AC 2008-410: CACHE MODULE DEVELOPMENT FOR INTRODUCING ENERGY INTO THE CHEMICAL ENGINEERING CURRICULUM: FUEL CELLS

Jason Keith, Michigan Technological University

Jason Keith is an Associate Professor of Chemical Engineering at Michigan Technological University. He received his B.S.ChE from the University of Akron in 1995, and his Ph.D from the University of Notre Dame in 2001. His current research interests include reactor stability, alternative energy, and engineering education. He is active within ASEE.

H. Scott Fogler, University of Michigan

H. Scott Fogler is the Ame and Catherine Vennema Professor of Chemical Engineering and the Thurnau Professor at the University of Michigan in Ann Arbor. His current research interests include the reaction and colloidal kinetics of asphaltene and wax deposition from crude oil. He is a member of the CACHE Corporation which is supporting this initiative of bringing energy modules into the undergraduate curriculum.

Valarie Thomas, University of Michigan

Valarie Thomas is an assistant research scientist in the Department of Chemical Engineering at the University of Michigan. She received her S.B. in chemical engineering from Massachusetts Institute of Technology and her Ph.D from the University of Michigan in the same field. Her current research interests are interdisciplinary and include surface chemistry, catalysis, alternative energy, novel uses of electrochemical reactors, vegetable oil hydrogenation chemistry and engineering education.

Don Chmielewski, Illinois Institute of Technology

Don Chmielewski is an Associate Professor of Chemical and Environmental Engineering at the Illinois Institute of Technology. He received his B.S. from the Illinois Institute of Technology in Electrical Engineering in 1991, and his M.S. (1993) and Ph.D (2000) in Chemical Engineering from the University of California, Los Angeles. His research interests are advanced process control and fuel cell system design and control.

Michael Gross, Bucknell University

Michael Gross is an Assistant Professor in the Chemical Engineering Department at Bucknell University. He has a B.S. Ch.E. from Bucknell University, and his M.S. Ch.E. and Ph.D Ch.E from the University of Pennsylvania. His teaching interests are materials science, fuel cells, and energy conversion, and his research interests are in electrochemistry and solide oxide fuel cells.

CACHE Module Development for Introducing Energy into the Chemical Engineering Curriculum: Fuel Cells

Abstract

In this paper we describe the development of modules that can be used to introduce fuel cells into existing chemical engineering courses. Course specific modules have been developed that apply fundamental chemical engineering principles to the analysis of fuel cell systems. The modules are currently located at the following website: http://www.chem.mtu.edu/~jmkeith/fuel_cell_curriculum, and after beta testing, will be available through the CACHE website http://www.cache.org. Each module contains a problem motivation, reference to material from textbooks widely used in the chemical engineering curriculum, an example problem statement, example problem solution, home problem statement, and home problem solution. To date modules have been developed for the following chemical engineering core courses: mass and energy balances, thermodynamics, fluid mechanics, heat and mass transfer, and kinetics and reaction engineering. In addition to presenting the modules, we will present some preliminary assessment on these educational modules.

Objectives and Motivation

The search for alternative energy sources is an area that has received great attention in the last few years, beginning with the January 2003 State of the Union address by President George W. Bush, approving federal funding for hydrogen fuel cell research for passenger vehicles. Similar announcements were made by state governors, most notably Michigan Governor Jennifer Granholm, stating "not only will we build these cars in Michigan, our Automotive Technology Corridor will help develop the fuel cell technology those cars will run on."

Inherent within the nation's initiative should be the development of educational programs related to fuel cells and other aspects of the hydrogen economy. Although it is common for engineering curricula to lag behind technology in emerging fields, there has been a thrust to develop course material for hydrogen technology research within the chemical undergraduate curriculum. This paper describes these efforts.

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.

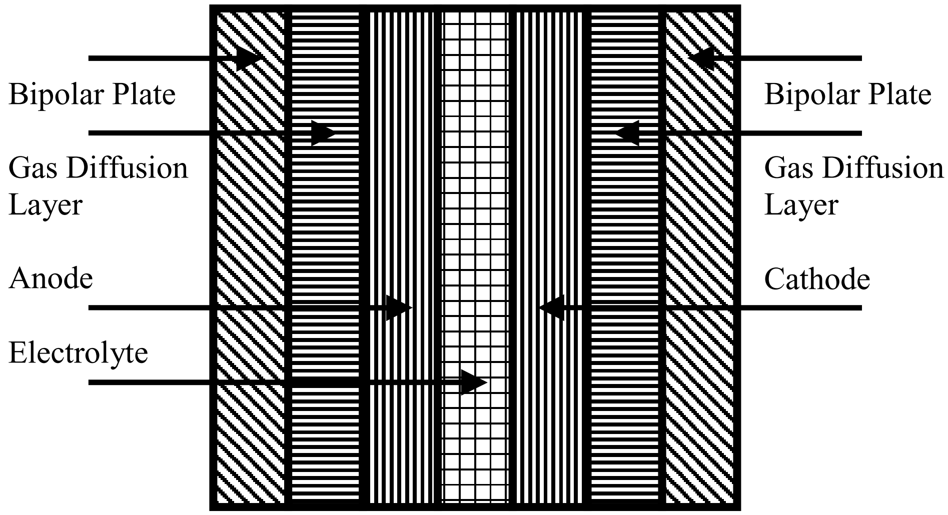


Figure 1. Schematic of one cell of a proton exchange membrane fuel cell. The slanted lines are the bipolar plates, the horizontal lines are the gas diffusion layer, the vertical lines are the electrodes (left block is the anode; right block is the cathode), and the grid represents the electrolyte.

