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

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Outline

- Introduction and Motivation
- What is in each module?
- Where are the modules?
- What are the modules?
- Module walk-through
- Conclusions / Acknowledgments

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Introduction and Motivation

- Alternative energy component missing from most departments
- Fuel Cells have been discussed in the political arena as an alternative energy solution
  - Need to educate ChE's in this area
- Growth in number of fuel cell textbooks
  - Most do not have homework problems
- Modules can rapidly infuse new technologies into the Chemical Engineering Curriculum

What is in each module?

- Problem motivation
- Reference to related sections and pages in popular ChE texts
- Example problem statement
- Example problem solution
- Home problem statement
- Home problem solution
- Link to web resources
- Non-ChE textbook resources
- Notes to instructor

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Where are the modules?

- Current beta test website:
  http://www.chem.mtu.edu/~jmkeith/fuel_cell_curriculum
- Currently available for use by anyone!
- Ultimately linked through CACHE website

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What are the modules?

- Mass and Energy Balances
  - Module 1: Heat of Formation for Fuel Cell Applications
  - Module 2: Material Balances in a Solid Oxide Fuel Cell
  - Module 3: Energy Balances in a Solid Oxide Fuel Cell
  - Module 4: Generation of Electricity Using Recovered Hydrogen

What are the modules?

- Thermodynamics
  - Module 5: Equation of State for Hydrogen Fuel
  - Module 6: Equilibrium Coefficient and Van’t Hoff Equation for Fuel Cell Efficiency
  - Module 7: Fuel Cell Efficiency
  - Module 8: Vapor Pressure / Humidity for Fuel Cell Gases
  - Module 9: Nernst Equation

What are the modules?

Some Modules Still Under Construction

- Fluid Mechanics
  - Module 10: Pressure Drop in Bipolar Plate Channel
  - Module 11: Finite Difference Method for Flow in a Fuel Cell Bipolar Plate
- Kinetics and Reaction Engineering
  - Reaction Kinetics in a Solid Oxide Fuel Cell
  - Reactor Design Applied to a Solid Oxide Fuel Cell
  - Tafel Equation and Fuel Cell Kinetic Losses
  - Hydrogen Adsorption and Catalyst Surface Coverage

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What are the modules?

Some Modules Still Under Construction

- Separations
  - Hydrogen Purification
  - Natural Gas Assisted Steam Electrolysis
  - Air Separation Module
- Heat and Mass Transport
  - Conduction and Convection Heat Transfer in Fuel Cells
  - Microscopic Balances Applied to Fuel Cells
  - Diffusion Coefficients for Fuel Cell Gases

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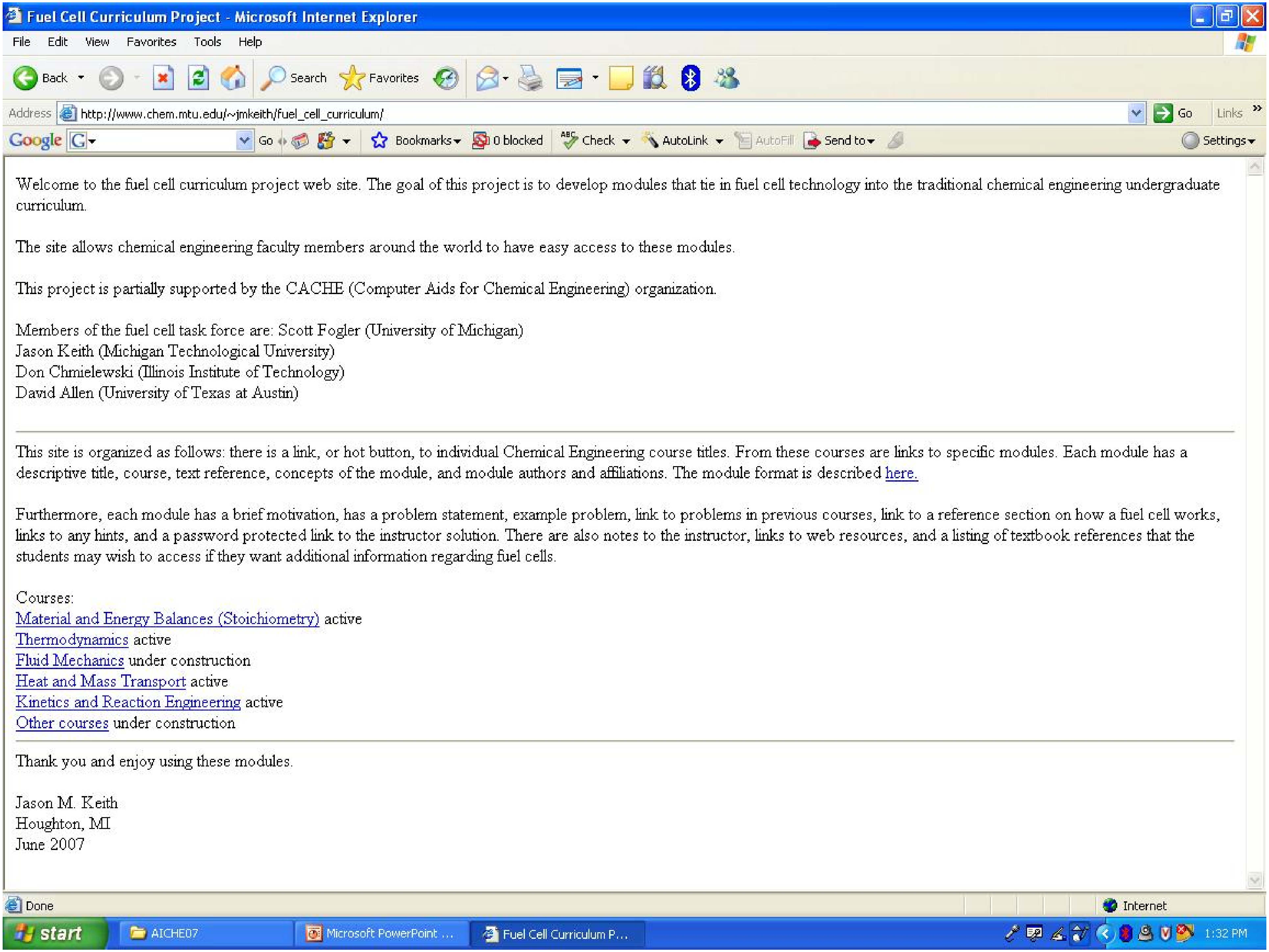


