COMSOL Conference 2015 Boston

Session: Optimization and Simulation Methods

Boston Marriott Newton
Boston, MA

Commonwealth Ballroom 1
1:00 PM – 2:30 PM

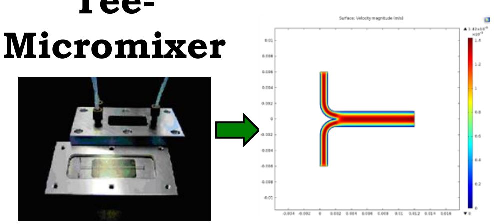
October 8, 2015

Moderator : Jeffrey Fong

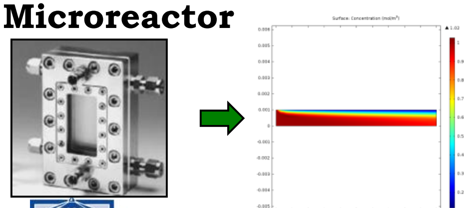
COMSOL CONFERENCE 2015

Novel Approach for Teaching Microchemical Systems Analysis to Chemical Engineering Students Using Graphical User Interfaces (GUIs)

Tee-Micromixer



Microreactor



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Background

- Next generation technologies must be developed that potentially change the chemical plants and process engineering giving rise to safe, compact, flexible, eco-friendly, energy efficient processes and plants.
- Traditional educational curriculum provide engineering students with a spectrum of theoretical knowledge, but generally provide limited exposure to more advanced technologies.
- Utilization of process simulators and design tools allow engineering students to gain useful exposure to advanced technologies.
- Microprocess systems is one of the key emerging technologies with applications ranging from discovery research through commercial processes.
- This technology was introduced as part of the NSF funded web-based learning resource called *Interlinked Curriculum Components* (ICCs) to educate undergraduate students*.

*P.L. Mills *et al.*, Development Of A Web Based Self Teaching And Module For Chemical Engineering Microchemical Systems, American Society for Engineering Education Conference Proceedings (2010).

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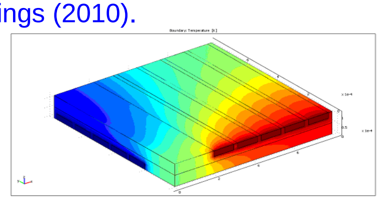
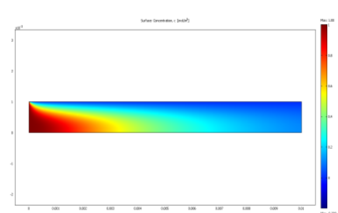
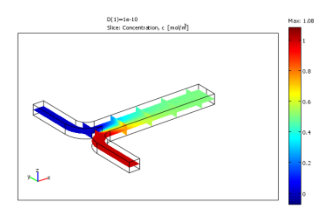






Microprocess Systems ICC

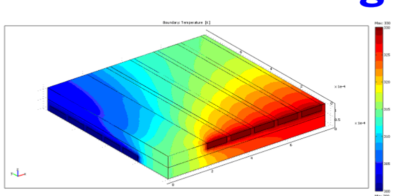
Objectives:

1. Introduce MEMS as applied to microreaction systems.
2. Broaden exposure to multi-scale type of analysis.
3. Strengthen understanding & insight into system behavior.

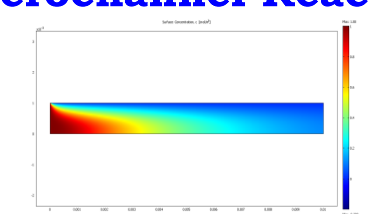
Focus Areas:

- **MEMS & microreactors** → **Components, materials, & fabrication processes**
- **Microfluidics** → **Fluid mechanics at the microscale**
- **Transport phenomena** → **Coupled momentum & energy transport**
- **Transport-kinetic effects** → **Coupled momentum, energy, & species transport**
- **Device & system design** → **Microprocess component & system performance**

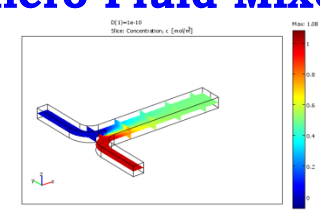
Micro Heat Exchanger



Microchannel Reactor



Micro Fluid Mixer



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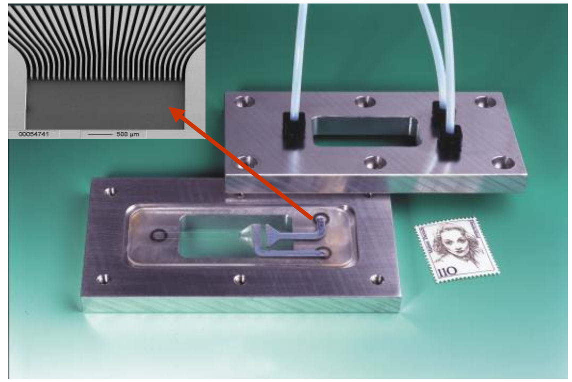
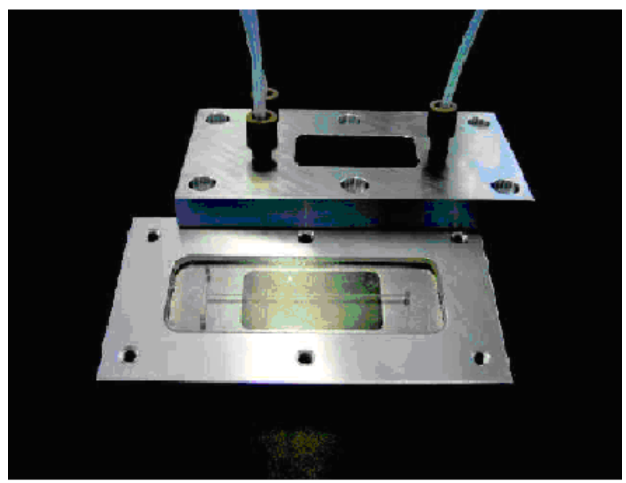
Microreactors & Microprocess Components Fabricated from Glass & Metal

Falling Film Gas-liquid Microreactor



Interdigitial Micromixer for Two-phase Systems



Tee-Micromixer (Glass)

Cross-flow Heat Exchanger

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Microchannel vs Conventional Reactors

-Typical Ranges for Design Parameters-

Design Parameter	Microchannel Reactor	Conventional Reactor
Internal volume	1-1000 μL	100 ml-30,000 L
Surface Area/Volume	10,000-50,000 m^2/m^3	100-1000 m^2/m^3
Heat transfer coeff.	10-25,000 $kW/m^2/K$	17-25 $kW/m^2/K$
Film thickness	~25 μL	~250 μL
Mixing time	< 1 sec	> 1 sec
Power input	10 X less	X

Angew. Chem. Int. Ed. 43,406,2004

Graphical User Interface (GUI)

- Readily allows users to modify key system parameters and to obtain graphical results.
- Advantages of GUI's in COMSOL
  - Reduces the complications with model development
  - Simplifies assigning boundary conditions
  - Allows visualization of various model parameters
  - Improves understanding of model physics *vs* details associated with the model development

