ME 140 | Advanced Thermal Systems

Project #5 & #6: PEM Fuel Cell Evaluation and Hydrogen Production Analysis

Jon Renslo, Frankie Willcox, Emily Bohl, Kendall Fagan, and Natasha Berk

PART A: PEM Fuel Cell Performance

Figure 1. Current vs. Load

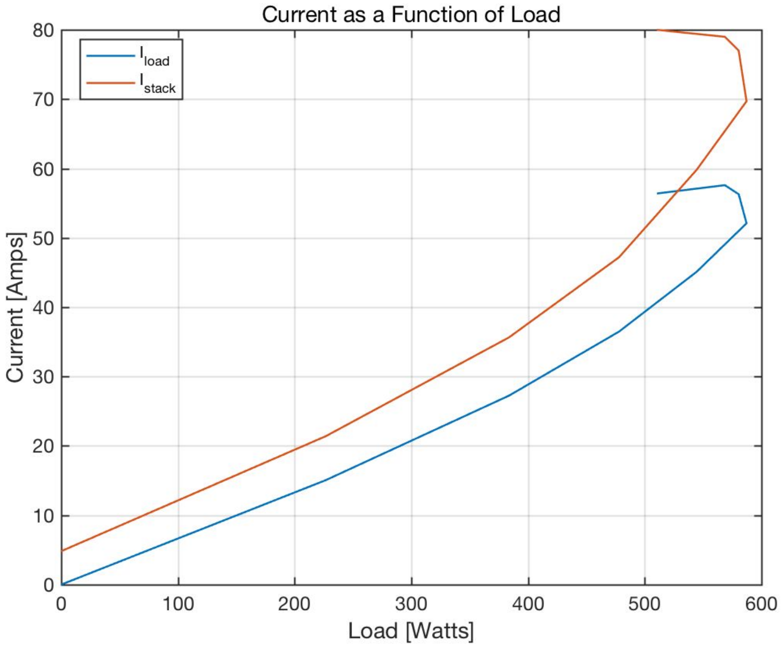


Figure 2. Voltage vs. Load

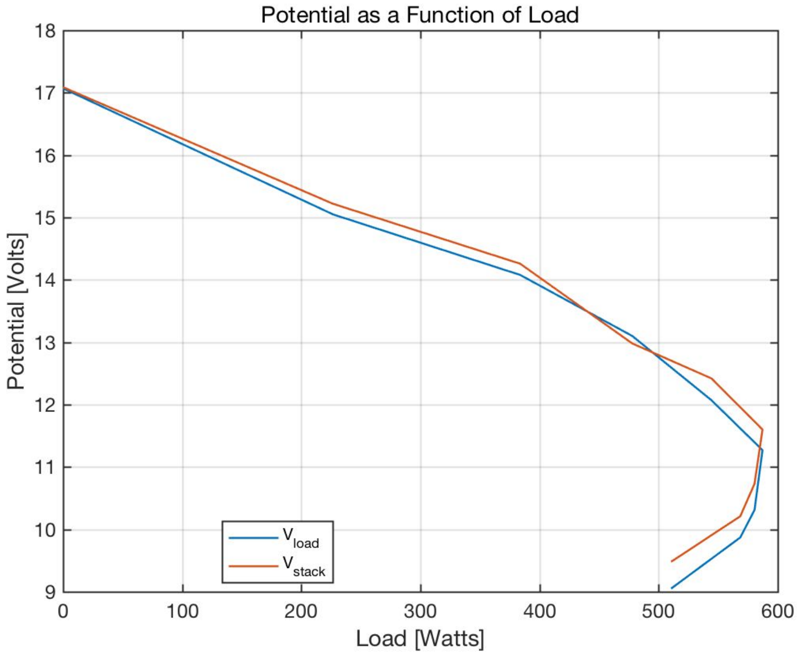


Figure 3. Power vs. Load

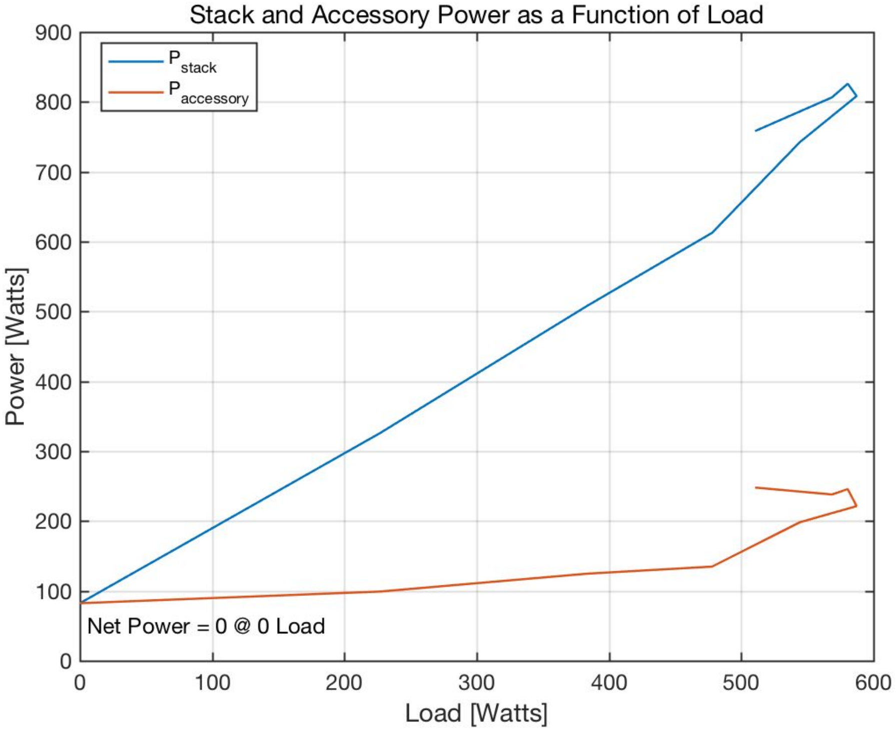


