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

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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 of this project involves the development of Interlinked Curriculum Components (ICCs). These are web-based learning sites that aim to strengthen student knowledge in the fundamental subjects that span all chemical engineering courses, and to broaden their exposure to emerging technologies and non-traditional applications.

This paper describes the development of an ICC that is focused on microprocess technology. This is a key emerging technology in chemical engineering that has applications ranging from discovery research of new catalysts and materials to small-scale manufacturing of high value-added products, toxic reagents, explosives, and other chemicals where point-of-use is preferred over a large-scale centralized manufacturing plant. The ICC module design follows a standardized protocol that includes five major sub-components: (1) pre-testing to quantitatively assess existing student knowledge on the module topic; (2) a set of topic notes so that students can perform a self-paced online review of the required subject matter; (3) examples that provide illustrations of various problems; (4) a series of exercises and problems having increasing complexity that allow the effect of various model equation set-ups and the effect of various model parameters to be studied in a conversational type of mode with graphical output; and (5) post-testing for quantitative assessment of student knowledge progression for validation of the desired modules outcomes.

The examples, exercises and problems mentioned above employ a software tool called COMSOL Multiphysics as the numerical engine to simulate various microprocess system components involving fluid flow, heat transfer, and species transport, such as micro-scale fluidics and fluid micro mixers, micro heat exchangers, and micro reactors. A library of various models was also created so that students can readily explore the effect of various model parameters on the physical system without worrying focusing on details of the numerical solution. 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 required courses on fluid mechanics, heat transfer, and mass transfer. To provide a more direct connection between the model equations and the calculated results, a user interface was also created that provides either a 2-D and 3-D visualization of the model simulations where the effect of various model parameters can be explored. Complex chemical engineering problems that are typically omitted in undergraduate training can now be readily studied and provide new opportunities for student learning.
Introduction

The projected decrease in the supply of petroleum-based feedstocks over the next several decades has been a key driver in renewed efforts on the discovery of sustainable feedstocks for manufacture of clean energy, chemicals, and advanced materials, and the invention of next-generation clean processes with minimal environmental impact. Evolutionary academic programs that can produce a new generation of scientists and engineers who can create unique and timely solutions to meet these and other related global challenges are essential for the stability and well-being of future generations. In addition, the rapid development of the internet and wireless-based communication systems has greatly contributed to an exponential growth in knowledge generation and technology transfer over the past decade, and will continue to play a major role in both education and technology development. Along these lines, the chemical engineering departments at Texas A&M University (TAMU), Prairie View A&M University (PVAMU), and Texas A&M University-Kingsville (TAMUK) are continuing their efforts to evolve their four-year undergraduate curricula so their graduates are equipped with the requisite fundamental and practical knowledge that will prepare them for either graduate-level studies or entry-level professional positions in these and other emerging technologies, such as nanotechnology, biotechnology, or pharmaceutical sciences. Particular broad-based educational objectives of these evolving curricula include the ability 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) to successfully 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. The 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 chemical engineering curricula
(iii) Using service learning in required chemical engineering courses;
(iv) Integrating assessment plans and processes throughout the chemical engineering curriculum;
(v) Offering faculty development activities to offer knowledge and development opportunities for chemical engineering faculty members; and
(vi) Implementation of dissemination plans to share experiences with an audience beyond the Texas A&M University system.

A detailed discussion of above the curricula objectives, the three strategies, and their implementation through each of these six mechanisms is provided in several recent publications. Of particular interest here is the concept of interlinked curriculum components (ICCs) and recent progress toward in the development of an ICC in the area of microchemical systems.

Interlinked curriculum components (ICCs) are web-based learning sites where undergraduate chemical engineering students may reinforce fundamentals and gain new knowledge about emerging technologies and non-traditional applications. They are intended to provide an additional source of knowledge that is gained outside of typical classroom lectures. Table 1 provides an overview of the various ICCs that are being developed and the key topics covered within a particular ICC.
Table 1. Overview of Interlinked Curriculum Components and Topical Coverage.

<table>
<thead>
<tr>
<th>ICC 1 - Conservation Principles</th>
<th>ICC 2 - Materials</th>
<th>ICC 3 - Continuum Principles</th>
<th>ICC 4: System Synthesis and Integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a: Conservation laws and accounting</td>
<td>2a: Equations of state</td>
<td>3a: Coordinate systems</td>
<td>4a: Mass and energy metrics</td>
</tr>
<tr>
<td>1b: Conservation of mass</td>
<td>2b: Energy properties</td>
<td>3b. Mass continuity</td>
<td>4b: Thermal management</td>
</tr>
<tr>
<td>1c: Conservation of energy; mechanical and thermal energy balances</td>
<td>2c: Entropy</td>
<td>3c: Equation of motion and momentum transport</td>
<td>4c: Heat exchange network pinch analysis</td>
</tr>
<tr>
<td>1d: Conservation of linear momentum</td>
<td>2d: Transport properties: 1) viscosity, 2) thermal conductivity, 3) diffusivity</td>
<td>3d: Energy conservation and energy transport</td>
<td>4d: Mass exchange networks</td>
</tr>
<tr>
<td>1e: Conservation of angular momentum</td>
<td></td>
<td>3e: Species conservation and multicomponent systems</td>
<td>4e: Chemical and biochemical reaction network pathways</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ICC 5: Microchemical Systems</th>
<th>ICC 6: Molecular Modeling</th>
<th>ICC 7: Nanotechnology</th>
<th>ICC 8: Environment and Sustainability</th>
</tr>
</thead>
<tbody>
<tr>
<td>5a: Fluid mechanics at the microscale</td>
<td>7a: Molecular-level energies and forces</td>
<td>8a: Scaling; what is important at the nanoscale?</td>
<td>8a: Sustainability</td>
</tr>
<tr>
<td>5b: Heat and mass transfer; influence on reaction engineering</td>
<td>7b: Property prediction from single-molecule modeling</td>
<td>8b: Soft particulate systems; compare to atomistic</td>
<td>8b: Sustainable energy</td>
</tr>
<tr>
<td>5c: Microfluidics device design and creation (lab component)</td>
<td>7c: Molecular simulation for property prediction</td>
<td>8c: Nanotechnology design (lab component)</td>
<td>8c: Chemical process designs, performance evaluation and improvement</td>
</tr>
<tr>
<td>5d: Process control and microsystems analysis</td>
<td>7d: Molecular modeling</td>
<td></td>
<td>8d: Life cycle analysis</td>
</tr>
</tbody>
</table>

