

## **AC 2010-2009: DEVELOPMENT OF A WEB-BASED SELF-TEACHING AND ASSESSMENT MODULE FOR CHEMICAL ENGINEERING MICROCHEMICAL SYSTEMS**

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## **Development of a Web-Based Self-Teaching and Assessment Module for Chemical Engineering Microchemical Systems**

### **Abstract**

The National Science Foundation (NSF) has supported an undergraduate curriculum reform project in chemical engineering with an overall objective of developing a web-based educational resource for teaching and learning. One aspect involves the development of Interlinked Curriculum Components (ICC's). These are web-based learning sites that aim to strengthen student knowledge in the fundamental chemical engineering subjects, and to broaden student exposure to emerging technologies. The ICC's can also be used to review existing concepts and applications, to gain additional exposure to new technologies that may not be part of any formal course, and to develop a more fundamental understanding of the common threads and methods that represent the underpinning of their chemical engineering education. The ICC's are also envisioned as an integrating tool that will help students better recognize the collection of courses in their program as a unified curriculum.

The development, teaching experience, and assessment of an ICC that is focused on microprocess technology are described. The latter is a key emerging technology in chemical engineering that has applications ranging from discovery research of new catalysts or materials to small-scale manufacturing of high value-added products or toxic reagents where point-of-use is preferred over a large scale plant. The ICC module design follows a standardized protocol that includes four major sub-components: (1) pre-testing to quantitatively assess existing student knowledge; (2) a set of topic notes so that students can perform a self-paced on-line review; (3) a series of exercises and problems that allow the effect of various model parameters to be studied in a conversational type of mode with graphical output; and (4) post-testing for quantitative assessment of student knowledge progression for validation of the desired modules outcomes. A model library is included in the module design for additional reinforcement and as a source of open-ended problems that can be used to help drive creativity and provide motivation.

The exercises that comprise step 3 defined above employ COMSOL Multiphysics to simulate various microprocess system components involving fluid flow, heat transfer, and species transport, such as micro-scale fluid mixers, micro heat exchangers, and micro reactors. A library of various models was created so that students can readily explore the effect of various model parameters on the physical system. This approach allows them to focus on developing better insight and understanding of the system physics, which helps to reinforce the fundamentals that are taught in typical required courses. To provide a more direct connection between the model equations and results, a user interface was created that provides either 2-D or 3-D visualizations where the effect of various model parameters can be explored. Complex chemical engineering problems that are typically ignored in undergraduate training owing to challenges in solving the associated non-linear system of partial differential equations can now be readily studied. A key result is this new approach provides new opportunities for student learning and faculty engagement, which is expected to provide the basis for future extension of the concepts to other aspects of both undergraduate and graduate engineering education.

## Introduction

Recent advances in science and engineering have contributed to the development of new technologies having greater complexity. Chemical processes, petroleum refining, pharmaceuticals, biotechnology, and other technologies involving molecular transformations of feedstocks and their associated manufacturing plants are no exception. The use of more advanced sub-systems for manufacturing processes, such as advanced sensors, new process control and automation hardware and software, and just-in-time production management tools, has reduced the generation of off-spec products, which has resulted in process systems having greater operational efficiency.<sup>(1-6)</sup> The rapid development of the internet and wireless-based communications has greatly contributed to an exponential growth in knowledge generation and technology transfer over the past two decades, and is expected to do so in the coming decade. Hence, the next-generation of engineers and technologists will have access to a significant knowledge pool, which will provide new opportunities to provide faster and more comprehensive solutions to complex problems.

Traditional educational curriculums provide undergraduate engineering students with a spectrum of theoretical knowledge, but generally provide limited exposure to more advanced technologies. This is partly due to limited space in the curriculum for electives, although development of curriculum “tracks” provides an opportunity for students to develop more focused expertise in a particular area. Utilization of process simulators, along with other engineering analysis and design tools, allow engineering students to gain useful exposure to advanced technologies. These design tools allow students to simulate complex lumped or distributed parameter systems under steady-state or transient conditions, and can help them develop deeper insights into the combined effects of system geometries and model parameters.

Over the past 4 years, three chemical engineering departments at Texas A& M University-College Station, Prairie View A & M University, and Texas A & M University-Kingsville have collaborated on a NSF-funded program on undergraduate curriculum reform.<sup>(7)</sup> The broad objectives of the program are to provide students with tools that allow them to: (1) apply fundamental ideas in chemical engineering over a greatly expanded range of temporal and length scales; (2) apply chemical engineering fundamentals to emerging technology applications; (3) construct novel solutions for more complex, open-ended problems and processes; and (4) translate fundamental concepts and knowledge to novel challenges.

To achieve the above curricula objectives, three major strategies have been identified and defined to facilitate implementation. These include: (1) curriculum content reform and development; (2) student assessment activities, and (3) faculty development initiatives.<sup>(7,8)</sup> These three strategies are being implemented through the following six key mechanisms:

- i. Identification and organization of curriculum development activities around four course strings to improve integration of learning outcomes and activities;
- ii. Development of interlinked curriculum components (ICC's) to organize and reinforce core ideas in the chemical engineering curricula;
- iii. Using service learning in required chemical engineering courses;
- iv. Integration of assessment plans and processes throughout the chemical engineering curriculum;

- v. Offering faculty development activities to expand knowledge and to provide development opportunities; and
- vi. Implementation of dissemination plans to share experiences with an audience beyond the Texas A&M University system.

Detailed discussion of these curricula objectives, the three strategies, and their implementation through each of these six mechanisms is provided in several publications.<sup>(7-10)</sup> Of particular interest here is recent progress toward in the development of an ICC in the area of microchemical process systems. Key aspects of this particular ICC are described below.

### Microchemical process systems ICC

The microchemical ICC consists of 4 key parts: (1) a pre-test to initially ascertain the students knowledge; (2) topic notes to provide the student with the required theory; (3) example problems to illustrate application of the simulation tools; (4) interactive exercises to strengthen understanding; and (5) a post-test to ascertain the knowledge they have obtained. The exercises and problems that comprise steps (3) and (4) employ COMSOL Multiphysics as the numerical engine to simulate various microprocess system components involving fluid flow, heat transfer, species transport, and chemical reaction.<sup>(11)</sup> Typical micro process components that have been analyzed include micro-scale fluidic devices, fluid-fluid micro-mixers, micro scale heat exchangers, and micro reactors. A library of various models is being created so students can explore the effect of various model parameters on the physical system. Calculated scalar or vector field model output variables, or various quantities derived from them, are linked to a user interface that provides either a 2-D and 3-D visualization of the model simulations.

The primary objective of this paper is to describe the development and application of various exercises for chemical engineering undergraduate students that are part of the microchemical ICC. These exercises are based upon COMSOL Multiphysics with MATLAB and illustrate transport principles involving fluid mechanics, energy transport, mass transport, and chemical reaction for distributed parameter models. The models involve coupled phenomena, such as fluid momentum and energy transport, or fluid momentum, energy, and species transport, so they expose students to the principles of multiphysics models. This aspect is a particular advantage for using COMSOL Multiphysics as the numerical engine since it includes model libraries for various types of transport laws that occur in various branches of science and engineering. A key part of any ICC involves developing an interactive modeling environment where students can visually examine the impact of various model parameters on model response variables. The creation of these interfaces is illustrated using a unique software tool called *MATLAB Guide*.

The other three key ingredients of an ICC are the pre-test, topic notes, and post-test. These are omitted here since they have been described in a previous publication with key documentation available in a recent MS thesis.<sup>(12)</sup> The focus here is on development of the interactive exercises that are used to provide students with an environment for visualization of results for transport models for selected microchemical systems. The model development for selected exercises are captured in the following sections by first providing a brief introduction to the problem. This section is then followed by a descriptions of the system geometry, governing equations, and interactive student interface along with a set of typical results.

## Example Applications

### Example 1. Tee-Micro Reactor

A general model is defined for a single-phase elementary reaction occurring in a T-shaped micro-reactor. The following general reaction stoichiometry is considered



This reaction is assumed follow mass action kinetics so it is 1<sup>st</sup> order with respect to A and 1<sup>st</sup> order with respect to B. It is also assumed that the reaction is homogeneous and occurs when reactant A and reactant B are contacted with each other. The reaction is assumed to be a single-phase liquid reaction with water being the carrier fluid, so that the fluid properties are based upon water for simplicity. This is not a restriction and can be easily modified. Reactant A enters the T-microreactor at a prescribed initial concentration from one of the inlets while reactant B enters from the other inlet at either the same or a different prescribed concentration.