Figure 4. Mass Flow Rate vs. Load

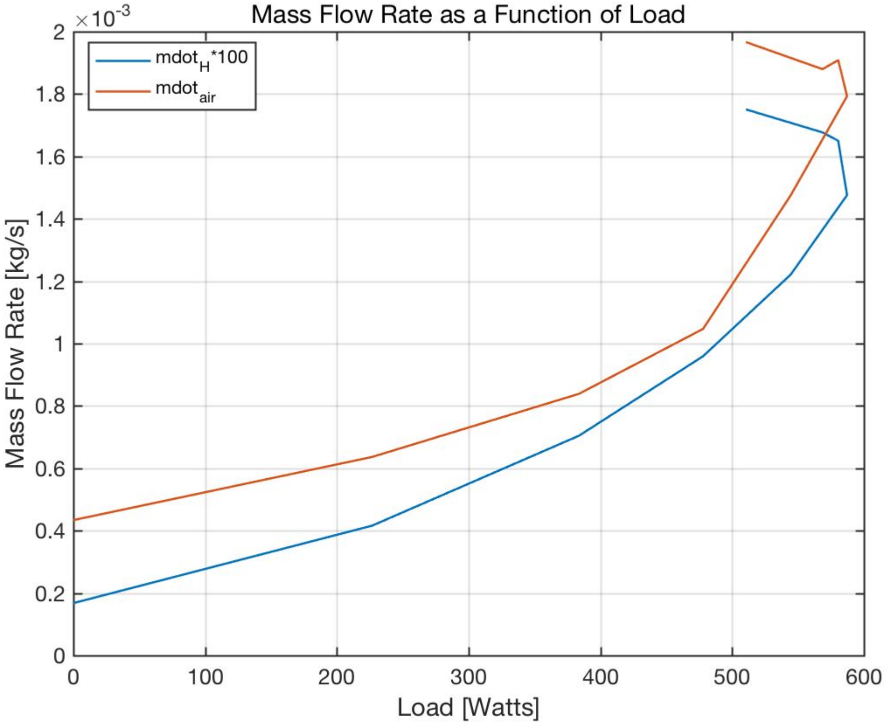


Figure 5. Excess Air Coefficient (Lambda) vs. Load

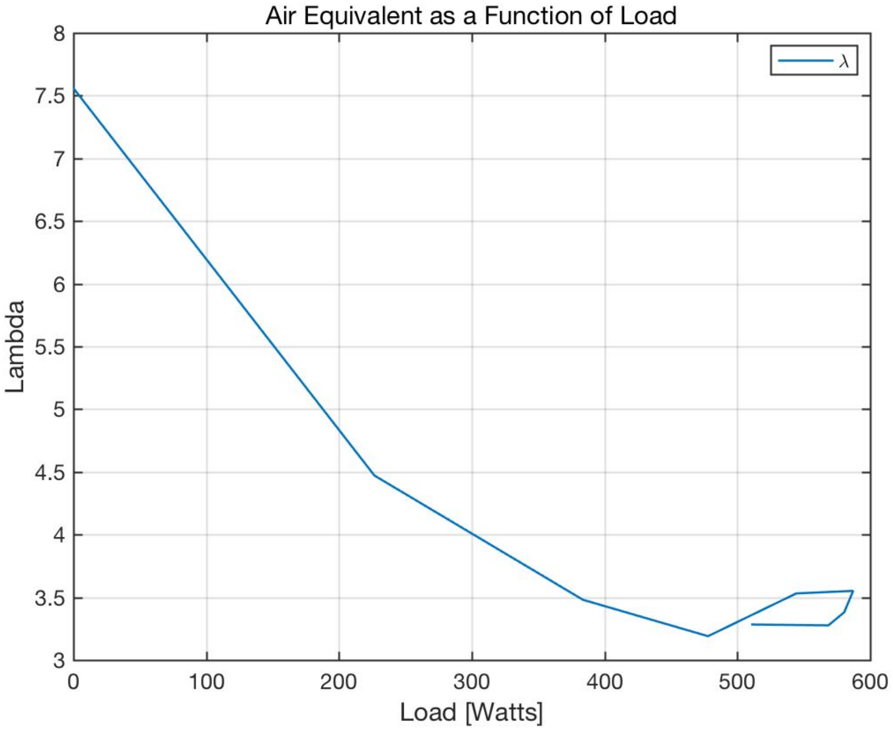


Figure 6. Efficiency (First and Second Law) vs. Load

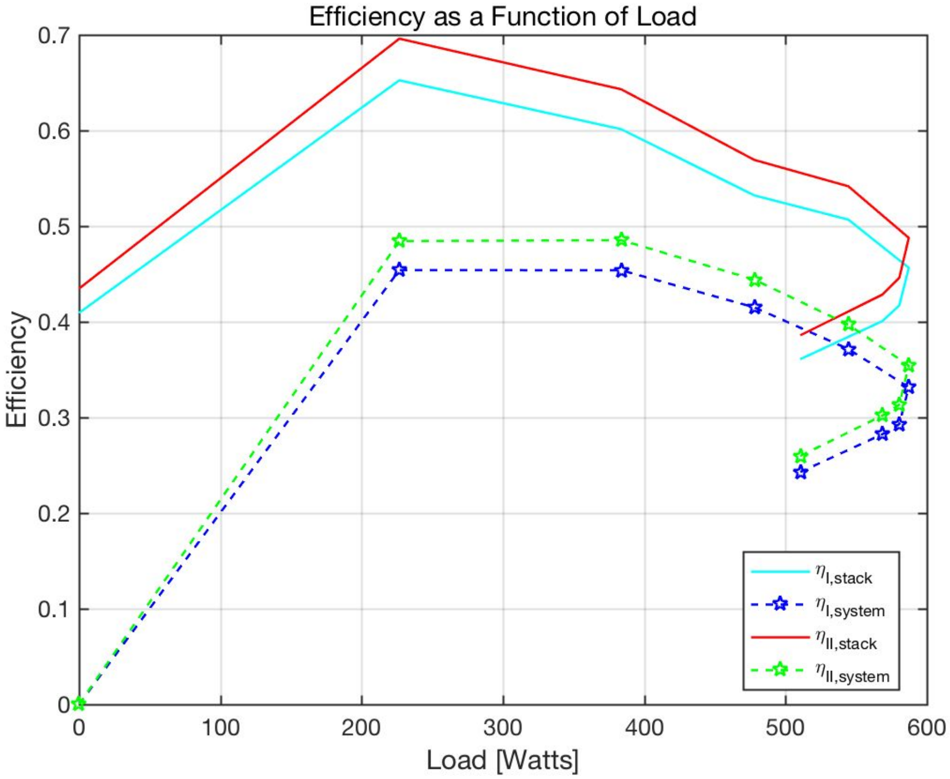


Figure 7. Power Loss (Inefficiency) vs. Load

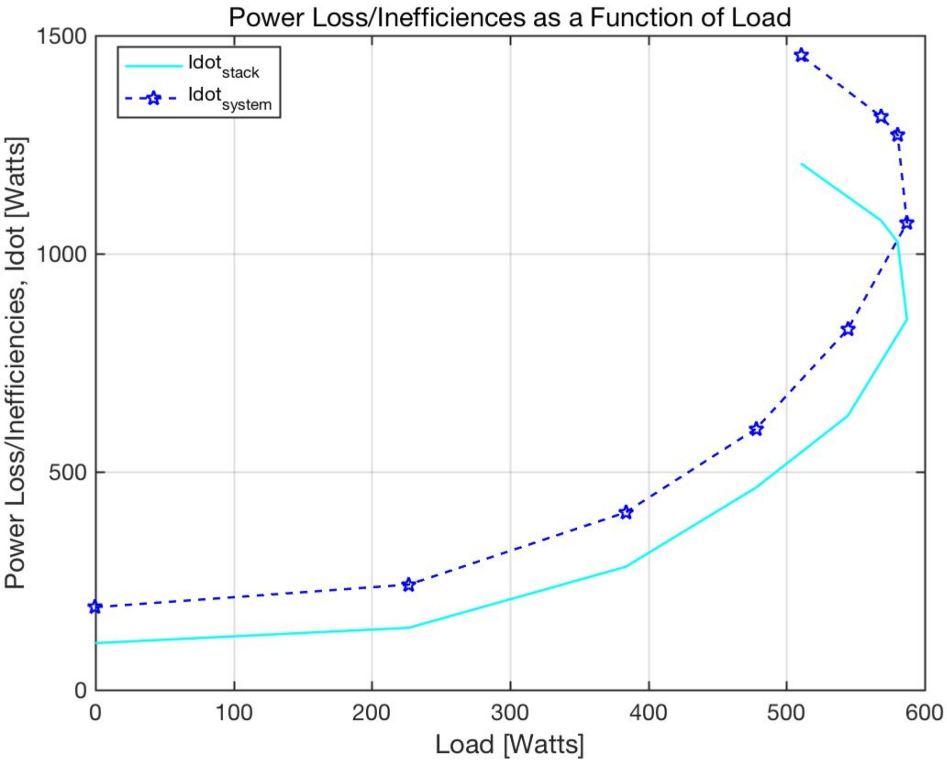
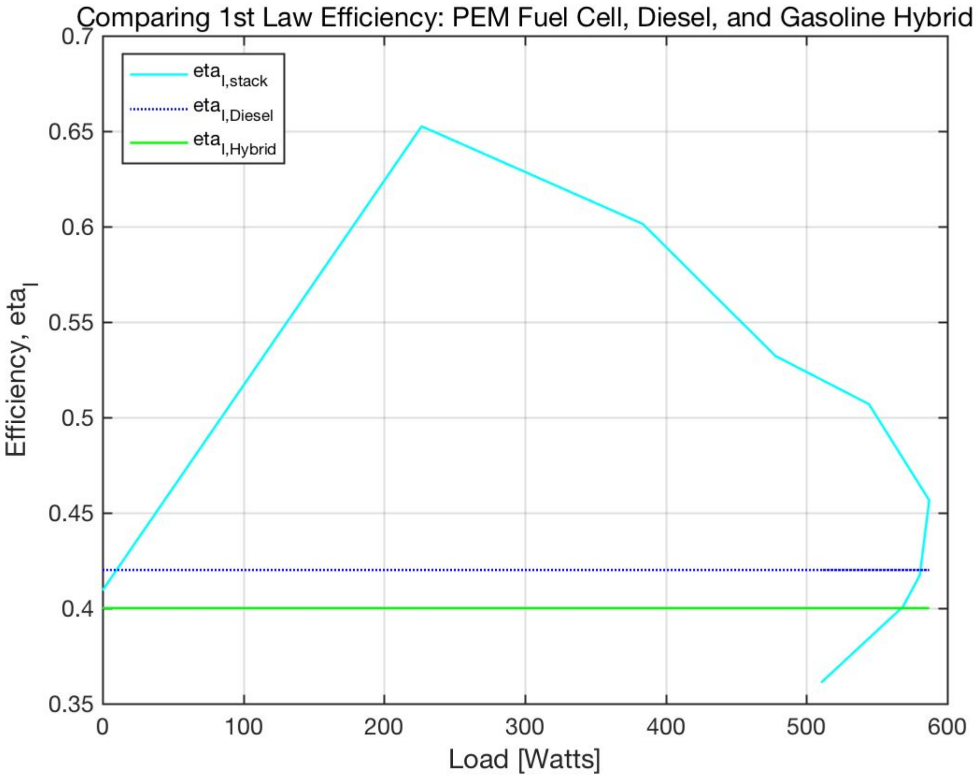


