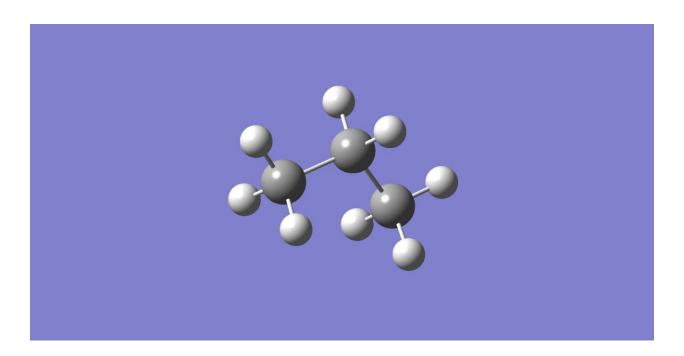
## Guilherme Bertola

Final Exam

I used gaussian to optimize the molecules described in the problem given for the final exam, each of the molecule's results are shown below with their thermochemistry results:

#### C3H8



- Thermochemistry -

Zero-point correction=

0.104122 (Hartree/Particle)

Thermal correction to Energy=

0.108635

Thermal correction to Enthalpy=

0.109580

Thermal correction to Gibbs Free Energy=

0.079118

Sum of electronic and zero-point Energies=

-119.040127

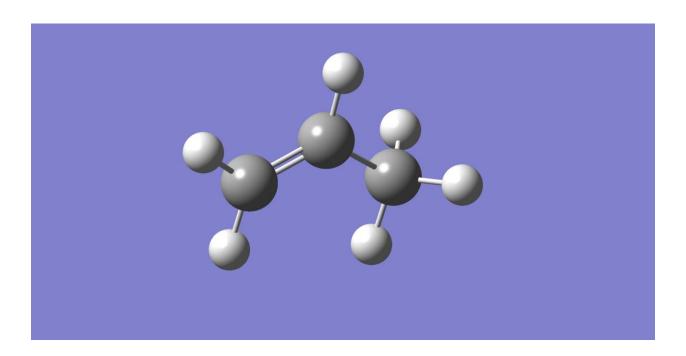
Sum of electronic and thermal Energies=

-119.035613

Sum of electronic and thermal Enthalpies=

-119.034669

### C3H6



- Thermochemistry -

-----

Zero-point correction= 0.080082 (Hartree/Particle)

Thermal correction to Energy= 0.084158

Thermal correction to Enthalpy= 0.085102

Thermal correction to Gibbs Free Energy= 0.055079

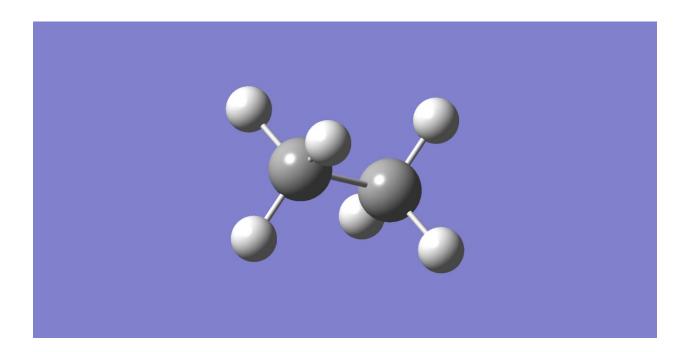
Sum of electronic and zero-point Energies -117.827475

Sum of electronic and thermal Energies= -117.823398

Sum of electronic and thermal Enthalpies = -117.822454

Sum of electronic and thermal Free Energies = -117.852477

### C2H6



-----

- Thermochemistry -

-----

Zero-point correction= 0.075229 (Hartree/Particle)

Thermal correction to Energy= 0.078698

Thermal correction to Enthalpy= 0.079642

Thermal correction to Gibbs Free Energy= 0.053810

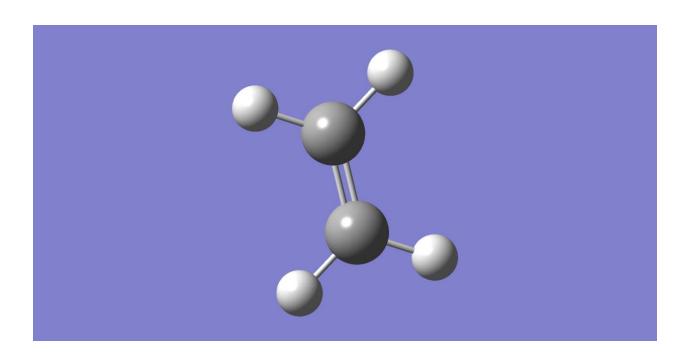
Sum of electronic and zero-point Energies -79.755188