The intrinsic reaction rate follows mass action kinetics and is defined as

$$r = k C_A C_B \quad (2)$$

Here, the rate constant  $k$  has units of  $[m^3 / (\text{moles} \cdot s)]$ . The rate expressions for each reactant are related to the intrinsic reaction rate defined by equation (2) by their respective stoichiometric coefficients where the latter are negative for reactants and positive for products.

$$r = \frac{r_A}{-1} = \frac{r_B}{-1} = \frac{r_C}{1} \quad (3)$$

#### i. Model Geometry

The geometric model and dimensions are the same as that of the T-micromixer. A 3-D diagram of the model is shown Figure 1.

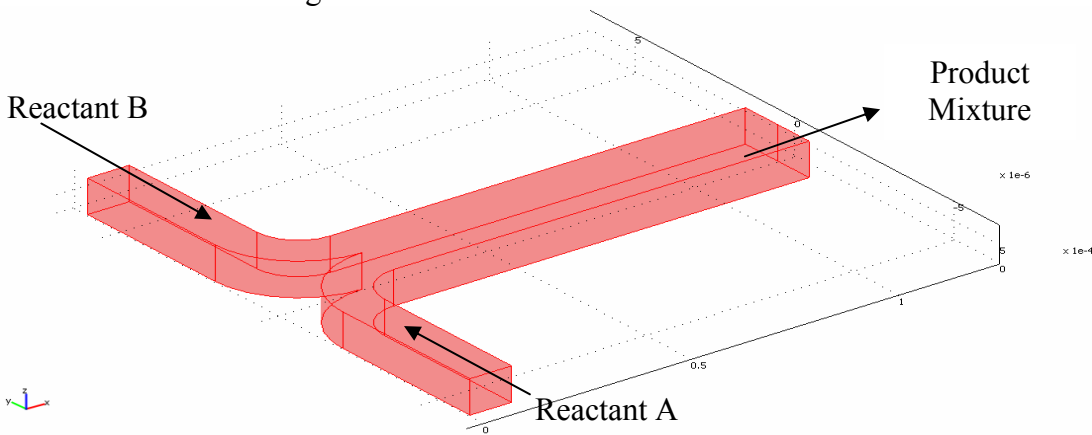


Figure 1. Geometric Model for T-Microreactor

The model dimensions are shown below in Table 1.

Table 1. Dimensions of the Tee-Microreactor

Parameter	Size,mm
Length	12
Inlet width	0.5
Outlet width	1
Height	0.5
Rectangular baffles	0.3 x 0.1 x 1
Circular baffles diameter	0.3

## ii. Modeling Equations

The velocity profiles required for the convective terms of the species mass transport equation were determined by solving the Navier-Stokes equations. The fluid density and viscosity in the Navier Stokes equations were both based upon the carrier fluid (water). Once the velocity profiles were determined, the concentration profiles for species A, B, C and D were calculated by solving the convection-diffusion equation. For this reason, it is implicitly assumed that changes in the local molar flows associated with the reaction do not alter the velocity profiles. If this was the case, then this sequential approach could not be used.

The x, y, and z components of the Navier-Stokes momentum transport equations are:

x-direction:

$$\rho \left[ \frac{\partial u_x}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right] + \frac{\partial p}{\partial x} = 0 \quad (4)$$

y-direction:

$$\rho \left[ \frac{\partial u_y}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right] + \frac{\partial p}{\partial y} = 0 \quad (5)$$

z-direction:

$$\rho \left[ \frac{\partial u_z}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right] + \frac{\partial p}{\partial z} = 0 \quad (6)$$

The convection-diffusion equation is a microscopic form of mass balance and defined by

$$D_{ij} \left( \frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2} \right) - \left( u_x \frac{\partial c_i}{\partial x} + u_y \frac{\partial c_i}{\partial y} + u_z \frac{\partial c_i}{\partial z} \right) + v_i r = \frac{\partial c_i}{\partial t} \quad (7)$$

In these equations,  $D_{ij}$  is the diffusion of component i in component j,  $v_i$  is the stoichiometric coefficient for species i, and r is the intrinsic reaction rate.

### iii. Boundary Conditions

For the Navier-Stokes equations, the boundary conditions include either specified pressures at the duct inlets and outlet, or specified fluid velocities at the inlet of each duct with specified fluid pressure at the exit. The no-slip condition was used for the fluid velocity at all solid walls. The boundary conditions for the convection-diffusion equation included specified solute concentrations at the inlet, no diffusive flux at the outlet, and zero flux (no solute permeation) at the walls. These boundary conditions are summarized below.

Boundary conditions for the Navier-Stokes equations:

The first set of boundary conditions for specified fluid pressures are:

$$\text{At the duct inlets,} \quad p = p_i \quad (8a)$$

$$\text{At the duct outlet,} \quad p = p_o \quad (8b)$$

The overall pressure drop is evaluated by difference.

$$\Delta P = p_o - p_i \quad (8c)$$

The second set of boundary conditions are:

$$\text{At the duct inlets,} \quad u = U_{in} \quad (9a)$$

$$\text{At the duct outlet,} \quad p = p_o \quad (9b)$$

At the walls, no-slip boundary conditions are used.

At  $y = 0$  and at  $y = h$ ,

$$\overline{u} = \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix} = 0 \quad (10)$$

The boundary conditions for the convection-diffusion equation are:

At inlet 1,

$$\text{Concentration of reactant A,} \quad C_A = C_{A0} \quad (11a)$$

$$\text{Concentration of reactant B,} \quad C_B = 0 \quad (11b)$$

$$\text{Concentration of reactant C,} \quad C_C = 0 \quad (11c)$$

At inlet 2,

$$\text{Concentration of reactant A,} \quad C_A = 0 \quad (12a)$$

$$\text{Concentration of reactant B,} \quad C_B = C_{B0} \quad (12b)$$

$$\text{Concentration of reactant C,} \quad C_C = 0 \quad (12c)$$

At the outlet, the diffusive flux is zero so that

$$N_D = -D \left( \frac{\partial c}{\partial x} + \frac{\partial c}{\partial y} + \frac{\partial c}{\partial z} \right) = 0 \quad (13)$$

At the walls, no solute reacts or permeates so that the combined convective and diffusive fluxes are zero.

$$N = -D \left( \frac{\partial c}{\partial x} + \frac{\partial c}{\partial y} + \frac{\partial c}{\partial z} \right) + c \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix} = 0 \quad (14)$$

#### iv. Results and Discussion

The reaction considered is a second order reaction where two reactants A and B react to form C.



The rate expression is

$$r = k C_A C_B \quad (16)$$

The concentration profiles for each of the reactants and products are shown below in Figures 2 to 4.



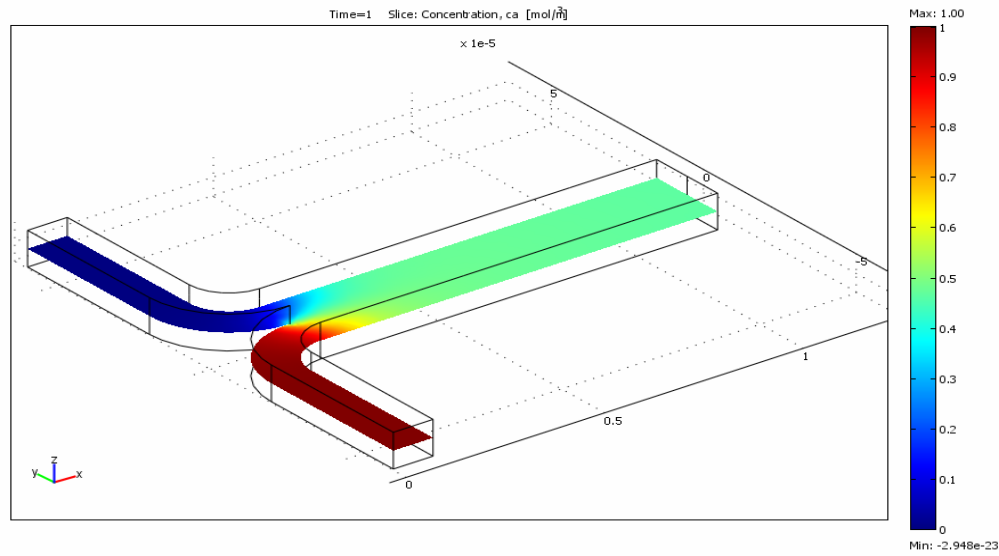


Figure 2. Concentration Profiles for Reactant A. Parameters:  $U_{in} = 1$  [m/s],  $C_{A0} = 1$  [mol/m<sup>3</sup>],  $C_{B0} = 1$  [mol/m<sup>3</sup>],  $\mu = 1.0 \times 10^{-3}$  [Pa-s],  $D_A = 1.0 \times 10^{-7}$  [m/s],  $D_B = 1.1 \times 10^{-7}$  [m/s].