Inspection of Table 1 shows that the ICCs are generally divided into fundamentals (Conservation Principles, Materials, Continuum Principles, Systems Synthesis and Integration) and selected emerging technologies (Microchemical Systems, Molecular Modeling, Nanotechnology, and Environment and Sustainability). As a result of this structure, the ICCs can be used by students to review fundamental concepts and how they are applied to solve problems, and to learn about emerging technologies. From a broader perspective, these two parallel learning opportunities allow them to develop a better appreciation and understanding of the common threads and methods that connect various courses in their curriculum. Thus, the ICCs are also envisioned as an integrating tool that will help students gain a better perspective of the course collection in their program as a unified curriculum. Another benefit is the ICCs allow faculty to review presentations of various curricula topics and to work towards better unification of their course lectures and course outcomes. The latter is especially important for any department where the same course may be taught by more than one faculty member.

Currently, eleven chemical engineering faculty members from the three departments, along with their students and associates, are working on development and implementation of the interlinked curriculum components. An ICC coordination committee was formed to coordinate the progress reports from ICC coordinators. ICC development may be reviewed at http://che.tamu.edu/orgs/NSFCR/ or at the new site http://ALChemE.tamu.edu/.

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The primary objective of this paper is to present and analyze the development of an ICC that is focused on microprocess technology (ICC 5 in Table 1). This 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, toxic reagents, explosives, or other chemicals where point-of-use is preferred over a large-scale centralized manufacturing plant. Some examples of microprocess system components that are used to conduct gas-liquid reactions, mix two heterogeneous or homogeneous fluids, or alter fluid temperatures are shown in Figure 1.

![Figure 1a. Falling-film gas-liquid reactor.](image1a)

![Figure 1b. Interdigital two-phase system mixer.](image1b)

![Figure 1c. T-micromixer for homogeneous fluids.](image1c)

![Figure 1d. Cross-flow heat exchanger.](image1d)

Figure 1. Various microchemical process components that are used to conduct gas-liquid reactions (Figure 1a), mix heterogeneous (Figure 1b) or homogeneous (Figure 1c) fluids, or alter the temperature of two streams using a cross-flow heat exchanger (Figure 1d).

The exercises and problems that comprise step 3 defined above employ COMSOL Multiphysics as the numerical engine to simulate various microprocess system components involving fluid flow, heat...
transfer, and species transport, such as micro-scale fluidics and fluid micro mixers, micro heat exchangers, and micro reactors. A library of various models was created so that students can explore the effect of various model parameters on the physical system. The 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.

Microchemical ICC

ICC Module Design

ICC modules are generally designed according to a standardized protocol that includes five major sub-components: (1) pre-testing to quantitatively assess existing student knowledge on the module topic; (2) a set of topic notes so that students can perform a self-paced on-line review of the required subject matter; (3) a series of examples that guide the student through the various steps involved in setting up and solving a particular problem along with illustrations of the solution; (4) a series of exercises and problems having increasing complexity that allow the effect of various model equation set-ups and the effect of various model parameters to be studied in a conversational type of mode with graphical output; and (5) post-testing for quantitative assessment of student knowledge progression for validation of the desired modules outcomes. In addition, a model library that contains additional exercises can also be included in the module design for additional reinforcement and as a source of open-ended problems that drive creativity and motivation. The structure of a typical ICC module is shown in Figure 2.

![Diagram of ICC Module Structure](image)

Figure 2. Structure of a typical ICC module showing the various components.

a. Webpage design. The web pages were developed using Dreamweaver software. A main template was designed so that all ICCs would follow a uniform format. The template is a copy of the
page on which the remaining website is based. Here, it is possible to establish zones that can be either edited or prevented from any additional modifications. It is not possible to modify the properties of a page that is based on a template, apart from the title. As shown in Figure 3, the template faceplate itself consists of a uniform design that includes a navigation bar with buttons that provide links to the appropriate web pages. The one shown here corresponds to the fluid mechanics sub-section for the microchemical ICC.

Figure 3. Navigation bar and index webpage.
Referring above to Figure 3, the index page is the home page of this particular web site that includes a brief written introduction on the module objectives. The top of the page contains a navigation bar that consists of six buttons, namely, Home, Pre-test, Topic Notes, Examples, Exercises, and Post-Test. This page also provides five images associated with the last five buttons. For instance, when the Pretest button in the navigation bar is clicked, a link is provided for the Pretest web page and the page is subsequently displayed. Since the main template is used for all web pages in the website, the navigation bar associated with the index webpage is also present on all other pages.

b. Pre-test sub-module. This sub-module is designed to quantitatively assess a student’s knowledge before the starting the module. It consists of twenty multiple choice questions. An abbreviated example that shows the first two pre-test questions is shown in Figure 4.

![Fluid Mechanics](image)

**Fluid Mechanics**

The following is only a pre-test. It is used to provide a basis for assessment of knowledge gained after completion of the Fluid mechanics module. When you are finished, please click submit at the bottom of the page.

1. Identify the condition based on the value of Knudsen number (Kn) for the following flow regimes
   a. The continuum regime for Navier-Stokes equation applies when
      - Kn < 0.001
      - 0.001 < Kn < 0.1
      - 0.1 < Kn < 10
      - Kn ≥ 10
   b. The transitional regime occurs when
      - Kn < 0.001
      - 0.001 < Kn < 0.1
      - 0.1 < Kn < 10
      - Kn ≥ 10
   c. The Navier-Stokes equation regime with slip-flow boundaries is valid from
      - Kn < 0.001
      - 0.001 < Kn < 0.1
      - 0.1 < Kn < 10
      - Kn ≥ 10

2. The characteristic dimension of micro electromechanical systems (MEMS) devices is of the order
   - 0.1 to 1μm
   - 0.1 to 10μm

Figure 4. Pre-test web page showing the arrangement of typical pre-test questions.