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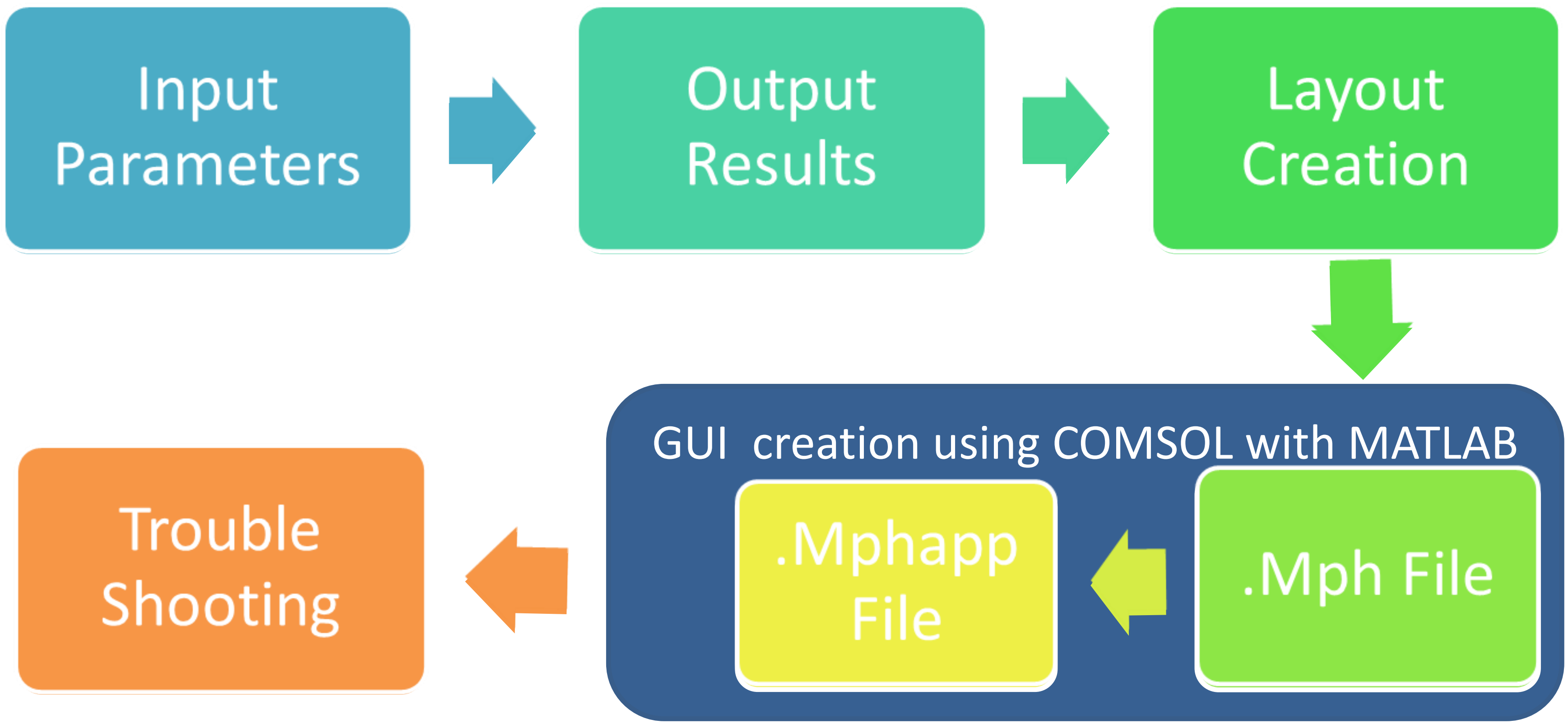
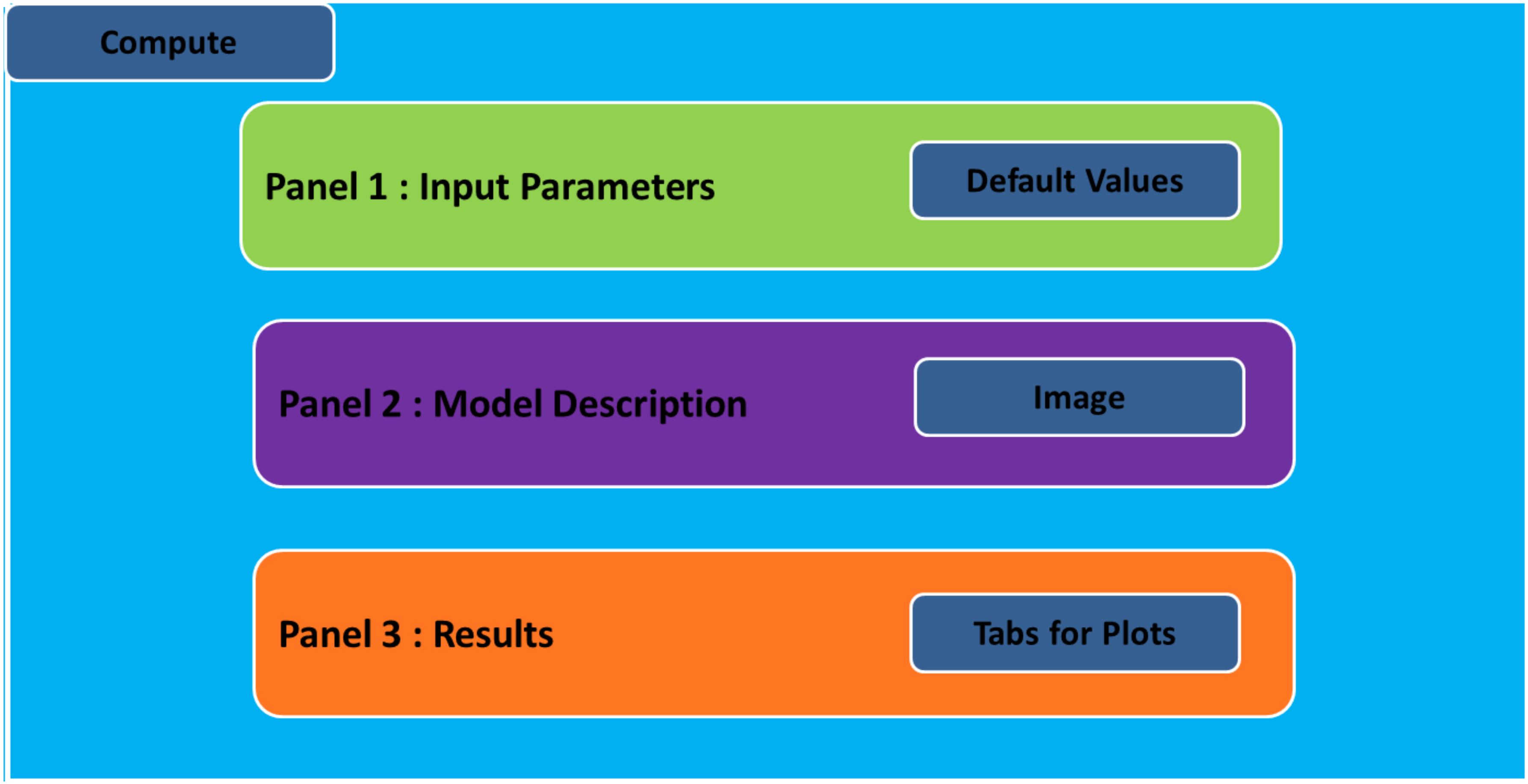
Steps Involved in GUI Creation



Example of Typical GUI Layout



Catalytic Wall Reactor

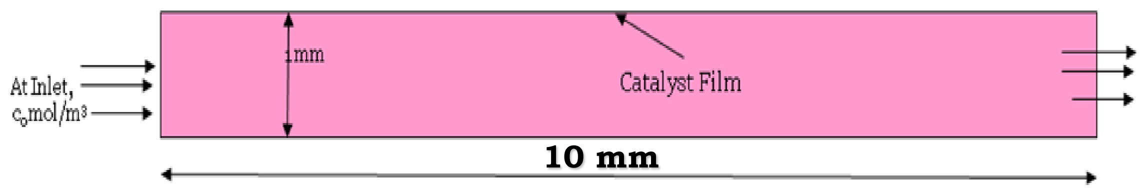
Objective

Illustrate the interactions between fluid transport and chemical kinetics for a steady-state model of a simple wall-microreactor with a first-order reaction

Channel Dimensions

Length: 10 mm

Height : 1 mm



Input Parameters

- Fluid density & fluid viscosity
- Inlet solute concentrations
- Two choices for boundary conditions
  - Specified inlet velocity & outlet pressure
  - Specified inlet & outlet pressure

Chemistry

A → B

Reaction Rate

$-r_A = k\,C_A$

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Model Equations and Kinetics

Model Equations:

Momentum Transport Equations

x- direction:

$$\rho\left[\frac{\partial u_x}{\partial t}\right]-\eta\left[\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2}\right]+\rho\left[u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y}\right]+\frac{\partial p}{\partial x}=F_x$$

y-direction:

$$\rho\left[\frac{\partial u_y}{\partial t}\right]-\eta\left[\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2}\right]+\rho\left[u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y}+\right]+\frac{\partial p}{\partial y}=F_y$$

Convection - Diffusion Equation:

$$D\left(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}\right)-\left(u_x\frac{\partial c}{\partial x}+u_y\frac{\partial c}{\partial y}\right)+\nu_i R=\frac{\partial c}{\partial t}$$

Reaction Kinetics:

$A \rightarrow B$ rate, $r_A = k\, C_A$

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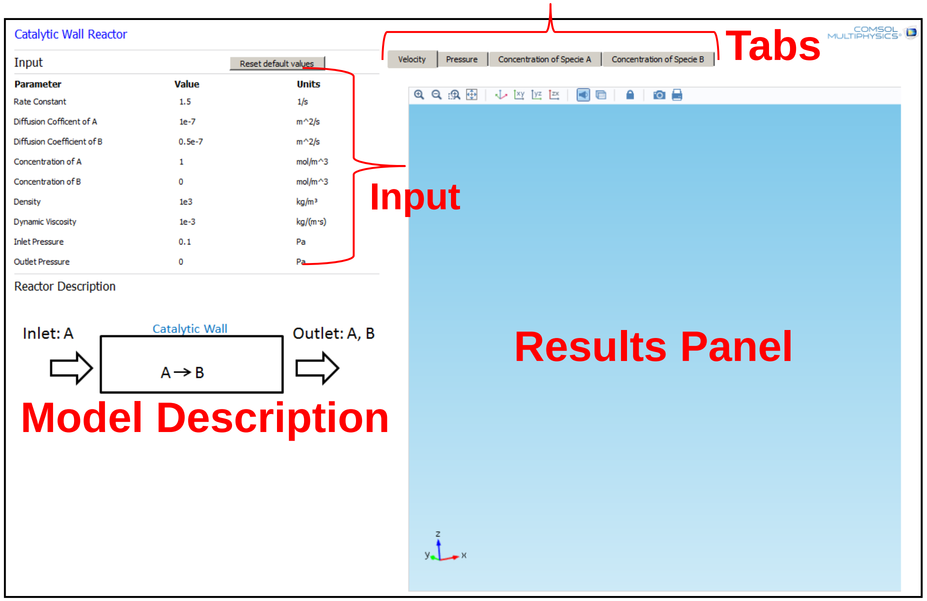
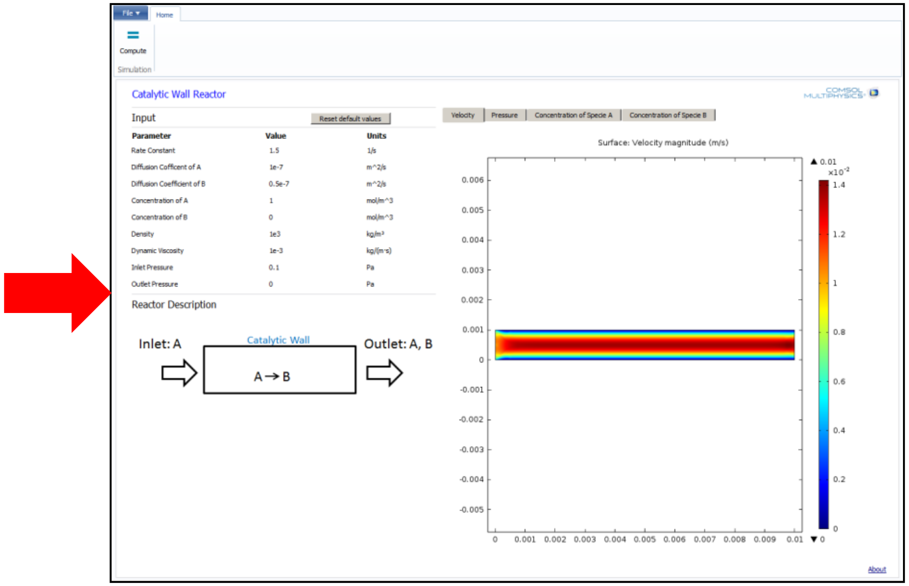
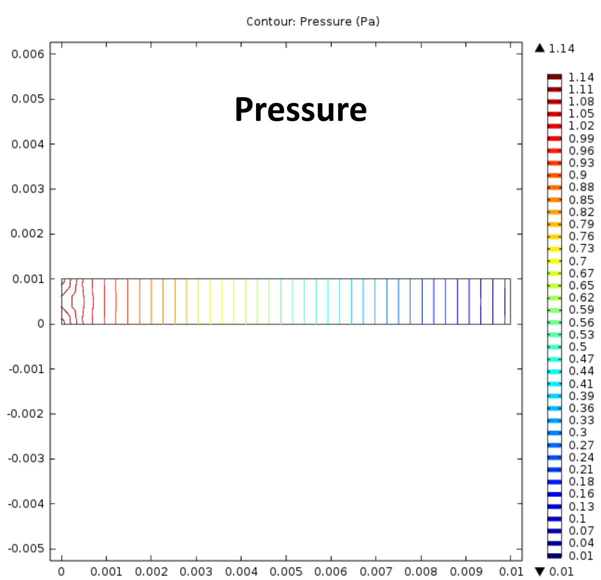
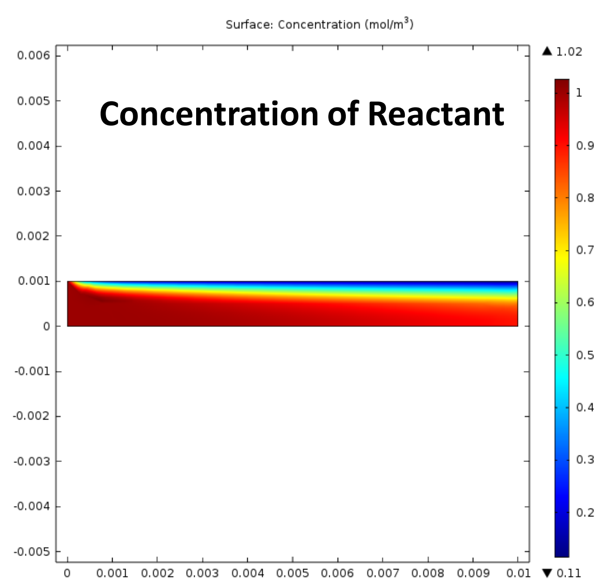
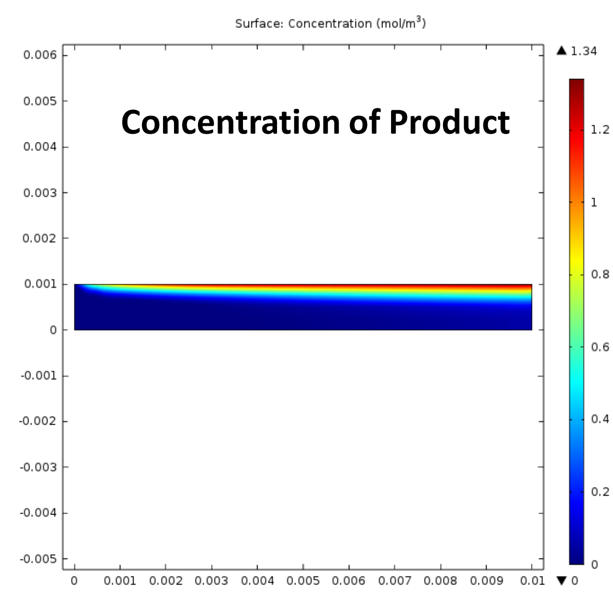
Catalytic Wall Microreactor Results











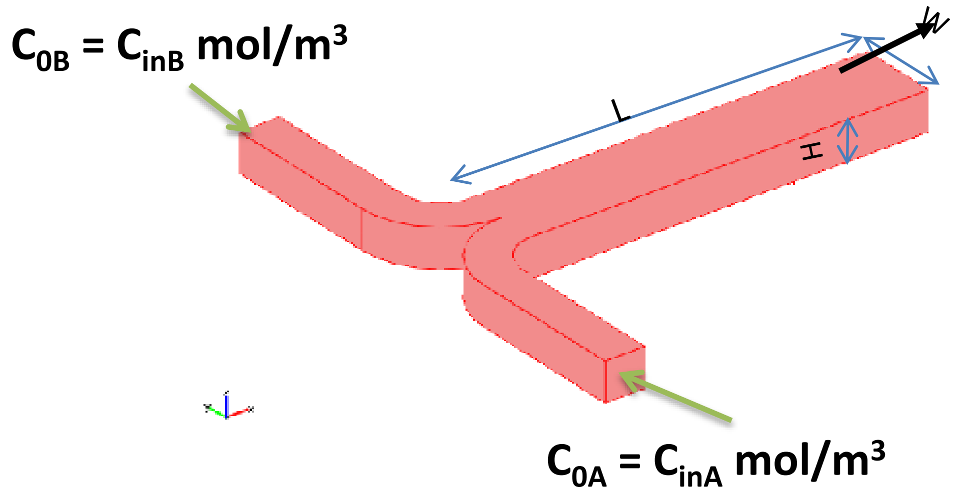
T-Micromixer

Objective

Illustrate the interactions between fluid transport and chemical kinetics for a steady-state model of a simple T-microreactor with a second-order reaction

Channel Dimensions

Length :	10 mm
Width :	1 mm
Height :	1 mm
Circular Baffles Diameter	0.3 mm



Input Parameters

- Fluid density & fluid viscosity
- Inlet solute concentration
- Two choices for boundary conditions
  - Specified inlet velocity & outlet pressure
  - Specified inlet & outlet pressure

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Model Equations and Kinetics

Model Equations:

Momentum Transport Equations

x- direction: $$\rho\left[\frac{\partial u_x}{\partial t}\right]-\eta\left[\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2}+\frac{\partial^2 u_x}{\partial y^2}\right]+\rho\left[u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y}+u_z\frac{\partial u_z}{\partial z}\right]+\frac{\partial p}{\partial x}=0$$

y-direction: $$\rho\left[\frac{\partial u_y}{\partial t}\right]-\eta\left[\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2}+\frac{\partial^2 u_y}{\partial z^2}\right]+\rho\left[u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y}+u_z\frac{\partial u_z}{\partial z}\right]+\frac{\partial p}{\partial y}=0$$

z-direction: $$\rho\left[\frac{\partial u_z}{\partial t}\right]-\eta\left[\frac{\partial^2 u_z}{\partial x^2}+\frac{\partial^2 u_z}{\partial y^2}+\frac{\partial^2 u_z}{\partial z^2}\right]+\rho\left[u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y}+u_z\frac{\partial u_y}{\partial z}\right]+\frac{\partial p}{\partial z}=0$$

Convection - Diffusion Equation:

$$D\left(\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}+\frac{\partial^2 c}{\partial z^2}\right)-\left(u_x\frac{\partial c}{\partial x}+u_y\frac{\partial c}{\partial y}+u_z\frac{\partial c}{\partial z}\right)+v_i R=\frac{\partial c}{\partial t}$$

Parameter Estimation:

Mixing Effectiveness

$$\tau=\frac{\tau_v}{\tau_D}=\frac{DL}{u_{avg} * W^2}$$

where ρ is the fluid density, η is the fluid viscosity, p is the fluid pressure, D is diffusivity, c is concentration, u_{avg} is average velocity and L, W, H are duct dimensions