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[1] or the Los Alamos National Laboratory fuel cell website[2].

Bringing Fuel Cell Concepts into Engineering Curricula

In this section we will briefly review our efforts in bringing fuel cell technology into the undergraduate and graduate chemical engineering curriculum.

At Michigan Tech, fuel cell concepts have been incorporated in several ways:

- Alternative Fuels Group Enterprise – this introduces students to alternative energy technology through project work. Projects have been sponsored by the United States Army Tank Automotive and Armaments Command (TACOM) and Army Research Laboratory (ARL), and have focused on integration of commercially available fuel cells into small and large vehicles. More information on this curriculum is available elsewhere[3-5].

- Fuel Cell Fundamentals Course – this is a 1 credit elective course introducing fuel cell technology to chemical, mechanical, and electrical engineering students. More information on this course is available elsewhere[3-5].
- Fuel Cell Problem Sets – these are problems for CM3120 Transport / Unit Operations 2 (heat and mass transfer and related unit operations). These include traditional homework problems and calculations using finite element software[6].

At the University of Michigan, fuel cell concepts have been incorporated via an advanced course in electrochemical engineering. At the Illinois Institute of Technology, fuel cell concepts have been incorporated through an advanced course on fuel cell system design and control.

Fuel Cell Module Development

In the summer of 2006, J. Keith initiated a collaboration with Prof. Scott Fogler of the University of Michigan and Prof. Don Chmielewski of the Illinois Institute of Technology. This "Fuel Cell Curriculum Development Project" has been partially funded by the CACHE Corporation (Computer Aids for Chemical Engineering), and the project status was presented by J. Keith during an invited session at the November 2007 American Institute of Chemical Engineers Annual Meeting[7].

To be most effective in teaching the students, each module consists of a problem motivation, example problem statement, example problem solution, home problem statement, and home problem solution. The modules also have additional information that lists the chemical engineering course that the problem can be used in, sections of popular textbooks to aid instructors in knowing when to use the problems, and common stumbling points for students (based upon beta-tests at Michigan Technological University). The modules are currently online at the following site[8]: http://www.chem.mtu.edu/~jmkeith/fuel_cell_curriculum/, but will eventually be moved over to the CACHE website[9]: (http://www.cache.org/). The CACHE site also contains a wealth of information for chemical engineering educators.

It is noted that bio-related online modules exist for the material and energy balance course at the bioengineering educational materials bank[10]: (http://www.bioemb.net), materials related online modules exist at the materials digital library pathway[11]: (http://matdl.org), and a significant amount of content for all of engineering can be found at the Massachusetts Institute of Technology open courseware site[12] (http://ocw.mit.edu) and the Multimedia Educational Resource for Learning and Online Teaching site[13] (http://www.merlot.org).

There are two example modules shown in the appendix at the end of this paper, for the material and energy balance course and for the transport phenomena course.

Current modules are available for the courses, and topic areas as seen in table 2 below. These modules are currently under peer review from leading educators around the nation as well as industrial members of the CACHE Corporation.

Chemical Engineering Core Course	**Module Title**
Material and Energy Balances	Application of Heat of Reaction: Hydrogen vs. Gasoline
Material and Energy Balances	Material Balances on a Fuel Cell
Material and Energy Balances	Energy Balances on a Fuel Cell
Material and Energy Balances	Generation of Electricity Using Recovered Hydrogen
Thermodynamics	Equation of State for Fuel Cell Gases
Thermodynamics	Thermodynamics and Fuel Cell Efficiency
Thermodynamics	Vapor Pressure / Humidity for Fuel Cell Gases
Heat and Mass Transport	Conduction and Convection Heat Transfer in Fuel Cells
Heat and Mass Transport	Microscopic Balances Applied to Fuel Cells
Heat and Mass Transport	Diffusion Coefficients for Fuel Cell Gases
Fluid Mechanics	Pressure Drop in Fuel Cell Bipolar Plates
Kinetics and Reaction Engineering	Nernst Equation and Fuel Cell Kinetics
Kinetics and Reaction Engineering	Using Plug Flow Reactor Equations for Fuel Cell Voltages

Table 2. Current chemical engineering fuel cell modules

Preliminary Assessment

During fall of 2007, twenty-three students enrolled in the Fuel Cell Fundamentals Course at Michigan Technological University. The homework assignments for this course are shown in the following list:

- Application of Heat of Reaction: Hydrogen vs. Gasoline (full module)
- Equation of State for Fuel Cell Gases (full module)
- Thermodynamics and Fuel Cell Efficiency (full module)
- Nernst Equation and Application in Chemical Kinetics (problem only)
- Fuel Cell Mass Balance (problem only)
- Vapor Pressure / Humidity for Fuel Cell Gases (full module)
- Conduction and Convection Heat Transfer in Fuel Cells (full module)

In five of these assignments, the full module was given (with the exception of the home problem solution). Examples of the full modules can be seen in the Appendix of this paper. In two of the homework assignments, only a problem statement was provided. The rationale behind assigning the problem only was to assess the value of providing an example problem and solution.

Institutional Review Board approval was granted (MTU protocol # M0243, Assessing New Learning Modules for Fuel Cell Instruction) to use human subjects in the classroom. A survey instrument was developed and distributed during the final class meeting. Participation in the survey was voluntary. Nineteen students participated out of an enrollment of twenty-three students. The questions on the survey and survey results, which were very positive, are summarized below.

