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

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TEXAS A&M UNIVERSITY KINGSVILLE

Falling Film Gas-Liquid Microreactor

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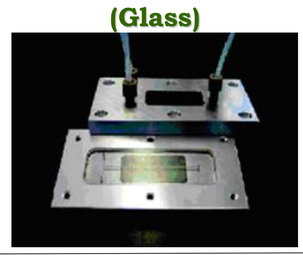
Tee-Micromixer (Glass)



Introduction

Next-generation technologies must be developed that result in safe, compact, flexible, eco-friendly, energy-efficient chemical processes and manufacturing plants. A need exists for future engineers to be exposed to these emerging technologies. *Microchemical Process Systems* are a key emerging technology with applications ranging from discovery research through small-scale commercial processes. Their characteristic length-scales usually range from 10 to 500 μm. To introduce this technology to students in the Department of Chemical Engineering at Texas A&M-Kingsville (TAMUK), special-purpose educational modules called *Interlinked Curriculum Components* (ICC's) were developed on Microchemical Process Systems as a part of the undergraduate curriculum reform program that was initially funded by NSF in 2008[1].

Chemical engineering models for this ICC describe fluid flow, heat transfer, species transport, and chemical reaction, which can be coupled phenomena. The GUI's that were developed allow students to readily modify key system parameters and obtain graphical results, which can either be scalar or vector model output variables or various derived quantities.

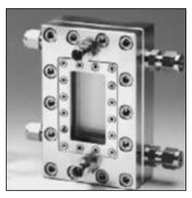
COMSOL Multiphysics™ was used as the numerical engine to simulate various microchemical process system components, such as fluid micro-mixers, micro heat-exchangers and micro reactors. *COMSOL Application Builder* was used to create various GUIs so students can readily modify key system parameters and view them in graphical form. This allows students to focus on the multiphysics versus numerical aspects.

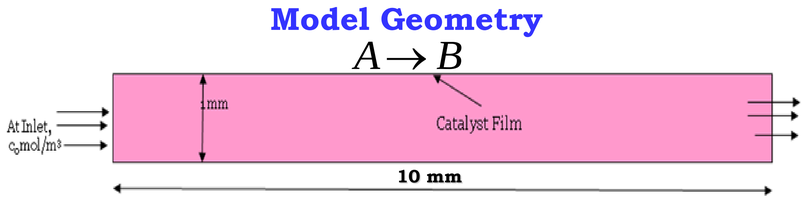
Objectives

- Create GUIs that allow users to readily interact with the model by varying selected parameters.
- Illustrate how COMSOL can be used to minimize the effort on setting up the problem so that more time can be allocated on understanding the interaction of various multiphysics.
- Develop an initial approach that provides a new method for teaching complex engineering systems to undergraduate students using an interactive approach.

Catalytic Wall Reactor

Model Geometry





Fluid & Species Transport - Kinetics Model

Momentum Balance:

$$\rho(\mathrm{u}\cdot\nabla)\mathrm{u} = \nabla\cdot\left[-\rho\mathrm{I}+\mu\left(\nabla\mathrm{u}+(\nabla u)^{\mathrm{T}}\right)\right]+\mathrm{F}$$

$$\rho\nabla\cdot(\mathrm{u}) = 0$$

where i = A, B

Mass Balance:

$$\nabla\cdot\left(-D_{\mathrm{i}}\nabla c_{\mathrm{i}}\right)+\mathrm{u}\cdot\nabla c_{\mathrm{i}} = R_{\mathrm{i}}$$

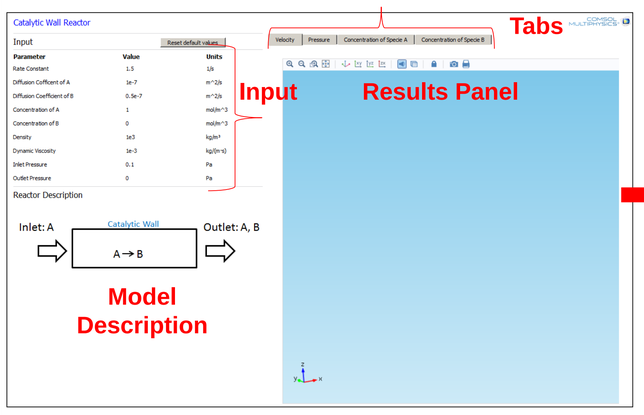
$$\mathrm{N}_{\mathrm{i}} = -D_{\mathrm{i}}\nabla c_{\mathrm{i}}+\mathrm{u}c_{\mathrm{i}}$$

