Understanding Transport Phenomena Concepts in Chemical Engineering with COMSOL Multiphysics®

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ABSTRACT

Transport Phenomena in Chemical Engineering involves three key aspects: Momentum, Heat and Mass Transport. These areas are described by differential equations which are solved for a particular problem using independent or a set of combined equations (e.g., water flowing in a heated pipe). At an undergraduate level class, the advanced mathematics of partial differential equations, tensors and the specific applications of conservations laws for a differential element are challenging concepts to understand. Nonetheless, Transport phenomena represent the basis of Chemical Engineering fundamentals. For example, fluid velocity distribution, temperature distribution, and fluxes (momentum flux, heat flux, and Mass/Molar Fluxes) are core concepts in Chemical Engineering.

Although analytical solutions exist for very simplified problems that are solved in class using mathematics, the students are usually eager to understand the effect of velocity change in more than one dimension and/or with respect to time. In this work, a unique approach is presented to develop an applied Transport Phenomena course that involves simulations using COMSOL Multiphysics®. The specific models from the applications library used for enhancing students learning are (a) shell and tube heat exchanger and (b) flow past a cylinder. Additionally, the Fluid Flow module, Heat Transfer module, and Chemicals species Transport modules are used to understand laminar/turbulent flow in a pipe. As an outcome, it is expected that a combination of analytical solutions and their representation in COMSOL Multiphysics® can be utilized to enhance students' learning. A survey has been developed to be used in the assessment of learning outcomes from this class.

The ultimate goal is to develop a project-based course so that the students can obtain a practical understanding of Transport Phenomena and connect the importance of computational tools in many Chemical Engineering processes.

Keywords: Engineering Education, Transport Phenomena, Student Creativity, Hands-on learning.

1. Introduction

Momentum, heat, and mass transfer are the three core concepts involved in Transport Phenomena. In Chemical Engineering, the fundamental concepts are usually taught using the traditional BS&L textbook.[1,2] Typically, at an undergraduate level in our institution, this subject is divided into two courses and a complementary laboratory. The first course involves 1-D and steady-state problems for the Navier-Stokes equation and the equation of energy, and Fick's 2nd law of Diffusion at steady state for Newtonian fluids. The second course involves unsteady state problems which are also solved mathematically with changes in one dimension. For example, when using the error function to predict heating of a semi-infinite slab. In the second course, additional emphasis is placed on interphase transport processes and turbulent flow. Lastly, the Transport Phenomena Laboratory involves measurements of flow, temperature, and mass concentration using a variety of instrumentation.

Recently, it has been shown that coupling computer simulations with theory lead to a better understanding of a topic.[3,4] Due to the required use of PDEs and various assumptions needed to solve Transport phenomena problems, COMSOL Multiphysics® is a potential tool that can enhance students' learning of this topic. In fact, other researchers have already focused on the implementation of COMSOL Multiphysics® to foster Transport Phenomena understanding.[5–8]

In this study, simple and easy-to-solve problems, including models from the application library, were implemented at the end of the second Transport Phenomena course at an undergraduate level. During a traditional lecture, analytical solutions of ODEs and PDEs are presented using a sequence of steps until a problem is solved. Hence, the students found a connection between the steps shown in class and on setting up a study with the software interface.

Students' surveys were used to assess the understanding of transport phenomena after computer simulations, and a preliminary discussion of these results along with the survey questions is discussed.

COMSOL Multiphysics® is a powerful tool for solving a multitude of research projects; here, it is shown that it can also be used to motivate students to understand the concepts of Momentum, Heat, and Mass Transport at an undergraduate level. Also, it gives a first-hand experience to computational tools that complement the lectures and the laboratory experiments.

2. Methods and Examples using COMSOL Multiphysics®

COMSOL Multiphysics® v.5.2 was used for all the class examples. The students had complete access to the software and performed the simulations with guidance from the instructor simultaneously. The following examples were implemented during class sessions [Note: * indicates a problem found in the application library]:

A. Flow in a pipe
B. Flow Between Parallel Plates
C. Heat Conduction through a plane
D. Flow Past a Cylinder*
E. Transient Diffusion or Tubular Reactor*.

For Examples A-C, the students learned the selection of space dimension, setup boundary conditions, steady vs. non-steady steady solutions, draw geometries, and define mesh types. This connection also helped the students to identify the steps followed in-class for simplified problems.

A project-type assignment was given to the students based on the shell and tube heat exchanger* simulation at the end of the course. The assignment consisted of changing one variable of their choice and compare it with the results provided originally. This assignment was left to connect concepts that are taught in following courses: Fluid Flow and Heat Transfer and the Chemical Engineering Unit Operations Laboratory.

