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Development of an Interlinked Curriculum Component Module for Microchemical Process Systems Components Using COMSOL Multiphysics

Abhijeet D. Mokal and Patrick L. Mills*
Department of Chemical and Natural Gas Engineering, Texas A&M University-Kingsville
*Corresponding author: 700 University Blvd, MSC 188, Kingsville, TX 78363, Patrick.Mills@tamuk.edu

Introduction

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 both emerging technologies and non-traditional applications. The ICCs 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 better appreciation and a more fundamental understanding of the common threads and methods that represent the underpinning of their chemical engineering education. In addition to these benefits, the ICCs are also envisioned as an integrating tool that will help students better recognize the collection of courses in their program as a unified curriculum. Besides enhancing student education, another benefit of the ICCs is that they will allow chemical engineering faculty to improve the quality of their lectures and to work towards better unification of topic coverage for a particular core course. The latter is especially important for any department where the same course may be taught by more than one faculty member.

This paper will discuss and analyze the development of an ICC that is focused on microprocess technology. 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, toxic reagents, explosives, or other chemicals where point-of-use is preferred over a large-scale centralized manufacturing plant. ICC modules are designed according to a standardized protocol that includes 4 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 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 (4) 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 be included in the module design for additional reinforcement and as a source of open-ended problems that drive creativity and motivation.

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 micromixers, 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.

Use of COMSOL Multiphysics

COMSOL Multiphysics was used to simulate the performance of the various microprocess devices mentioned above. The example given here for illustration purposes consists of a MEMS-type of heat exchanger where hot and cold water are as the heat transfer fluids. To characterize the effectiveness of the heat exchanger, several variations in the fluid contacting configuration and system geometry were analyzed. Simulations were performed for various process configurations so that the heat exchanger effectiveness factor could be evaluated for ranking purposes.

a. System geometry. A diagram of the system geometry is shown in Figure 1. Two rectangular slabs, each containing five microchannels and constructed of Type 316 SS, are stacked over each other so the channels form right angles to create a cross-flow type of 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 machined within the slabs can be readily varied as part of an effort to identify the effect of these parameters on heat exchanger effectiveness for a particular application.

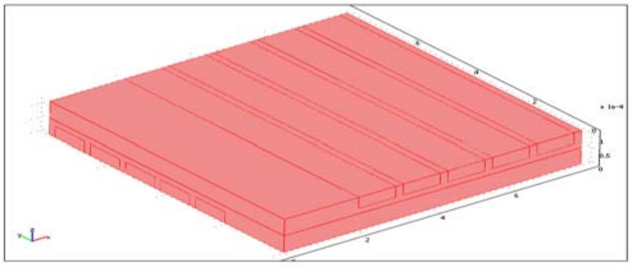

Figure 1. 3-D model for the MEMS heat exchanger consisting of two laminated layers. Slab dimensions: Length (L) = 800 μm, width (W) = 800 μm, Height (H) = 60 μm; Individual microchannel dimensions: Length (L) = 800 μm, width (w) = 100 μm, Height (h) = 30 μm

b. Model equations. Momentum transport for the heat transfer fluids flowing through the microchannels is accurately described by the incompressible Navier-Stokes equations. The range of Reynolds numbers indicates that the flow regime is well within the laminar-flow region. The primitive forms of the equations that are solved for the x, y and z components of the fluid velocity vector **u** = [u_x u_y u_z) in the microchannels are given below.

x-momentum

$$\rho\left[\frac{\partial u_x}{\partial t}\right]-\eta\left[\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2}+\frac{\partial^2 u_x}{\partial z^2}\right]+\rho\left[u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y}+u_z\frac{\partial u_x}{\partial z}\right]+\frac{\partial p}{\partial x}=0 \qquad (1)$$

y-momentum

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

z-momentum

$$\rho\left[\frac{\partial u_z}{\partial t}\right]-\eta\left[\frac{\partial^2 u_z}{\partial x^2}+\frac{\partial^2 u_z}{\partial y^2}+\frac{\partial^2 u_z}{\partial z^2}\right]+\rho\left[u_x\frac{\partial u_z}{\partial x}+u_y\frac{\partial u_z}{\partial y}+u_z\frac{\partial u_z}{\partial y}\right]+\frac{\partial p}{\partial z}=0 \qquad (3)$$

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 conduction-convection equation in 3-D.

$$\left(k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2}\right) - \rho C_p \left(u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z}\right) + Q = \rho C_p \frac{\partial T}{\partial t} \qquad (4)$$

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 where $u_x = u_y = u_z = 0$. 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. 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 used in this work.