Standard HTML form components, such as radio buttons and checkboxes, are used to implement the multiple choices. Two buttons named Submit and Reset are displayed at the bottom of the web page (not shown for brevity). When the Submit and Reset are displayed at the bottom of the web page (not shown for brevity). When the Submit button is clicked, the form is validated and number of correct answers is evaluated. The Reset button is used to reset the form, that is, all the checked components of the form will be unchecked. Javascript code is used for the validation of the form. The code is written to evaluate the questions and display the number of correct answers. When the Submit button is clicked, an alert box that contains a message indicating the number of correct answers.
answers is displayed. This script is embedded in the web page, and the results are logged in a database for assessing metrics of student progress on both an individual and group basis.

c. **Topic notes sub-module.** The *Topic Notes* are intended to provide complete technical information on the module subject matter for self-study. This sub-module consists of several web pages. When the *Topic Notes* button is clicked, the web page associated with it is displayed and with a focused description of the topics given in the selected sub-module. A hierarchical structure is designed using the Flash software tool where the root node of the tree structure is the main topic and the branch nodes are the sub topics. Buttons are used to represent topics. When the button is clicked, the appropriate page is displayed. This Flash media file enables students to open the web page of the topic without being redirected to the main topic notes webpage.

d. **Examples sub-module.** This sub-module allows students to learn skills through simulation of various models using COMSOL Multiphysics (see www.comsol.com). When the *Examples* button from the navigation bar is clicked, a webpage is opened that shows a descriptive illustration of all the examples. Links for each example are provided in this page as shown below in Figure 5. The problems are self-explanatory and provide a scope on the various phenomena that can be analyzed.

![Fluid Mechanics](image)

**Figure 5.** Main web page of the examples for the microchemical ICC module.

Each example consists of a video tutorial that provides step-by-step guidance on how to design and simulate the selected model. This video tutorial is a Flash media file embedded in the webpage. Since all of the video tutorials in the web pages are Flash media files, Adobe flash player software is needed to run these media files. The web page also provides links to all the steps involved in designing and simulating the model as shown below in Figure 6. When the link for each step is
clicked, the web page containing detailed descriptions of that step is subsequently displayed as shown in Figure 7.

Figure 6. Webpage for example 2 of the ICC microchemical module.
e. Exercises sub-module. This sub module is designed to enable students to obtain in depth knowledge of each step involved in design and simulation of a model and work through complex models in COMSOL Multiphysics using the web-based approach. When the Exercises button from the navigation bar is clicked, the web page that consists of all the exercises is opened. Links for each exercise are provided in this page as shown below in Figure 8.

Each exercise also contains a video tutorial and detailed description of the steps required to setup and solve a problem are shown in the video. The video tutorial is embedded in the web page and the steps involved are described as shown in Figure 9. When the link for the step is clicked, the web page containing the complete information about the step is displayed as shown in Figure 10. The video cannot be shown here but will be available in the future once an official version of the software is more fully tested and released.

f. Post test sub-module. This sub-module is designed to assess a student’s knowledge after completion of the module. The sub module consists of one web page. This web page displays the same twenty multiple choice question used in the pretest web page as shown in Figure 11. The same questions are used in both the pre-test as well as the post-test webpage to assess improvement in student knowledge after completion of the module. The design technique used is the same as that used in the Pretest sub-module.

Internet Browsers, such as Internet Explorer or Firefox, are needed to browse the website. Since Flash media files are embedded in the web ages, Adobe flash player software is needed. Adobe flash
player is free software that could be downloaded from the official website of Adobe www.adobe.com. The detailed screen shots are shown in Appendix A.

Figure 8. Exercises main web page of the ICC microchemical module.

Figure 9. Web page for exercise 1 of the ICC microchemical module.
Figure 10. 1-D geometry web page of the ICC microchemical module.

Figure 11. Post-test web page of the ICC microchemical module.

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COMSOL Multiphysics Modeling Platform

The web pages described in the previous section where examples, exercises, and problems are illustrated for various microchemical system components (e.g., Figure 5) require simulation tools to produce numerical results. This section provides a description of the methodology used in this project, although it represents a work-in-progress so a snapshot of the current state-of-the-art is provided.

The model equations that describe the performance of microchemical process system components are the microscopic forms of the conservation laws for continuity of mass, momentum, energy, and species along with appropriate constitutive equations, initial conditions, boundary conditions, and other supporting physico-chemical, thermodynamic and transport property parameters. Currently, several commercially available numerical codes are available that can be used to solve these model equations, which greatly reduces the effort in creating a specific model code. Some examples of these codes include FLUENT (www.fluent.com), CFD-ACE+ (www.cfdrc.com), CoventorWare (www.coventor.com) and COMSOL Multiphysics (www.comsol.com). COMSOL Multiphysics was selected in this work as the numerical modeling platform due to its ease of use, classes of generalized ODE and PDE equations that can be solved, incorporation of robust numerical solvers, and attractive graphical interface. The ability of COMSOL to interface with other powerful CAD software packages makes it straightforward to import CAD models into the COMSOL modeling interface. This is a very useful feature for modeling since many microprocess system components consist of complex geometries that are not easily described by a conventional orthogonal coordinate system. Single or multiple reactions can also be included using the Reaction Engineering Lab, which is an add-on toolbox for COMSOL Multiphysics that allows the user to create reaction kinetic models using either the law of mass action or user-defined non-elementary reaction kinetic equations. COMSOL Multiphysics also has other add-on toolboxes, such as COMSOL Script, that can also be used to create user-interfaces. It also has bi-directional interfaces with both MATLAB and SIMULINK (www.mathworks.com). These software tools can be used to introduce realistic process simulation interfaces in a microprocess system component, or in coupled system of microprocess components that execute a particular process sequence. Additional details on COMSOL Multiphysics are available in electronic form from both their software package as well as user conferences that have been held on an annual basis since 2004 (www.comsol.com). One advantage of this approach in this particular application is that undergraduate students can focus on examining the effect of various microprocess component and system parameters for fairly complex systems without spending significant time in creating numerical algorithms and computer codes. The end result is that new insights are gained on the behavior of more realistic systems that otherwise are not possible using simpler models that are contained in most undergraduate textbooks were microchemical process systems are introduced. A few introductory lectures on the finite element method provide undergraduate students with sufficient background that they can grasp the concepts required to produce reliable solutions.