3. Governing Equations and Numerical Model

Stationary and Time-Dependent studies were implemented in the class. Laminar flow and Turbulent flow (k-ϵ) were used to demonstrate the different velocity profiles obtained in fluid flow. Heat transport was illustrated only using conduction through a wall. For Diffusion studies, transport of diluted species was utilized. Materials were selected from the applications library and are specified for each example in the next sections. The primary equations used for each problem are the following:

Continuity Equation

$$\rho\nabla.(\mathbf{u}) = 0 \tag{1}$$

Navier-Stokes Equation

$$\rho(\mathbf{u}.\nabla)\mathbf{u} = \nabla.[\mathrm{p}\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T] + \mathrm{F} \tag{2}$$

Fourier's law of Heat Conduction

$$\mathbf{q} = -k\nabla\mathbf{T} \tag{3}$$

Energy Equation

$$\rho C_p\frac{\partial\mathbf{T}}{\partial t} + \rho C_p\mathbf{u}.\nabla\mathbf{T} + \nabla.\mathbf{q} = \mathrm{Q} + \mathrm{Q}_{\mathrm{ted}} \tag{4}$$

Fick's Laws

$$\mathbf{N}_{\boldsymbol{i}} = -D_i\nabla c_i \tag{5}$$

$$\frac{\partial c_i}{\partial t} + \nabla.(-D_i\nabla c_i) = R_i \tag{6}$$

4. Simulation Results and Major Transport Concepts Illustrated in Class.

4.1 Flow in a pipe

Laminar flow was illustrated using flow in a pipe (Fig. 1). For this example, a Newtonian fluid was selected at a constant temperature. The primary goal of this example consisted of identifying the velocity profile, the maximum velocity at the center of the pipe, and the symmetry of the solution based on defining an average velocity at the entrance of the pipe. The same examples was solved in class analytically. However, using simulations, students were able to see the importance of assumptions and the effects on the results from a 3-D point of view.

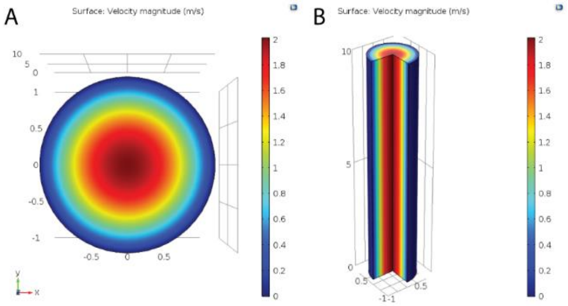

Figure 1. A) Top view of a pipe with a maximum velocity of 2 m/s and B) isometric view of the velocity profile.

4.2 Flow between parallel plates

A second concept illustrated with COMSOL Multiphysics® involves pressure drop between parallel plates (Fig. 2). In this example, students defined different boundary conditions such as inlet and outlet pressure and determine the velocity profile at different sections of the system. Overall, the students gained a better understanding of the relationship between pressure drop and fluid flow, which is typically covered by the Hagen-Poiseuille equation for flow in a pipe. This example also illustrated fluid flow transitions between laminar and turbulent velocity profiles based on the gap between the plates and the inlet pressure.

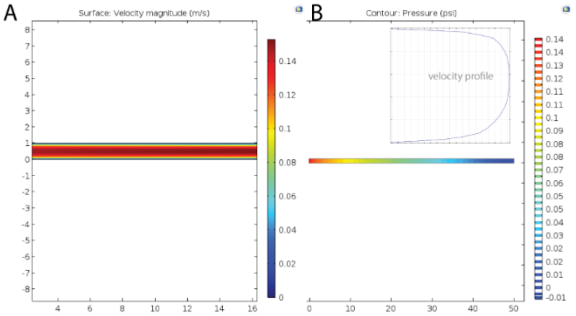

Figure 2. A) Velocity magnitude for flow between parallel plates and B) Turbulent velocity profile (inset) and pressure drop illustration.

4.3 Heat conduction through a plane

This example was used to illustrate Fourier's law of heat conduction in one direction by defining the necessary boundary conditions. By using a plane geometry, the students were able to connect the importance of defining a coordinate system that correlates with the direction of the heat flow. In this example (Fig. 3), the x-direction was used to illustrate the temperature drop across a plane. In addition, the linear temperature drop obtained in class for panels was demonstrated. Another concept illustrated with this example includes the calculation of heat flux and heat flow through an area using simulations. The students were able to observe the convenience and the powerful use of computational simulations when predicting these quantities.

