Finite Element Modules for Enhancing Undergraduate Transport Courses: Application to Fuel Cell Fundamentals

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Abstract

The transport phenomena courses (momentum, heat, and mass transfer) in chemical engineering typically contain many mathematical derivations and may often lack practical applications. The use of finite element software can help students visualize solutions and see how parameter changes affect velocity, temperature, and concentration profiles and their corresponding fluxes for design of practical systems.

Alternative energy is a rapidly growing research area yet is lacking in available course content for chemical engineering transport phenomena. In this paper we illustrate the use of the finite element method using Comsol Multiphysics[1] (formerly known as FEMLAB) for problems related to the design of fuel cells and their components. As such, we present ready-made tutorials for use in undergraduate transport courses.

Introduction and Motivation: The Typical Transport Course

As is the case with many core courses in the undergraduate curriculum, courses in fluid mechanics, heat transfer, and mass transfer can be categorized into three generic classifications:

1. Transport phenomena approach – a highly theoretical approach focusing on the derivation of microscopic conservation equations and their solutions, such as that contained in the text of Bird, Stewart, and Lightfoot[2].
2. Unit operations approach – a highly practical approach focusing on macroscopic balance equations and using them for the design of pumps, heat exchangers, and membranes, such as that contained in the text of McCabe, Smith, and Harriott[3].
3. A balance between the transport phenomena and unit operations, such as that contained in the text of Geankoplis[4].

At Michigan Technological University, students must complete a two-semester sequence of lecture courses (CM 3110 Transport / Unit Operations 1; CM 3120 Transport / Unit Operations 2). Based upon the title of the course we typically follow the third classification; however, content can vary depending on the instructor.

In a recent ASEE paper, Krantz discussed that the above textbooks often focus on simple problems with analytical or numerical solutions, but the development of software for performing computational analysis has allowed instructors of transport phenomena to focus on model development by introducing more complex problems[5]. An additional advantage of the software is that it allows the students to visualize the transport processes taking place.

Other studies have also used computers to help students learn concepts in chemical engineering education. This includes that of Thompson[6], who has used the partial differential equation (PDE) toolbox within MATLAB to visualize steady laminar flow in a finned heat exchanger, transient and steady heat transfer in a finned heat exchanger, and wave propagation in a heterogeneous material. Sinclair[7] has used FLUENT computational fluid dynamics software within the undergraduate curriculum. Besser[8] has used EXCEL spreadsheets to study two-dimensional heat conduction in solid materials. Zheng and Keith[9-10] have developed JAVA applets for unsteady and steady state transport problems.

As such, we present a handful of problems developed with the Comsol Multiphysics (formerly known as FEMLAB) finite element method modeling software[1]. We also use the "Chemical Engineering Module" which allows for quick access to the typical governing equations of momentum, heat, and mass transport. Additional modules are also available.

As the authors are working on a National Science Foundation project to develop new materials for fuel cell bipolar plates, many of the modules developed here focus solving a variety of fluid mechanics, heat transfer, and mass transfer problems applied to the relatively modern field of fuel cells.

After a very brief overview of fuel cells, six modules are presented that may be of use to instructors of transport phenomena courses.

Fuel Cell Overview

A fuel cell is device that converts a fuel into electricity with heat as a byproduct. There are several types of fuel cells, with the most likely fuel cell to be used for transportation applications being the proton exchange membrane fuel cell. In this device, the hydrogen fuel reacts with oxygen from the air and produces water. A single cell of a fuel cell produces about 0.7 V of potential; for many applications the cells are "stacked" together to give a higher voltage to power an electric motor. As such, the majority of design and analysis of fuel cell systems focuses on a single cell. A cartoon is shown in figure 1 below.