Example Applications

Several examples are now given where COMSOL Multiphysics is used to simulate the performance of selected microprocess component devices. These include a MEMS heat exchanger and a T-micro mixer used for blending two fluids. They are provided to illustrate the types of models that can be analyzed and typical results that can be generated from the model solutions. Additional examples and details are provided in the MS theses of Mokal and Adapa.15,16
1. MEMS Heat Exchanger

The first example consists of a MEMS-type of heat exchanger where hot and cold water are used as the heat transfer fluids. To characterize the effectiveness of the heat exchanger, several variations in the fluid contacting configuration and system geometry are analyzed. Simulations are performed for various process configurations so that the heat exchanger effectiveness factor can be evaluated for ranking purposes. This represents a fairly complex model that could not be readily analyzed in a typical undergraduate chemical engineering course on heat transfer. Here, it is been defined as a relatively complex system of fundamental transport equations whose solution is readily generated for various assumed parameters using COMSOL Multiphysics.

a. System geometry. A diagram of the system geometry is shown in Figure 12. Two rectangular slabs, each containing five microchannels and constructed of Type 316 stainless steel, are stacked over each other so the channels form right angles to create a cross-flow type of contacting configuration. The dimensions of the slabs and microchannels are provided in the figure caption. The geometrical shape, material, and dimensions of the slabs and microchannels that are machined within the slabs can be readily varied as part of an exercise to identify the effect of these parameters on heat exchanger effectiveness for a particular application.

Figure 12. 3-D model for the MEMS heat exchanger consisting of two laminated layers. Slab dimensions: Length (L) = 800 μm, width (W) = 800 μm, Height (H) = 60 μm; Individual microchannel dimensions: Length (L) = 800 μm, width (w) = 100 μm, Height (h) = 30 μm

b. Model equations. The incompressible Navier-Stokes equations are used to describe momentum transport for the heat transfer fluids flowing through the heat exchanger microchannels. The range of Reynolds numbers suggests that the flow regime is well within the laminar-flow region (Re <2100). The primitive forms of the equations that are solved for the x, y and z components of the fluid velocity vector \( \mathbf{u} = [u_x \ u_y \ u_z] \) in the microchannels are summarized below where \( \rho \) is the fluid density, \( \eta \) is the fluid viscosity, and \( p \) is the fluid pressure.

\[
\begin{align*}
\text{x-momentum} & \\
\rho \left[ \frac{\partial u_x}{\partial t} \right] & - \eta \left[ \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right] + \frac{\partial p}{\partial x} = 0 \\
\text{y-momentum} & \\
\rho \left[ \frac{\partial u_y}{\partial t} \right] & - \eta \left[ \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right] + \rho \left[ u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right] + \frac{\partial p}{\partial y} = 0
\end{align*}
\]
The temperature profiles in both the fluid and the solid walls are obtained by solving the energy balance equation, which is defined below by the generalized form of the conduction-convection equation in 3-D.

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

The various components of the velocity vector that appear in eq. (4) are obtained from the solution of the Navier-Stokes equations defined earlier by eqs. (1) – (3). When solving the energy balance within the solid wall sub-domains, conduction is the primary mode of thermal energy transport so eq (4) reduces to the conduction equation by setting \( u_x = u_y = u_z = 0 \). The conductivities of fluid and solid materials can be considered to be either isotropic, \( i.e. k_x = k_y = k_z = k \) or non-isotropic. For the case considered here, isotropic behavior is assumed. The numerical method in COMSOL can solve the system defined by eqs. (1) – (6) by either a sequential or simultaneous type of algorithm. The sequential approach was found to provide converged solutions in this case. The total amount of CPU time on a Dell Precision M20 desktop is less than 60 seconds.

**c. Boundary conditions.** The boundary conditions for the Navier-Stokes equations are specified velocities at the cold and hot fluid inlets, specified fluid pressure at the outlets, and zero velocity gradient (no slip) at all solid walls. The boundary conditions for the energy balance equation include specified temperatures for the hot and cold fluid inlets, no conductive flux at the hot and cold fluid outlets, continuity of temperature and flux at all solid-solid interfaces, and zero heat flux at all other external boundaries owing to assumed perfect insulation at these surfaces. Here, the steady-state solution is obtained so the transient terms in all of the above equations are set to zero. Transient solutions can be readily generated, which allows real-time visualization of the phenomena and insight into the problem physics.

**d. Performance parameters.** The effectiveness factor of a heat exchanger is generally defined as the ratio of the actual rate of heat transfer to the maximum possible rate of heat transfer. The maximum heat rate is that which would occur in a counter-current flow heat exchanger having infinite heat-transfer area. In this ideal heat exchanger, one of the inlet fluid streams will either gain or lose heat (energy) until its outlet temperature is equivalent to the inlet temperature of the other inlet stream. The fluid that experiences this maximum temperature change is the one having the smaller value of the specific thermal energy parameter \( C = mC_P \) where \( m \) is the mass flow rate and \( C_P \) is the heat capacity of the fluid. If the hot fluid has a lower value of \( C \), then the maximum total rate of heat flow \( q_{max} \) in terms of the hot fluid whose outlet temperature will be equal to the inlet temperature of cold fluid \( (T_{hot, out} = T_{cold, in}) \) can be expressed as

\[
q_{max} = mC_p (T_{hot, in} - T_{cold, in})
\]

The heat exchanger effectiveness factor \( \varepsilon \) is then given as the following ratio of the actual rate of heat flow to the maximum possible rate of heat flow:

\[
\varepsilon = \frac{q_{actual}}{q_{max}}
\]
The outlet temperatures that appear in eqs. (5) and (6) are typically based upon cross-sectional averaged values. Average outlet temperatures for both the hot and cold outlets can be readily calculated using the boundary integration feature of COMSOL Multiphysics.

\[ T = \frac{\int T \, dA}{\int dA} \]  
\[ \varepsilon = \frac{q}{q_{\text{max}}} = \frac{m \cdot c_p \left( T_{\text{hot-in}} - T_{\text{hot-out}} \right)}{m \cdot c_p \left( T_{\text{hot-in}} - T_{\text{cold-in}} \right)} \]  

\[ (6) \]

**e. Results and discussion.** The performance of the 3-D MEMS heat exchanger was evaluated using COMSOL Multiphysics to illustrate the effect of stream direction on heat exchanger performance. The same 3-D MEMS heat exchanger configuration that was defined above in Figure 12 with a microchannel height of 30 µm was used as the basis for the simulation. Generally, the flow direction of the streaming fluids can be defined as being either cocurrent, countercurrent, or cross-current.