Reaction Kinetics:

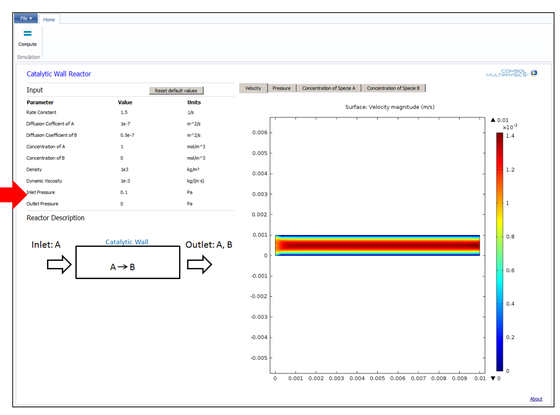
$$R = \mathrm{k}C_{\mathrm{A}}$$

Application Results

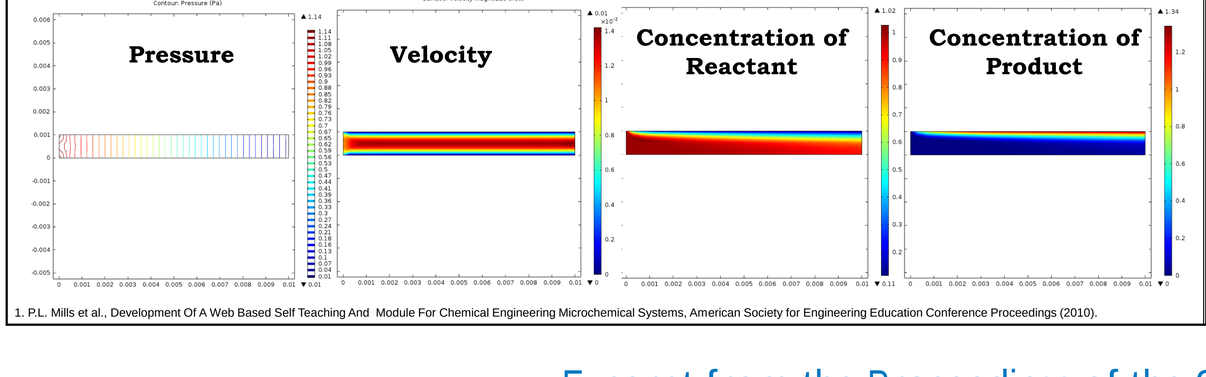
User Interface



Model Application



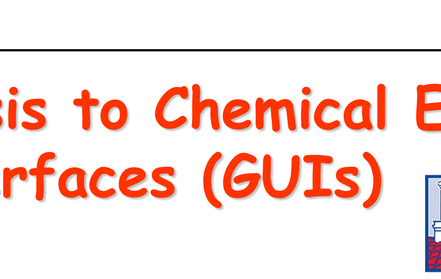
Fluid Pressure, Fluid Velocity and Species Concentration Profiles



1. 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).

T-Micromixer

Model Geometry



Parameter	Size, mm
Length (L)	12
Inlet width	0.5
Outlet width (W)	1

Fluid & Species Transport - Kinetics Model

Momentum Balance:

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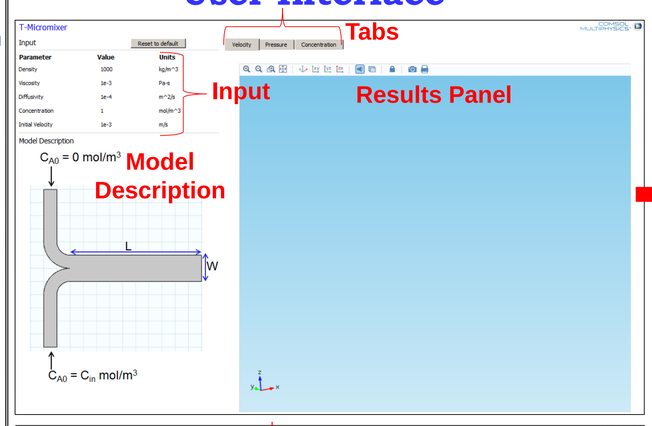
Application Results

