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

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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*.

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
Microreactors & Microprocess Components Fabricated from Glass & Metal

- Tee-Micromixer (Glass)
- Interdigital Micromixer for Two-phase Systems
- Falling Film Gas-liquid Microreactor
- Cross-flow Heat Exchanger
## Microchannel vs Conventional Reactors

- Typical Ranges for Design Parameters-

<table>
<thead>
<tr>
<th>Design Parameter</th>
<th>Microchannel Reactor</th>
<th>Conventional Reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal volume</td>
<td>1-1000 μL</td>
<td>100 ml-30,000 L</td>
</tr>
<tr>
<td>Surface Area/Volume</td>
<td>10,000-50,000 m²/m³</td>
<td>100-1000 m²/m³</td>
</tr>
<tr>
<td>Heat transfer coeff.</td>
<td>10-25,000 kW/m²/K</td>
<td>17-25 kW/m²/K</td>
</tr>
<tr>
<td>Film thickness</td>
<td>~25 μL</td>
<td>~250 μL</td>
</tr>
<tr>
<td>Mixing time</td>
<td>&lt; 1 sec</td>
<td>&gt; 1 sec</td>
</tr>
<tr>
<td>Power input</td>
<td>10 X less</td>
<td>X</td>
</tr>
</tbody>
</table>

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
Steps Involved in GUI Creation

1. Input Parameters
2. Output Results
3. Layout Creation
4. Trouble Shooting

GUI creation using COMSOL with MATLAB

- .Mphapp File
- .Mph File
Example of Typical GUI Layout

Panel 1: Input Parameters
Panel 2: Model Description
Panel 3: Results

Compute

Default Values
Image
Tabs for Plots
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

\[ \text{A} \rightarrow \text{B} \]

Reaction Rate

\[ -r_A = k C_A \]
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:
\[
D \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) - \left( u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} \right) + v_y R = \frac{\partial c}{\partial t}
\]

Reaction Kinetics:
\[
A \rightarrow B \quad \text{rate, } r_A = k \ C_A
\]
Catalytic Wall Microreactor Results

- **Input**
- **Results Panel**
- **Tabs**

**Model Description**

**Results Panel**

**Surface Concentration**

**Surface Velocity Profiles**

**Pressure**

**Concentration of Reactant**

**Concentration of Product**
**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

\[
C_{OB} = C_{inB} \text{ mol/m}^3
\]

\[
C_{OA} = C_{inA} \text{ mol/m}^3
\]
Model Equations and Kinetics

Model Equations:

Momentum Transport Equations

\[ \begin{align*}
\text{x- direction:} & \quad \rho \left[ \frac{\partial u_x}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right] + \frac{\partial p}{\partial x} = 0 \\
\text{y-direction:} & \quad \rho \left[ \frac{\partial u_y}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right] + \frac{\partial p}{\partial y} = 0 \\
\text{z-direction:} & \quad \rho \left[ \frac{\partial u_z}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right] + \frac{\partial p}{\partial z} = 0
\end{align*} \]

Convection - Diffusion Equation:

\[ D \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) - \left( u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} + u_z \frac{\partial c}{\partial z} \right) + \nu_R = \frac{\partial c}{\partial t} \]

Parameter Estimation:

Mixing Effectiveness

\[ \tau = \frac{\tau_y}{\tau_D} = \frac{DL}{u_{\text{avg}} * W^2} \]

where \( \rho \) is the fluid density, \( \eta \) is the fluid viscosity, \( p \) is the fluid pressure, \( D \) is diffusivity, \( c \) is concentration, \( u_{\text{avg}} \) is average velocity and \( L, W, H \) are duct dimensions.
**Regular T-Micromixer**

**Tabs:**
- Input
- Results Panel

**Model Description:**
- \( C_{A0} = 0 \text{ mol/m}^3 \)
- \( C_{A0} = C_{A0} \text{ mol/m}^3 \)

**Results Panel:**
- Velocity
- Pressure
- Concentration

**Velocity:**
- Surface Velocity magnitude (m/s)

**Pressure:**
- Contour Pressure (Pa)

**Concentration:**
- Surface Concentration (mol/m\(^3\))
T-Micromixer with Circular Baffles

- Model Description
- Input
- Results Panel
- Tabs

- Velocity
- Pressure
- Concentration
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
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:

<table>
<thead>
<tr>
<th>term</th>
<th>definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>flow rate</td>
<td>viscosity</td>
</tr>
<tr>
<td>Reynolds number</td>
<td>Knudsen number</td>
</tr>
<tr>
<td>flow regime</td>
<td>Navier-Stokes equation</td>
</tr>
<tr>
<td>newtonian fluid</td>
<td>non-newtonian fluid</td>
</tr>
<tr>
<td>boundary settings</td>
<td>subdomain settings</td>
</tr>
</tbody>
</table>

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 confident to simulate various complicated models related to fluid mechanics.

• 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

GUI Creation using COMSOL Application Builder

Input Parameters → Output Results → Layout Creation

Trouble Shooting

GUI Creation using COMSOL Application Builder

Example of Typical GUI Layout

Panel 1: Input Parameters
Panel 2: Model Description
Panel 3: Results

Compute
Default Values
Image
Tabs for Plots
Catalytic Wall Microreactor Results

Model Description:
- Input: A → B
- Outlet: A, B

Tabs:
- Input
- Results Panel

Results Panel:
- Pressure
- Concentration of Reactant
- Concentration of Product

Contour: Pressure (Pa)
- Surface: Concentration (mol/m³)
Regular T-Micromixer

Model Description

Velocity

Pressure

Concentration
T-Micromixer with Circular Baffles

Model Description

Input

Results Panel

Velocity

Pressure

Concentration
T-Micromixer with Rectangular Baffles

Graphical User Interface
- Velocity Profile
- Heat Exchanger Cross Current
- Simple T-Micromixer
- Heat Exchanger Co Current
- T-Micromixer With Obstacles
- Heat Exchanger Counter Current
- T-Micromixer Rectangular Baffles
- T-Micromixer Ellipsoidal Baffles
- Catalytic Wall Reactor

Surface Velocity Profiles

Surface Concentration