Sum of electronic and thermal Energies= -79.751720

Sum of electronic and thermal Enthalpies= -79.750776

Sum of electronic and thermal Free Energies -79.776607

C2H4



\_\_\_\_\_

- Thermochemistry -

-----

Zero-point correction= 0.050845 (Hartree/Particle)

Thermal correction to Energy= 0.053888

Thermal correction to Enthalpy= 0.054832

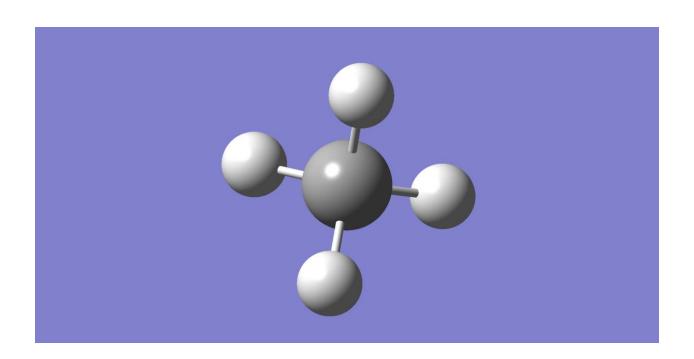
Thermal correction to Gibbs Free Energy= 0.029321

Sum of electronic and zero-point Energies -78.556112

Sum of electronic and thermal Energies= -78.553069

Sum of electronic and thermal Enthalpies= -78.552125

Sum of electronic and thermal Free Energies= -78.577636



-----

- Thermochemistry -

-----

Zero-point correction= 0.045214 (Hartree/Particle)

Thermal correction to Energy= 0.048078

Thermal correction to Enthalpy= 0.049022

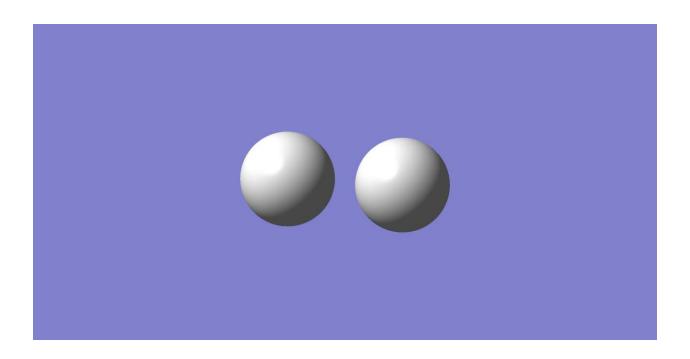
Thermal correction to Gibbs Free Energy= 0.027890

Sum of electronic and zero-point Energies -40.473175

Sum of electronic and thermal Energies= -40.470311

Sum of electronic and thermal Enthalpies= -40.469367

Sum of electronic and thermal Free Energies= -40.490499



-----

- Thermochemistry -

-----

Zero-point correction= 0.010145 (Hartree/Particle)