Welcome to the fuel cell curriculum project web site. The goal of this project is to develop modules that tie in fuel cell technology into the traditional chemical engineering undergraduate curriculum.

The site allows chemical engineering faculty members around the world to have easy access to these modules.

This project is partially supported by the CACHE (Computer Aids for Chemical Engineering) organization.

Members of the fuel cell task force are: Scott Fogler (University of Michigan)
Jason Keith (Michigan Technological University)
Don Chmielewski (Illinois Institute of Technology)
David Allen (University of Texas at Austin)

This site is organized as follows: there is a link, or hot button, to individual Chemical Engineering course titles. From these courses are links to specific modules. Each module has a descriptive title, course, text reference, concepts of the module, and module authors and affiliations. The module format is described here.

Furthermore, each module has a brief motivation, has a problem statement, example problem, link to problems in previous courses, link to a reference section on how a fuel cell works, links to any hints, and a password protected link to the instructor solution. There are also notes to the instructor, links to web resources, and a listing of textbook references that the students may wish to access if they want additional information regarding fuel cells.

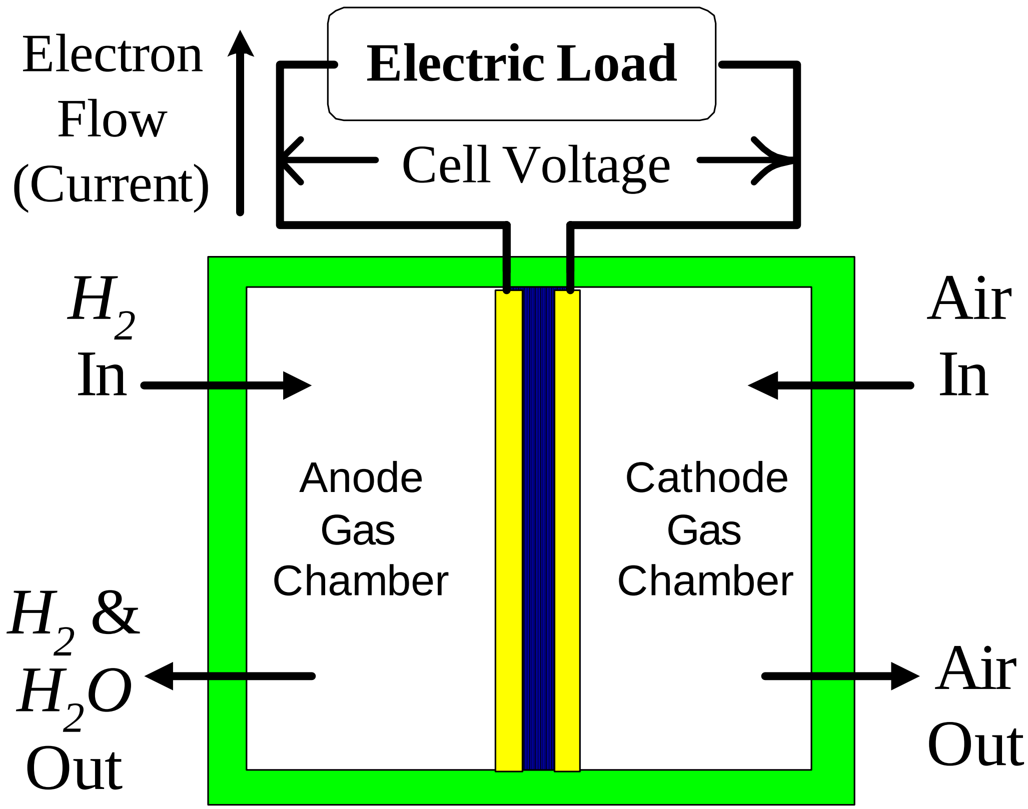
Courses:
Material and Energy Balances (Stoichiometry) active
Thermodynamics active
Fluid Mechanics under construction
Heat and Mass Transport active
Kinetics and Reaction Engineering active
Other courses under construction