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 outlet, and zero velocity gradient (no slip) at the 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.

d. Calculated quantities. 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 such a heat exchanger, one of the fluid streams will either gain or lose heat until its outlet temperature is equivalent to the inlet temperature of the other 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

$$q_{max} = mC_p (T_{hot-in} - T_{cold-in}) \ldots\ldots(5)$$

The heat exchanger effectiveness factor ε is then given as the following ratio of actual to maximum heat flow parameters:

$$\varepsilon = \frac{q}{q_{max}} = \frac{mC_p (T_{hot-in} - T_{hot-out})}{mC_p (T_{hot-in} - T_{cold-in})} \ldots\ldots(6)$$

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.

$$T = \frac{\int T dA}{\int dA} \ldots\ldots(7)$$

The above model is just one example of several that will be described in the proposed presentation. A fairly complex model that could not be readily analyzed in a typical undergraduate chemical engineering course on heat transfer has been reduced to a set of equations whose solution is readily generated for various assumed parameters using COMSOL Multiphysics.

Preliminary Results

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 1 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 2 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 3. As expected, the countercurrent system has a temperature distribution leads to higher outlet temperatures.

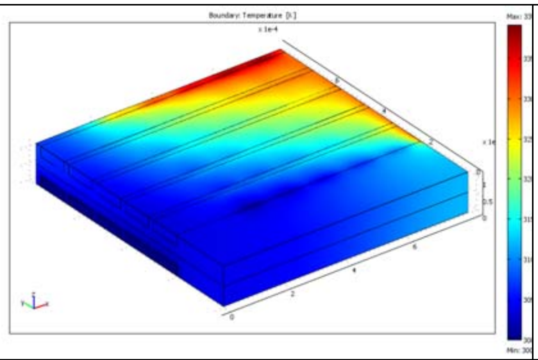	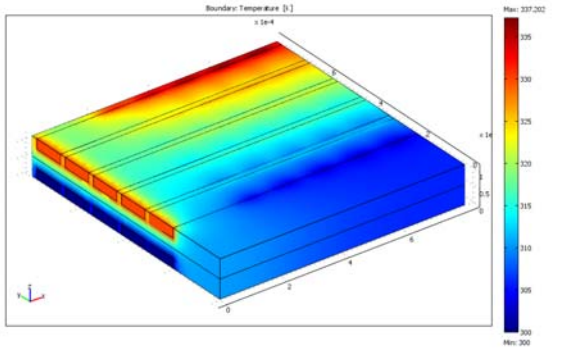
Figure 2. Temperature distribution for counter-current flow in a 3-D MEMS heat-exchanger.	Figure 2. Temperature distribution for cocurrent flow in a 3-D MEMS heat-exchanger.

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 1. 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.

Table 1. Effectiveness (ε) 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: $T_{cold\text{-}in} = 300$ K; $T_{hot\text{-}in} = 330$ K

Flow Type	**Height (h)**	**T_{hot_out}**	**T_{cold_out}**	**Effectiveness**
	μm	K	K	ε
Cross-flow	30	212.17	317	0.5943
Counter-flow	30	304.62	325.19	0.8460
Co-current	30	318.19	318.18	0.3937

Conclusions

COMSOL Multiphysics provides a powerful numerical platform where various models for microchemical process technology components can be readily created for both education and research. This modeling tool allows chemical engineering students to focus on understanding the effects of various microchemical system component design and operational parameters versus coding and debugging of the numerical methods. Models of various microprocess system components allows students to study the effect of various system design and operation parameters in a conversational type of mode from which much greater insight can be obtained on the system physics versus other approaches. The development of a user interface that works between the COMSOL engine and the student will also be described. This interface minimizes the amount of time spent on setting up the problem while also keeping the problem specifications within reasonable bounds so that feasible solutions are obtained.