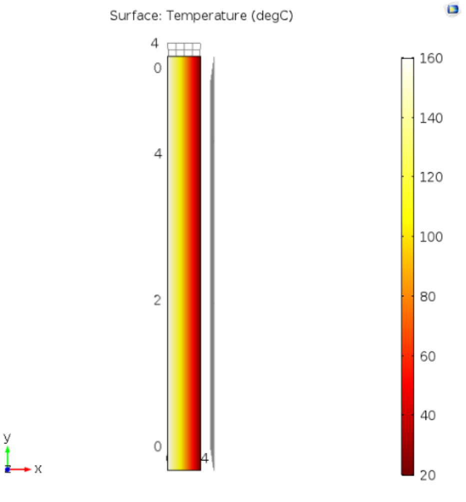

Figure 3. Temperature distribution across a concrete plane from 160° to 20 °C.

After illustrating basic concepts and how to use COMSOL Multiphysics® in the classroom, the students were introduced to transient/unsteady state studies using two examples.

4.4 Flow past a cylinder

The concepts of streamlines, boundary layers, eddies, and turbulent flow were explained using an example from the application library: Flow past a cylinder. The students demonstrated understanding on this topic after running the simulations (Fig.4). Moreover, the students also changed the size or the position of the cylinder to obtain a better idea of the effects of disturbances in fluid flow. While these topics enhanced students understanding, the most interesting outcome from this simulation was the generation of small video that showed the fluid flow as a function of time. This example fulfilled the expectations of students on getting a better understanding of transient fluid flow from a simulation point of view. Without experiments to confirm transitional regimes—laminar to turbulent flow—simulations are an excellent alternative for these topics.

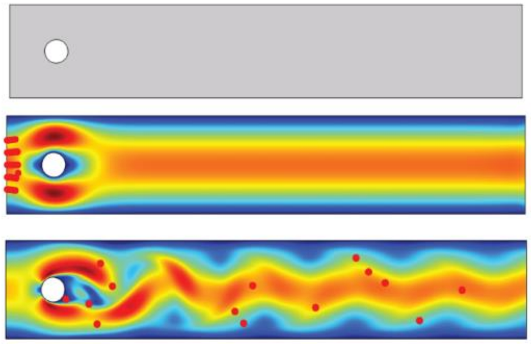

Figure 4. Fluid Flow past a cylinder at different Re numbers.

4.5 Transient Diffusion

Diffusion in 1- and 2-Dimensions was analyzed using COMSOL Multiphysics®. These examples illustrated concentration gradients as a function of time in more than one dimension (Fig. 5). In fact, the importance of Fick's first and second law of diffusion was emphasized. In the classroom, the students learned about the effects of 2-D concentration gradients as illustrated in Fig. 5C. Moreover, the students were able to generate concentration profiles with respect to time which is comparable to mathematical models for 1-D examples (Fig. 5B). Similar to the previous transient example, the students were fascinated about the generation of a small video to illustrate transient transport phenomena processes.

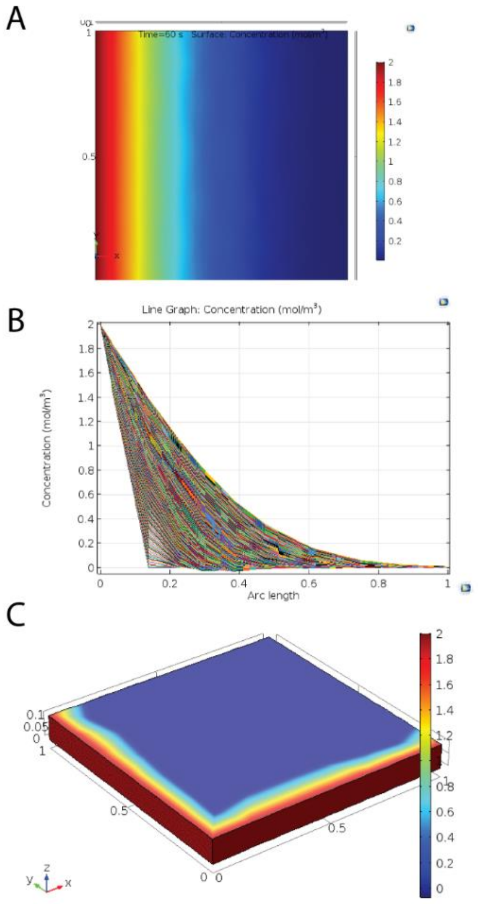

Figure 5. A) 1-D concentration drop as function of time, B)Concentration profiles for 1-D simulations and C) 2-D concentration drops for a plane.