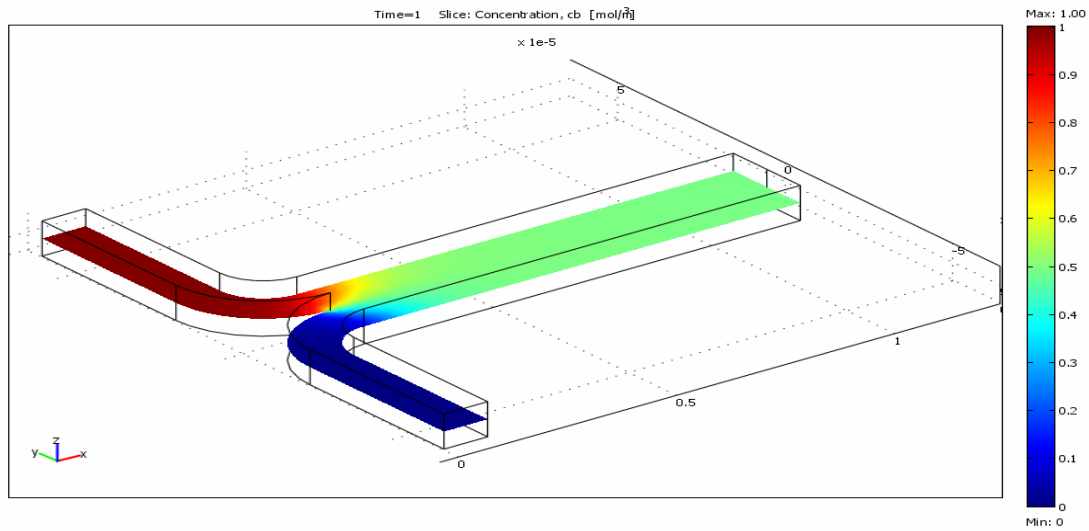


Figure 3. Concentration Profiles for Reactant B. Parameters:  $U_{in} = 1$  [m/s],  $C_{A0} = 1$  [mol/m<sup>3</sup>],  $C_{B0} = 1$  [mol/m<sup>3</sup>],  $\mu = 1.0 \times 10^{-3}$  [Pa-s],  $D_A = 1.0 \times 10^{-7}$  [m/s],  $D_B = 1.1 \times 10^{-7}$  [m/s].

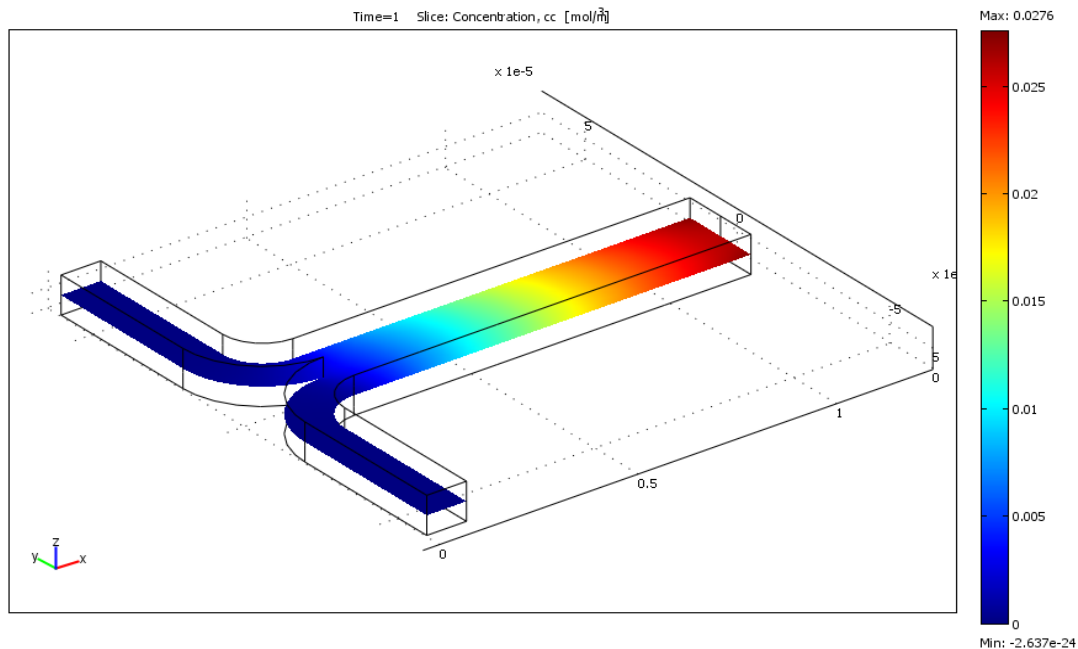


Figure 4. Concentration Profiles for Product C. Parameters:  $U_{in} = 1$  [m/s],  $C_{A0} = 1$  [mol/m<sup>3</sup>],  $C_{B0} = 1$  [mol/m<sup>3</sup>],  $\mu = 1.0 \times 10^{-3}$  [Pa-s],  $D_A = 1.0 \times 10^{-7}$  [m/s],  $D_B = 1.1 \times 10^{-7}$  [m/s].

#### v. Graphical User Interface

Figure 5 shows the screenshot of the GUI for this exercise. Here, the student can change the values of the fluid density and viscosity of the carrier fluid, inlet concentrations of A and B, and the diffusivity coefficients for each solute and study the variation of the concentration profiles. The resulting fluid velocity profiles and concentration profiles for each of the reaction species A, B, C can be observed. Typical profiles are shown in Figure 6 to 9 for a selected set of parameters.

**Tee-microreactor**

**Reaction Parameters**

Parameter	Reactant-A	Reactant-B	Product-C	Units	Range of Operation
Rate Constant	20			[ $\text{m}^3/\text{mol.s}$ ]	( $1\text{e-}2$ to $1\text{e}2$ )
Diffusivity	$6.32\text{e-}6$	$8.99\text{e-}6$	$5.06\text{e-}6$	[ $\text{m}^2/\text{s}$ ]	( $1\text{e-}11$ to $1\text{e-}5$ )
Initial Concentration	1	1	0	[ $\text{mol}/\text{m}^3$ ]	(1 to 100)

**Solvent Properties**

Parameter	Description	Value	Units	Range of Operation
$\rho$	Density	1000	[ $\text{kg}/\text{m}^3$ ]	( $800 < \rho < 1300$ )
$\eta$	Viscosity	$1\text{e-}3$	[ $\text{Pa.s}$ ]	( $1\text{e-}5 < \eta < 1\text{e-}2$ )

**Boundary Conditions**

Pressure

Parameter	Description	Value	Units	Range of Operation
$P_{\text{in}}$	Inlet Pressure	2	[Pa]	( $1 < P_{\text{in}} < 1500$ )
$P_{\text{out}}$	Outlet Pressure	1	[Pa]	( $1 < P_{\text{out}} < 1500$ )

**Buttons:** Solve, A-Concentration , Profiles, Default Values

Figure 5. Tee-Microreactor GUI at the Parameter Entry Stage.