Thermal correction to Energy= 0.012505

Thermal correction to Enthalpy= 0.013450

Thermal correction to Gibbs Free Energy= -0.001342

Sum of electronic and zero-point Energies = -1.165337

Sum of electronic and thermal Energies= -1.162977

Sum of electronic and thermal Enthalpies= -1.162033

Sum of electronic and thermal Free Energies = -1.176825

### MATLAB CODE:

```
%Final Exam%
%Guilherme Bertola%
% C3H8 -> 0.3 C3H6 + 0.065 C2H6 + 0.6675 C2H4 + 0.635 CH4 + 0.3 H2
% A -> 0.3 B + 0.065 C + 0.6675 D + 0.635 E + 0.3 F
%Letter | Molecule
% A | C3H8
% B
     | C3H6
% C
     C2H6
응 D
     | C2H4
% E
     | CH4
% F
     | H2
%stoic table
% Species | Fi0 | Exit (Fi) | Exit (Ci) |
%----|---|
       | F0 | F0 - z | F0-F0*Xa / v |
    % B
응 C
% D
응 E
% F
%-----
% Total | F0 | Ft | F0-0.9855*F0*Xa/v|
% Fa0 = F0
% Fa = F0 - F0*Xa
% Fa = F0 - z
% then
% z = F0*Xa (extent of reaction)
%stoic indexes
vA = 1;
vB = 0.3;
vC = 0.065;
vD = 0.6675;
vE = 0.635;
vF = 0.3;
%known parameters
%conversion
Xa = 0.8;
%Initial Temperature
T0 = 1100; %F
T0 = (T0-32) * 5/9 + 273.15; %K
%Inital Pressure
P0 = 60; % psia
```

```
P0 = P0 * 6894.76; %Pa
%molar mass of propane
Ma = 44.097; %q/mol
Ma = Ma/1000; %kg/mol
%Feed Rate (mass)
M0 = 7000; % lb/h
M0 = M0/2.205; %Kg/h
M0 = M0/3600; %Kg/s
%Feed Rate (mol)
F0 = M0/Ma; %mol/s
%R gas constant
R = 8.31446261815324; %m3?Pa?K?1?mol?1
%concentration
c = P0/(R*T0); %mol/m3
%volumetric flow
v0 = F0/c; %m3/s
%Heat flux
Q = 2.52e6; %cal/(h*ft2)
Q = Q*10.764; %cal/(h*m2)
Q = Q/3600; %cal/(s*m2)
%pipes data
%2 inch diameter pipe
di 2 = 2.07; %in
                        Internal diameter
                        Internal Transverse Area
ai 2 = 3.36; %in2
do 2 = 2.375; %in
                        External Diameter
wpft 2 = 3.65; %lb/ft
                        Weight per length
di 2 = di 2 / 39.37; %m
do 2 = do 2 / 39.37; %m
ai 2 = ai 2 / 1550; %m2
ff 2 = 0.0050;%
                        Friction factor
%4 inch diameter pipe
di 4 = 4.03; %in
                        Internal diameter
                        Internal Transverse Area
ai 4 = 12.73; %in2
do 4 = 4.500; %in
                        External Diameter
wpft 4 = 10.79; %lb/ft
                        Weight per length
di 4 = di 4 / 39.37; %m
do^{4} = do^{4} / 39.37; %m
ai 4 = ai 4 / 1550; %m2
ff 4 = 0.0044; %
                        Friction factor
%6 inch diameter pipe
di 6 = 6.07; %in
                        Internal diameter
                        Internal Transverse Area
ai 6 = 28.89; %in2
do 6 = 6.625; %in
                        External Diameter
wpft 6 = 18.97; % lb/ft
                        Weight per length
di 6 = di 6 / 39.37; %m
do 6 = do 6 / 39.37; %m
ai 6 = ai 6 / 1550; %m2
ff 6 = 0.0044; %
                        Friction factor
%heats of reactions
%gaussian calculated (298 K)
```

```
dH H2 gau = -1.162033; %Hartrees
dH CH4 gau = -40.469367; %hartrees
dH C3H8 gau = -119.034669; %hartrees
dH C3H6 gau = -117.822454; %hartrees
dH C2H6 gau = -79.750776; %hartress
dH C2H4 gau = -78.552125; %hartress
dH prod = vB*dH C3H6 gau + vC*dH C2H6 gau + vD*dH C2H4 gau +
vE*dH CH4 gau + vF*dH H2 gau; %hartrees
dH reac = vA*dH C3H8 gau; %hartrees
dH Gau 298 = dH prod - dH_reac; %hartrees
dH Gau 298 = dH Gau 298 * 627.5095; %Kcal/mol
dH Gau 298 = dH Gau 298 * 1000; %cal/mols
%length of the reactor (m)
len span = linspace(0,426,400); %426 \text{ m} \sim 1400 \text{ ft}