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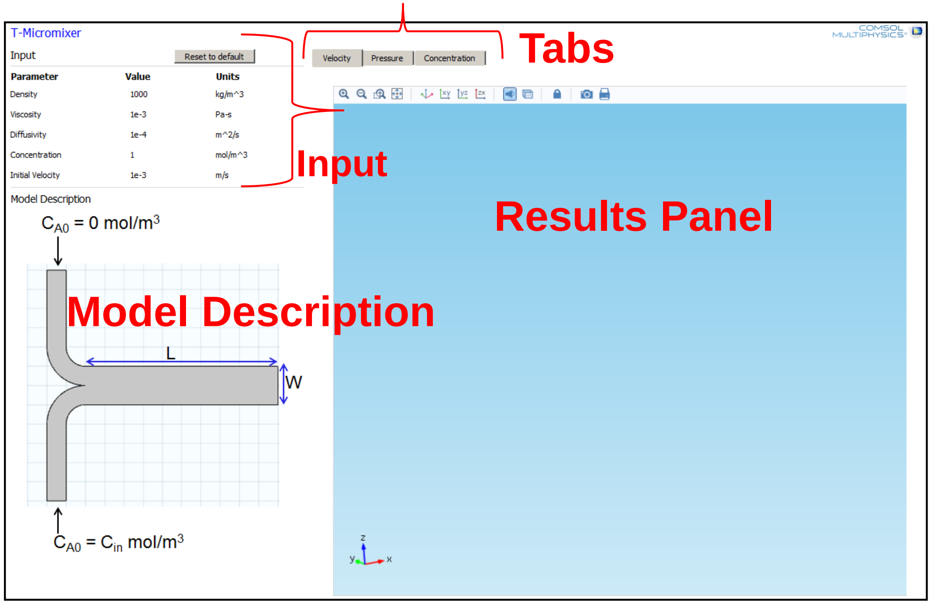
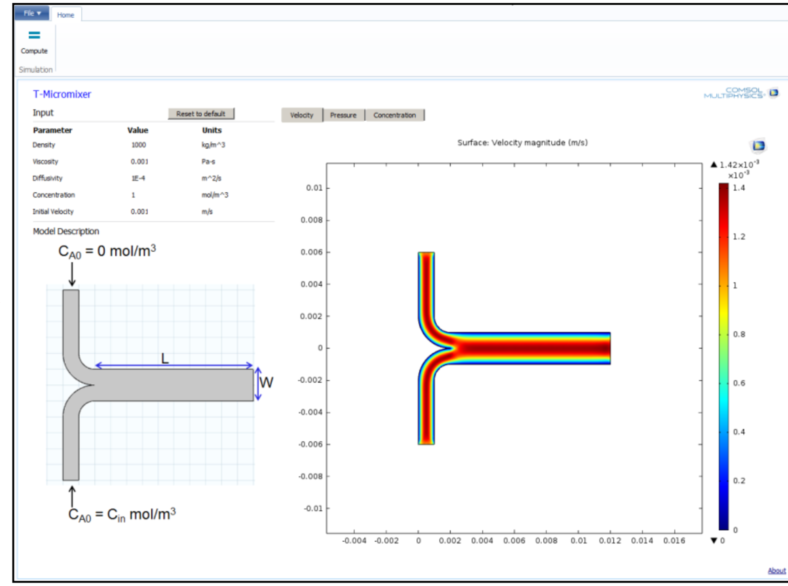
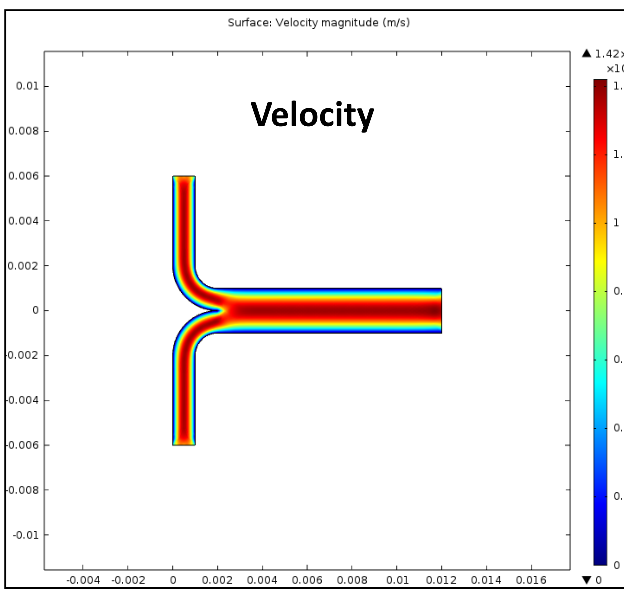
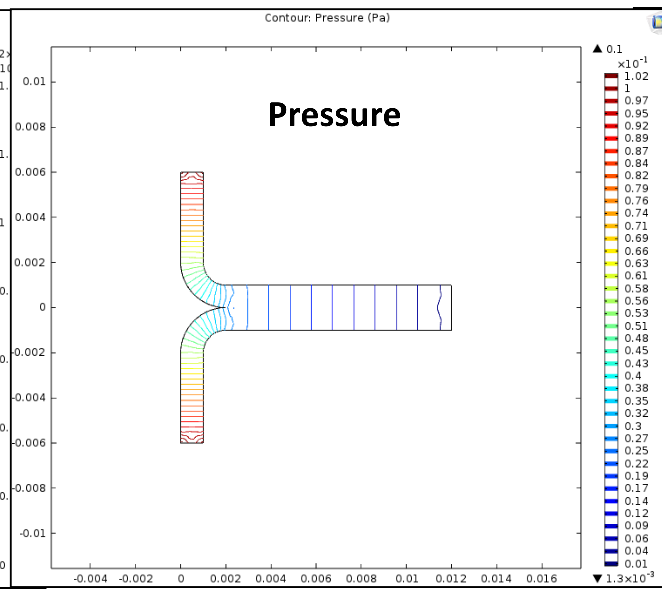
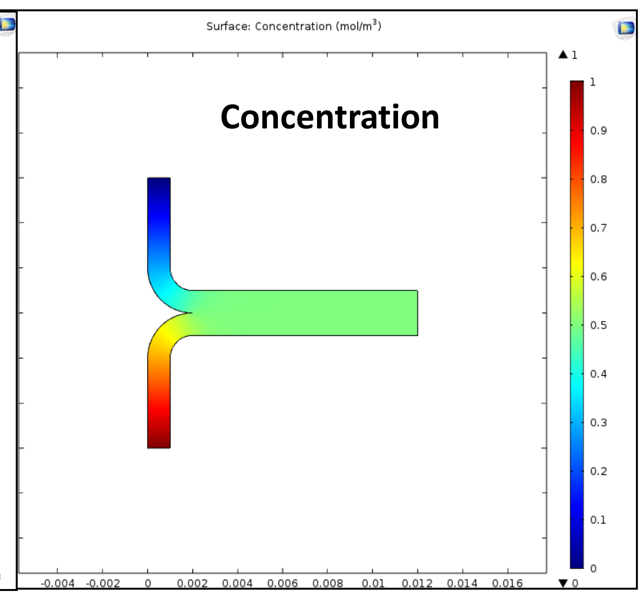
Regular T-Micromixer