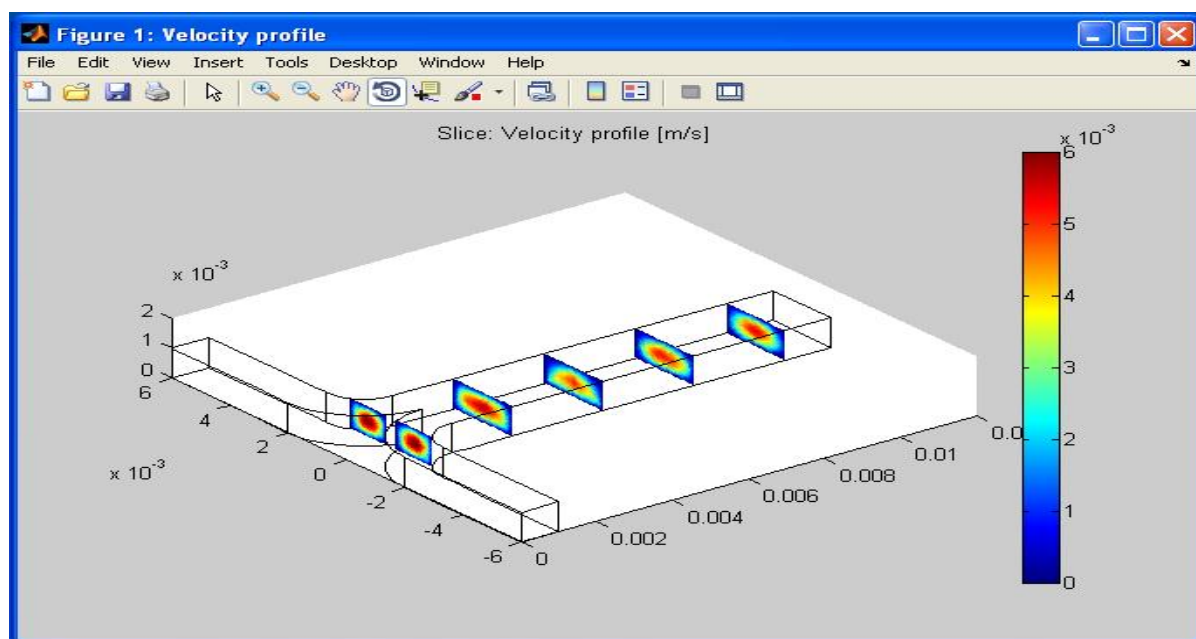


Figure 6. Slice Plots Showing the Carrier Fluid Velocity Profiles at Different Locations in the Duct.

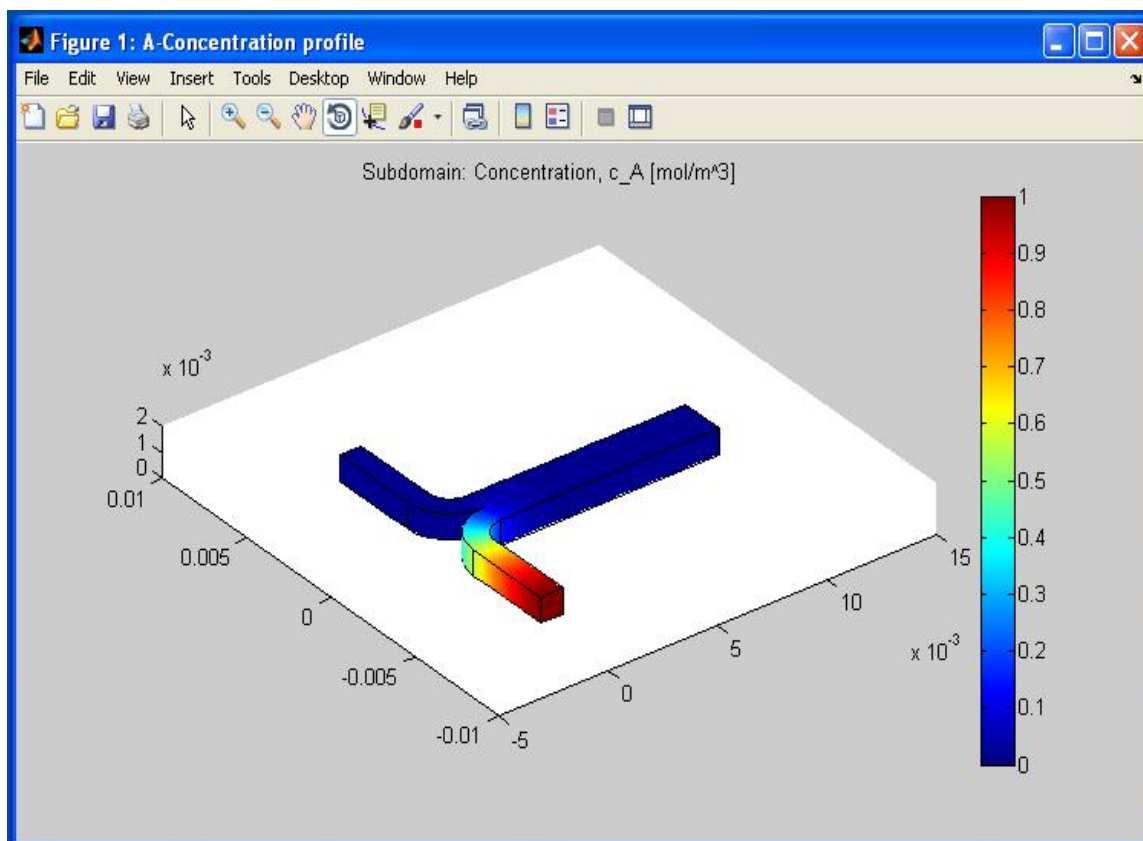


Figure 7. Concentration Profiles for Reactant A.

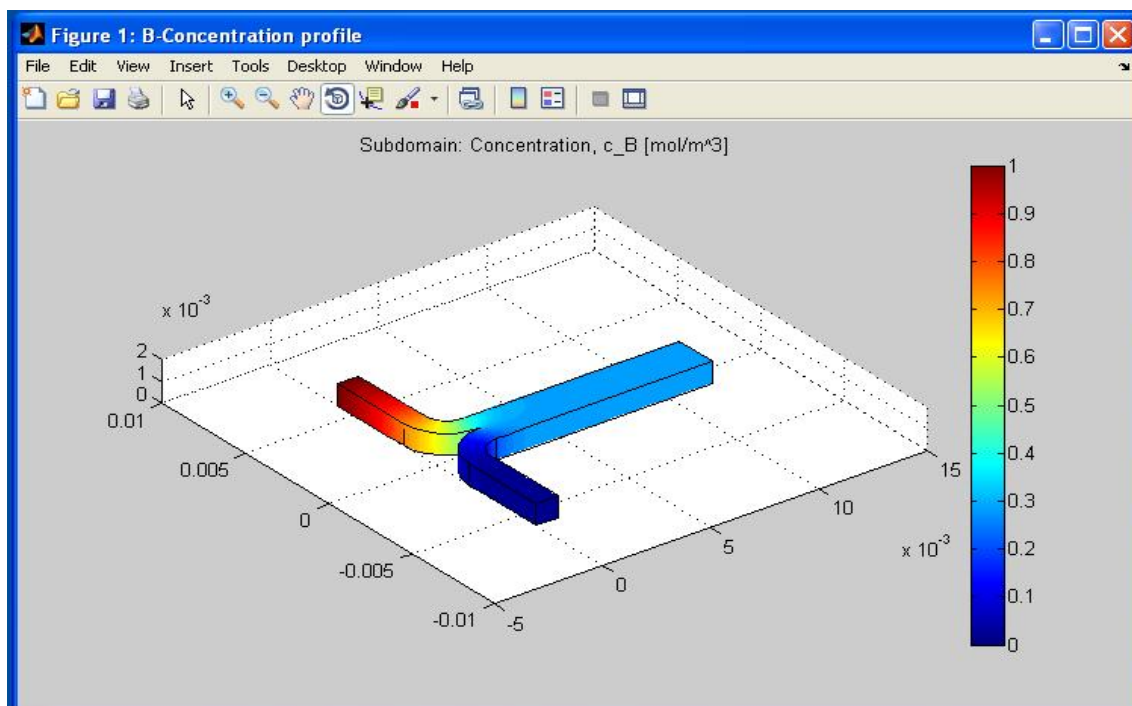


Figure 8. Concentration Profiles for Reactant B.