User Interface



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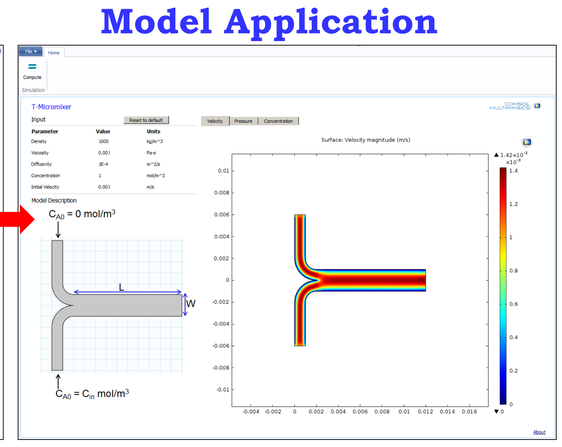

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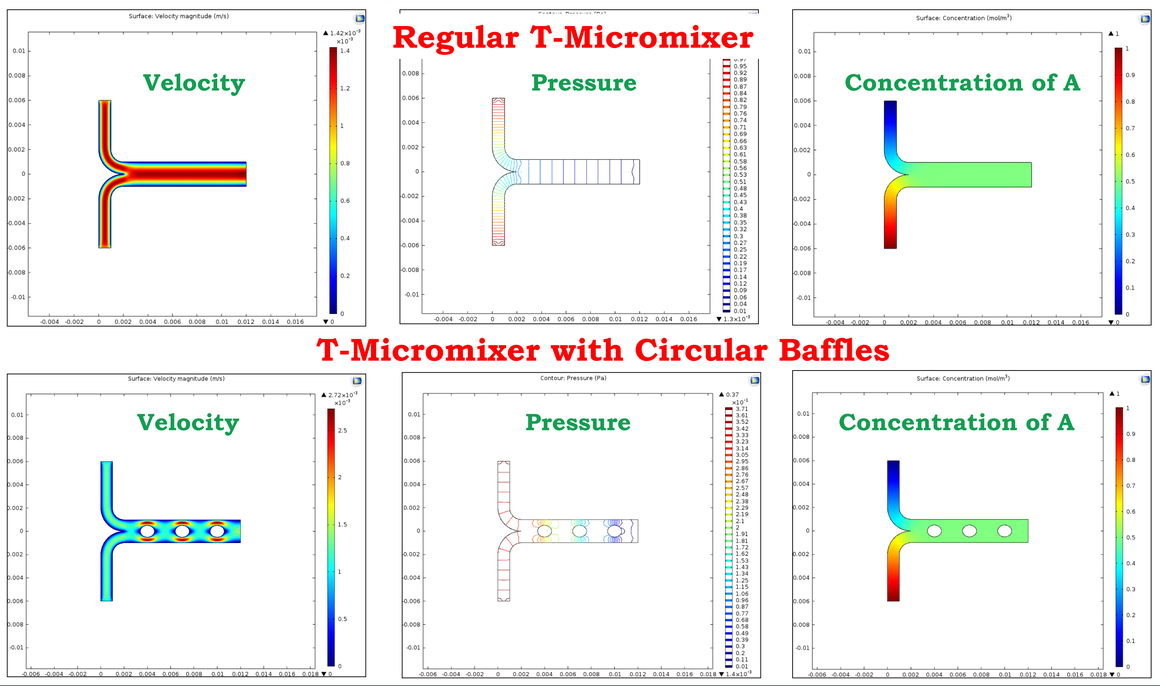

Conclusions

- The GUIs enables students to readily study the effect of various design parameters.
- These applications not only reduce the complexity of model setup and computational time, but also emphasize understanding of multiphysics in multi-dimensions that is otherwise not possible with simple 1-D models.
- This approach helps undergraduate students to understand complex chemical systems using a interactive approach versus laborious manual calculations or using other software tools.