Figure 8. Comparison with Gas and Diesel



Challenges with Scaling Up H-Power System

A large amount of cooling would be required to scale up a hydrogen powered system for use in a car. Components like the humidifier and heat exchanger would have to require a significant amount of power to run and dissipate the necessary amount of heat.

We would need anywhere from 508 to 1316 fuel cells to be equivalent to a diesel engine. We would need 154 to 398 fuel cells to be equivalent to a gasoline hybrid engine, which makes sense because it is less power intensive.

The accessories and auxiliary components of the cell are also a significant consideration. The table full of heat exchangers, humidifiers, water pumps, and fuel regulators during lab gave a sense for the size of all the accessories. While scaling up the accessories would see some economies of scale given a 50gph pump is smaller than 50 - 1gph pumps, scaling up all these devices would still be a considerable increase in size, expense, and weight.

Figure 9. Table of Typical and Theoretical First Law Efficiencies

	Fuel Cell	Diesel Engine	Gasoline Hybrid Engine
First Law Efficiency	65%	42%	40%

Note: All sources are listed in our Matlab code in the appendix.

PART B: Hydrogen Forming Reactions

Figure 10. Equilibrium Constants vs. Temperature for SMR and WGS Reactions

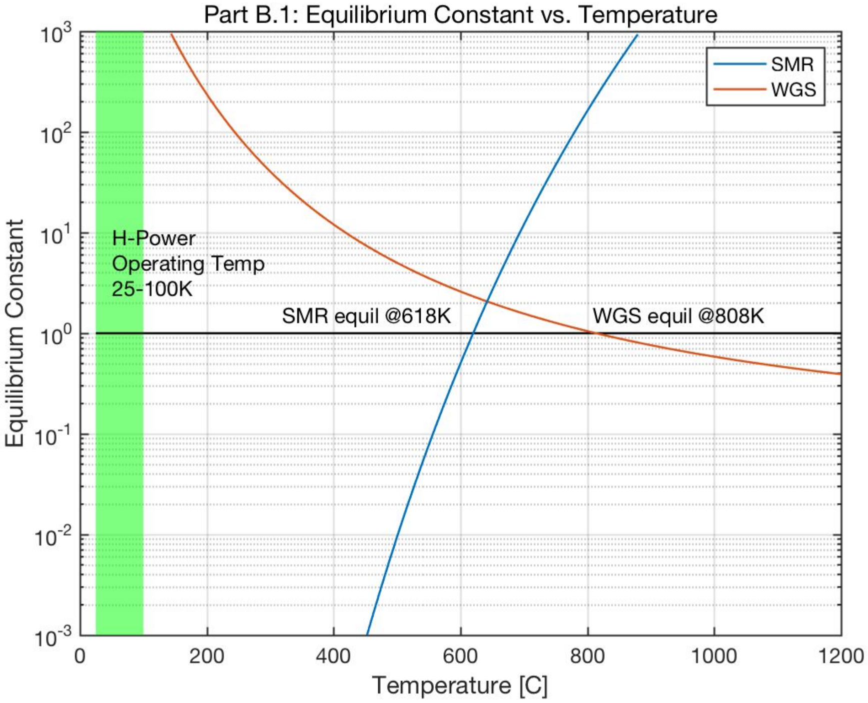


Figure 11. Equilibrium Mole Fractions (SMR) vs. Temperature

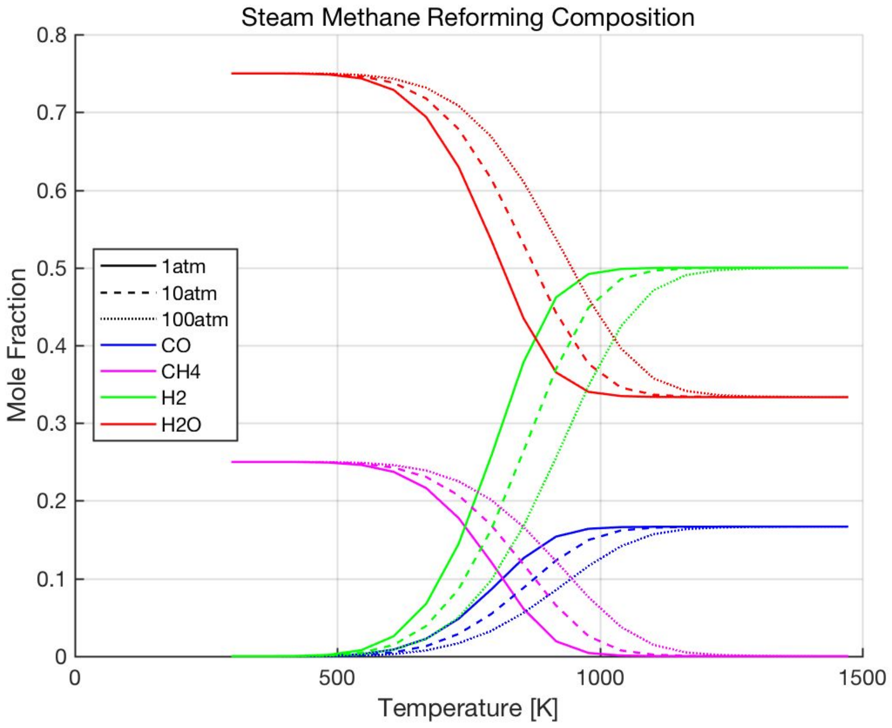


Figure 12. Equilibrium Mole Fractions (WGS) vs. Temperature

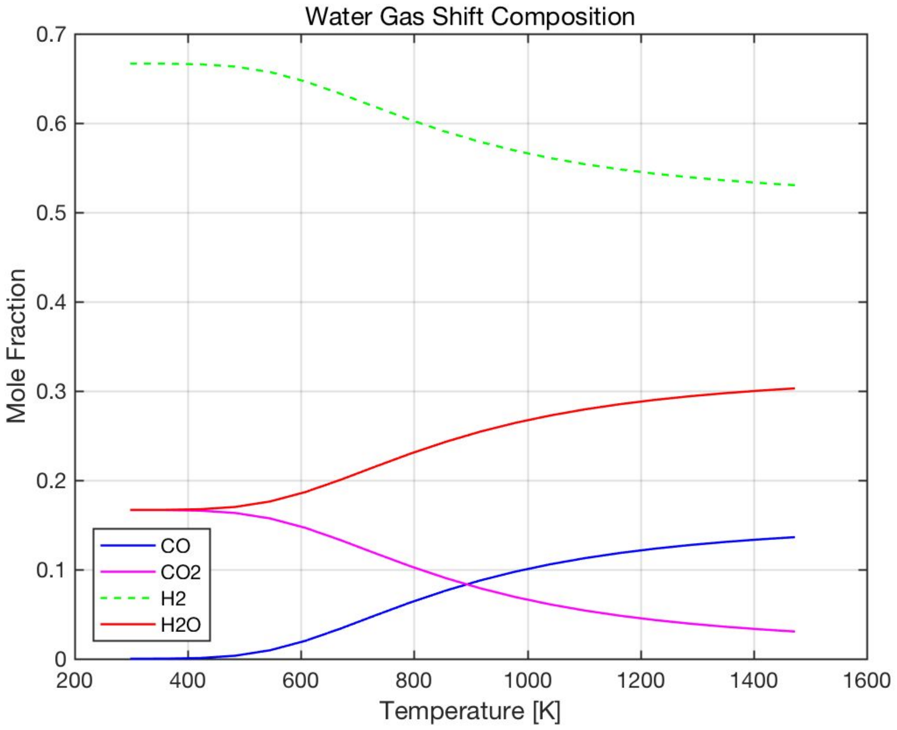


Figure 13. Exit Composition vs. Station (Adiabatic & Isothermal)

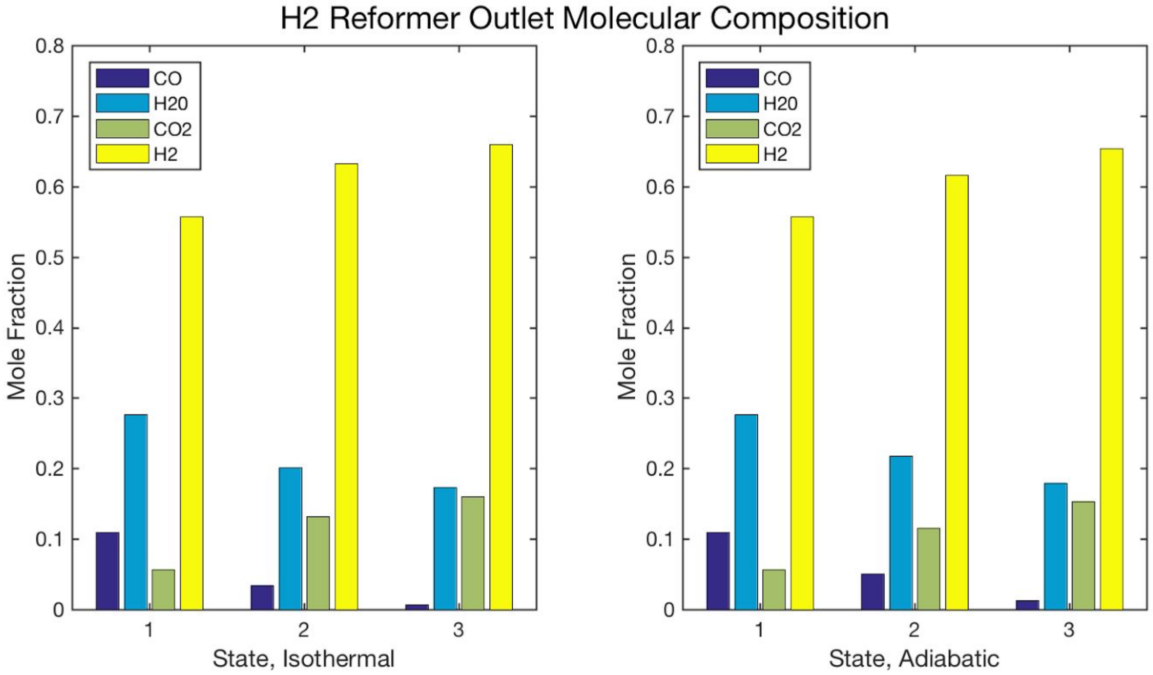


Figure 14. Table of Metrics at Each Station

	Reformer	**1st Shift Reactor**		**2nd Shift Reactor**	
	Isothermal	Isothermal	Adiabatic	Isothermal	Adiabatic
Inlet Temperature [C]	800	400	400	250	250
Exit Temperature [C]	800	400	467.4	250	295.7