Thank you and enjoy using these modules.

Jason M. Keith
Houghton, MI
June 2007

Module walk-through

- Mass Balances on a Solid Oxide Fuel Cell



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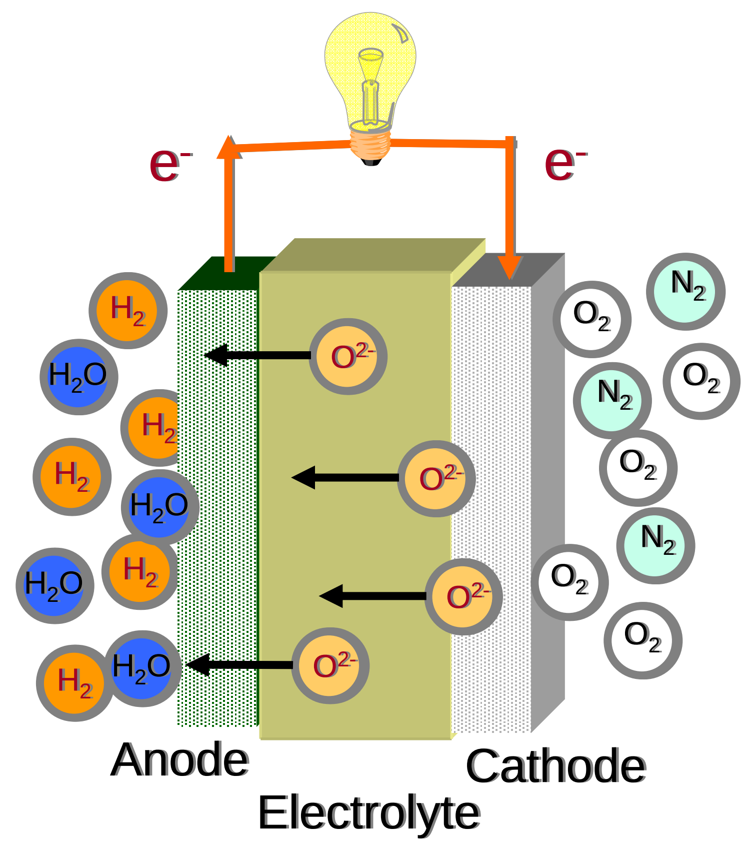
Module walk-through

- Mass Balances on a Solid Oxide Fuel Cell



The SOFC reactions are:

Anode: $H_2 + O^{-2} \rightarrow H_2O + 2\,e^-$

Cathode: $\frac{1}{2}\,O_2 + 2\,e^- \rightarrow O^{-2}$

Overall: $H_2 + \frac{1}{2}\,O_2 \rightarrow H_2O$

Module walk-through

Course: Material and Energy Balances (Stoichiometery)

Title: Mass Balances on a Solid Oxide Fuel Cell

Motivation: Use mass balance concepts and "fuel utilization" to determine mass flow rates, current, and power in a solid oxide fuel cell

Reference: Felder and Rousseau, Section 4.7(3rd ed.)