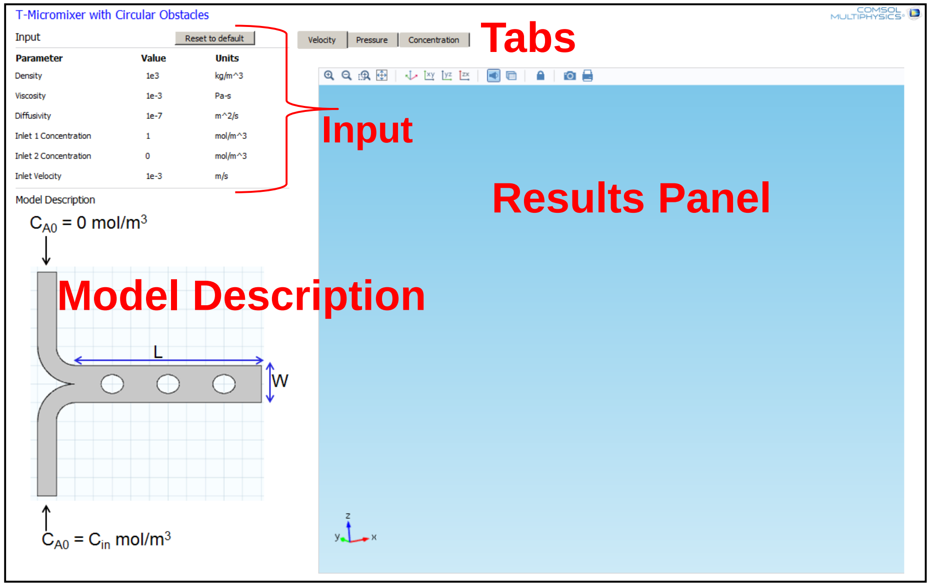


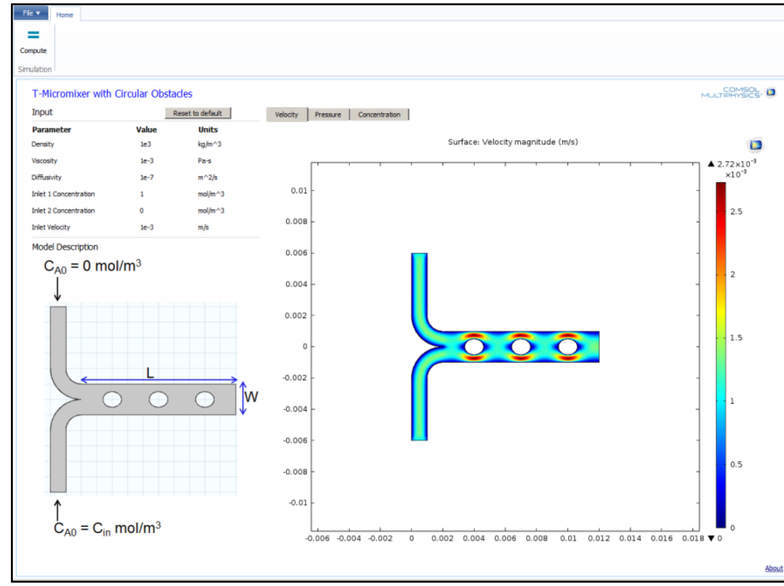


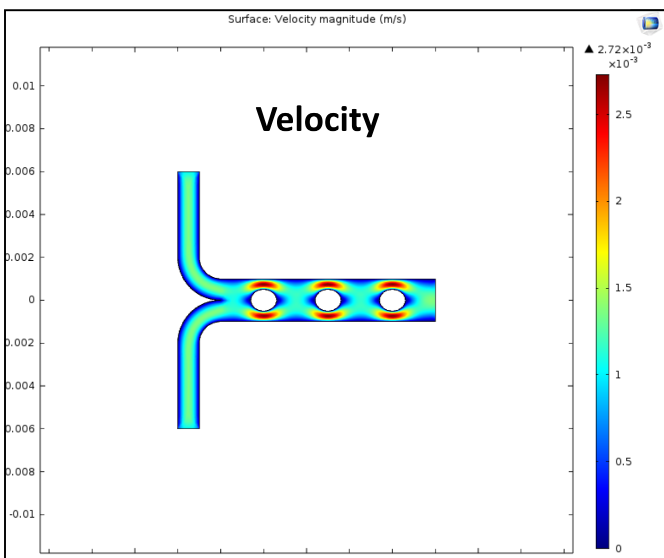


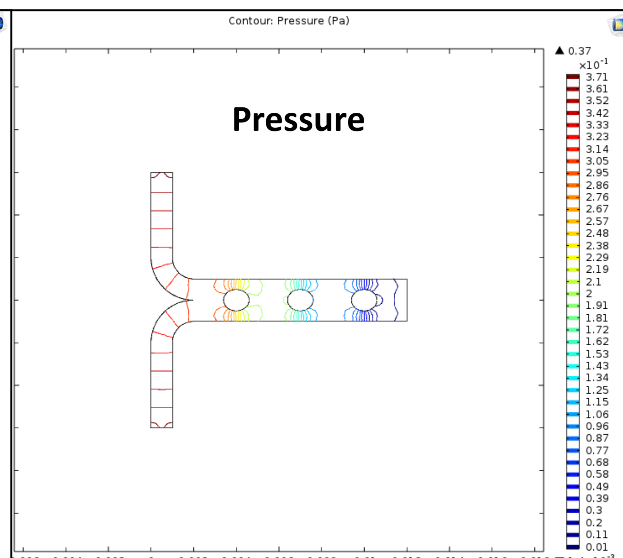


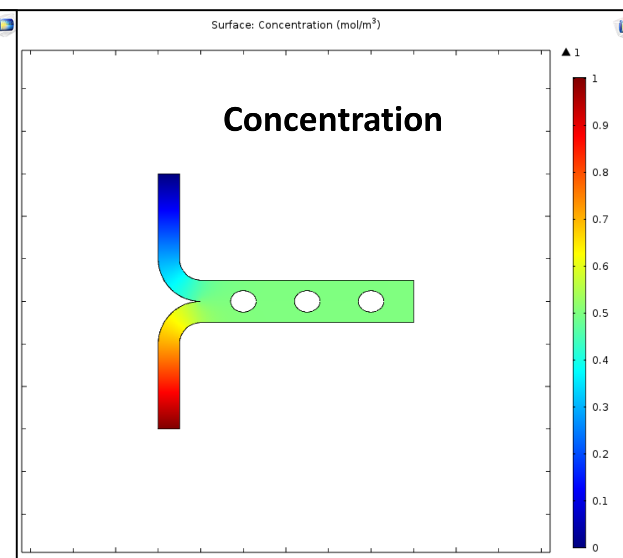
T-Micromixer with Circular Baffles











Conclusions

- COMSOL Multiphysics provides a powerful numerical platform where various models for *microchemical process technology* components can be readily created for both education and research.

- This modeling tool allows chemical engineering students to focus on understanding the *effects of various system design and operational parameters* instead of coding and numerical method debugging.

- The GUIs enable students to readily study the *effect of various design parameters.*

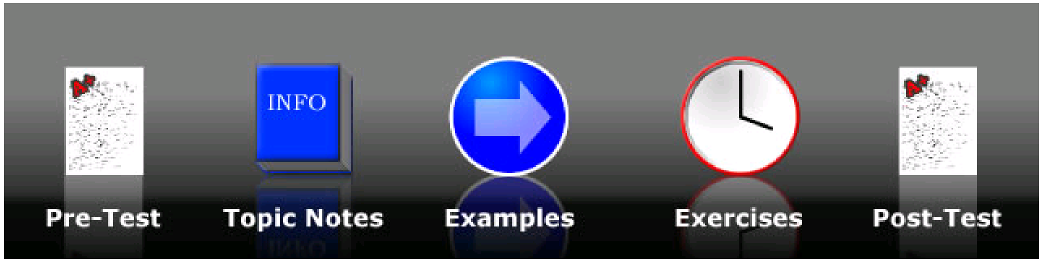
- These applications reduces the *complexity* of model setup and computational time and emphasize understanding of multiphysics in multi-dimensions.

- This approach helps students to understand complex chemical systems using an *interactive approach* vs laborious manual calculations or using other software tools.

Additional Supporting Documentation

Fluid Mechanics

Home | Pre-test | Topic Notes | Examples | Exercises | Post-Test



Introduction

In this section, you will learn basic principles of flow regimes, and the basic knowledge of simulating models in microchemical systems.

Learning objectives (bold words correspond to indicators in Bloom's taxonomy)

1. You will be able to **define** the terms in the table below.

flow rate	viscosity
Reynolds number	Knudsen number
flow regime	Navier-Stokes equation
newtonian fluid	non-newtonian fluid
boundary settings	subdomain settings

2. You will be able to **create** a concept map that demonstrates the relationships among the terms defined in Objective (1).
3. You will be able to **explain** the difference between
   - conventional flow and micro-scale flow
   - Newtonian fluids and Non-newtonian fluids

   and **give examples** of each.
4. **Learn** more about the effect of subdomain settings and boundary settings on the given geometrical figure.
5. **Become more confiden**t to simulate various complicated models related to fluid mechanics.

Home | Pre-test | Topic Notes | Examples | Exercises | Post-Test

The development of this page is sponsored by the National Science Foundation through an Engineering Departmental Level Reform grant.