Figure 13a shows the steady-state temperature distributions that are obtained from COMSOL Multiphysics when a countercurrent flow direction is used for the stream contacting pattern. The temperature distributions generated when the streams are contacted using a cocurrent flow pattern are compared in Figure 13b. As expected, the countercurrent system has a temperature distribution leading to higher outlet temperatures.

The effectiveness of each flow orientation was then calculated using the formula for the effectiveness factor as defined above by eq. (6). The results are compared in Table 2. It can be seen that the counter-current flow provides the best effectiveness factor, which is followed by the cross-current and then finally the co-current orientation. The use of the effectiveness factor approach allows the student or designer to readily assess the effect of changing various heat exchanger design parameters.

![Figure 13a. Temperature distribution for counter-current flow in a 3-D MEMS heat-exchanger.](image1)

![Figure 13b. Temperature distribution for cocurrent flow in a 3-D MEMS heat-exchanger.](image2)

Figure 13. Comparison of temperature distributions in a microprocess heat exchanger with counter-current (Figure 13a) and cocurrent (Figure 13b) flow.
Table 2. Effectiveness ($\varepsilon$) of 3-D MEMS heat-exchangers based on fluid contacting patterns.
Parameters: Cold and hot fluid inlet velocities: $u_x = 0.005$ m/s, $u_y = u_z = 0$; Outlet pressures $p_{out} = 0$ Pa; Inlet temperatures: $T_{cold-in} = 300$ K; $T_{hot-in} = 330$ K

<table>
<thead>
<tr>
<th>Flow Type</th>
<th>Height, h</th>
<th>$T_{hot_out}$</th>
<th>$T_{cold_out}$</th>
<th>Effectiveness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cross-flow</td>
<td>30 $\mu$m</td>
<td>212.17</td>
<td>317</td>
<td>0.5943</td>
</tr>
<tr>
<td>Counter current</td>
<td>30 $\mu$m</td>
<td>304.62</td>
<td>325.19</td>
<td>0.8460</td>
</tr>
<tr>
<td>Cocurrent</td>
<td>30 $\mu$m</td>
<td>318.19</td>
<td>318.18</td>
<td>0.3937</td>
</tr>
</tbody>
</table>

2. Tee-Micro mixer
The second example considers mixing of two fluid streams having the same density and viscosity. The degree of mixing is largely controlled by solute diffusion. Two transport equations are used to describe the fluid mixing. The Navier-Stokes equations are first used to determine the velocity profiles for a pressure-driven flow. Once the velocity profiles are determined, they are substituted into the convection-diffusion equation to determine the local species concentration profiles. A 3-D spatial coordinate system is used. The control volume for the 3-D model is created in COMSOL Multiphysics by first drawing a 2-D model in the x-y plane and then extruding this geometry into the z-plane. The geometry and process conditions of the T-mixer are within the specifications where the continuum regime applies.

a. System geometry. A diagram of the system geometry is shown in Figure 14. It consists of two inlet ducts that converge to form a single duct. The dimensions are provided in the figure caption.

![Figure 14. Geometry for the T-micro mixer. Model dimensions: Length = 12 mm; Width of inlet = 0.5 mm; Width of outlet = 1 mm; Height of the channel = 0.5 mm](image-url)
b. Model equations. The fluids to be mixed are assumed to be incompressible with constant density and viscosity and follow Newtonian fluid behavior. For simplicity, it is also assumed that the process of diffusion does not significantly affect the density and viscosity of the fluid. The incompressible Navier-Stokes equations are used to describe momentum transport for all fluids flowing through the ducts of the T-micro mixer. The range of Reynolds numbers suggests that the flow regime is well within the laminar-flow region (Re < 2100). The primitive forms of the equations that are solved for the x, y and z components of the fluid velocity vector  in the ducts are summarized below where  is the fluid density,  is the fluid viscosity, and  is the fluid pressure.

**x-momentum**

\[
\rho \left( \frac{\partial u_x}{\partial t} \right) - \eta \left( \frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) + \rho \left[ u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} \right] + \frac{\partial p}{\partial x} = 0 \tag{8}
\]

**y-momentum**

\[
\rho \left( \frac{\partial u_y}{\partial t} \right) - \eta \left( \frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right) + \rho \left[ u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} \right] + \frac{\partial p}{\partial y} = 0 \tag{9}
\]

**z-momentum**

\[
\rho \left( \frac{\partial u_z}{\partial t} \right) - \eta \left( \frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right) + \rho \left[ u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} \right] + \frac{\partial p}{\partial z} = 0 \tag{10}
\]

The convection-diffusion equation represents a microscopic form of the species mass balance and is defined by eq. (11).

\[
D \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right) - \left( u_x \frac{\partial c}{\partial x} + u_y \frac{\partial c}{\partial y} + u_z \frac{\partial c}{\partial z} \right) = \frac{\partial c}{\partial t} \tag{11}
\]

The various components of the velocity vector that appear in eq. (11) are obtained from the solution of the Navier-Stokes equations defined by eqs. (8)–(10). The diffusivity of the solute was be considered to be isotropic, i.e., \( D_x = D_y = D_z = D \) with a constant value of \( 1 \times 10^{-11} \text{ m}^2/\text{s} \). The numerical method in COMSOL can solve the system defined by eqs. (8)–(11) by either a sequential or simultaneous type of algorithm. The sequential approach was found to provide converged solutions in this work within less than 60 seconds on a Dell Precision M20 laptop.