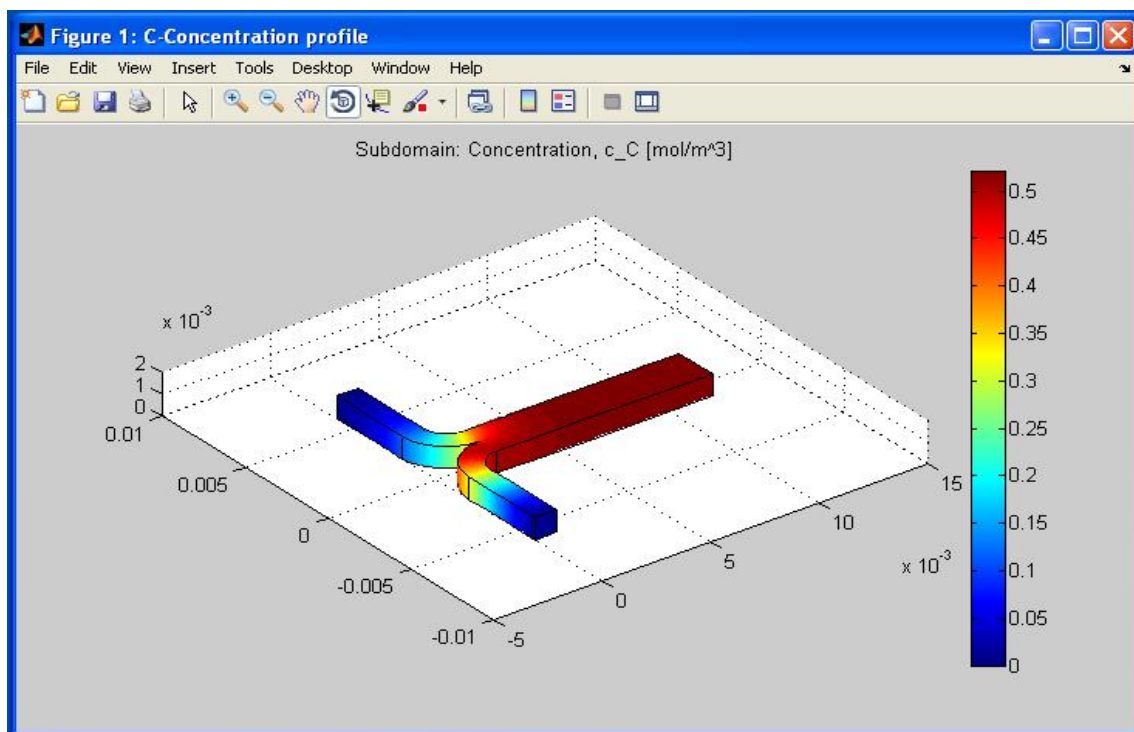


Figure 9. Concentration Profiles for Product C.

#### vi. Pedagogical Aspects

The pedagogical aspects of this example are similar to those for the tee-micro mixer except chemical reaction is now simultaneously occurring along with the fluid mixing. The student gains additional knowledge of the following concepts: (1) coupling of single phase, isothermal fluid momentum transport with simultaneous dilute solute transport and bulk-phase chemical reaction using the microscopic forms of the continuity, momentum, and convection-diffusion equations in two and three spatial dimensions; (2) understanding of the various types of boundary conditions that describe isothermal fluid flow in 3-D conduits with solute transport and chemical reaction; (3) insight into the role of various parameters that characterize solute mixing and chemical reaction, and their relation to fluid velocity profiles and solute concentration profiles; and (4) ability to directly examine the effect of fluid properties (density and viscosity), solute properties (solute inlet concentration and solute diffusivity), and reaction rate constant on calculated velocity profiles and solute concentration profiles in a 3-D geometry.

### Example 2. Micro-Scale Heat Exchanger

This example describes the performance of a micro scale heat exchanger where both fluids are identical except they enter the system at different temperatures. This is a fairly complex model that could not be easily solved in a typical undergraduate heat transfer course. The key assumptions are that temperature variations in the fluid density and viscosity are negligible. This assumption could be readily relaxed to provide another parametric case for study. Here, the complexity is reduced while retaining the 3-D forms of the convective transport and energy transport equations. Various configurations of the heat exchanger, such as cross flow, co-current flow and concurrent flow, can be studied by the variation of flow rate of the fluid.

### i. System Geometry

The geometry of the micro heater considered is shown in Figure 10 and consists of two copper blocks with dimensions  $800\ \mu\text{m} \times 800\ \mu\text{m} \times 60\ \mu\text{m}$  in height. Each of these blocks contains five type 316 stainless steel conduits. The blocks are placed such that they are at right angles to the conduits in the other block, thereby forming a cross-flow heat exchanger. The fluid flowing through these conduits can be changed and the corresponding effects in physical properties on heat transfer can be studied.

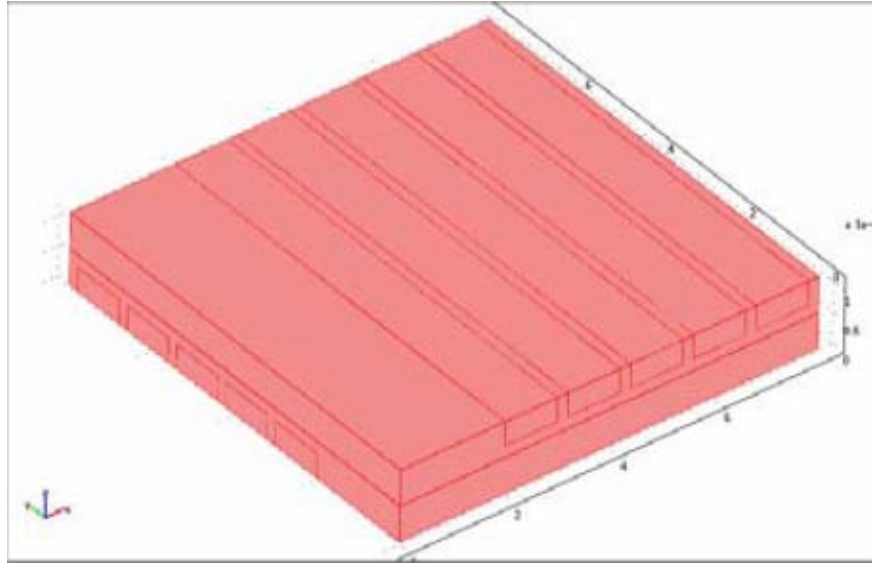


Figure 10. Geometry of the 3-D Micro Heat-Exchanger

### ii. Model Equations

The velocity field of the fluid flowing in the small ducts can be calculated using the incompressible Navier-Stokes equations. The fluids are assumed to have negligible variations in fluid density and fluid viscosity so these parameters are constant. The flow rates, channel dimension, and fluid properties result in fluid Reynolds numbers that are well within the laminar flow region ( $N_{Re}=200$  to  $500$ ). The  $x$ ,  $y$ , and  $z$  components of the incompressible Navier-Stokes Equation for the 3-D flow field are

x-momentum:

$$\rho \left[ \frac{\partial u_x}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right] + \frac{\partial p}{\partial x} = 0 \quad (17)$$

y-momentum:

$$\rho \left[ \frac{\partial u_y}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right] + \frac{\partial p}{\partial y} = 0 \quad (18)$$

z-momentum:

$$\rho \left[ \frac{\partial u_z}{\partial t} \right] - \eta \left[ \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right] + \frac{\partial p}{\partial z} = 0 \quad (19)$$

Heat transfer in the flowing fluids occurs by both convection and conduction. The energy balance for the flowing fluids in the pipes is:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \left( u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z} \right) = \left( k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} \right) + Q \quad (20)$$

After obtaining the components of the velocity vector by solving the Navier-Stokes equations, the energy balance equation can be solved and the temperature profiles can be determined.

### iii. Boundary Conditions

For the Navier-Stokes equations, the boundary conditions include either specified pressures at the inlets and outlets, or specified fluid velocities at the inlet of each stream with specified fluid pressures at the fluid exits. The no-slip condition was used for the fluid velocities at all solid walls. The boundary conditions for the conduction-convection equation include specified fluid temperatures at the respective hot and cold fluid inlets with specified convective fluxes at the fluid outlets. All exterior walls were assumed to be thermally insulated. These boundary conditions are summarized below.