4.6 Students' projects: Shell and tube heat exchanger

Problem solving and creativity are key components in an engineering class.[9] In this study, the creativity of the students was tested by allowing them to switch parameters of their choice using the shell and tube heat exchanger application library example. While no major modifications were done on the geometry of the system, interesting results were obtained when other materials were used or the fluid allocation (hot to cold) was switched. For example, instead of using air to cool the system, Freon was selected from the materials library. As a result, a new temperature profile and a different heat transfer coefficient were obtained. Examples of the temperature streamlines results are shown in Fig. 6. As expected, Heat was transferred a faster rate with this fluid.

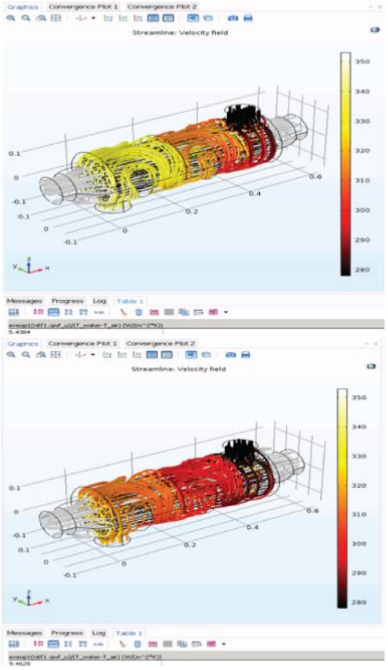

Figure 6. Shell and tube heat exchanger simulations showing temperature streamline with air(top) and Freon(bottom) as the materials under the same conditions.

5. Students Assessment and Feedback

After spending class time and a take-home project using COMSOL Multiphysics®, a survey was provided to the student for the assessment of the efficacy of using this software in a Transport Phenomena Course (Table 1).

The main learning objective pursued in this course was to use a modeling software to help the students understand Transport phenomena topics using an interactive platform. To develop the survey, a series of questions were introduced to the students in the following order: (1) importance of computational simulation in Transport phenomena (Q1-Q3), (2) Specific questions regarding COMSOL Multiphysics ® as a software (Q4-Q7), and (3) examples evaluation of the concepts illustrated in class and in their project (Q8-Q11). The specific questions are listed in Table 1.

Results from this survey (Table 1) were mostly agree and/or strongly agree for the majority of the questions. However, some exceptions included neutral answers, which were obtained mostly for question 4 (Table 1). In this survey, it is clear that the students could not connect some of the mathematical predictions and translate the use of simulations for the design of an equipment.

Table 1. Students survey to evaluate their experience of learning Transport Phenomena with COMSOL Multiphysics®

	Strongly Disagree	Disagree	Neutral	Agree	Strongly Agree
1. Transport Phenomena helped me to connect various topics learned in my previous Eng. Classes					
2. Simulations helped me to obtain a better understanding of Transport Phenomena					
3. The in-class examples helped me to visualize results in 3-D					
4. COMSOl® modeling helped me to understand the relationship between actual experiments and equipment design/ mathematical predictions					
5. COMSOL® results are easy to understand and manipulate					
6. COMSOL® is a software with a user friendly interface					
7. By using COMSOL®, I am more interested in Transport phenomena					
8. Simulations/videos were useful to connect with the theory and understand multidimensional flow					
9. The following modules were useful for my learning:					
a. flow in a pipe/ flow between two plates/ Heat conduction through a plane					
b. Flow past a cylinder					
c. Diffusion/Tubular reactor					
10. The project (Shell and tube HX) was effective in connecting new concepts in Chemical Engineering					
11. The instructor should spend more class time with computer simulations to enhance my learning					

6. Conclusions

Overall, the students surveyed in this course were satisfied by the implementation of a modeling software in the Transport Phenomena class. One of the major concerns when implementing this type of simulations involves the ability to work with a user-friendly software interface. For this study, the students were completely satisfied on using COMSOL Multiphysics® for this class based on the survey results (Q6; Table 1). In future courses, both simulations and mathematical results will be covered at the same time to compare mathematical or experimental results with simulation values. Similarly, as part of the suggestions, COMSOL Multiphysics® could potentially be used for modeling the equipment in the Transport Phenomena laboratory and in the Unit Operations laboratory in order to validate simulations results. These suggestions will be implemented in future sections as part of the outcomes arising from this study.

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