c. Boundary conditions. The boundary conditions for the Navier-Stokes equations are specified velocities at the duct inlets and specified fluid pressure at the outlet and zero velocity gradients (no slip) at the solid walls. The boundary conditions for the convection-diffusion equation include specified solute concentration for the fluid inlets, no diffusive flux at the fluid outlet, and zero flux at the walls since the solute does not react and the wall is impermeable. Here, the steady-state solution is obtained so the transient terms in all of the above equations are set to zero. The specific mathematical representations of these boundary conditions are defined below for both the Navier-Stokes and convection-diffusion equation.
For the Navier-Stokes equations,

At the inlet of both fluid ducts: \( p_{in} = 2 \text{ Pa} \) \hspace{1cm} (12a)

At the outlet of both fluid ducts: \( p_{out} = 0 \text{ Pa} \) \hspace{1cm} (12b)

At the walls, the no slip condition applies so that

\[
\eta \cdot \mathbf{u} = n \cdot \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix} = 0
\]

(13)

For the convection-diffusion equation,

At the first fluid inlet tee \( i.e., \) pure solvent is assumed so that \( c = 0 \text{ mol/m}^3 \) \hspace{1cm} (14)

At the second inlet tee, \( i.e., \) species B enters so that \( c = 1 \text{ mol/m}^3 \) \hspace{1cm} (15)

At the fluid outlet, pure convective flow is assumed so that

\[
N_D = -D \left( \frac{\partial c}{\partial x} + \frac{\partial c}{\partial y} + \frac{\partial c}{\partial z} \right) = 0
\]

(16)

At the walls, the species does not react or permeate through it so the net diffusive and convective flux is zero.

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

(17)

d. Results and discussion. Figure 15 shows the velocity profiles obtained for a steady-state pressure-driven flow, while Figure 16 shows the corresponding concentration profiles for the diffusing species. The concentration profile is solved sequentially after solving the velocity profile to obtain faster convergence. It is possible to solve the two equations simultaneously if good initial guesses are possible; otherwise it is better to solve the two equations sequentially and then use the sequential solution as the initial values for simultaneous solution of the coupled problems.

The effect of different solute diffusivities can also be easily studied. The concentration profiles for different diffusivities can be solved by using parametric linear or non-linear solver settings and choosing the solute diffusivity (D) as the varying parameter and evaluating the concentration profiles for the varying diffusivities. Several simulations were performed to study the effects of changes in the operating and design parameters on flow dynamics and quality of mixing. These results are provided in the next sub-section, which are also included in Example 6 of the examples web page (see Figure 5).
Figure 15. Velocity profile obtained for the T-micro mixer with an assumption of a steady state pressure driven flow.

Figure 16. Concentration profiles obtained for T-micro mixer for the pressure driven flow.

e. Performance parameters. Several key parameters can be derived from the computed velocity and concentration profiles that provide students with knowledge on how the effectiveness of various devices for fluid mixing can be quantified. These include the mixing effectiveness factor and the measure of mixing. The basis for both of these parameters is outlined below.
1. Mixing effectiveness factor, $\tau$

The time it takes for the solute to travel the length of the channel by pure convection in the absence of any other transport effects, such as axial or radial dispersion, is called the mean residence time, $\tau_v$.\(^{17}\)

$$\tau_v = \frac{L}{v}$$  \hspace{1cm} (18)

where $v$ is the fluid velocity and $L$ is the channel length.

The time it takes for the solute to diffuse across the characteristic channel width due to pure diffusion in the absence of convection is called the characteristic time for solute diffusion, $\tau_D$.\(^{17}\)

$$\tau_D = \frac{h^2}{D}$$  \hspace{1cm} (19)

where $h$ is the characteristic width of the channel and $D$ is the diffusivity of the solute in the fluid. The ratio of the above two parameters can be used to make predictions for the mixing effectiveness factor of the system, $\tau$.\(^{17}\)

$$\tau = \frac{\tau_v}{\tau_D} = \frac{DL}{vh^2}$$  \hspace{1cm} (20)

A low value for $\tau$ implies that the characteristic time for diffusion is large compared to the characteristic time for convection and vice-versa. To design effective mixing devices, a large value of $\tau$ is desired since

2. Measure of mixing ($\psi$)

To compare the mixing quality for different values of $\tau$, it is necessary to have some measure of mixing. For systems described in 2-D models, the variance of the concentration distribution is used as a measure of mixing.\(^{17}\) It is defined as

$$\psi = 1 - \int_0^h \left( \frac{c(y) - c_0}{2Li*c_0} \right) dy = 1 - \Sigma$$  \hspace{1cm} (21)

where $Li$ is the length-scale of the inlet of the mixing channel, and $c_0$ is the initial concentration for the mixing channel.

The parameter $\Sigma$ is defined by the following ratio

$$\Sigma = \int_0^h \left( \frac{c(y) - c_0}{2Li*c_0} \right) dy.$$  \hspace{1cm} (22)
The time constant $\tau$ in eq. (20) is found to be a good measure of the effectiveness of mixing imparted within a particular channel. Here, it was evaluated by varying the fluid velocity from $10^{-3}$ m/s to $10^{-2}$ m/s in steps of $10^{-3}$ m/s and then calculating both the mixing effectiveness factor and measure of mixing at the channel outlet. The diffusivity was kept constant at $1 \times 10^{-7}$ m$^2$/s and only the inlet velocity is varied. The data shown below in Table 3 were generated in this fashion.

Figure 17 is a plot of the integral term of the measure of mixing ($\Sigma$) as defined by eq. (22) versus the mixing effectiveness ($\tau$) as defined by eq. (20). Figure 18 compares the measure of mixing quantity ($\psi$) versus the mixing effectiveness ($\tau$). The results show that an increase in the fluid velocity decreases the mixing effectiveness factor since the contribution of convection increases relative to solute diffusion. As a result, the solute doesn’t have sufficient time to diffuse across the channel width and create a more uniform concentration.

