MICROMIXER:

Mixing two fluids or particle suspensions in fluids in micro or nanoscale devices can be a challenge as the velocities are very low (typically 0.1 mm/s in a micro device) compared to the viscosities of the fluids (for water 0.001 Pa.s). The Reynolds number for a channel with 10 micrometer width is:

\[ Re = \frac{\rho UL}{\mu} \]
\[ = 0.001 \]

where the density \( \rho \) is 1000 kg/m^3. Thus the flow regime is laminar and mixing is diffusion dominated. The primary control over mixing of two constituents is via designing the proper geometry to increase the effective “area” over which diffusion can take place.

Theory:

We will be solving the Navier-Stokes (NS) equations (mass and momentum conservation for the fluid) and the mass conservation equation for the second species which is mixing with the first (main) fluid. The NS equations are:

- \[ \rho(u \cdot \nabla)u = \nabla \cdot (-\rho I + \mu (\nabla u + (\nabla u)^T)) + F \quad \text{Eq. 1} \]
- \[ \rho \nabla \cdot (u) = 0 \quad \text{Eq. 2} \]

Panel 1.

In Eq. 1, due to the low Reynolds number, the convective part on the left hand side can be neglected and there are not external forces other than the pressure gradient. Hence, the only terms the equations are the pressure gradient and viscous terms (highlighted in red). This is solved in combination with the continuity equation (mass conservation for the main fluid). Once the velocity of the main species is determined, the predominantly diffusive transport (Fickian diffusion; mixing) is determined via the mass conservation via a “dilute species” approximation (Eq. 3 in Panel 2). We justify the approximation by the fact that the second species constitutes a
small fraction of the first (main) species and the second species interacts almost exclusively with
the “main” species.

\[ \nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \nabla \cdot = -D_i \nabla c_i + \mathbf{u} \cdot \nabla c_i \quad \text{Eq. 3} \]

Panel 2.

**COMSOL INSTRUCTIONS --- Micromixer -- 2D**

In this problem, we model a “H-cell” with a view to assess the mixing efficiency of the H-Cell.
This is a two physics problem: (i) Fluid Flow and (ii) Chemical Diffusion.

1. Click on “Model Wizard”
2. Choose 2D
3. Under “Select Physics” choose
   a. Fluid Flow → Single-Phase Flow → Laminar Flow (spf) ; click “add”
   b. Chemical Species Transport → Transport of Diluted Species (tds); click “add”
4. Click on “Study”
5. Choose “Stationary”; Click “Done”

**Global Definitions:**

1. In the “Model Builder” window, right click on Global definitions and choose Parameters.
2. Fill in the parameters as in Figure 1.
Geometry:

1. In the model builder ("Model Build") panel, click on Geometry 1.
2. In the Settings window, click under Length Unit and choose μm.
3. We will build the H-Cell geometry as a union of three rectangles. To do this, we need to build 3 rectangles.

Rectangle 1:

1. Right click on Geometry, choose Rectangle.
2. In the settings panel for “Rectangle 1”, fill in as follows.
3. Under “Size” in the Settings window:
   a. Width: 10
   b. Height: 120
4. Under Position:
   a. x: 0
   b. y: -60
5. Click on “Build Selected” at the top.

Rectangle 2:

1. Right click on Geometry, choose Rectangle.
2. In the settings panel for “Rectangle 2”, fill in as follows.
3. Under “Size” in the Settings window:
   a. Width: 10
   b. Height: 120
4. Under Position:
a. x: 130
b. y: -60

5. Click on “Build Selected” at the top.

Rectangle 3:

1. Right click on Geometry, choose Rectangle.
2. In the settings panel for “Rectangle 3”, fill in as follows.
3. Under “Size” in the Settings window:
   a. Width: 140
   b. Height: 20
4. Under Position:
   a. x: 0
   b. y: -10
5. Click on “Build Selected” at the top.

Boolean Union:

1. Right click on Geometry, under “Booleans and Partitions” choose “Union”.
2. Select all rectangles (i.e. click on all the three rectangles).
3. Uncheck “Keep interior boundaries”.
4. Click on “Build All Objects” at the top.

