlet.
4. Locate the **Initial Position** section. From the **Initial position** list, choose **Density**.
5. In the **N** edit field, type 3000.
6. In the **ρ** edit field, type **spf \cdot U**.
7. Locate the **Initial Velocity** section. From the **u** list, choose **Velocity field (spf/fp1)**.

**Outlet 1**
1. In the **Model Builder** window, right-click **Particle Tracing for Fluid Flow** and choose **Outlet**.
2. Select Boundary 20 only.

**Particle Properties 1**
1. In the **Model Builder** window, click **Particle Properties 1**.
2. Go to the **Settings** window for Particle Properties.
3. Locate the **Particle Properties** section. From the **Particle property specification** list, choose **Specify particle density and diameter**.
4. In the **dp** 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. Go to the **Settings** window for Time Dependent.
3. Locate the **Physics Selection** section. In the table, enter the following settings:

<table>
<thead>
<tr>
<th>PHYSICS INTERFACE</th>
<th>USE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laminar Flow (spf)</td>
<td>×</td>
</tr>
</tbody>
</table>

4. Click to expand the **Values of Dependent Variables** section.
5. Select the **Values of variables not solved for** check box.
6. From the **Method** list, choose **Solution**.
7. From the **Study** list, choose **Study 1, Stationary**.
8 Locate the **Study Settings** section. Click the **Range** button.
9 Go to the **Range** dialog box.
10 In the **Step** edit field, type 0.2.
11 In the **Stop** edit field, type 5.
12 Click the **Replace** button.
13 In the **Model Builder** window, right-click **Study 2** and choose **Compute**.

**RESULTS**

**Particle Trajectories (fpt)**
1 Go to the **Settings** window for 3D Plot Group.
2 Click to expand the **Color Legend** section.
3 From the **Position** list, choose **Bottom**.
4 Click to expand the **Title** section.
5 From the **Title type** list, choose **None**.
6 In the **Model Builder** window, expand the **Particle Trajectories (fpt)** node, then click **Particle Trajectories 1**.
7 Go to the **Settings** window for Particle Trajectories.
8 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Line**.
9 Find the **Point style** subsection. From the **Type** list, choose **None**.
10 In the **Model Builder** window, expand the **Particle Trajectories 1** node, then click **Color Expression 1**.
11 Go to the **Settings** window for Color Expression.
12 In the upper-right corner of the **Expression** section, click **Replace Expression**.
13 From the menu, choose **Laminar Flow>Shear rate (spf.sr)**.
14 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 **Particle 2** and choose **Add Selection**.
4 Go to the Settings window for Selection.

5 Locate the Geometric Entity Selection section. From the Geometric entity level list, choose Boundary.

6 Select Boundary 20 only.

_Derived Values_

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

2 Go to the Settings window for Global Evaluation.

3 Locate the Data section. From the Data set list, choose Particle 2.

4 From the Time selection list, choose Last.

5 In the upper-right corner of the Expression section, click Replace Expression.

6 From the menu, choose Particle Tracing for Fluid Flow>Transmission probability (fpt.alpha).

7 Click the Evaluate button.

_Data Sets_

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

2 Go to the Settings window for Cut Plane.

3 Locate the Data section. 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 Go to the Settings window for 3D Plot Group.

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

4 Click to expand the Color Legend section.

5 From the Position list, choose Bottom.

6 Click to expand the Title section.

7 From the Title type list, choose None.

8 Right-click Results>3D Plot Group 4 and choose Poincaré Map.
9 Go to the Settings window for Poincaré Map.
10 Locate the Data section. From the Cut plane list, choose Cut Plane 1.
11 Locate the Coloring and Style section. Select the Radius scale factor check box.
12 In the associated edit field, type 6E-5.
13 Click the Plot button.
14 Right-click Poincaré Map 1 and choose Color Expression.
15 Go to the Settings window for Color Expression.
16 Locate the Expression section. In the Expression edit field, type at(0,qx<0).
17 Locate the Coloring and Style section. Clear the Color legend check box.
18 In the Model Builder window, right-click 3D Plot Group 4 and choose Surface.
19 Go to the Settings window for Surface.
20 Locate the Data section. From the Data set list, choose Cut Plane 1.
21 Locate the Expression section. In the Expression edit field, type 1.
22 Locate the Coloring and Style section. From the Coloring list, choose Uniform.
23 From the Color list, choose Gray.
24 Click the Go to Default 3D View button on the Graphics toolbar.
25 Click the Plot button.

2D Plot Group 5
1 In the Model Builder window, right-click Results and choose 2D Plot Group.
2 Go to the Settings window for 2D Plot Group.
3 Locate the Plot Settings section. 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 Go to the Settings window for Phase Portrait.
7 Locate the Expression section. 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 Phase Portrait 1 and choose Color Expression.

16 Go to the Settings window for Color Expression.

17 Locate the Coloring and Style section. 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.

21 Go to the Settings window for 2D Plot Group.

22 Locate the Data section. 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.