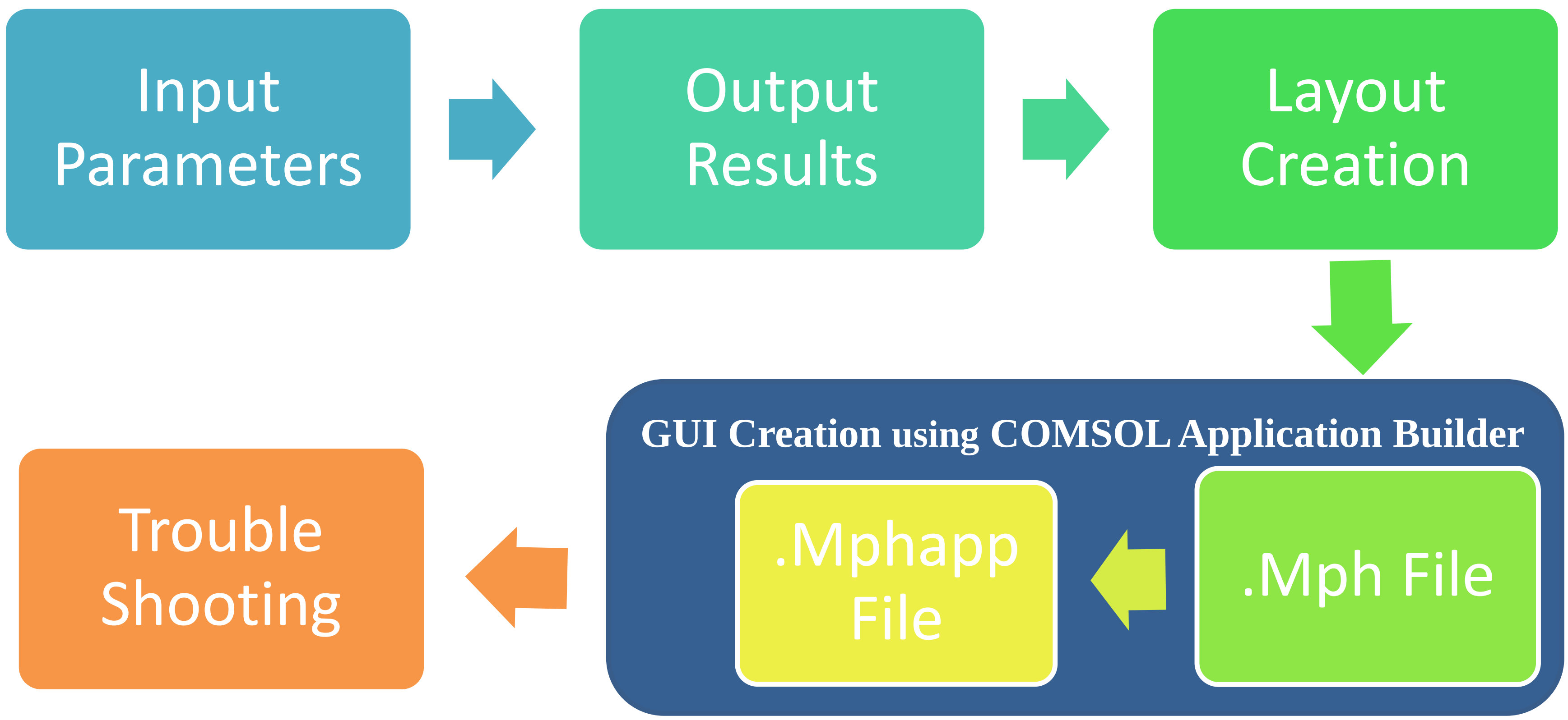
Main Template for an ICC Module

- Provides topical overview on a given subject.
- Directs user to subsections
  - Pre test
  - Topic notes
  - Examples
  - Exercises
  - Post assessment
- Same format for all ICC's
- Navigation bar with buttons provides links to web pages
- Based on *Dreamweaver* and *Flash 8* software tools.

COMSOL Multiphysics as the Numerical Engine

- Finite Element Method analysis modeling tool
- Equation oriented: Physical systems are described in terms of governing microscopic forms of transport laws
- Predefined equations ("Application modes") are available covering a wide range of physics/multiphysics
- User-defined equations can be added for post calculations
- Modules: Optional application-specific add-ons
- Complete Modeling Package provides:
  - Integrated tools for import of 2D or 3D CAD drawings
  - Automatic or user-controlled meshing of subdomains
  - State-of-the-art solvers for resulting systems of equations
  - Postprocessing / Data Import / Export Capabilities

Steps Involved in GUI Creation



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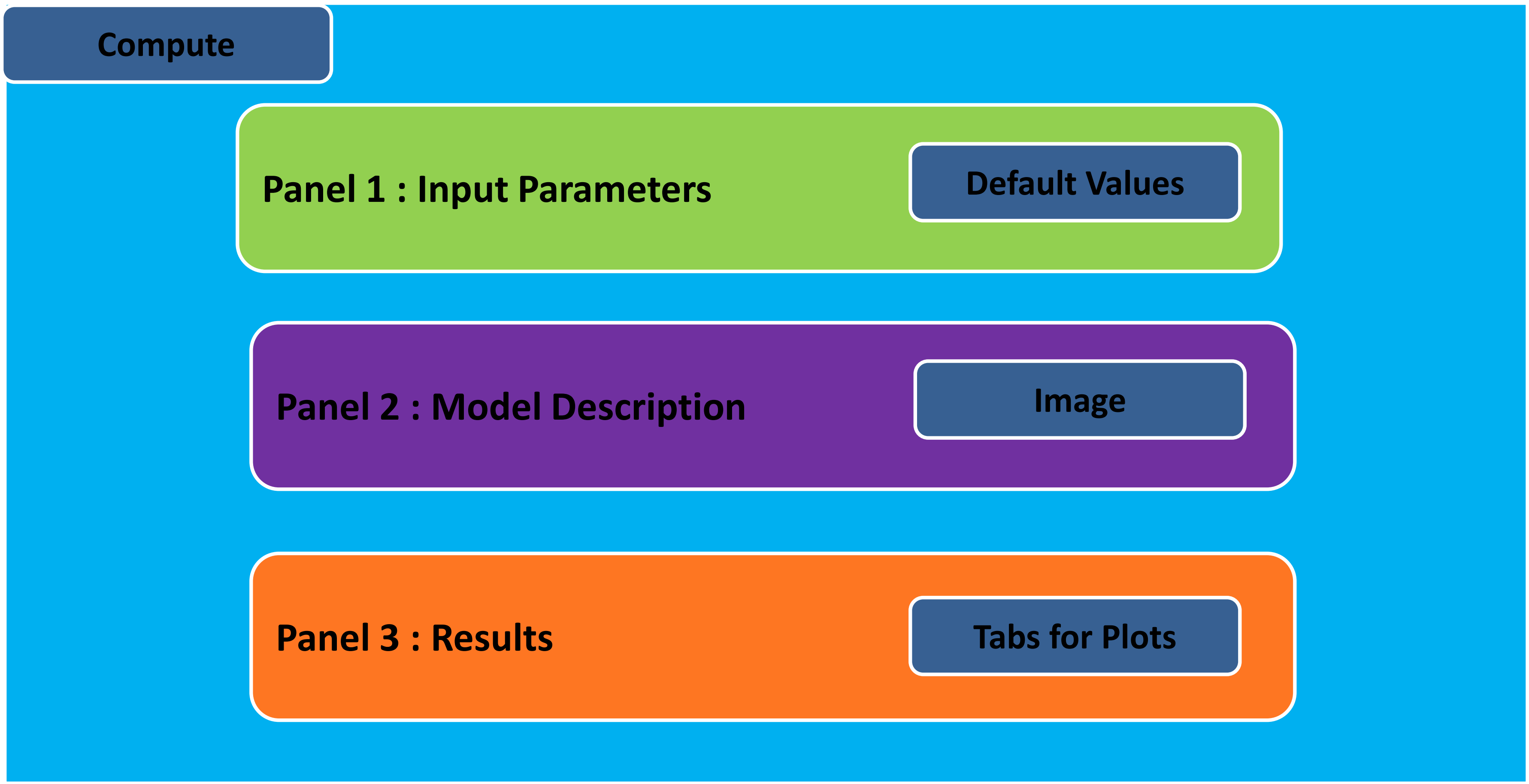
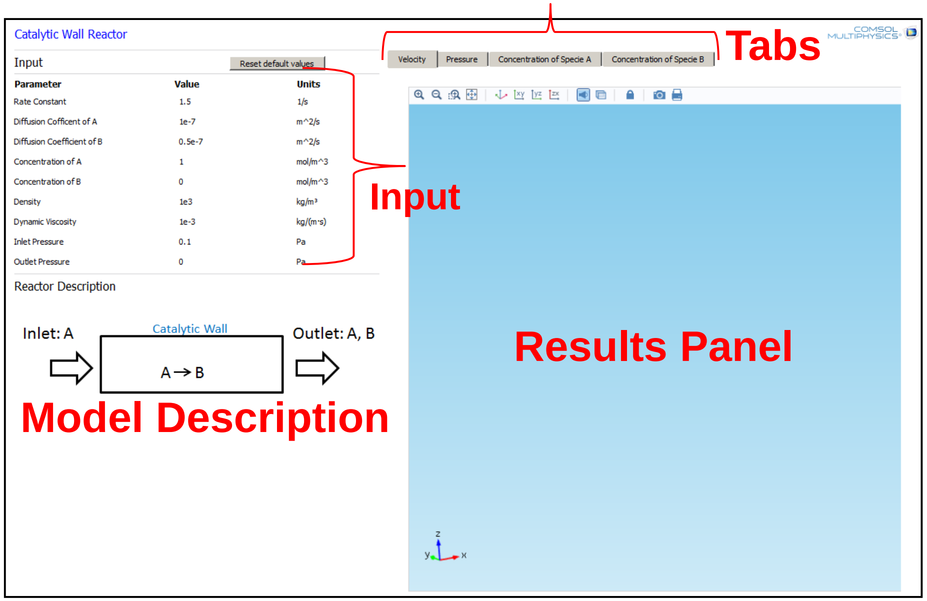
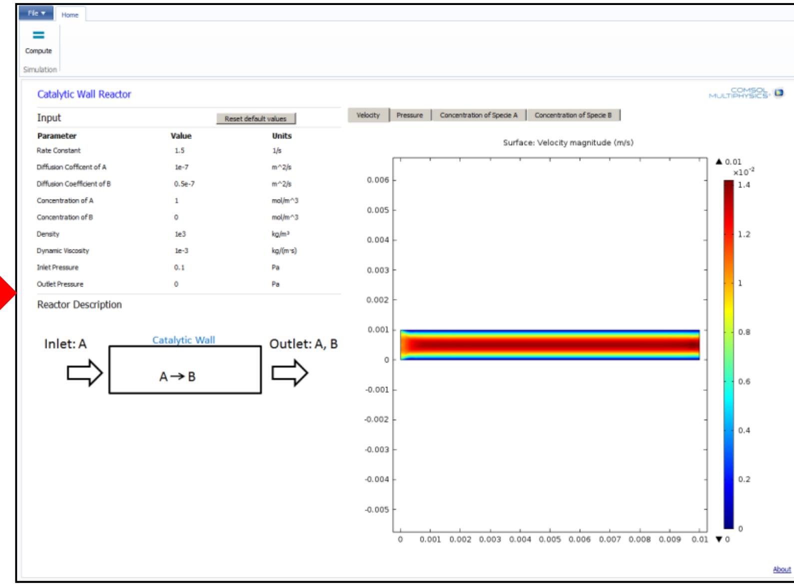
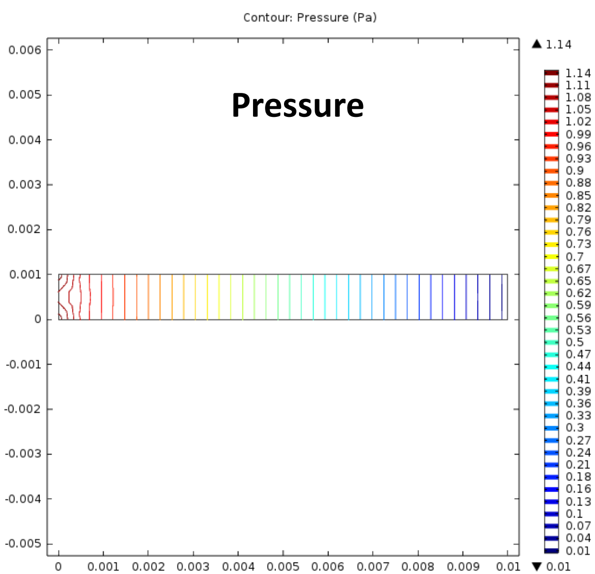
Example of Typical GUI Layout