Mole % CO2	0.0570	0.1321	0.1159	0.1599	0.1537
Mole % H2O	0.2763	0.2012	0.2174	0.1735	0.1796
Mole % CO	0.1096	0.0345	0.0507	0.0068	0.0130
Mole % H2	0.5570	0.6321	0.6159	0.6599	0.6537
Heat Addition for Isothermal Reaction [MJ/kg reactants]	3.06	-0.247	NA	-0.095	NA
Methane Burned to Heat (%)	21.09	NA	NA	NA	NA
Efficiency: LHV H2/CH4 used	NA	NA	NA	94.14	93.26

Individual Reflections

- Kendall: I spent 14 hours on this project. I was surprised by how many fuel cells it would take to power a car using this calculation, given there are cars that currently run on fuel cells, they must be using much more effective fuel cells and it would interesting to go over these fuel cells and how they differ.

- Frankie: I spent 14 hours on this project. I would like to learn more of the specifics of what would required to implement a hydrogen fuel cell in a vehicle and innovative ways that this might be done.

- Emily: I spent 14 hours on this project. I liked how this project pulled together a lot of thermo and chemistry concepts! It was also cool to be able to see the fuel cell in the lab. I would like to have a better understanding of how humidifiers work, because I thought it was interesting that we were able to run one backwards.

- Jon: I spent 20 hours on this project. I enjoyed the modeling problems of the equilibrium reactions, particularly the method using atom balances and the nernst equation as a system to find compositions under different pressure and temperature conditions. I'd like to understand how we might solve two, or multiple equilibrium reactions simultaneously (i.e. without assuming the SMR goes to completion in the first reactor). I'd also like to see the fuel cell working. :-((perhaps a demo later on?)

- Natasha: I spent 15 hours on this project. I thought understanding how a fuel cell works in this much detail was interesting. I thought it required a bit too much depth in chemistry though - beyond what is useful to me.