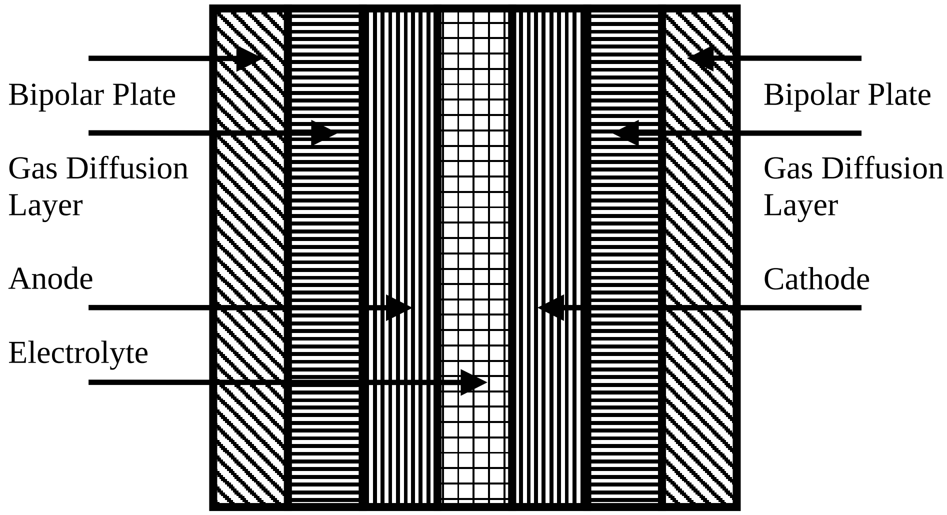

Figure 1. Schematic of one cell of a proton exchange membrane fuel cell. The slanted lines are the bipolar plates, the horizontal lines are the gas diffusion layer, the vertical lines are the electrodes (left block is the anode; right block is the cathode), and the grid represents the electrolyte.

Within a single cell of a fuel cell are bipolar plates which function to separate one cell from the other. The bipolar plates have channels etched on either side to allow for reactant and product gases to flow. The plates also need to have low hydrogen permeation, high thermal conductivity, and high electrical conductivity. Within the channels the chemicals reach a gas diffusion layer, and are transported through this layer, after which where they encounter the electrodes. The electrodes contain a platinum catalyst which facilitates the conversion of the fuel into protons and electrons. The protons pass through a sulfonated polymer electrolyte membrane. Meanwhile, the electrons are conducted back through the gas diffusion layer, bipolar plate, and electric load where they react with the protons and oxygen to form water. For more information regarding fuel cell construction, the reader is referred to the text of Larminie and Dicks[11] or the Los Alamos National Laboratory fuel cell website[12].

Finite Element Problems

In this paper we develop five modules in the following areas:

- Fluid Flow
    - The first module concerns the flow of polymer melts in a capillary rheometer. We note that rheology needs to be understood for compression molding analysis of complex bipolar plate designs. The objective of the module is to determine the velocity profile for laminar and power-law fluids, measure the pressure drop, and compare with published correlations. The users can also calculate Reynolds numbers and entrance lengths for the velocity profile to develop.

  - The second module concerns the flow of gases in bipolar plate channels. We note that pressure drop and reactant uniformity is important in fuel cell systems to improve overall fuel conversion efficiency. The objective of the module is to create a model of a channel with complicated flow geometry (U-shaped section) and determine the pressure drop over this channel. The users are then asked to consider multiple sections and the design of plates with multiple flow channels.
- Heat Transfer
  - The third module concerns steady-state one-dimensional heat conduction in a composite slab with reaction. We note that thermal analysis can allow for design of low or high temperature fuel cells. The objective of the module is to model multi-phase heat transfer and compare simulation results with the analytical solution.
- Mass Transfer
  - The fourth module concerns one- and two-dimensional unsteady state diffusion in a slab. We note that bipolar plates have low hydrogen permeation, but a complete analysis allows for estimates of fuel cell overall efficiency. The objective of the module is to model mass transfer and compare simulation results with a cumbersome analytical Fourier series solution. The users are then asked to solve the unsteady-state diffusion equation in a complex geometry that applies to a real fuel cell bipolar plate.
- Transport Effects on Kinetics
  - The fifth and final module concerns diffusion and reaction in a porous solid. We note that transport effects can have a large impact on fuel cell performance and catalyst design. This is the classical Thiele modulus problem where the user calculates concentration profiles and catalyst effectiveness factors for a cube-shaped and for a cone-shaped catalyst pellet.

Typical problems, shown here as separate appendices, walk the user through an example so they can become acquainted with how the software works. Many of these examples have analytical solutions so one can determine accuracy of the numerical model. This allows for discussions on computational methods and convergence.

At the conclusion of the modules there is often a question or portion where the users apply their knowledge to a more complex problem that usually cannot be solved analytically. It is noted that the first module includes several figures to illustrate the set up of the model geometry. All modules include figures which illustrate the results.

Conclusions

We present several ready-to-use modules using Comsol Multiphysics finite element software for the undergraduate transport courses. The topics can easily be integrated into a momentum, heat, or mass transfer course. Students using the finite element method benefit from enhanced visualization of the physical processes occurring and also benefit from seeing practical applications of the complex partial differential equations that are typically derived in these courses.

To date these modules have only been developed and some are currently being used in our courses. In a future paper we will assess student learning skills with these tools.

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