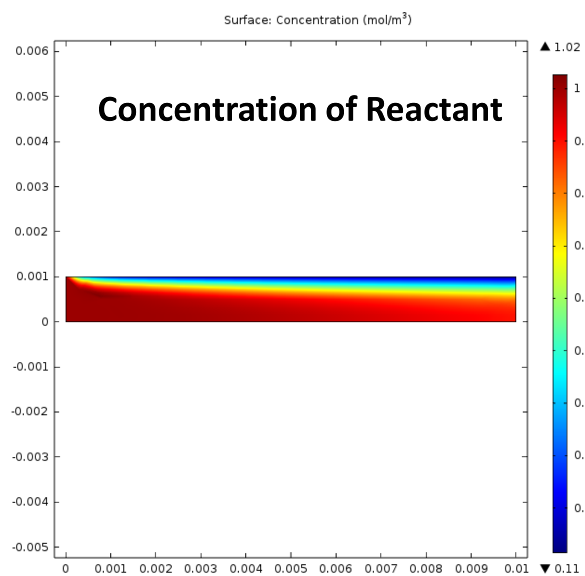


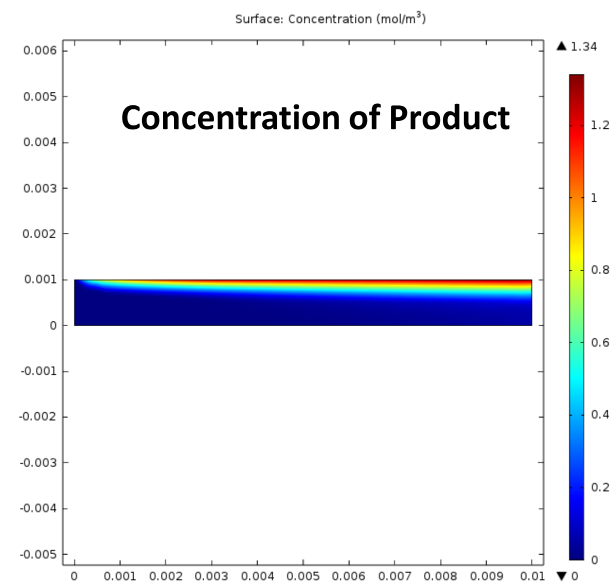
Catalytic Wall Microreactor Results



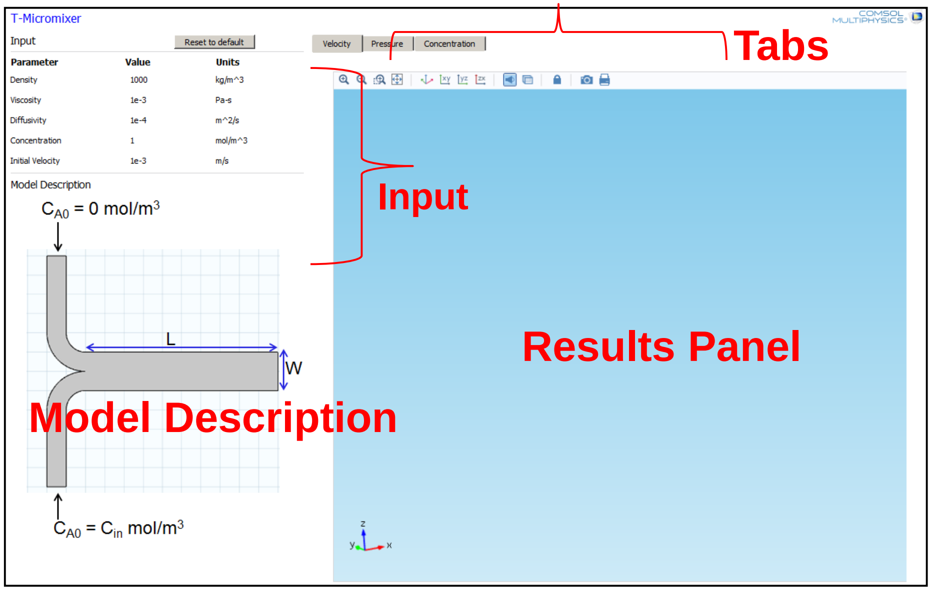


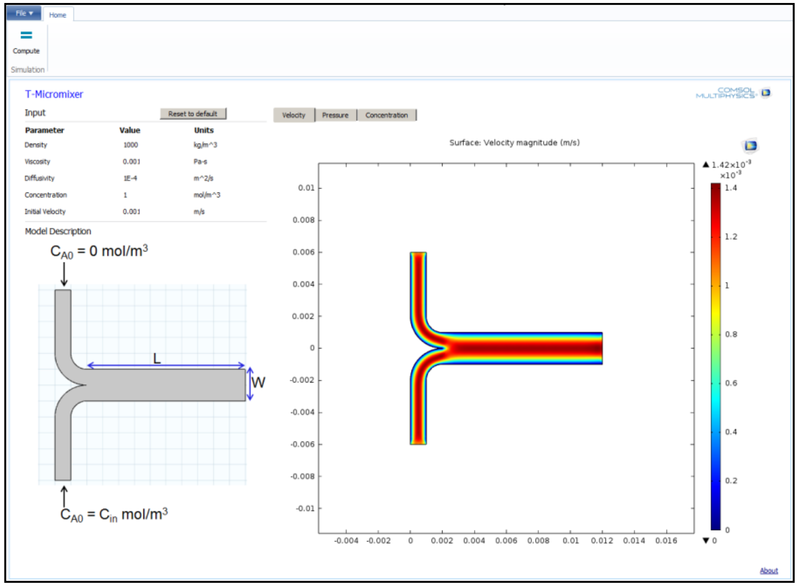


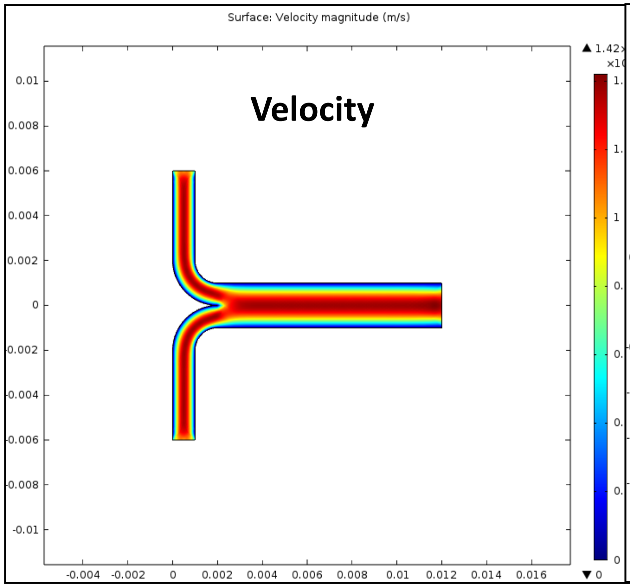


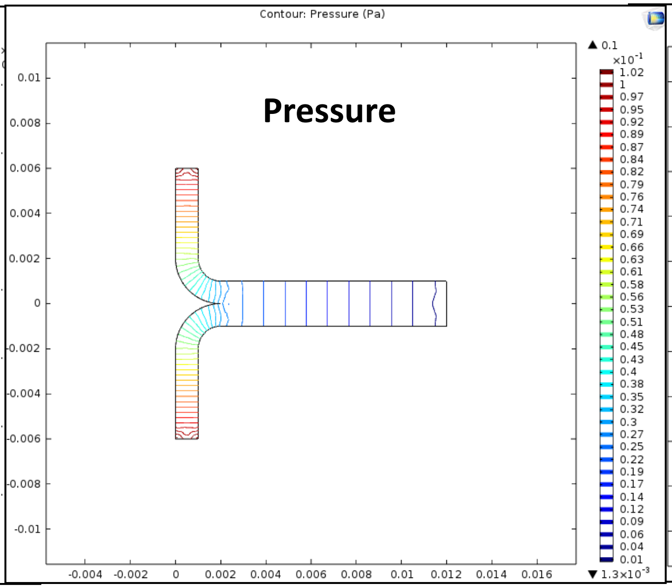


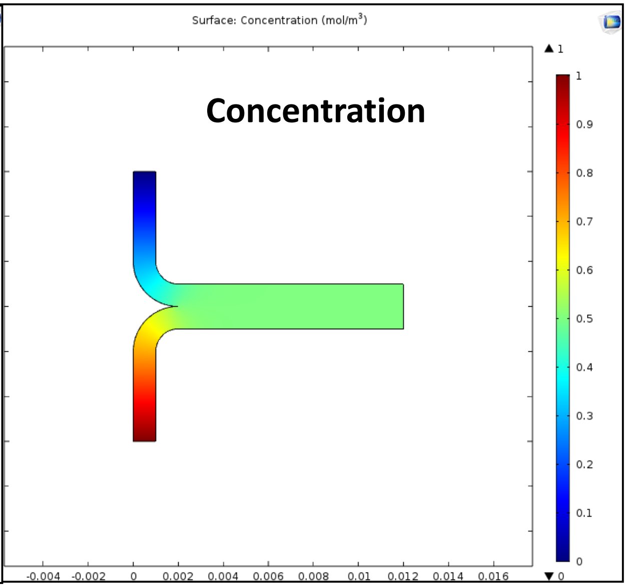