Each module has reference to popular text(s) for the course

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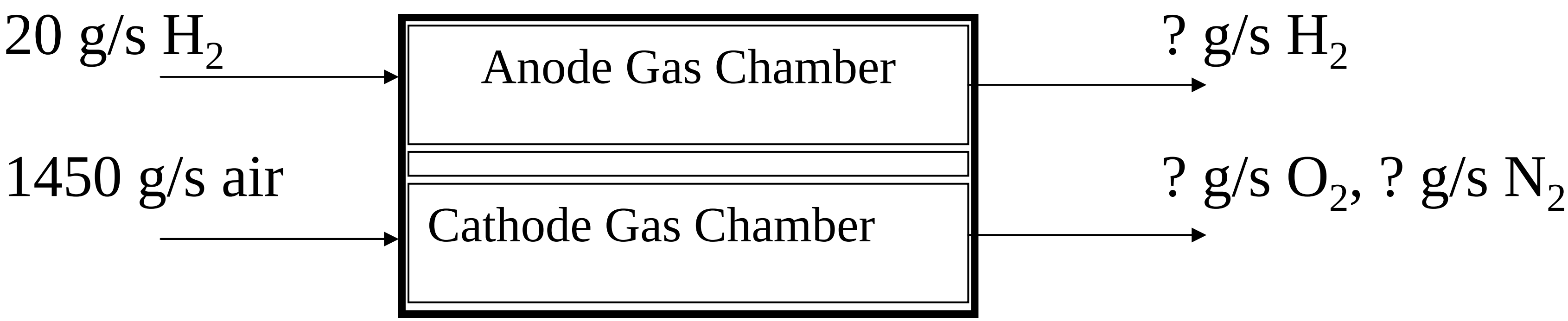
Module Example Problem

Each example has an easy to follow step-by-step approach

Example Problem: A SOFC is operated with an inlet flow of 20 g/s H_2 to the anode and 1450 g/s air to the cathode. The fuel utilization is 50%.



Determine the current and power delivered for a cell voltage of 0.8 V

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Module Example Solution

- **Part 1**) *Determine mass flow rate out of anode*
- Step 1) *Convert mass to moles*

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

- Step 2) *Determine hydrogen consumption*

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

Step 3) *Unconverted hydrogen is 10 – 5 = 5 mol/s*

Exiting water is 5 mol/s

Module Example Solution

- Step 4) *Convert moles to mass*

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

and

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

Step 5) *Total cathode exit flow rate = 100 g/s*

Module Example Solution

- **Part 2**) *Determine mass flow rate out of cathode given an oxygen mass fraction of 0.233*
- Step 1) *Convert mass to moles*

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

and

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

Step 2) *Oxygen conversion is 5(0.5) = 2.5 mol/s*

Exit oxygen rate = 10.6 – 2.5 = 8.1 mol/s

Module Example Solution

- Step 3) *Convert moles to mass*

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

and

$$\frac{39.7\,mole\ N_2\ exiting}{s} \times \frac{28\ g\ N_2}{mole\ N_2} = \frac{1112\ g\ N_2\ exiting}{s}$$

Step 4) *Determine oxygen utilization*

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

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Module Example Solution

- Step 5) *Determine exiting mass flow rate of 259 + 1112 = 1369 g/s*
- **Part 3**) *Determine Current*
- Step 1) *There are 2 moles of electrons formed per mole of hydrogen reacted*
- Step 2) *Using Faraday's constant find the current (1 A = 1 Coulomb / s)*

$$\frac{10\ mole\ e^-}{s} \times \frac{96{,}485\ coulombs}{mole\ e^-} = \frac{964{,}850\ coulombs}{s}$$

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Module Example Solution

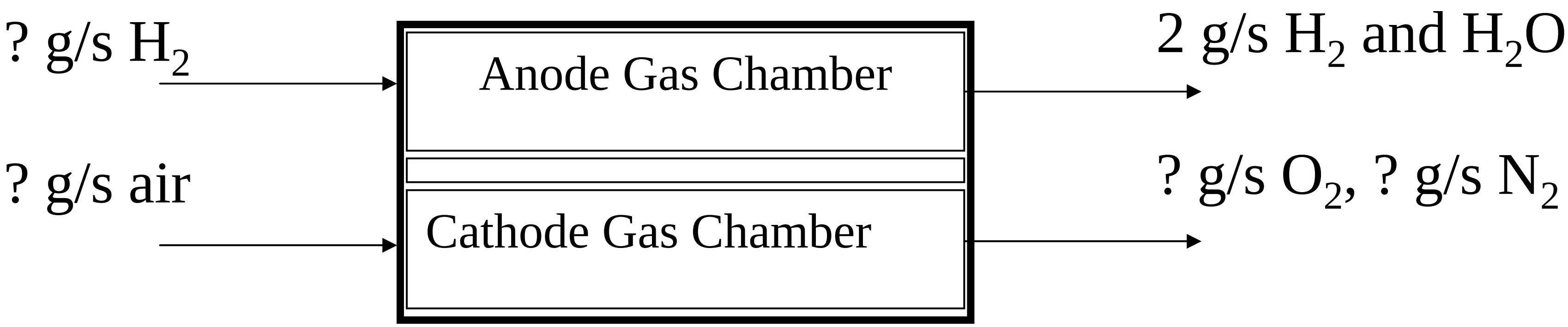
- **Part 4**) *Determine Power*
- Step 1) *Noting that Power = Current (Voltage) yields:*