Boundary conditions for the Navier-Stokes equations:

The first set of boundary conditions are:

$$\text{At the cold fluid inlet, } u_x = u_{\text{cold}} \quad (21a)$$

$$u_y = u_z = 0 \quad (21b)$$

$$\text{At the hot fluid inlet, } u_y = u_{\text{hot}} \quad (21c)$$

$$u_x = u_z = 0 \quad (21d)$$

$$\text{At both fluid outlets, } p = p_{\text{out}} \quad (21e)$$

The second set of boundary conditions are:

$$\text{At the cold fluid inlet, } p = p_{\text{in}} \quad (22a)$$

$$\text{At the hot fluid inlet, } p = p_{\text{in}} \quad (22b)$$

$$\text{At both fluid outlets, } p = p_{\text{out}} \quad (22c)$$

At the solid-fluid interface boundary, no slip boundary conditions are used.

$$\bar{\mathbf{u}} = \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix} = 0 \quad (23)$$

The boundary conditions for the conduction-convection equation are:

$$\text{At the cold fluid inlet,} \quad T = T_{\text{cold}} \quad (24a)$$

$$\text{At the hot fluid inlet,} \quad T = T_{\text{hot}} \quad (24b)$$

At the fluid outlets, the convective heat flux is zero.

$$\mathbf{n} \cdot \mathbf{q}_{\text{cond}} = \mathbf{n} \cdot k_1 \left( \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z} \right) = 0 \quad (25)$$

Similarly, continuity of thermal energy transport is applied at common boundaries so that

$$\mathbf{n} \cdot \mathbf{q}_{\text{fluid}} = \mathbf{n} \cdot \mathbf{q}_{\text{wall}} \quad (26a)$$

In the above equations,  $\mathbf{q}_{\text{fluid}}$  and  $\mathbf{q}_{\text{wall}}$  are defined as

$$\mathbf{q}_{\text{fluid}} = -k_1 \left( \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z} \right) + \rho_1 C_{p1} T \mathbf{u} \quad (26b)$$

$$\mathbf{q}_{\text{wall}} = -k_2 \left( \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z} \right) \quad (26c)$$

At the external surfaces, the blocks outer surfaces are assumed to be thermally insulated so that

$$\mathbf{q}_{\text{solid}} = -k_2 \left( \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z} \right) = 0 \quad (27)$$

#### iv. Results and Discussion

Due to the complex nature of the geometry, the problem is solved sequentially. First, the velocity profiles are calculated by solving the Navier-Stokes equation using the corresponding boundary conditions. Figure 11 shows the velocity profiles that occur in the micro channels. Once the velocity profiles are known, they are used to evaluate the temperature profiles for the entire MEMS heater. A typical set of results are shown in Figure 12 for the cross flow case. Other results are provided in the thesis of Seelam. <sup>(12)</sup>



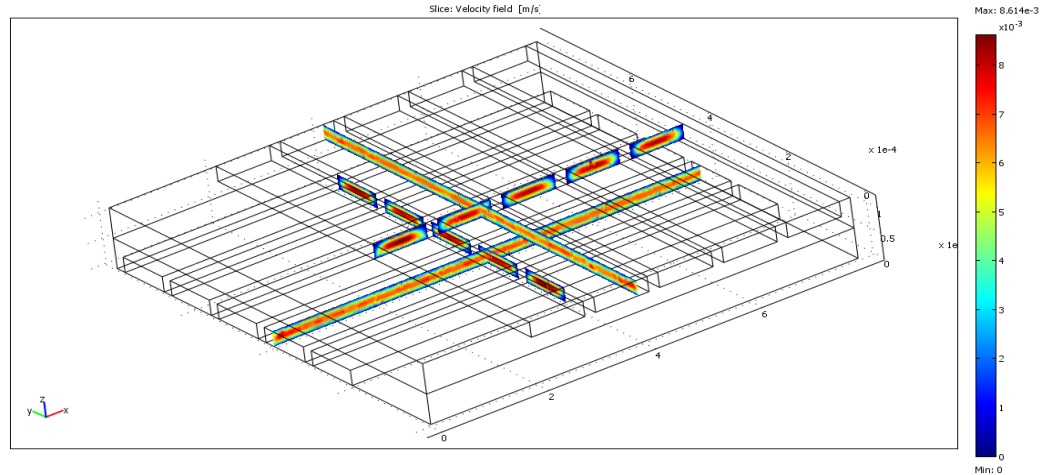


Figure 11. Slice Plots of the Fluid Velocity Profiles in the Conduits.

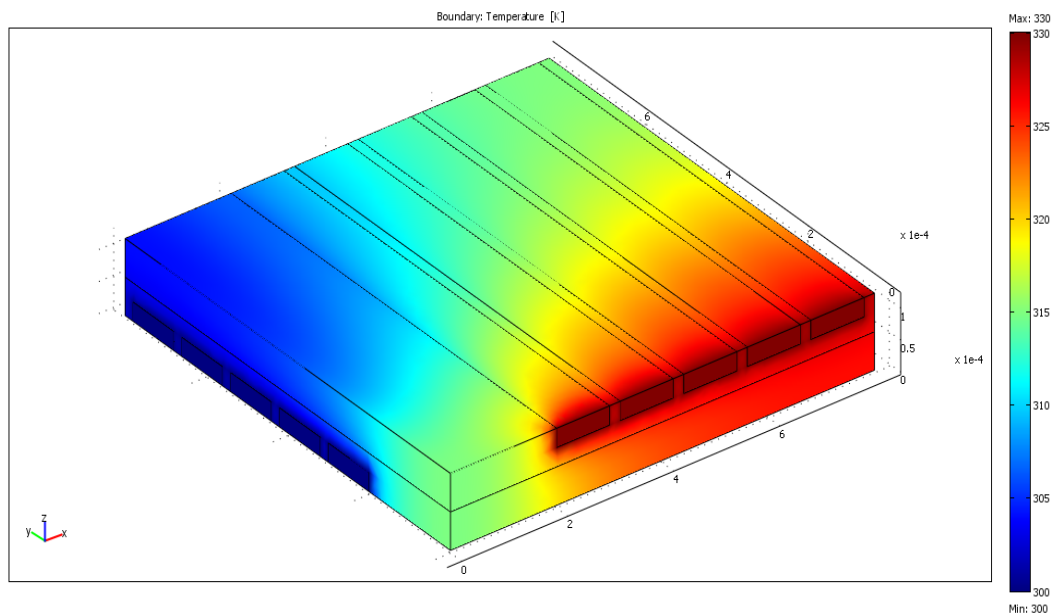


Figure 12. Temperature Profiles in the 3-D Micro Scale Heat Exchanger with Cross-Flow.

#### v. Graphical User Interface

A screenshot of the GUI that is used to solve the above problem is shown below in Figure 13. The parameters available for the user to modify include the fluid density, fluid viscosity, hot inlet fluid temperature, cold inlet fluid temperature, and the boundary conditions. As discussed previously, the differential equations are solved and the results are shown in the form of boundary plots for both the fluid velocity and fluid temperature. Typical screen shots for the fluid velocity and temperature profiles are shown below in Figures 14 and 15. The GUI also allows the heat exchanger effectiveness to be calculated over a user-specified velocity range. The results of this calculation are shown in Figure 16. While COMSOL Multiphysics runs in the background, the buttons are disabled so as to prevent the user from clicking the buttons multiple times. As discussed earlier, the 'Plot' button plots the graphs while the 'Default value' button sets the default values for the parameters.

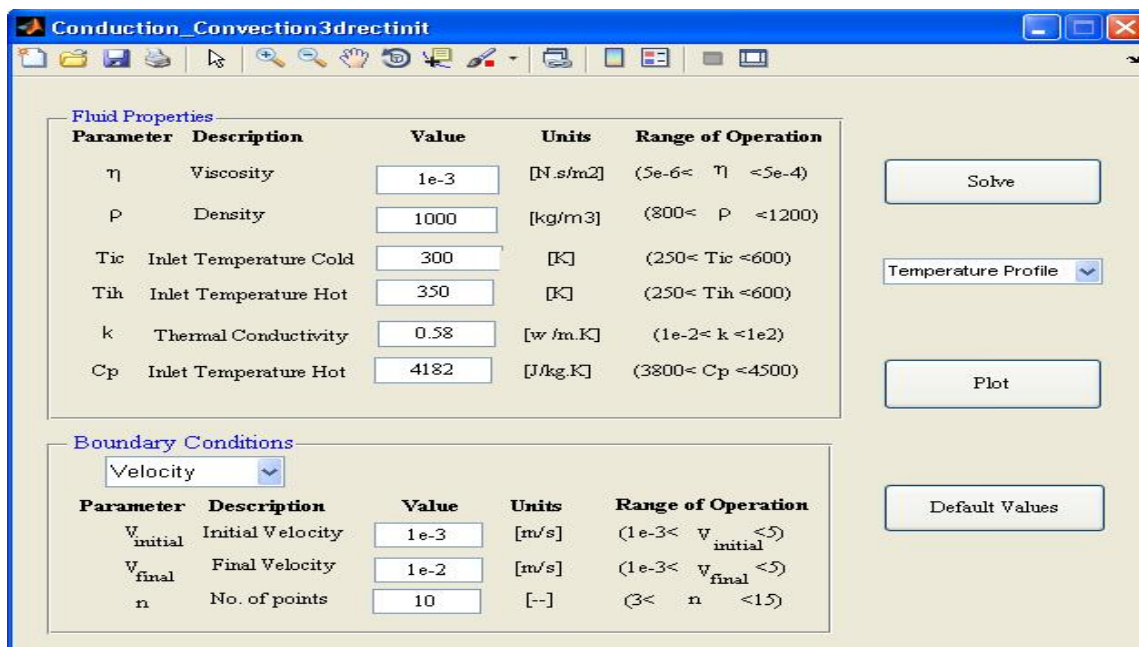


Figure 13. GUI for the 3-D Micro Scale Heat Exchanger with Cross Flow.