Appendix: Matlab Scripts

```
% ME 140 Project #5
% FUEL CELL EVALUATION & HYRDOGEN PRODUCTION ANALYSIS
% Frankie Willcox, Jon Renslo, Kendall Fagan, Emily Bohl, Natasha Berk

%Jon's todo list
% double check power loss (inefficiencies)
% ask about starting from STP (extra methane used?)

% ASSUME:
% (i)  mol_H2 = 1
clear; close all; clc;
format compact;
entireTime = tic;

global PERMIN_TO_PERSEC PERHR_TO_PERSEC G_PER_KG LHV F N_TO_O
 SCF_TO_MOLS ...
    C_TO_K PSI_TO_PA MM_h MM_h2 MM_o MM_n MM_ch4 MM_h2o MM_air PATM
 HORSEPOWER_TO_W
defineGlobals();
mol_H2 = 1;
savePlots = 0;
                % 1,2,3,4,5,6,7,8,9,10,11

supressplots =   [1,      1,     1,   1];         % supresses plots by
 section

% Part A, Section 1
% Currents (load & stack)
i_load =  [0.00 15.06 27.25 36.48 45.1 52.1 56.3 57.6 56.4];       %
 [Amps]
i_stack = [4.82 21.40 35.65 47.20 59.8 69.7 77.0 79.0 80.0];


% Potentials (load & stack)
v_load =  [17.07 15.05 14.08 13.10 12.07 11.27 10.31 9.87  9.05 ]; %
 [Volts]
v_stack = [17.09 15.22 14.26 12.98 12.42 11.60 10.73 10.21 9.48];


% Temperatures from Thermocouple Readings [C]
% KEY: (Kendall please fill in with photo you took)
T1_C = [42.8 42.9 46.1 48.5 50.5 52.8 54.8 55.8 56.5];
T2_C =     [42.5 45.8 45.8 48.4 50.3 51.9 53.3 53.9 54.3];
Tstack_C = [40.7 41.3 42.5 42.9 44.6 45.6 46.9 46.9 47.6];

T1 = T1_C + C_TO_K;                                                 %
 [K],  T1, air into stack
T2 = T2_C + C_TO_K;                                                 %
 [K],  T2, air out of stack
Tstack = Tstack_C + C_TO_K;                                         %
 [K],  metal plates on the stack
```

```
% NOTE: T3-T5 are not needed for now
% T3_C =     [48.0 47.1 48.6 48.9 50.4 51.1 51.2 51.1 51.1];       %
 T3, water reservoir DON'T USE!
% T3 = T3_C + C_TO_K;
T4_C =     [48.0 47.2 48.2 48.9 50.4 51.1 51.2 51.1 51.1];
T5_C =     [40.7 41.3 42.5 42.9 44.6 45.6 46.9 46.9 47.6];
T4 = T4_C + C_TO_K;                                                %
 T4, water into stack
T5 = T5_C + C_TO_K;                                                %
 T5, water into heat exchanger


% Mass Flow Rates (TODO: check what units the mdots should be in)
mdot_total_scf = [0.75 1.10 1.45 1.81 2.55 3.10 3.30 3.25 3.40];   %
 [scf/min]
mdot_fuel_scf =  [2.50 6.20 10.5 14.3 18.2 22.0 24.6 25.0 26.1];   %
 [scf/hr] (standard cubic feet/hour)

mdot_total = mdot_total_scf * SCF_TO_MOLS * PERMIN_TO_PERSEC *
 ( MM_air / G_PER_KG);  % [kg/s]
mdot_fuel = mdot_fuel_scf * SCF_TO_MOLS * PERHR_TO_PERSEC * (MM_h2  /
 G_PER_KG);      % [kg/s]
mdot_h2o = 40 /G_PER_KG;
                % [kg/s]

% Pressures
Pfuel_psi =  [2.9 2.9 3.1 3.3 3.30 3.20 3.00 3.0 3.1];              %
 [psi] (gauge)
Ptotal_psi = [0.2 0.3 0.6 0.7 1.15 1.25 1.35 1.3 1.5];              %
 [psi] (gauge), pressure of combined air and H2O after humidifier
Pfuel =  Pfuel_psi  .* PSI_TO_PA + PATM;                            %
 [Pa]
Ptotal = Ptotal_psi .* PSI_TO_PA + PATM;                            %
 [Pa]

% CALCULATIONS
% ------------
% Power (USE: p = i*v)
% NOTE: "Accessories" include H2O pump, air pump, H2 vent, &
 controller
p_load =  i_load  .* v_load;                                        %
 [W] = [kg*m^2*s^-3], a.k.a. "load" (power delivered to resistor bank)
p_stack = i_stack .* v_stack;
p_access = p_stack - p_load;                                        %
 [W], Acessory Power, i.e. power used to run controls. Pstack-Pload
if(~supressplots(1))
    hold off;
    f1 = figure(1);
    plot(p_load,i_load,p_load,i_stack);
    title('Current as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Current [Amps]');
    legend('I_{load}','I_{stack}','Location','best'); grid on;

    f2 = figure(2);
    plot(p_load,v_load,p_load,v_stack);
    title('Potential as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Potential [Volts]');
    legend('V_{load}','V_{stack}','Location','best'); grid on;

    f3 = figure(3);
    plot(p_load,p_stack,p_load,p_access);
    title('Stack and Accessory Power as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Power [Watts]');
    text(5,50,'Net Power = 0 @ 0 Load');
    legend('P_{stack}','P_{accessory}','Location','best'); grid on;

    f4 = figure(4);
    plot(p_load, mdot_fuel*100, p_load, mdot_total);
    title('Mass Flow Rate as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Mass Flow Rate [kg/s]');
    legend('mdot_{H}*100','mdot_{air}','Location','best'); grid on;

end

% Part A, Section 2

% SOURCE: LEC 8, SLIDES 21 & 22

% 1st & 2nd Law Efficiencies (eta_I & eta_II) & Inefficiencies (Idot)
% Stack
[etaI_stack ,etaII_stack, Idot_stack,lambda_stack,dGstack] =
 findEtas(mdot_total, mdot_fuel, Ptotal, Pfuel, T2, p_stack);

% Entire System (Load)
[etaI_load ,etaII_load, Idot_load,lambda_load,dGload] =
 findEtas(mdot_total, mdot_fuel, Ptotal, Pfuel, T2, p_load);
if(~supressplots(2))
    f6 = figure(6);
    plot(p_load,lambda_load);
    title('Air Equivalent as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Lambda');
    legend('\lambda','Location','best');  grid on;

    f5 = figure(5);
    plot(p_load,etaI_stack,'c',p_load,etaI_load,'bp--',...
        p_load,etaII_stack,'r',p_load,etaII_load,'gp--');
    title('Efficiency as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Efficiency');
    legend('\eta_{I,stack}','\eta_{I,system}',...

  '\eta_{II,stack}','\eta_{II,system}', 'Location','Best');grid on;

    f7 = figure(7);
    plot(p_load,-dGstack-p_stack,'c',p_load,-dGload-p_load,'bp--');
    title('Power Loss/Inefficiences as a Function of Load');
    xlabel('Load [Watts]'); ylabel('Power Loss/Inefficiencies, Idot
 [Watts]');
    legend('Idot_{stack}','Idot_{system}','Location','best'); grid on;
```

```
end

% Part A, Section 3
% Comparing First Law Efficiencies of PEM Fuel Cell with Diesel &
 Hybrid Engines

% Typical modern Diesel engine (eta_disel = 42%) (chose diesel truck
 because it's better than a car and worse than a freight ship)