1. I felt that the instructional material helped facilitate my learning.

Strongly Agree	Agree	Ambivalent	Disagree	Strongly Disagree
9 responses	10 responses	0 responses	0 responses	0 responses

2. I felt that the homework problems allowed me to apply my engineering principles to fuel cell and / or fuel cell system design.

Strongly Agree	Agree	Ambivalent	Disagree	Strongly Disagree
8 responses	11 responses	0 responses	0 responses	0 responses

3. Please provide any additional comments you may have on this course and/or the instructional modules:

Sample responses:

- "It was nice to see one worked out… it conceptualized and gave better background."
- "I thought the content and pace of this course were ideal for providing an interesting course which was not bogged down with an overwhelming amount of coursework."
- "The example problems helped a lot in figuring out how to do each problem. Even when the problems weren't exactly the same as the assignment the examples were still helpful."
- "Wish the material could be more advanced."

During fall of 2007, two of the modules were used in ChE 202 Material and Energy Balances at the Illinois Institute of Technology:

- Material Balances on a Fuel Cell (full module) as a homework assignment
- Energy Balances on a Fuel Cell (full module) as an extra credit assignment

The following observations were made by the instructor: "My general impression is favorable for the modules; they are relevant and useful to the class, taking the concepts given in Felder & Rousseau and applying them to a practical application with the added complexity of an electron transfer reaction and current*voltage = power. For the students it is a good way of applying (and stretching) their mastery of the material / energy balance principles."

Future Directions

In the future, we aim to develop modules for the following courses, with problem descriptions in italics:

- Fundamentals of Engineering (freshman engineering courses within or outside of chemical engineering departments): *unit conversions, basic engineering calculations, graphing*
- Fundamentals of Chemical Engineering: *material and energy balances in fuel cells and fuel reformers*
- Transport / Unit Operations 1 (Fluid Mechanics): *pressure drop in bipolar plate channels, sizing air compressors for fuel cells, sizing cooling fans for fuel cell systems*
- Transport / Unit Operations 2 (Heat and Mass Transfer): *design of membranes for use in fuel cell vehicles, thermal management, mass transfer through fuel cell electrodes, hydrogen leakage through fuel cell bipolar plates, finite element modeling of mass transfer in fuel cell applications*
- Chemical Engineering Thermodynamics: *theoretical efficiency of fuel cells, and hydrogen reformers, comparison with internal combustion engines*
- Chemical Reaction Engineering: *impact of heat and mass transfer on reactor design, catalysts for hydrogen processing, catalyst for fuel cells*
- Chemical Process Analysis and Design: *design of alternative energy production facilities, including hydrogen reforming stations*

New module ideas are also welcome to be included in this initiative and anyone that would like to participate in this CACHE task force should contact one of the authors.

Conclusions

This paper has described modules to introduce fuel cell technology into the undergraduate chemical engineering curriculum. Each module contains a problem motivation, example problem statement, example problem solution, home problem statement, and home problem solution. Preliminary assessment of the modules indicates that they are very effective in teaching students about fuel cells. It is hoped that these modules can enhance interest in alternative energy technology.

Acknowledgments

The CACHE Corporation is acknowledged for partial support of this project. JMK is supported by the United States Department of Energy (DE-FG02-04ER63821), National Science Foundation , and the Michigan Space Grant Consortium. DJC is supported by Argonne National Laboratory. HSF and VT are supported by the Vennema and Thurnau Professorships at the University of Michigan.

Bibliography

1. Larminie, J.; Dicks, A. Fuel Cell Systems Explained, 2nd Edition, Wiley, West Sussex, England, 2003.
2. Los Alamos National Laboratory fuel cell website, http://www.lanl.gov/orgs/ee/fuelcells/index.shtml, accessed February 2008.
3. J. M. Keith, "A Student-Driven Enterprise in Fuel Cells and Alternative Fuels," ASEE Conference Proceedings, 2004.
4. J. M. Keith, K. C. Opella, M. G. Miller, J. A. King, G. D. Gwaltney, C. A. Green, J. S. Meldrum, and S. A. Bradley, "Engineering Education in Alternative Energy," ASEE Conference Proceedings, 2006.
5. J. S. Meldrum, C. A. Green, G. D. Gwaltney, S. A. Bradley, J. M. Keith, and T. F. Podlesak, "Fuel Cell Powered Unmanned Ground Vehicle," SPIE Conference Proceedings, 2007, Orlando, FL.
6. J. M. Keith, F. A. Morrison, and J. A. King, "Finite Element Method for Enhancing Undergraduate Transport Courses: Application to Fuel Cell Fundamentals," ASEE Conference Proceedings, 2007.
7. J. M. Keith, D. J. Chmielewski, H. S. Fogler, and V. Thomas, "CACHE Modules on Energy in the Curriculum: Fuel Cells," presented at the AIChE Annual Meeting, 2007, Salt Lake City, UT.
8. Fuel Cell Curriculum website, http://www.chem.mtu.edu/~jmkeith/fuel_cell_curriculum, accessed February 2008.
9. CACHE website, http://www.cache.org, accessed February 2008.
10. Bioengineering Educational Materials Bank website, http://www.bioemb.net, accessed February 2008.
11. Materials Digital Library Pathway website, http://matdl.org, accessed February 2008.
12. Massachusetts Institute of Technology Open Courseware website, http://ocw.mit.edu, accessed February 2008.
13. Multimedia Educational Resource for Learning and Online Teaching website, http://www.merlot.org, accessed February 2008.