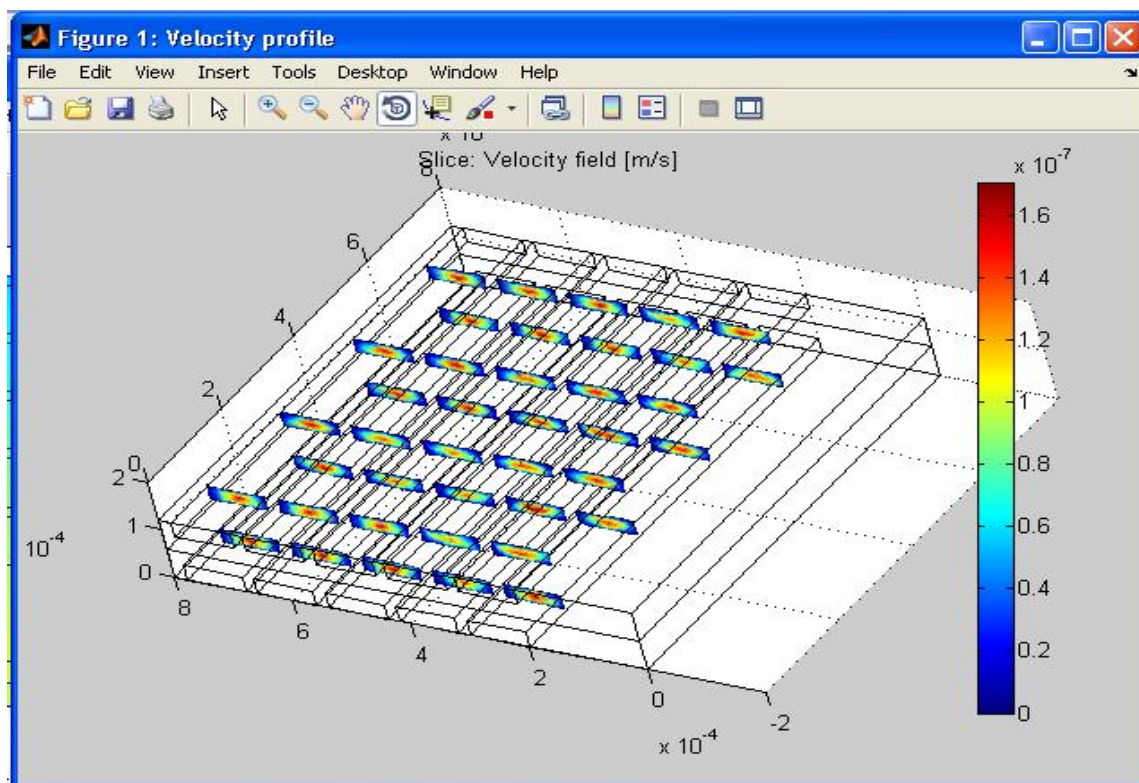


Figure 14. Velocity Profiles in the 3-D Micro Scale Heat Exchanger with Cross Flow.

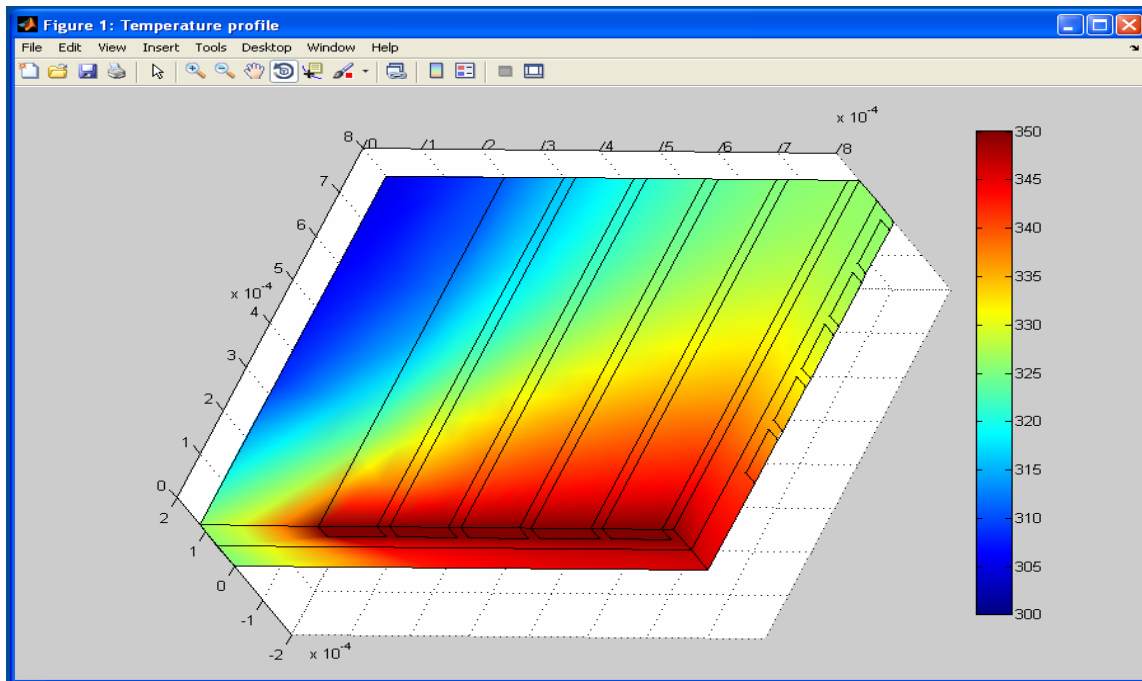


Figure 15. Temperature Profiles in the 3-D Micro Scale Heat Exchanger with Cross Flow.

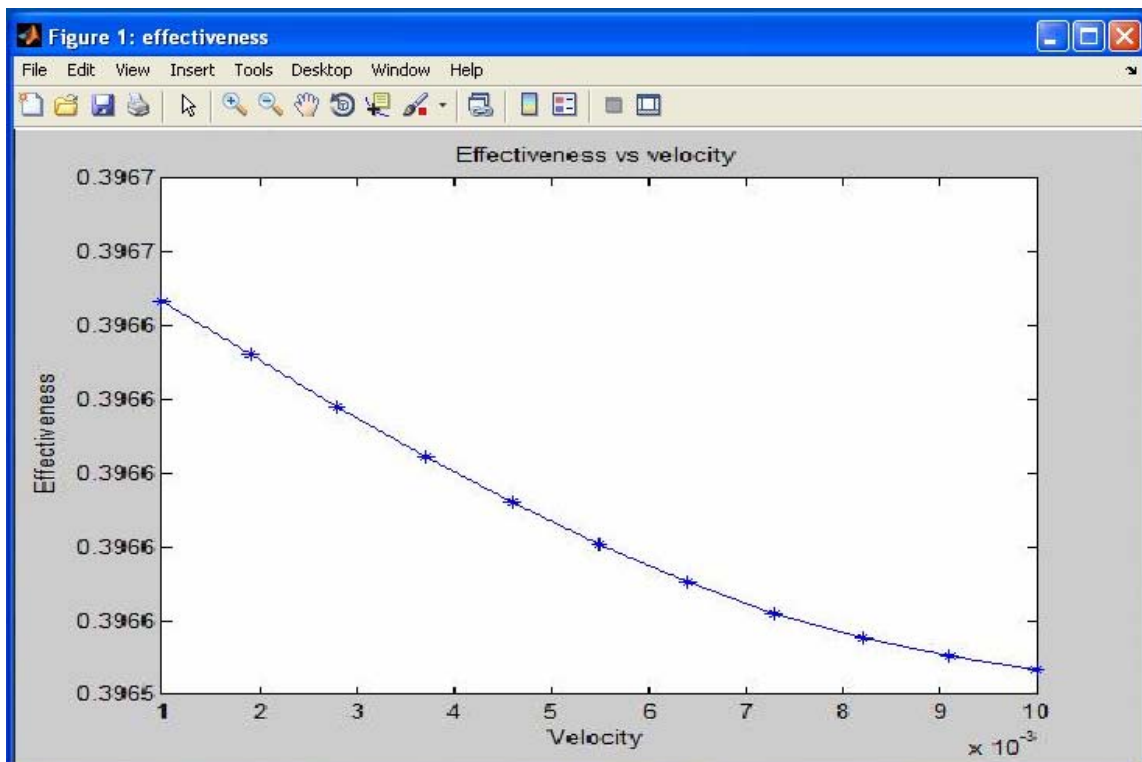


Figure 16. Effectiveness vs. Velocity for the 3-D Micro Scale Heat Exchanger with Cross Flow.