% Source Efficiency: Slide 3, http://www.sae.org/events/gim/
presentations/2011/RolandGravel.pdf
% Source Horsepower: https://cumminsengines.com/isx15-heavy-duty-
truck-2013#overview
eta_diesel = 0.42;
eta_diesel = linspace(eta_diesel, eta_diesel, length(p_load)); %Make
 it a line instead of points
Wdot_diesel = 400 * HORSEPOWER_TO_W;  % [W]

% Typical gasoline hybrid engine (eta_hybrid = max of 40%)
% Source Efficiency & Horsepower: Toyota Hybrid Vehicles, http://
www.toyota-global.com/innovation/environmental_technology/hybrid/
eta_hybrid = 0.40;
eta_hybrid = linspace(eta_hybrid, eta_hybrid, length(p_load)); % Make
 it a line
Wdot_hybrid = 121 * HORSEPOWER_TO_W;  % [W]

% Calcuate Heat Removal (Qdot) --> 40 g/s necessary only for
% intensive/extensive conversion
Qdot_fuelCell = zeros(length(T4));
for i = 1:length(T4)
    Qdot_fuelCell(i) = hEng(T4(i),'h2o') - hEng(T5(i),'h2o');
end
Qdot_fuelCell_max = max(Qdot_fuelCell);

% Theoretical Number of Fuel Cells Needed
% Finding total power of cell out = load power plus Qdot
powerOut = p_load + Qdot_fuelCell_max;

num_fuelCells_diesel = Wdot_diesel ./ powerOut;
num_fuelCells_hybrid = Wdot_hybrid ./ powerOut;

if(~supressplots(3))
    % Overall First Law Efficiency of the PEM Fuel Cell = Stack
 Efficiency
    f8 = figure(8);
    plot(p_load, etaI_stack, 'c', p_load, eta_diesel, 'b:', p_load,
 eta_hybrid, 'g');
    title('Comparing 1st Law Efficiency: PEM Fuel Cell, Diesel, and
 Gasoline Hybrid');
    xlabel('Load [Watts]'); ylabel('Efficiency, eta_{I}');

 legend('eta_{I,stack}','eta_{I,Diesel}', 'eta_{I,Hybrid}','Location','northwest')
  grid on;
end
```

```
% Comments: To scale this up, we would need somewhere between 280-540
 fuel
% cells to equal the diesel output, and 85-165 fuel cells to equal the
% hybrid output.

% Part B, Section 1
% Part B, Section 1 - Emily & Kendall
% Calculating Kp Values
% SOURCE Kp Formula: LECTURE 14, SLIDE 4

% SMR: CH4 + H2O --> CO + 3H2
% v values are stoichiometric coefficients
v_CO_SMR = 1;
v_H2_SMR = 3;
v_H2O_SMR = 1;
v_CH4_SMR = 1;

% Calculating Kp for SMR
% Nv_CO = mm
% SMRnumKp =

% WGS: H2O + CO --> H2 + CO2
v_H2_WGS = 1;
v_CO2_WGS = 1;
v_H2O_WGS = 1;
v_CO_WGS = 1;

T_B1 = linspace(25, 1200, 100); %Temperature for part B1 = T_B1
T_B1 = T_B1 + C_TO_K;
%NOTE: Standard pressure, is usually defined as 100,000, however in
 energyF
%we have standard presssure as 101300. Because the pressure needs to
%cancel out, I have changed this pressure to 101300, however, we
 should
%perhaps consider changing the reference pressure in energyF to
 100,000Pa.
P_ref = 101300; %This is the pressure defined for standard conditions.
% Standard conditions are what we need because that is what
% the little zero indicates in the equation for g.
R_u = 8.314; %Universal gas constant

%G_reaction = G_products - G_reactants
g_SMR = (gEng(T_B1, P_ref, 'co',v_CO_SMR) + gEng(T_B1,
 P_ref, 'h2',v_H2_SMR)) - ...
    (gEng(T_B1, P_ref, 'h2ovap',v_H2O_SMR) + gEng(T_B1,
 P_ref, 'ch4',v_CH4_SMR));

g_WGS = (gEng(T_B1, P_ref, 'h2',v_H2_WGS) + gEng(T_B1,
 P_ref, 'co2',v_CO2_WGS)) - ...
    (gEng(T_B1, P_ref, 'h2ovap',v_H2O_WGS) + gEng(T_B1,
 P_ref, 'co',v_CO_WGS));

%Lecture 13 - Slide 15
kp_SMR = exp(-g_SMR ./ (R_u .* T_B1)); %increases with temp
```

```
kp_WGS = exp(-g_WGS ./ (R_u .* T_B1)); %decrease with temp


%functions for convenience
f_kp_SMR = @(T_B1) exp(-((gEng(T_B1, P_ref, 'co',v_CO_SMR) ...
    + gEng(T_B1, P_ref, 'h2',v_H2_SMR))  ...
    - (gEng(T_B1, P_ref, 'h2ovap',v_H2O_SMR) ...
    + gEng(T_B1, P_ref, 'ch4',v_CH4_SMR)))...
    ./ (R_u.*T_B1));

f_kp_WGS = @(T_B1) exp(-((gEng(T_B1, P_ref, 'h2',v_H2_WGS) ...
    + gEng(T_B1, P_ref, 'co2',v_CO2_WGS)) ...
    -(gEng(T_B1, P_ref, 'h2ovap',v_H2O_WGS) ...
    + gEng(T_B1, P_ref, 'co',v_CO_WGS))) ...
    ./ (R_u.*T_B1));

%Prep for plot
%convert back to celcius
T_B1 = T_B1 - C_TO_K;
%find index of where kp=10^-3 and kp = 10^3, as the problem asks that
 we
%limit the graph to this range
[~,i_min_SMR] = min(abs(kp_SMR - 10^-3));
[~,i_max_SMR] = min(abs(kp_SMR - 10^3)); %yes, this is supposed to use
 min() to find the max ;P
[~,i_min_WGS] = min(abs(kp_WGS - 10^3));
[~,i_max_WGS] = min(abs(kp_WGS - 10^-3));

[zero_smr,izero_smr] = min(abs(log(kp_SMR)));
[zero_wgs,izero_wgs] = min(abs(log(kp_WGS)));

%Plot
if(~supressplots(3))
    f9 = figure(9);
    kpIsOne = ones(size(T_B1));
    semilogy(T_B1(i_min_SMR:i_max_SMR),
 kp_SMR(i_min_SMR:i_max_SMR), ...
        T_B1(i_min_WGS:i_max_WGS),
 kp_WGS(i_min_WGS:i_max_WGS),T_B1,kpIsOne,'k');
    xlabel('Temperature [C]')
    ylabel('Equilibrium Constant')
    text(T_B1(izero_smr) -300 , 1.5,...
        strcat('SMR equil @ ',num2str(round(T_B1(izero_smr))),'K'));
    text(T_B1(izero_wgs), 1.5,...
        strcat('WGS equil @ ',num2str(round(T_B1(izero_wgs))),'K'));
    legend('SMR', 'WGS')
    title('Part B.1: Equilibrium Constant vs. Temperature')
    ylim([0.001,1000]);
    text(50,5,{'H-Power','Operating Temp','25-100K'})
    grid on
    patch([25,100,100,25],
[10^-3,10^-3,10^3,10^3],'g','FaceAlpha',.5,'EdgeAlpha',0);
    set(gca,'children',flipud(get(gca,'children'))) %puts shading
 beneath lines
```

```
end
% Part B No. 2
% Find the Equilibrium Composition (Mol Fractions) of the Steam
 Methane
% Reformation(SMR) Reaction
% SOURCE Nernst Atom Balance: LECTURE 14, SLIDE 4 (equation in lower
 right corner)
npts = 20;
syms nco nch4 nh2 nh2o;
warning('off','symbolic:numeric:NumericalInstability');

temps = linspace(25,1200,npts);
temps = temps + C_TO_K;
pres = [1,10,100];
soln = zeros(length(temps),4,length(pres));
tic
for i =  1:length(temps)
    t = temps(i);
    parfor j = 1:length(pres)
        p = pres(j);

        warning('off','symbolic:numeric:NumericalInstability');
        eqs = [1  == nco   + nch4;...             carbon atom balance
            10 == nh2*2 + nch4*4 + nh2o*2; ... hydrogen atom balance