Appendix: Sample Module for Material and Energy Balances

Module Title: Material Balance in a Solid Oxide Fuel Cell
Module Author: Donald J. Chmielewski
Author Affiliation: Center for Electrochemical Science and Engineering
Department of Chemical and Biological Engineering
Illinois Institute of Technology, Chicago, IL 60616

Course: Material and Energy Balances

Text Reference: Felder and Rousseau (2000), Section 4.7

Concept Illustrated: Material balances on a reactive process with complex geometry; Extension of balance and stoichiometry concepts to electrons.

Problem Motivation: Fuel cells are a promising alternative energy technology. One type of fuel cell, the Solid Oxide Fuel Cell (SOFC) uses hydrogen as a fuel. The fuel reacts with oxygen to produce electricity. Fundamental to the design of an SOFC is an understanding of the fuel and oxidant utilization as well as the amount of current generated.

The SOFC reactions are:

	Anode:	$H_2 + O^{-2} \rightarrow H_2O + 2\,e^-$
	Cathode:	$O_2 + 2\,e^- \rightarrow O^{-2}$
	Overall:	$H_2 + 1/2O_2 \rightarrow H_2O$

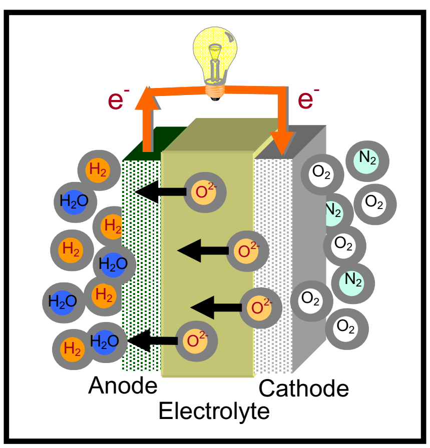


Figure 1: Reactions within SOFC

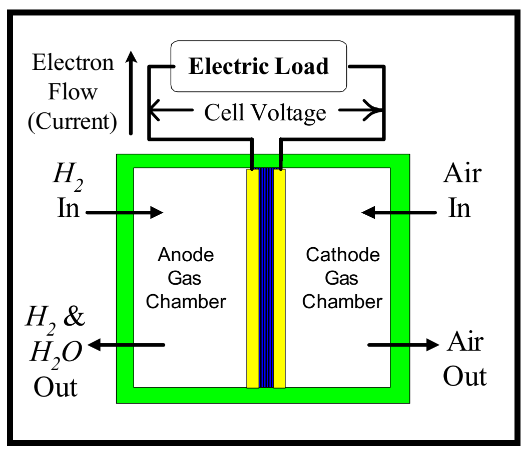


Figure 2: Flow Diagram for SOFC

For each mole of hydrogen consumed, two moles of electrons are passed through the electric load. To convert electron flow (moles of electrons/s) to electrical current (coulombs/s or amps), one would use Faraday's constant: $F = 96{,}485$ coulombs / mole of electrons. The primary objective of a fuel cell is to deliver energy to the electric load. To calculate the energy delivery rate (also know as power) one would multiply the current times the cell voltage: *Power* = *Current* * *Voltage*. (Recall the unit conversions: $coulomb \cdot volt = joule$ and $joule / s = watt$).

Problem Information

Example Problem Statement: A SOFC is operated with an inlet flow of 20 g/s of pure hydrogen and an inlet flow of 1450 g/s of air. If the fuel utilization is 50%, then determine the following:

1) The mass flow out of the anode gas chamber.
2) The mass flow out of the cathode gas chamber and the oxygen utilization.
3) The current through the electric load.
4) If the cell voltage is 0.8 volts, determine the power delivered to the load.

Example Problem Solution:

1) We begin by converting the anode inlet mass flow rate to molar flow:

$$\frac{20\, g\ H_2\ fed}{s} \times \frac{1\, mole\ H_2}{2\, g\ H_2} = \frac{10\ mole\ H_2\ fed}{s}$$

The term utilization is synonymous with the percent conversion, as defined in section 4.6 of Felder and Rousseau (2000). Thus, a 50% utilization of hydrogen indicates

$$\frac{0.5\ mole\ H_2\ reacted}{mole\ of\ H_2\ fed} \times \frac{10\ mole\ H_2\ fed}{s} = \frac{5\ mole\ H_2\ reacted}{s}$$

Thus, 5 moles / sec of H_2 will be converted to H_2O. The remaining 5 moles/sec of H_2 will then exit with the generated steam. Converting back to mass flows, we have:

$$\frac{5\ mole\ H_2\ exiting}{s} \times \frac{2\, g\ H_2}{1\ mole\ H_2} = \frac{10\ g\ H_2\ exiting}{s}$$

$$\frac{5\ mole\ H_2O\ exiting}{s} \times \frac{18\, g\ H_2O}{1\ mole\ H_2O} = \frac{90\ g\ H_2O\ exiting}{s}$$

for a total of 100 g/s exiting the anode.