$$\frac{964{,}850\ coulombs}{s} \times 0.8\ volts = \frac{770{,}000\ coulomb\ volts}{s}$$

- *Total power = 0.77 MW*

Module Home Problem

Home Problem: A SOFC has a feed of pure H_2 and an anode exit flow of 2 g/s (hydrogen and water vapor). The cell voltage is 0.75 V and the power is 10 kW.



Determine:

1) The mass flow rate into the anode chamber

2) The mass flow rate into the cathode chamber if 20% oxygen utilization is desired

Module Assessment

- During fall 2007, 27 MTU students took CM3974 Fuel Cell Fundamentals
- 7 homework problems
  - 5 were full module
  - 2 were home problem only
- IRB Approval through MTU #M0243 for student survey
- 2 Problems used in a MEB course at IIT, very positive comments from instructor

Module Assessment

- I felt the instructional material helped facilitate my learning
  - Strongly Agree (9), Agree (10), Ambivalent (0), Disagree (0), Strongly Disagree (0)
- I felt that the homework problems allowed me to apply my engineering principles to fuel cell and / or fuel cell system design
  - Strongly Agree (8), Agree (11), Ambivalent (0), Disagree (0), Strongly Disagree (0)
- Additional comments very positive

Conclusions / Acknowledgments

- Fuel Cell Modules are for your use!
- Contact one of the authors to participate
- Acknowledgments of Partial Support:

  - CACHE Corporation
  - JMK: DOE(DE-FG02-04ER63821 and DE-FG36-08GO18108), NSF(DMI-0456537), and the Michigan Space Grant Consortium
  - DJC: Argonne National Laboratory
  - HSF / VT: Vennema Professorship and Thurnau Professorship

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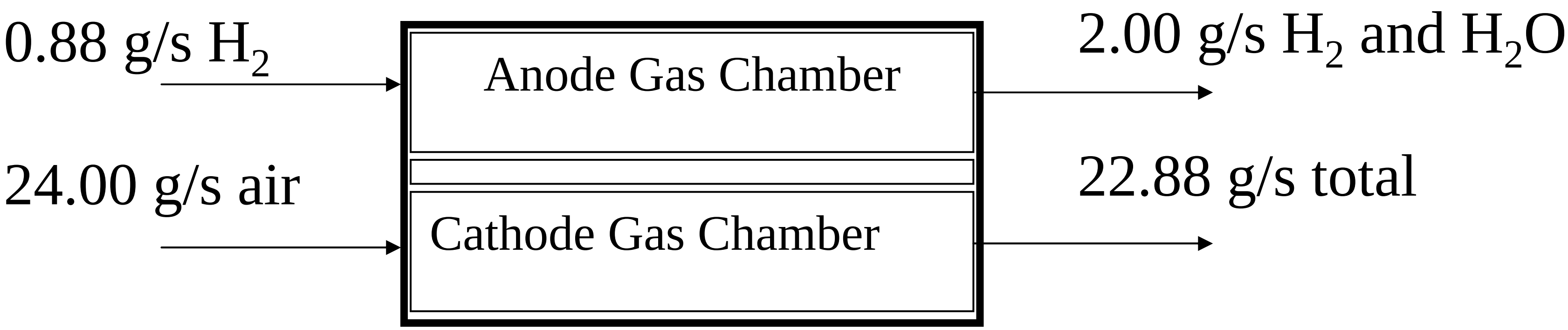
Module Home Problem Solution

Home Problem: A SOFC has a feed of pure H_2 and an anode exit flow of 2 g/s (hydrogen and water vapor). The cell voltage is 0.75 V and the power is 10 kW.



1) Determine current, convert to mol/s electrons (and hydrogen)
2) Control volume balance to determine inlet air rate
3) With oxygen mol/s reacted, find feed amounts (and nitrogen)
4) Overall balance to get cathode exit