            3  == nco   + nh2o;...                oxygen atom balance
            nco.*nh2.^3./(nch4.*nh2o).* ...    Nernst atom balance
            (p ./ (nco + nch4 + nh2 + nh2o).^2) ...
            == f_kp_SMR(t)];
        % 4 eq, 4 unknown
        assume([nco,nch4,nh2,nh2o],'real');
        assumeAlso([nco,nch4,nh2,nh2o] > 0);
        assumeAlso([nco,nch4,nh2,nh2o] < 20);
        [a,b,c,d] = vpasolve(eqs,[nco,nch4,nh2,nh2o],[1,1,1,1]);

        nco_sol(i,j) = double(a);
        nch4_sol(i,j) = double(b);
        nh2_sol(i,j) = double(c);
        nh2o_sol(i,j) = double(d);
        %          soln(i,:,j) = max(double(real([a,b,c,d]));

    end
end
% toc;
%calculate mole fractions from nmols in composition
ntot = nch4_sol + nh2_sol + nh2o_sol + nco_sol;
ych4 = nch4_sol./ntot;
yh2 = nh2_sol./ntot;
yh2o = nh2o_sol./ntot;
yco = nco_sol./ntot;

if(~supressplots(4))
    %unneeded but cool looking plot
    f10 = figure(10);
 plot(temps,nco_sol,'b',temps,nch4_sol,'m',temps,nh2_sol,'g',temps,nh2o_sol,'k');
    legend('CO','CH4','H2','H2O');

    %plot mole fractions
    f11 = figure(11);
    linestyle = {'-','--',':'};
    hold on
    plot(1,0,'-k',1,0,'--k',1,0,':k');
    hold on
    for i = 1:length(pres)
        plot(temps,yco(:,i),strcat(linestyle{i},'b'),...
            temps,ych4(:,i),strcat(linestyle{i},'m'),...
            temps,yh2(:,i),strcat(linestyle{i},'g'),...
            temps,yh2o(:,i),strcat(linestyle{i},'r'));
        hold on
    end
    hold off
    xlabel('Temperature [K]');
    ylabel('Mole Fraction');
    title('Steam Methane Reforming Composition');

 legend('1atm','10atm','100atm','CO','CH4','H2','H2O','location','West');
    %ylim([0.001,1]);
    grid on;
end

% Part B No. 3
% % Equations we'll need:
%  eqs = [       1  == nco2   + nco;...          carbon atom balance
%                4  == nco2*2 + nco + nh2o; ...  hydrogen atom balance
%                6  == nh2*2   + nh2o*2;...      oxygen atom balance
%                nco.*nh2o.^3./(nco2.*nh2).* ... Nernst atom balance
%                   == f_kp_SMR(t)];
%          % 4 eq, 4 unknown
%          [a,b,c,d] = vpasolve(eqs,[nco,nh2o,nco2,nh2],[1,1,1,1]);
syms nco nco2 nh2 nh2o;
%soln_wgs = zeros(length(temps),4,length(pres));
tic
% ***BROKEN***
parfor i = 1:length(temps)
    warning('off','symbolic:numeric:NumericalInstability');
    t = temps(i);

    eqs = [        1  == nco2   + nco;...carbon atom balance
        3  == nco2*2 + nco + nh2o; ...  oxygen atom balance
        10  == nh2*2   + nh2o*2;...       hydrogen atom balance
        (nco2.*nh2)./(nco.*nh2o) ... Nernst atom balance
        == f_kp_WGS(t)];        %(note no pressure term, as nmols same
 on RHS and LHS)
    % 4 eq, 4 unknown
    assume([nco,nh2o,nco2,nh2],'real');
    assumeAlso([nco,nh2o,nco2,nh2] > 0);
    assumeAlso([nco,nh2o,nco2,nh2] < 20);
    [a,b,c,d] = vpasolve(eqs,[nco,nh2o,nco2,nh2],[1,1,1,1]);
    nco_wgs(i) = double(a);
    nh2o_wgs(i) = double(b);
    nco2_wgs(i) = double(c);
    nh2_wgs(i) = double(d);
    %          soln(i,:,j) = max(double(real([a,b,c,d]));

end
% toc;
ntot_wgs = nco_wgs + nh2_wgs + nh2o_wgs + nco2_wgs;
yco2_wgs = nco2_wgs./ntot_wgs;
yh2_wgs = nh2_wgs./ntot_wgs;
yh2o_wgs = nh2o_wgs./ntot_wgs;
yco_wgs = nco_wgs./ntot_wgs;

if(~supressplots(4))

    f12 = figure(12);
    plot(temps,yco_wgs,'b',...
        temps,yco2_wgs,'m',...
        temps,yh2_wgs,'--g',...
        temps,yh2o_wgs,'r');
    legend('CO','CO2','H2','H2O','location','southwest');
    xlabel('Temperature [K]');
    ylabel('Mole Fraction');
    title('Water Gas Shift Composition');
    %ylim([0.001,1]);
    grid on;
end


% Part B No. 4
% Plot exit composition (mol fractions) vs. 3 system stations
 (Reformer,
% Shift Reactor 1, Shift Reactor 2)
% Note: do this for 2 Different Assumptions: (1) isothermal, (2)
 adiabatic
% SMR: CH4 + 3*H2O --> CO + 3*H2 + 2*H2O <-known because all assume
 all
% methane is used
% WGS: CO  + 2*H2O + 3*H2--> ?CO2 + (3+?)H2 + ?CO + ?H2O <- unknown
 because WGS
% doens't go all the way to completition


% NAMING CONVENTIONS:
% Station Location: 1=Reformer, 2 = 1st Shift Reactor, 3 = 2nd Shift
% Assumption:       iso = isothermal, adi = adiabatic
% Inlet/Exit:       in = inlet, ex = exit

% PSEUDO CODE
% Start with Nernst atom balance for WGS reaction to get composition
% "Start with isothermal cases - adiabatic is a whole different beast"
% Assume first WGS uses up all CH4 and goes fully to completion
% Figure out the products from the WGS
% Use isothermal temperature values given to figure out Qdot
% Go step by step through and get products for each following
 reaction, ...
% Take those products and do isothermal calcs on them

% Inlet Temperatures
Tin_C = [800 400 250];     % [C]
Tin = Tin_C + C_TO_K; % [K]

% Exit Temperatures
Tex_iso_C = [800 400 250];
Tex_adi_C = [800 NaN NaN]; %TODO: solve for Tin_adi_C(2) & (3)
Tex_iso = Tex_iso_C + C_TO_K;
Tex_adi = Tex_adi_C + C_TO_K;

% Heat Addition for Isothermal Reaction (Qin, ASSUME: isothermal)
Qin_iso = [NaN NaN NaN];             % [MJ/(kg of reactants)]

% Percent Methane Burned to Heat Reformer (pct_CH4, ASSUME: adiabatic)
pct_CH4 = [NaN]; % Note: only applies to Reformer! Not Shift Reactors!


% Part 1: Isothermal
% find exit compositions
compositions = zeros(4,3); %co;h2o;c02;h2
for i = 1:3
    compositions(:,i) = compositionsFun(f_kp_WGS(Tin(i)));
end

% find heat addition for each component
% WGS: CO  + 2*H2O + 3*H2--> ?CO2 + (3+?)H2 + ?CO + ?H2O
% SMR: CH4 + 3*H2O --> CO + 3*H2 + 2*H2O
% comps[species, stage]. Species order: CO, H20, CO2, H2
Qin = zeros(1,3);
N_H20_in = 3;
N_CH4_in = 1;
h_react =  hEng(Tin(1), 'h2ovap', N_H20_in) + hEng(Tin(1), 'ch4',
 N_CH4_in);
for s = 1:3 % three stages: reformer and two reactors
    h_prod = hEng(Tin(s), 'co', compositions(1,s)) +
 hEng(Tin(s), 'h2ovap', compositions(2,s)) + hEng(Tin(s), 'co2',
 compositions(3,s)) + hEng(Tin(s), 'h2', compositions(4,s));
    Qin(s) = h_prod - h_react;