Table 3  Effect of velocity on mixing parameters. The following data were generated from COMSOL Multiphysics and used to construct the plots of the integral term $\Sigma$ versus mixing effectiveness $\tau$ (Figure 17) and the measure of mixing $\psi$ versus mixing effectiveness $\tau$ (Figure 18).

<table>
<thead>
<tr>
<th>Inlet velocity ($v_{in}$) (m/s)</th>
<th>Integral term ($\Sigma$) (Evaluated using COMSOL)</th>
<th>Measure of mixing ($\psi$) $= 1 - \Sigma$</th>
<th>Mixing Effectiveness ($\tau$) $= \frac{\tau_v}{\tau_D}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>1.60E-04</td>
<td>0.9998</td>
<td>0.050000</td>
</tr>
<tr>
<td>0.002</td>
<td>0.004159</td>
<td>0.9958</td>
<td>0.025000</td>
</tr>
<tr>
<td>0.003</td>
<td>0.013025</td>
<td>0.9870</td>
<td>0.016667</td>
</tr>
<tr>
<td>0.004</td>
<td>0.02318</td>
<td>0.9768</td>
<td>0.01250</td>
</tr>
<tr>
<td>0.005</td>
<td>0.032755</td>
<td>0.9672</td>
<td>0.010000</td>
</tr>
<tr>
<td>0.006</td>
<td>0.041184</td>
<td>0.9588</td>
<td>0.008333</td>
</tr>
<tr>
<td>0.007</td>
<td>0.048408</td>
<td>0.9516</td>
<td>0.007143</td>
</tr>
<tr>
<td>0.008</td>
<td>0.054538</td>
<td>0.9455</td>
<td>0.006250</td>
</tr>
<tr>
<td>0.01</td>
<td>0.064146</td>
<td>0.9359</td>
<td>0.005000</td>
</tr>
</tbody>
</table>

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Figure 17. Plot of the integral term $\Sigma$ in the measure of mixing versus $\tau$.

Figure 18. Plot of the measure of mixing versus $\tau$. 
Summary and Conclusions

Development of the microchemical interlinked curriculum component has encountered a number of challenges during the implementation stages. To create realistic examples and exercises, it is necessary to employ models that describe transport phenomena using geometries that in 2 or 3 spatial dimensions. This requires the use of advanced numerical methods for generating solutions that are reliable over realistic ranges of parameters and spatial coordinates where students can explore phenomena without having advanced knowledge on the underlying computer codes. Otherwise, one is limited to relatively simple systems that provide a reduced level of intellectual stimulation and development of physical insight. The availability of COMSOL Multiphysics provides a reliable numerical engine and flexible user interface that can be used to describe a broad range of continuum phenomena. However, one challenge with using this package in an educational environment is that it must be resident on the computer system that is being used for running the ICC. Hence, whereas some computer software suppliers allow a single user license to be installed on a student’s laptop, COMSOL Multiphysics can only be installed on the instructor’s laptop and on the university server used for supporting multi-student usage. Consequently, students must be physically present in the computer lab that connects to the local server in order to utilize the ICC. This represents a detractor to using the code, since unlimited access on a user’s laptop would allow students to run the ICC at their convenience in any location. This could be overcome by allowing students to access the code through remote access, which is feasible and has been explored by one of the authors (PLM) through a virtual private network (VPN).

Experience is using the microchemical ICC by students is limited as of this writing since most emphasis has been on development of the required user interface and creation of realistic examples, exercises, and problems. However, data will be collected in the Spring 2009 semester on student experience in using the ICC so this will provide valuable feedback for future improvements. The experience so far with a small subset of graduate students having no previous knowledge of microchemical systems has been very positive and enthusiastic. It is also evident that the developer of COMSOL Multiphysics must be engaged in the near future to provide an exchange of particular features that would facilitate future ICC development and integration.

In terms of creating graphical user interfaces (GUI’s) using COMSOL Script, the process has been very tedious owing to lack of examples to use as building blocks. However, momentum is being developed on this aspect since our group at TAMUK has recently focused on learning this language and has successfully created several GUI’s for several complex problems. For those cases that have been developed, it has proven to be very revealing since the user has to simply select parameters from drop-down menus and then the geometry is modified and solutions are instantly generated in graphical form. We expect to gain more experience with this feature in the near future and also connect it to data modeling problems where parameter estimation in nonlinear models is desired.

A final challenge will be broad implementation of the ICCs in the chemical engineering undergraduate curriculum and their continuous improvement. A plan to do this is in the early stages of implementation at TAMU-CS and those at partner institutions, such as TAMUK and Prairie View A&M, are expected to follow suit.

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References


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Appendix A. Screenshots Showing Details of Example 3 from the Microchemical ICC

**Example 3**: Model for Convection and Diffusion with Narrow Channels

- **Step 1**: Define Application mode.
- **Step 2**: Draw Geometry of the model.
- **Step 3**: Define Subdomain settings.
- **Step 4**: Define Boundary settings.
- **Step 5**: Initialize and Refine mesh for the model.
- **Step 6**: Solve the model.
- **Step 7**: Result is shown in chosen plot parameter.

Figure A-1. Example 3 Web page of the ICC Module

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*Copyright © 2009, American Society for Engineering Education*
Step 1: Define Application Mode

Application Mode is selected to describe type of physics. It provides modeling interfaces where you can create models using material properties, boundary conditions, and initial conditions. Each of the application modes comes with a template that automatically supplies the appropriate underlying PDE. In this example, Convection and Diffusion mass balance application mode with an Incompressible Navier-Stokes application mode are used. The interaction is a one-way coupling using the velocity described by the Navier-Stokes equations as part of the convective mass transfer. Refer example 01 for details about Incompressible Navier-Stokes application mode.

The Convection and Diffusion application mode solves for Concentration as dependent Variable.
**Step 2 : Define Geometry**

In this example, Hybrid modeling is used. A rectangle of height 100 μm, and width of 500 μm is created. A point is specified at coordinate (0, 0, 5). Ellipse with A-semi axes of 100 μm and B-semi axes of 30 μm is created at coordinate (2e-4, 0). Second Ellipse with A-semi axes of 100 μm and B-semi axes of 30 μm is created at coordinate (2e-4, 1e-4). All geometries are selected and boolean operation difference is performed to create a composite object.