2) Assuming the mass fraction of air is 76.7% N_2 and 23.3% O_2, we find the cathode inlet molar flows to be:

$$\frac{1450\, g\ of\ air\ fed}{s} \times \frac{0.767\, g\ N_2}{g\ of\ air} \times \frac{mole\ N_2}{28\ g\ N_2} = \frac{39.7\ mole\ N_2\ fed}{s}$$

$$\frac{1450\, g\ of\ air\ fed}{s} \times \frac{0.233\, g\ O_2}{g\ of\ air} \times \frac{mole\ O_2}{32\ g\ O_2} = \frac{10.6\ mole\ O_2\ fed}{s}$$

Since 5 moles/s of H_2 are converted in the anode, 2.5 moles/s of O_2 must be consumed in the cathode. Thus, only 8.1 moles/s of O_2 remain, and the oxygen utilization is calculated as:

$$Utilization = 100 \times \frac{2.5\ moles\ of\ O_2\ reacted}{10.6\ moles\ of\ O_2\ fed} = 23.6\%$$

Converting back to mass flows, we have:

$$\frac{8.1\ mole\ O_2\ exiting}{s} \times \frac{32\ g\ O_2}{1\ mole\ O_2} = \frac{259\ g\ O_2\ exiting}{s}$$

Adding this to the inert flow of N_2 (1112 g/s), gives a total of 1371 g/s exiting the cahode gas chamber.

3) Looking at the anode stoichiometry, we find that 2 moles of electrons are sent to the load for every mole of hydrogen consumed. Thus, the electron flow is 10 moles / sec. If we now employ Faraday's constant, $F = 96{,}485$ coulombs / mole of electrons, for unit conversion, we find the current to be 964,850amps (1 amp = 1 coulomb/sec).

4) Application of the relation: *Power* = *Current* * *Voltage*, yields a power of 770,000 J/s or 0.77 mega-watts (MW)

Home Problem Statement:

A SOFC is operated with an anode exit flow of 2 g/sec and an inlet of pure hydrogen. If the cell is operated at 0.75 volts and delivers 10kW of power, determine the following:

1) The mass flow into the anode gas chamber.
2) The mass flow into the cathode chamber if a 20% oxygen utilization is desired.

Home Problem Solution:

First, we will need some preliminary calculations. From the delivered power and operating voltage, we find the current as:

$$Current = \frac{10{,}000 J/s}{0.75\ volts} = 13{,}330\ amps = 13{,}330\ coulombs/s$$

Using Faraday's constant, this is equal to 0.14 moles of electrons/s. Using the SOFC stoichiometry this translates to 0.07 moles of H_2 reacted / s, 0.07 moles H_2O produced / s and 0.035 moles of O_2 reacted / s.

1) If we define a control volume around the anode gas chamber, we find the balance:

$$
\begin{aligned}
\dot{m}_{a,in} &= \dot{m}_{a,out} - (\dot{m}_{a,produced} - \dot{m}_{a,consumed}) \\
&= \frac{2g\ of\ H_2}{s} - \left(\frac{0.07 mole\ of\ H_2O}{s} \times \frac{18g\ H_2O}{mole\ H_2O} - \frac{0.07 mole\ of\ H_2}{s} \times \frac{2g\ H_2}{mole\ H_2} \right) \\
&= 0.88 g/s
\end{aligned}
$$

As an additional note, these numbers indicate a 15% utilization of the hydrogen feed.

2) From the preliminary calculations, 0.035 moles of O_2 are reacted / s. To achieve the desired 20% oxygen utilization the flow oxygen to the cathode is calculated as:

$$
\frac{mole\ of\ O_2\ fed}{0.2\ mole\ O_2\ reacted} \times \frac{0.035\ mole\ O_2\ reacted}{s} = \frac{0.175\ mole\ O_2\ fed}{s}
$$

Assuming the mole fraction of air is 79% N_2 and 21% O_2, we find that the required inlet flow of N_2 to be:

$$
\frac{0.175\ mole\ O_2\ fed}{s} \times \frac{0.79\ mole\ of\ N_2}{0.21\ mole\ of\ O_2} = \frac{0.658\ mole\ N_2\ fed}{s}
$$

Finally, the mass flow into the cathode is calculated as:

$$
\begin{aligned}
\dot{m}_{c,in} &= \dot{m}_{O_2,in} + \dot{m}_{N_2,in} \\
&= \frac{0.175\ mole\ of\ O_2}{s} \times \frac{32g\ O_2}{mole\ O_2} + \frac{0.658\ mole\ of\ N_2}{s} \times \frac{28g\ N_2}{mole\ N_2} \\
&= 24 g/s
\end{aligned}
$$

As an additional note, the exit flow from the cathode should be 21.7 g/sec.

Appendix: Sample Module for Transport Phenomena

Module Title: Microscopic Energy Balance in Fuel Cells
Module Author: Jason Keith
Author Affiliation: Department of Chemical Engineering
Michigan Technological University, Houghton, MI 49931

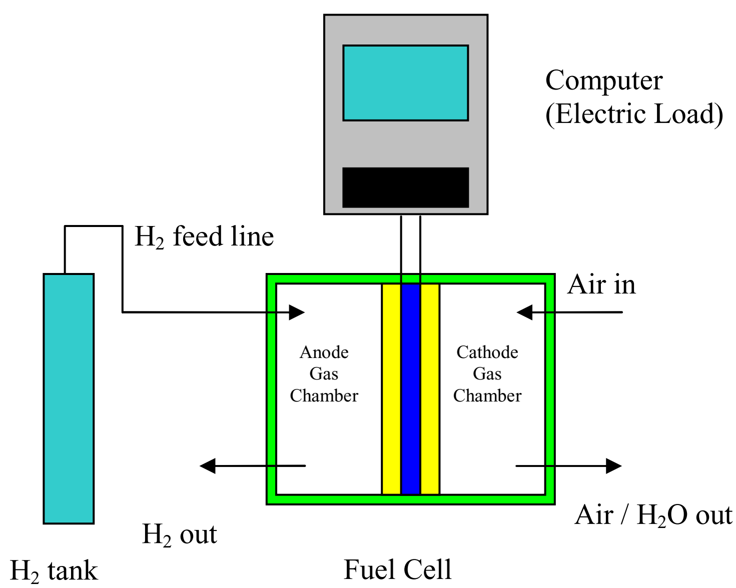
Course: Transport Phenomena (Heat Transfer)