Regular T-Micromixer



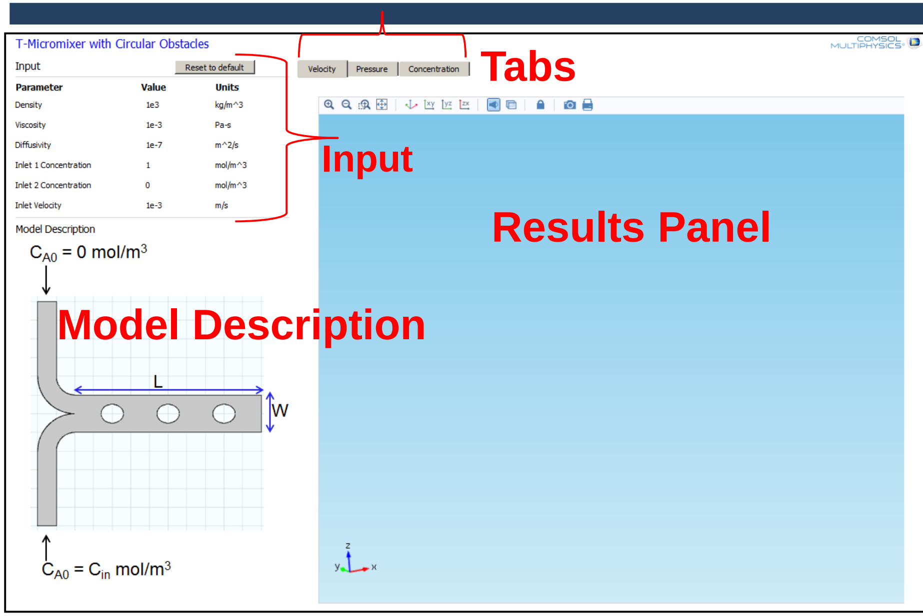


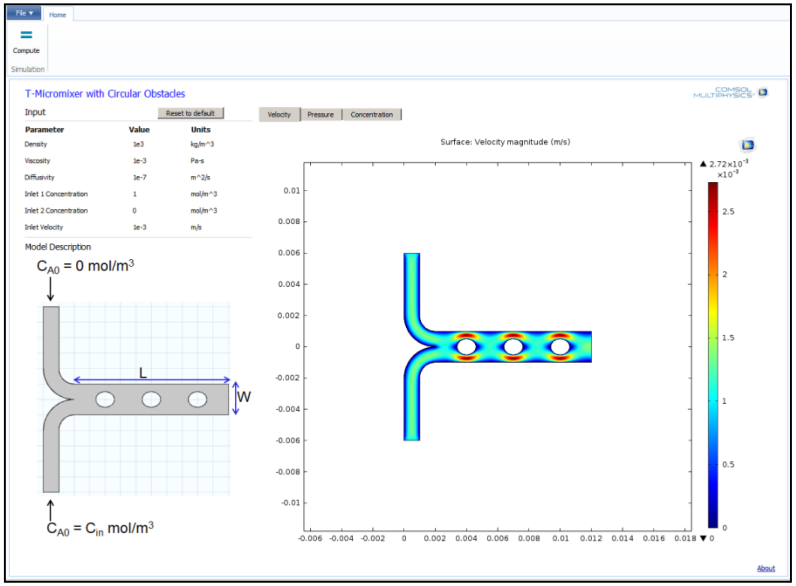


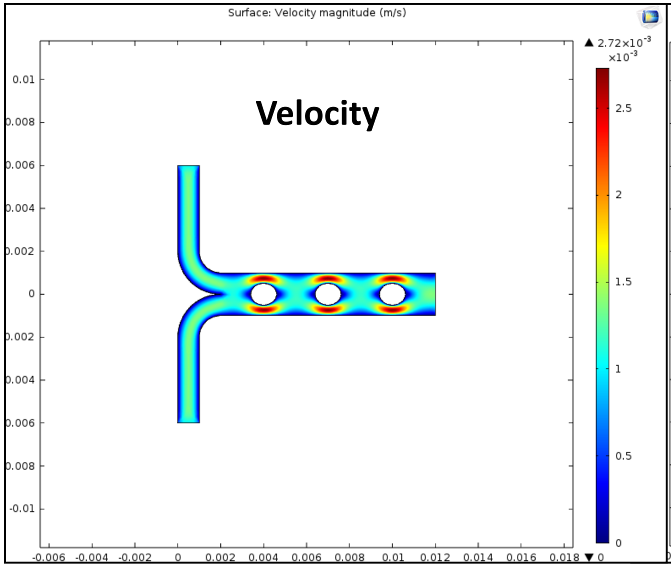


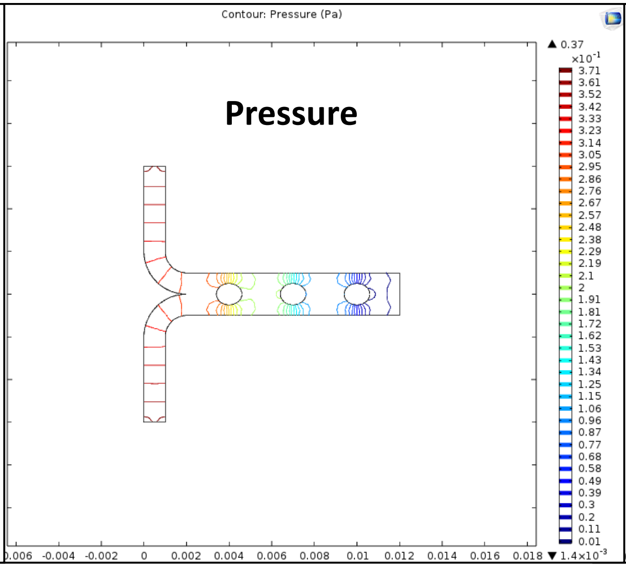


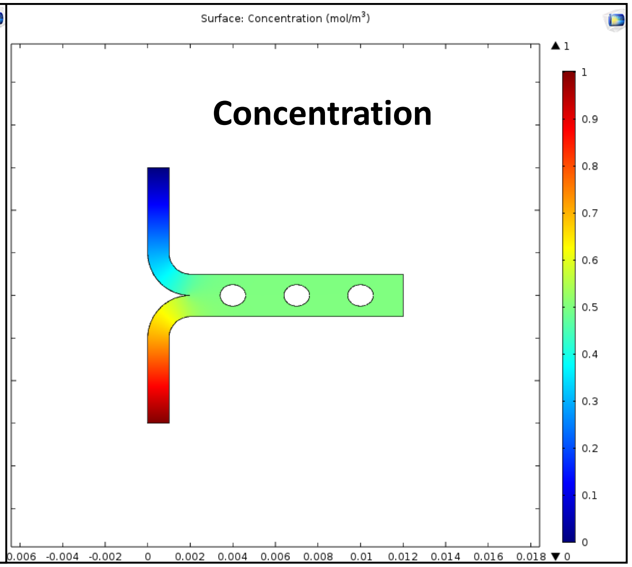
T-Micromixer with Circular Baffles











T-Micromixer with Rectangular Baffles