Form Union (not sure this is needed, but no harm in doing this):

1. Click on “Form Union” under “Geometry 1” and select Build All. The resulting geometry is in shown in Figure 2.
Materials:

1. Under “Component 1” in the Model Builder, right click on Materials and choose “Blank Material”.
2. Click on “Material 1”. In the “Settings” window, enter the following values for Density (rho) and Dynamic viscosity (mu).
   a. Density: 1000
   b. Dynamic Viscosity: 1e-3

Physics and Boundary Conditions:

1. We now need to specify the boundary conditions at all the boundaries for the two physics problems: a) Laminar Flow and b) Transport of Diluted Species.
Laminar Flow:

1. The velocities at all boundaries are by default set to zero. We need to override this by setting inlet and outlet boundary conditions.

Inlets:

1. Right click on “Laminar Flow” and choose Inlet.
2. In the settings window, select (by clicking) the two inlets a and b (see Figure 2).
3. Under “Boundary Condition” section in the Settings window, choose “Laminar Inflow” and check the “Flow Rate” button. Set \( V_0 \) to “fr” (Note fr is specified in the global parameters), \( L_{\text{entr}} \) to 100[um], and \( D_z \) to 10 micrometers. \( L_{\text{entr}} \) is the entry length for flow development and \( D_z \) is the thickness at entrance.

Outlets:

1. Right Click on “Laminar Flow” and choose Outlet.
2. In the Settings window, select the boundaries by clicking on the outlet boundaries c and d (See Figure 2).
3. Leave the default “Boundary Condition” at Pressure and the value at 0.

Transport of Diluted Species:

Transport Properties 1

1. Click on Transport properties. In the settings window, under “Velocity Field”, change the setting from “User Defined” to “Velocity Field (spf)”. This way, we couple the mass transport to laminar flow.
2. Under “Diffusion Coefficient”, set the diffusion coefficient to D (Recall D has been defined under Global Parameters).

Concentration 1: We now specify concentration at inlet boundary a

1. Right click on “Transport of Diluted Species” and choose “Concentration”.
2. In the settings window for “Concentration 1”, select the boundary by clicking on the lower left inlet boundary a (see Figure 2).
3. Under “Concentration”, check “Species c” and enter c0 (c0 has been defined under Global parameters).

Concentration 2: Concentration at inlet boundary b is set to zero.

1. Right click on “Transport of Diluted Species” and choose “Concentration”.
2. In the settings window, select the upper left hand inlet boundary (boundary b in Figure 2).
3. Under “Concentration”, check “Species c” and leave the concentration as 0.

Outlets:
1. Right click on “Transport of Diluted Species” and choose “Outflow”.
2. In the “Settings” window, select the outflow boundaries c and d (Figure 2).

Meshing:
1. Now we discretize the computational domain. As this is a 2-dimensional domain made up of rectangular shapes, let us choose quadrilateral elements.
2. Right click on “Mesh 1” in the Model Builder and choose “Free Quad”.
3. Under “Mesh 1”, click on “Size”. In the settings window, under “Element Size”, click under “Calibrate for” and choose “Fluid Dynamics”. Set the mesh size to “Normal” on Predefined and click on “Build All” at the top.

Study 1:
1. Right click on “Study 1” and choose “Compute”. As this is a 2D study with simple regular geometry, the computations should finish in a few seconds.
2. If the computation successfully completes, three plots are produced by default: 1) Velocity 2) Pressure and 3) Concentration.
3. The most interesting quantity in this study is concentration. Click on “Concentration” under results to display the concentration of the species that was input at entrance a (Figure 3).
4. It is clear that the two species mix pretty rapidly. here are a few questions to ponder:
   a. What are the quantities that determine how rapidly the two species mix?
   b. Given a species (with its properties fixed), what are the variables you can control that allow for proper mixing.
   c.

H-Cell (3D): Armed with the experience with the 2D geometry, you can now tackle (on your own) the 3D model in the COMSOL library:

Figure 3