Text Reference: Bird, Stewart, and Lightfoot (2nd edition) section 10.2
Welty, Wicks, Wilson, and Rorrer (4th edition) section 17.2

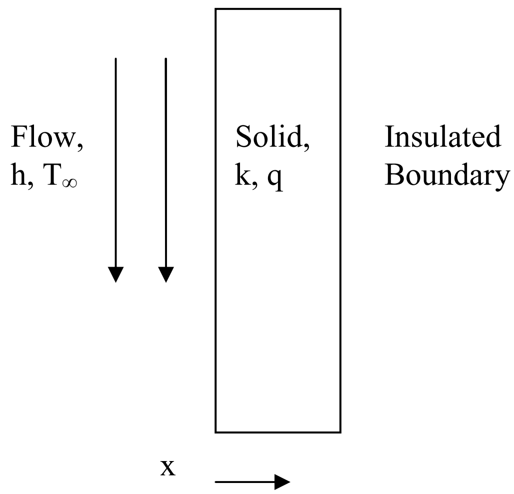
Concepts: Solving differential equations to obtain the temperature profile

Problem Motivation:
Fuel cells are a promising alternative energy technology. One type of fuel cell, a proton exchange membrane fuel cell reacts hydrogen and oxygen together to produce electricity. Fundamental to the design of fuel cells is an understanding of heat transfer mechanisms within fuel cells. Heat removal from fuel cells is critical to their scaleup for large power applications.

Consider the schematic of a compressed hydrogen tank feeding a proton exchange membrane fuel cell, as seen in the figure below. The electricity generated by the fuel cell is used here to power a laptop computer. In this module we will solve microscopic equations to determine the temperature profile within one cell of a fuel cell.



Example Problem Statement: In this example we will apply principles of microscopic energy balances to the design of a fuel cell system. For simplicity, we will consider the rectangular geometry shown below, which describes flow over and heat conduction through a solid plate, with a heat source (due to reaction).



The governing equation describing the thermal energy conservation equation is given by:

$$k\frac{d^2T}{dx^2} = -q \tag{1}$$

Note that in equation 1 there is a uniform heat generation rate q within the solid. Equation 1 is subject to the boundary conditions:

$$-k\frac{dT}{dx} = h(T_\infty - T)\text{, at } x = 0 \tag{2}$$

and

$$\frac{dT}{dx} = 0 \text{ at } x = L \tag{3}$$

It is noted that equation 2 condition can be derived from an energy balance at the gas/solid interface and that equation 3 is due to the insulated boundary.

The following parameters are available: q = 48 W/cm^3, L = 0.5 cm, T_∞ = 293 K, k = 0.20 W/cm-K.

Your tasks are the following:

1) Integrate the equation to determine T as a function of x.
2) Determine the value of the heat transfer coefficient h (in units of W/cm^2-K) needed to keep the maximum temperature in the solid below 358 K.
3) Plot the temperature distribution T as a function of the spatial coordinate x under the conditions of part 2.

Example Problem Solution:
We begin by doing some mathematical manipulation and then solve the ordinary differential equation of equation 1. For more information, please consult a differential equations text.

Part 1)
Step 1) Manipulation. We divide both sides of equation 1 by k and write the second derivative as the derivative of the first derivative to obtain:

$$\frac{d}{dx}\left(\frac{dT}{dx}\right) = -\frac{q}{k} \tag{4}$$

Step 2) Integration. We can then multiply both sides by dx, and integrate to obtain:

$$\left(\frac{dT}{dx}\right) = -\frac{q}{k}x + c \tag{5}$$

where c is an integration constant.

Step 3) Boundary condition. Applying the no-flux boundary condition at $x = L$ we can solve to show that:

$$c = \frac{qL}{k} \tag{6}$$

We also note that at $x = 0$ the derivative $\left(\frac{dT}{dx}\right) = \frac{qL}{k}$ or $-k\left(\frac{dT}{dx}\right) = -qL$. This will be used later in the other boundary condition.

Step 4) Another integration. Since the derivative *dT/dx* is already isolated, we can integrate equation 5 to solve for the temperature distribution:

$$T = -\frac{q}{k}\left(\frac{x^2}{2} - Lx\right) + d \tag{7}$$

where d is an integration constant. We note that at x = 0, $T = d$.