## Summary and Conclusions

The development of computer codes for education applications in chemical engineering has been an ongoing effort since the advent of analog and digital computer systems. More recently, a number of web-based educational tools have been developed<sup>(15-22)</sup> for specific areas, such as process control, laboratory experimentation, thermodynamics, and process design. To obtain realistic solutions for multiphysics problems in two or three spatial dimensions, one must use more advanced approaches for solving coupled systems, which are usually based on the finite element method. This requires a good understanding of the basic theory behind the method, a solid knowledge of linear algebra, and a host of other supporting techniques that are related to discretization, mesh generation, nonlinear equation solvers, numerical stability, to name a few, along with computer science skills for implementation. These skills are often beyond the scope of the typical engineering undergraduate student so one must rely upon computer packages to facilitate the process. On the undergraduate level, it is more important that students are first exposed to various technologies and then develop some insight into the behavior of more complex systems versus constructing computer codes that can solve complex models. The latter can be developed through other means, such as pursuit of an advanced degree, continuing education, and on-the-job training.

The ICC that is described here for microchemical systems is a first attempt at bridging the gap between simple analysis and more realistic systems that involve multiphysics phenomena. By creating the user interfaces, students do not get bogged down in details of using a fairly complex finite element code. Instead, they can gain a more global perspective of computer code capabilities and then work through some exercises to gain exposure to the type of results that such tools can generate. More important, the interactive nature of the interfaces allows them to quickly establish a "conversation" with the model, and start to ask questions that are answered in graphical form using 3-D visualization methods.

The assessment results thus far are somewhat limited owing to the recent development of these tools but work is ongoing to obtain metrics. Experience so far suggests that the pre-test and post-test results are quite different since low scores (*e.g.*, 2 correct out of 20) are typical for a pre-test while high scores (*e.g.*, 18 out of 20) are typical for a post-test. Additional data are being collected during the Spring semester of 2010 and will be presented at the conference.

## References

1. Albertazzi, S., Basile, F., Brandin, J., Einvall, J., Hulteberg, C., Fornasari, G., Rosetti, V., Sanati, M., Trfiro, F. & Vaccari, A. "The technical feasibility of biomass gassification for hydrogen production." *Catalysis Today International Conference on Gas-Fue-05*, 106(1-4), 297-300, (2005).
2. Chheda, J. N., and Dumesic, J. A. "An overview of dehydration, aldo-condensation & hydrogenation processes for production of liquid alkanes from biomass-derived carbohydrates." *Catalysis Today*, 123, 59-70, (2007).
3. Fleisch, T. H. "Emergence of the gas-to-liquids industry: A review of global GTL developments." *Journal of Natural Gas Chemistry*, 11(1-2), 1-14, (2002).
4. Kaufmann, T. G., Kaldor, A., Stuntz, G. F, Kerby, M.C., & Ansell, L.L. "Catalysis science and technology for cleaner transportation fuels." *Catalysis Today*, 62, 77-90, (2000).

5. Katada, N., Woo, S. I., Okamoto, Y. and Niwa, M. "Advances in catalysis & catalytic materials for energy and environmental protection." *Catalysis Today : Japan-Korea Symposium on Catalysis* . Matsue, Japan: Catalysis Today, 111(3-4), 145-146, (2005).
6. Bader, R. A. Catalysis in agrochemicals and pharmaceuticals industry: Frontiers and future developments. *Applied Catalysis A: General* 113(2), 141-146, (1994).
7. Froyd, J. E., & Ohland, M. Integrated engineering curricula. *Journal of Engineering Education*, 94(1), 147-164, (2005).
8. Glover, C. J., & Erdman, C. A. *Overview of the Texas A&M/NSF Engineering Core Curriculum*. Paper presented at the Frontiers in Education Conference (1992).
9. Yurttas, L., Christensen, J., Haney, J. S., El-Halwagi, M., Froyd, J. E., & Glover, C. Enhancement of Chemical Engineering Introductory Curriculum through Service-Learning Implementation. Paper presented at the *ASEE Annual Conference & Exposition*. Retrieved December 5, 2008, from <http://papers.asee.org/conferences/paper-view.cfm?id=4246> (2007).
10. Yurttas, L., Kraus, Z., Froyd, J. E., Layne, J., El-Halwagi, M., & Glover, C., A Web-based Complement to Teaching Conservation of Mass in a Chemical Engineering Curriculum. Paper presented at the *ASEE Annual Conference & Exposition*. Retrieved December 5, 2008, from <http://papers.asee.org/conferences/paper-view.cfm?id=3510> (2007).
11. COMSOL Multiphysics Chemical Engineering User Guide, 2009.
12. Srivenu, S.. "Design of Graphical User Interfaces for Interlinked Curriculum Component Modules for Microchemical Systems and Modeling of T-shaped Microchemical Reactor" Thesis, Department of Chemical and Natural Gas Engineering, Texas A& M University- Kingsville, Kingsville, (December 2009).
13. Wong, S.H., Ward, M.C.L., & Wharton, C.W. "Micro T-mixer as a rapid mixing micromixer" *Sensors and Actuators B: Chemical*, 100(3), 359-379, (2004.).
14. Christensen, A. E., "Numerical Simulation of Microfluidic Mixing", MIC – Institute of Micro and Nanotechnology Technical, University of Denmark, (2005).
15. Rafael, A. C., Bernardo, F., Ferreira, L. M., Rasteiro, M. G., & Teixeira, J. C. "Virtual Applications Using a Web Platform to Teach Chemical Engineering: The Distillation Case. *Education for Chemical Engineers*, 20-28,(2007).
16. Selmer, A., Kraft, M., Moros, M., & Colton, C. K. "Weblabs in Chemical Engineering Education." *Education for Chemical Engineers*, 38-45,( 2007).
17. Marlin, M., & Hough, T. "Web-based interactive learning modules for process control." *Computers & Chemical Engineering*, 1485-1490, (2000).
18. Stanford University - Library and Academic Information Resources. *SWAIN CHEMISTRY AND CHEMICAL ENGINEERING LIBRARY*.2009. <http://www-sul.stanford.edu/depts/swain/help/subjectguides/general/desk/toolbox.html> , (accessed 2009).
19. Rasteiro, M. G., Ferreira, L., Teixeira, J., Bernardo, F. P., Carvalho, M. G., Ferreira, A., Ferreira, R. Q., Garcia, F., Baptista, C. M. S. G., Oliveira, N., Quina, M., Santos, L., Saraiva, P. A., Mendes, A., Magalhães, F., Almeida, A. S. , Granjo, J., Ascenso, M., Bastos, R. M., & Borges, R. "LABVIRTUAL--A virtual platform to teach chemical processes." *Education for Chemical Engineers* , 1 ,e9-e19, (2009).
20. Shin, D., Yoon, E. S., Park, S. J., & Lee, E. S. "Web-based interactive virtual laboratory system for unit operations and process systems engineering education." *Computers & Chemical Engineering*, 1381-1385, ( 2000).
21. Koretsky, M. *VirtualCVD Reactor*. 2004-2006. <http://cbee.oregonstate.edu/education/VirtualCVD/>, (accessed 2009)
22. Koresky, M., & Connelly, B. *Thermosolver*. <http://cbee.oregonstate.edu/education/Thermosolver/>,(accessed 2009).