    if (s == 3) break; end
    h_react = hEng(Tin(s+1), 'co', compositions(1,s)) + hEng(Tin(s
+1), 'h2ovap', compositions(2,s)) + hEng(Tin(s+1), 'co2',
 compositions(3,s)) + hEng(Tin(s+1), 'h2', compositions(4,s));
end
% Qin_MJkg = ?
% TODO: GET Qin IN MJ/KG (CURRENTLY IN J. STORE IN NEW VARIABLE B/C
 Qin IS USED BELOW)
```

```
% PSEUDOCODE APPROACH
% Determine composition of each (CO H20vap CO2 H2) where we calculate
 Qin
% Use molar mass to get kg of each
% Divide Qin by kg total
% Convert J to MJ by dividing by a constant (10^6)

% currently in J/mol of methane reacted
%should be 3Mj/kg
Qin_perkg = Qin / (MM_ch4 / G_PER_KG) /1e6; % J/mol --> MJ/kg


% Part 2: Adiabatic (only shift reactors)
error = 0.0001;
speedFactor = 1000;
T_guess = zeros(1,3);
comps_out_adi = zeros(4,3);
tic
% PROBLEM IS THAT TEMPS ARE JUST CONVERGING TO TEMP AT H_IN - MISSING
% SOMETHING CONCEPTUAL.
% temps = linspace(273,800,40);
% comps_out = zeros(length(temps),4);
% for i = 1:length(temps)
%    comps_out(i,:) = compositionsFun(f_kp_WGS(temps(i)))';
%    h_out(i) = hEng(temps(i),   'co',    comps_out(i,1)) ...
%             + hEng(temps(i), 'h2ovap',comps_out(i,2)) ...
%             + hEng(temps(i), 'co2',   comps_out(i,3)) ...
%             + hEng(temps(i), 'h2',    comps_out(i,4));
% end

% H_in occurs at stage 2
% comps[species, stage]. Species order: CO, H20, CO2, H2
comps_in(:) = compositions(:,1);
tol = 0.0001;
step = 1;
for s = 2:3 % two stages: hot shift reactor, cold shift reactor
    t = Tin(s);
    h_in = hEng(t, 'co', comps_in(1)) ...
        + hEng(t, 'h2ovap', comps_in(2)) ...
        + hEng(t, 'co2',comps_in(3)) ...
        + hEng(t, 'h2', comps_in(4));
    T_guess(s) = Tin(s) + 20;
    comps_out_adi(:,s) = compositionsFun(f_kp_WGS(T_guess(s)));
    h_out = hEng(T_guess(s),   'co',    comps_out_adi(1,s)) ...
          + hEng(T_guess(s), 'h2ovap',comps_out_adi(2,s)) ...
          + hEng(T_guess(s), 'co2',   comps_out_adi(3,s)) ...
          + hEng(T_guess(s), 'h2',    comps_out_adi(4,s));
    dh = h_out - h_in;
    % set up newton raphson variables
    % need to remember previous state for newton raphson
    tlast = Tin(s);
    dhlast = T_guess(s) - tlast;

    while abs(dh/h_in) > tol %use percentage error for robustness
```

```
        dhprime = (dh - dhlast) ./(T_guess(s) - tlast);
        tlast = T_guess(s);
        T_guess(s) = T_guess(s) - dh ./ dhprime;
        comps_out_adi(:,s) = compositionsFun(f_kp_WGS(T_guess(s)));
        dhlast = dh;
        h_out = hEng(T_guess(s), 'co',comps_out_adi(1,s)) ...
            + hEng(T_guess(s), 'h2ovap',comps_out_adi(2,s)) ...
            + hEng(T_guess(s), 'co2',comps_out_adi(3,s)) ...
            + hEng(T_guess(s), 'h2',comps_out_adi(4,s));
        dh = h_out-h_in;
    end
    comps_in = comps_out_adi(:,s);
end
% toc
pctCO = comps_out_adi(1,:)./sum(comps_out_adi);
comps_out_adi(:,1) = compositions(:,1);
y_out_adi = comps_out_adi./repmat(sum(comps_out_adi),4,1);
y_iso = compositions./repmat(sum(compositions),4,1);
% ^SHOULD GET 740, 569 K FOR T_guess

% plot of exit composition vs system station (2x, isothermal and
 adiabatic)
if(~supressplots(4))
f13 = figure(13);
subplot(1,2,1);
bar(y_iso');
xlabel('State, Isothermal');
ylabel('Mole Fraction');
ylim([0,0.8]);
legend('CO', 'H20', 'CO2', 'H2','location','northwest');

subplot(1,2,2);
bar(y_out_adi');
xlabel('State, Adiabatic');
ylabel('Mole Fraction');
legend('CO', 'H20', 'CO2', 'H2','location','northwest');
ylim([0,0.8]);
set(f13, 'Position', [0 0 400 200])

annotation('textbox', [0 0.8 1 0.2], ...
    'String', 'H2 Reformer Outlet Molecular Composition', ...
    'EdgeColor', 'none', ...
    'HorizontalAlignment', 'center',...
    'FontSize',18); % add title to plot manually, subplots don't
 include an overall title
set(f13, 'Position', [300 800 800 400]) %resize plot
end


% Part 3: Heating reformer w/ methane
% find methane used by reformer - CHECK!
molar_mass_meth = 16.043/1000; % [kg/mol]
molar_mass_h2 = 2.016/1000; % [kg/mol]
LHV_meth = 50050e3*MM_ch4/G_PER_KG; % [J/mol]
```

```
LHV_h2 = 120000e3*molar_mass_h2; %[J/mol]
N_meth_burned = Qin(1)/LHV_meth; %moles of methane burned
perc_meth_burned = N_meth_burned./(N_meth_burned+1) * 100; %1 is the
 mole used for the actual reaction

% find LHV ratio - CHECK!
N_meth_rxn = 1;
LHV_ratio_isoth = LHV_h2*compositions(4,3)/(LHV_meth*(N_meth_burned +
 N_meth_rxn)) * 100;
LHV_ratio_adia = LHV_h2*comps_out_adi(4,3)/(LHV_meth*(N_meth_burned +
 N_meth_rxn)) * 100;


% NEED FOR TABLE:
% isothermal:
% -composition of gases exiting reformer and reactors
% -heat addition reqd for isothermal (do delta h energy balance on
 either
% side of each component)
% adiabatic:
% -adiabatic outlet temperatures of last two reactors
% -exit composition for shift reactors (and reformer, but same as
 above)
% heat part:
% -methane burned to heat reformer
% -LHV ratio (efficiency)
%
% PLOT: exit composition for isothermal and adiabatic at each station

if(sum(supressplots)~=4)
    plotfixer();
end
if(savePlots ==1)
     plotfixer();
    if(~supressplots(1))
        saveas(f1,'../plots5/1-CurrentbyLoad','png');
        saveas(f2,'../plots5/2-VbyLoad','png');
        saveas(f3,'../plots5/3-PowerbyLoad','png');
        saveas(f4,'../plots5/4-massbyload','png');
    end
    if(~supressplots(2))
        saveas(f5,'../plots5/5-Eff','png');
        saveas(f6,'../plots5/6-lambda','png');
        saveas(f7,'../plots5/7-PowerLoss','png');
    end
    if(~supressplots(3))
        saveas(f8,'../plots5/8-CompareToGasoline','png');
        saveas(f9,'../plots5/9-KeqbyT','png');
    end
    if(~supressplots(4))
        saveas(f10,'../plots5/10-SMRcompmol','png');
        saveas(f11,'../plots5/11-SMRcomp','png');
        saveas(f12,'../plots5/12-WGScomp','png');
        saveas(f13,'../plots5/13-ReformerComp','png');
    end
end
% toc(entireTime);
```

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