Step 5) Other boundary condition. Applying the mixed boundary condition at x = 0 we can show that $-k\frac{dT}{dx} = h(T_\infty - T)$ can be manipulated to give:

$$-qL = h(T_\infty - d) \tag{8}$$

and upon solving for $d = T_\infty + \frac{qL}{h}$ we can write down the temperature distribution as:

$$T = T_\infty - \frac{q}{k}\left(\frac{x^2}{2} - Lx\right) + \frac{qL}{h} \tag{9}$$

Part 2)
Step 1) Manipulation. We first note that the maximum temperature T_{max} will occur at the insulated boundary, where $x = L$. Performing this substitution into equation 9 gives:

$$T_{\max} = T_\infty + \frac{qL^2}{2k} + \frac{qL}{h} \tag{10}$$

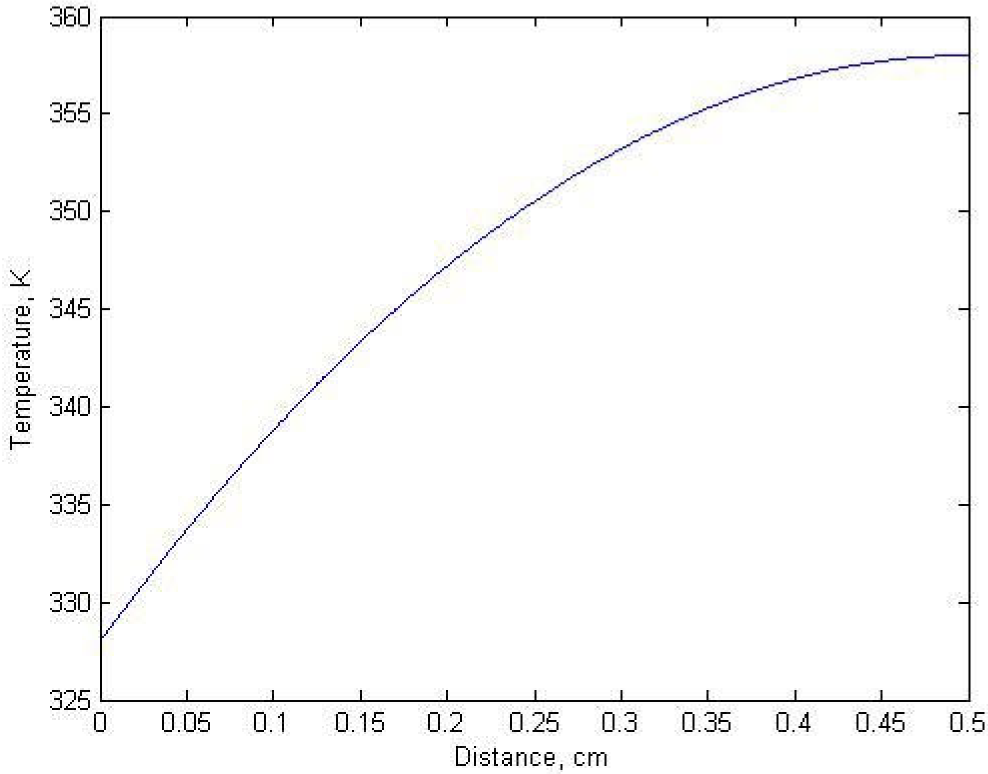
Step 2) Algebra. Solving equation 10 for h we obtain:

$$h = \frac{qL}{T_{\max} - T_\infty - \frac{qL^2}{2k}} \tag{11}$$

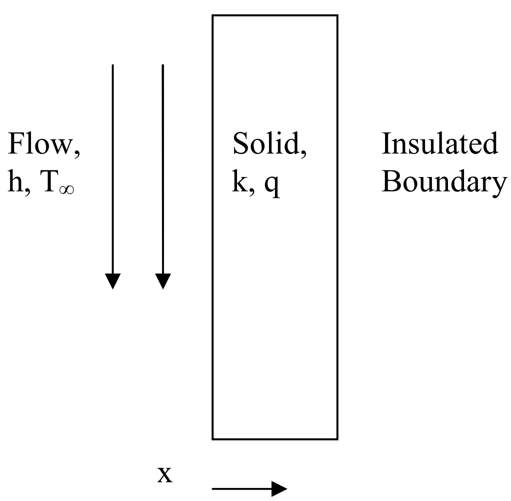
Step 3) Calculation. We can now substitute the known parameters to determine the value of the heat transfer coefficient. Equation 11 becomes:

$$h = \frac{48\frac{\text{W}}{\text{cm}^3}0.5\text{cm}}{358\text{K} - 293\text{K} - \frac{48\frac{\text{W}}{\text{cm}^3}(0.5\text{cm})^2}{2\times\frac{0.2\text{W}}{\text{cmK}}}} = 0.686\frac{\text{W}}{\text{cm}^2\text{K}} \tag{12}$$

Part 3)
The following is a plot of equation 9, showing T as a function of x. Note that the shape of the graph is parabolic. This makes sense since the second derivative is equal to a constant. The slope of the graph at $x = L$ is zero as it is expected to be for an insulated boundary.



Home Problem Statement: In this example we will apply principles of microscopic energy balances to the design of a fuel cell system. For simplicity, we will consider the rectangular geometry shown below:



Let us assume a nonuniform source, with more reaction near the insulated boundary, such that equation 1 of the example problem can be modified as:

$$k\frac{d^2T}{dx^2} = -qx \qquad (13)$$

Equation 13 is subject to the boundary conditions

$$-k\frac{dT}{dx} = h(T_\infty - T)\text{, at x = 0} \tag{14}$$

and

$$\frac{dT}{dx} = 0 \text{ at x = L} \tag{15}$$

The following parameters are available: q = 100 W/cm^4, L = 0.5 cm, T_∞ = 293 K, k = 0.20 W/cmK, and h = 1 W/cm^{2}K.