![Diagram showing the geometry defined in Step 2](image)

Figure A-3. Example 3, Step 2 Web page of the ICC Module
Step 3: Define Subdomain Settings

In this example, one group of subdomain sections is applied for the model. First, incompressible Navier-Stokes application mode is used. Physics for the model is defined by the following equations:

\[ \rho (u \cdot \nabla) u = - \nabla p + \eta \nabla \cdot \nabla u + \nabla (u \cdot (u \cdot \nabla u)) + \text{F} \]

\[ \nabla \cdot u = 0 \]

- \( \rho \) is the dynamic viscosity.
- \( p \) is the density.
- \( u \) is the velocity field
- \( \eta \) is the pressure
- \( \text{F} \) is a volume force field such as gravity
- \( \nabla \cdot \) is the diffusion coefficient.
- \( R \) is the Reaction rate.
- \( u \) is the velocity.

The values of both \( \rho \) and \( \eta \) are constants (using SI units),

\[ \rho = 1 \times 10^3 \text{ kg/m}^3 \]

\[ \eta = 1 \times 10^{-2} \text{ Pa.s} \]

After solving incompressible Navier-Stokes application mode then Convection and Diffusion application mode is used. Physics for the model is defined by the following equations:

\[ \nabla \cdot (-D \nabla c) = R \cdot u \cdot V \]

\( c \) is concentration.

D isotropic is the Diffusion coefficient.

- \( R \) is the Reaction rate.
- \( u \) is the velocity.

The values of both D, Isotropic, R, and c are constants (using SI units),

- \( D \) is isotropic = 1 \times 10^{-7} \text{ m}^2/\text{s} \)
- \( R = 0 \text{ mol/(m}^3\cdot \text{s}) \)

The initial condition is defined by the equations,

\[ \nabla \cdot (-D \nabla c) = R \cdot u \cdot c \]

\( c \) = concentration

\( c(0) = 1 \text{ mol/m}^3 \)
Step 4: Define Boundary Settings

There are eleven boundaries for the geometrical section. For each boundary selected, condition is defined. Since, two application modes are used boundary settings are defined for both the modes. when Incompressible Navier-Stokes mode is used:

For Boundary 1: The boundary type is Inlet.

Inflow/Outflow velocity condition is defined using equation,

\[ u = u_0 \]

\( u_0 \) is defined as constant,

\( u_0 = 0.3 \text{ m/s} \)

For Boundary 2: The boundary type is Wall.

No Slip condition is defined using equation,

\[ u = 0 \]
This condition is normally used for walls.

For Boundary 3: The boundary type is **Inlet**.

**Inflow/Outflow velocity** condition is defined using equation,

\[ u = u_0 \]

\[ u_0 \] is defined as constant,

\[ u_0 = 0.3 \text{ m/s} \]

For Boundary 4: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

For Boundary 5: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

For Boundary 6: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

For Boundary 7: The boundary type is **Outlet**.

**Normal flow/Pressure** condition is defined using equation,

\[ t \cdot u = 0, \quad n \cdot [-p + \eta \left( \nabla u + \left( \nabla u \right)^T \right) n] = -p_0 \]

\[ p_0 \] is the pressure,

\[ p_0 \] is defined as constant (SI unit is pa),

\[ p_0 = 0 \]

This condition is used for outlet.

For Boundary 8: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

For Boundary 9: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

For Boundary 10: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

For Boundary 11: The boundary type is **Wall**.

**No Slip** condition is defined using equation,

\[ u = 0 \]

When Convection and Diffusion application mode is used:

For Boundary 1: **Concentration** condition is defined using equation,

\[ c = c_0 \]

\[ c_0 \] is defined as constant,

\[ c_0 = 2 \text{ mol/m}^3 \]
For Boundary 2: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 3: **Concentration** condition is defined using equation,
\[
c = c_0
\]
\[
c_0 \text{ is defined as constant},
\]
\[
c_0 = 0 \text{ mol/m}^3
\]

For Boundary 4: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 5: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 6: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 7: **Convective flux** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c
\]

For Boundary 8: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 9: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 10: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]

For Boundary 11: **Insulation/Symmetry** condition is defined using equation,
\[
\mathbf{n} \cdot \mathbf{N} = 0
\]
\[
N = -\nabla c + cu
\]
Step 5: Initialize and Refine Mesh

After defining subdomain and boundary settings for given geometry, finite elements mesh is initialized. FEM (Finite Element Method) is used for finding approximate solutions for PDEs. Initialized mesh for this geometry consists of 499 elements.

After refining, mesh consists of 1995 elements.
**Step 6 : Simulation of Model**

After refining mesh, the model is solved for given input values for steady state flow. This model has two coupled application modes. Incompressible Navier-Stokes application mode is solved first since, the velocity described by the Navier-Stokes equations is used as part of the convective mass transfer. Then Convection and Diffusion application mode is solved. Stationary solver is used to solve this model. In Postprocessing mode, the simulated model is as shown below.

![Simulation of Model](image)

Figure A-7. Example 3, Step 6 Web page of the ICC Module
Step 7: Results Using Typical Plot

After Postprocessing, the result is displayed as a surface plot for the concentration field. Different Plot parameters could be used to display the simulated result. For this model, the interpolated coloring, filled fill style, and jet colormap for surface color is used.

The result is as shown below:

![Surface Concentration Plot](image)

Figure A-8. Example 3, Step 7 Web page of the ICC Module
Figure A-9. Exercises Main Web page of the ICC Module
Geometry of Model

COMSOL Multiphysics provides various possibilities to create geometry modeling in 1D, 2D, and 3D space dimensions such as solid modeling, boolean operators, and CAD tools.

1D geometry modeling.

2D geometry modeling.

3D geometry modeling.

---

Figure A-10. Exercise 1 Webpage of the ICC Module

---

Fluid Mechanics

In 1D geometry modeling **point** and **Line** are created.

The following video provide information about creating a point.
The following video provides information about creating a line.

Figure A-11. 1-D geometry Webpage of the ICC Module.

Figure A-12. Custom User Interface for the ICC Module.