Your tasks are the following:
1) Integrate the equation to determine T as a function of x.
2) Determine the maximum temperature in the solid.
3) Plot the temperature distribution T as a function of the spatial coordinate x

Home Problem Solution:
Part 1)
Step 1) Manipulation. We divide both sides of equation 1 by k and write the second derivative as the derivative of the first derivative to obtain:

$$\frac{d}{dx}\left(\frac{dT}{dx}\right) = -\frac{q}{k}x \tag{16}$$

Step 2) Integration. We can then multiply both sides by dx, and integrate to obtain:

$$\left(\frac{dT}{dx}\right) = -\frac{q}{k}\frac{x^2}{2} + c \tag{17}$$

where c is an integration constant.

Step 3) Boundary condition. Applying the no-flux boundary condition at $x = L$ we can solve to show that:

$$c = \frac{qL^2}{2k} \tag{18}$$

We also note that at $x = 0$ the derivative $\left(\frac{dT}{dx}\right) = \frac{qL^2}{2k}$ or $-k\left(\frac{dT}{dx}\right) = -\frac{qL^2}{2}$. This will be used later in the other boundary condition.

Step 4) Another integration. Since the derivative dT/dx is already isolated, we can integrate equation 17 to solve for the temperature distribution:

$$T = -\frac{q}{2k}\left(\frac{x^3}{3} - L^2 x\right) + d \tag{19}$$

where d is an integration constant. We note that at x = 0, $T = d$.

Step 5) Other boundary condition. Applying the mixed boundary condition at $x = 0$ we can show that $-k\frac{dT}{dx} = h(T_\infty - T)$ can be manipulated to give:

$$-\frac{qL^2}{2} = h(T_\infty - d) \tag{20}$$

and upon solving for $d = T_\infty + \frac{qL^2}{2h}$ we can write down the temperature distribution as:

$$T = T_\infty - \frac{q}{k}\left(\frac{x^3}{6} - \frac{L^2}{2}x\right) + \frac{qL^2}{2h} \tag{21}$$

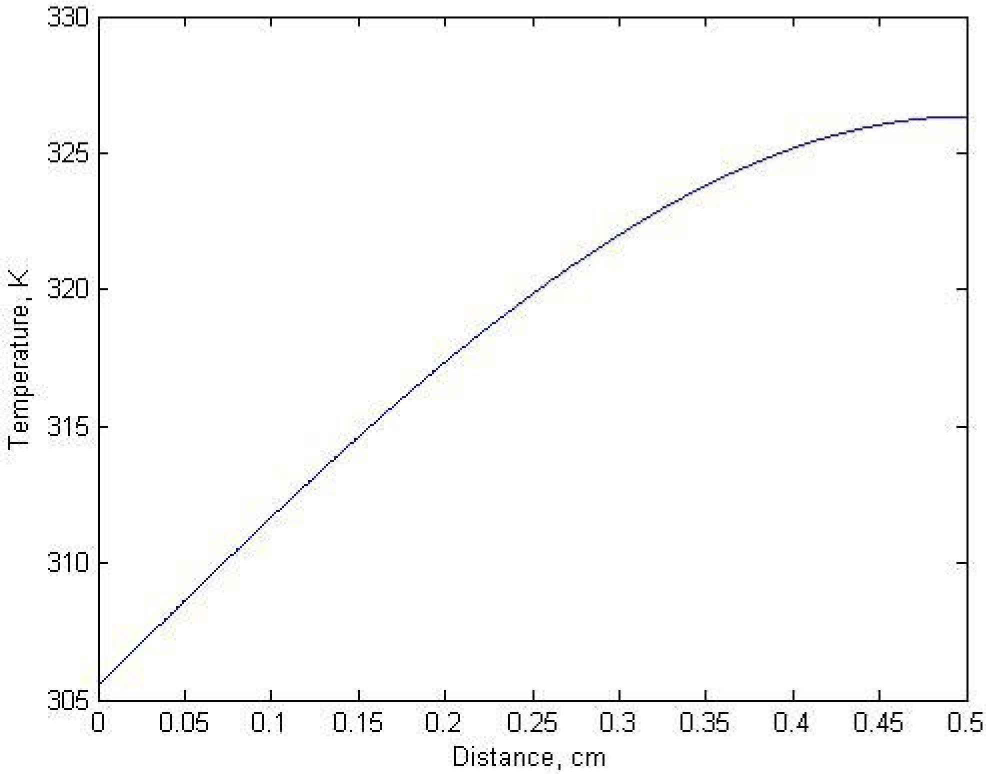
Part 2)
Step 1) Manipulation. We first note that the maximum temperature T_{max} will occur at the insulated boundary, where $x = L$. Performing this substitution into equation 21 gives:

$$T_{\max} = T_\infty + \frac{qL^3}{3k} + \frac{qL^2}{2h} \tag{22}$$

Step 2) Calculation. We can now substitute the known parameters to determine the value of the heat transfer coefficient. Equation 22 becomes:

$$T_{\max} = 293\text{K} + \frac{100\frac{\text{W}}{\text{cm}^4}(0.5\text{cm})^3}{3\times\frac{0.2\text{W}}{\text{cmK}}} + \frac{100\frac{\text{W}}{\text{cm}^4}(0.5\text{cm})^2}{2\times\frac{1\text{W}}{\text{cm}^2\text{K}}} = 326\text{K} \tag{23}$$

Part 3)
The following is a plot of equation 21, showing T as a function of x. Note that the shape of the graph is cubic, but still retains a zero slope at $x = L$ for the insulated boundary.


Temperature, K
330
325
320
315
310
305
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
Distance, cm