%initial conditions
y0 = [F0, 0, 0, 0, 0, 0, T0, P0];
%RUNS%
%Gaussian dH
%2 in
Tr = 298; %K
dH ref = dH Gau 298; %cal/mol
%Pipe data:
A = ai 2;
D = di 2;
DO = do 2;
ff = ff 2;
%ODE run
[l,x] =
ode15s(@(L,x)PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0),len span,y0
);
T 2 in = x(:,7); %K
P 2 in = x(:,8); %Pa
P 2 in = P 2 in./6895; psia
Fa 2 in = x(:,1); %mol/s
Xa 2 in = (F0-Fa 2 in)./F0;
Xa_2_{in} = Xa_2_{in} * \overline{100}; % (%)
L 2 in = 1 * 3.281; % ft
%Plots
figure;
subplot(2,2,1);
plot(L 2 in,T 2 in);
title ("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
subplot(2,2,2);
plot(L 2 in, P 2 in);
title("Pressure vs Length");
```

```
xlabel("Length (ft)");
ylabel("Pressure (psia)");
subplot(2,2,[3,4]);
plot(L 2 in, Xa 2 in);
title ("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
sgtitle("2 inches diameter pipe");
%4 in
Tr = 298; %K
dH ref = dH Gau 298; %cal/mol
%Pipe data:
A = ai 4;
D = di 4;
DO = do 4;
ff = ff 4;
%ODE run
[1,x] =
ode15s(@(L,x)PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0),len span,y0
T 4 in = x(:,7); %K
P 4 in = x(:,8); %Pa
P 4 in = P 4 in./6895; %psia
Fa 4 in = x(:,1); %mol/s
Xa \ 4 \ in = (F0-Fa \ 4 \ in)./F0;
Xa \ 4 \ in = Xa \ 4 \ in*100; % (%)
L 4 in = 1 * 3.281; % ft
%Plots
figure;
subplot(2,2,1);
plot(L 4 in, T 4 in);
title("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
subplot(2,2,2);
plot(L 4 in,P 4 in);
title("Pressure vs Length");
xlabel("Length (ft)");
ylabel("Pressure (psia)");
subplot(2,2,[3,4]);
plot(L 4 in, Xa 4 in);
title("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
sgtitle ("4 inches diameter pipe");
%6 in
Tr = 298; %K
dH ref = dH Gau 298; %cal/mol
%Pipe data:
A = ai 6;
```

```
D = di 6;
DO = do 6;
ff = ff 6;
%ODE run
[1,x] =
ode15s(@(L,x)PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0),len span,y0
);
T 6 in = x(:,7); %K
P 6 in = x(:,8); %Pa
P_6_{in} = P_6_{in./6895}; %psia
Fa 6 in = x(:,1); %mol/s
Xa 6 in = (F0-Fa 6 in)./F0;
Xa 6 in = Xa 6 in * \overline{100}; % (%)
L 6 in = 1 * 3.281; %ft
%Plots
figure;
subplot(2,2,1);
plot(L 6 in, T 6 in);
title("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
subplot(2,2,2);
plot(L 6 in,P 6 in);
title ("Pressure vs Length");
xlabel("Length (ft)");
ylabel("Pressure (psia)");
subplot(2,2,[3,4]);
plot(L 6 in, Xa 6 in);
title("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
sgtitle("6 inches diameter pipe");
%grouped plots
figure;
subplot(2,2,1);
hold on;
plot(L 2 in, T 2 in, "k-");
plot(L 4 in, T 4 in, "k--");
plot(L 6 in, T 6 in, "k:");
title("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
legend("2 in","4 in","6 in");
hold off;
subplot(2,2,2);
hold on;
plot(L 2 in, P 2 in, "k-");
plot(L 4 in, P 4 in, "k--");
plot(L 6 in, P 6 in, "k:");
title("Pressure vs Length");
xlabel("Length (ft)");
```

```
ylabel("Pressure (psia)");
legend("2 in","4 in","6 in");
hold off;
subplot(2,2,[3,4]);
hold on;
plot(L 2 in, Xa 2 in, "k-");
plot(L 4 in, Xa 4 in, "k--");
plot(L 6 in, Xa 6 in, "k:");
title("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
legend("2 in","4 in","6 in");
hold off;
sgtitle("Grouped plots");
%6 in - DH exam
Tr = 8.6648333333333333322; %K
dH ref = 21.96*1000; %cal/mol
%Pipe data:
A = ai 6;
D = di 6;
DO = do 6;
ff = ff 6;
%ODE run
[l,x] =
ode15s(@(L,x)PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0),len span,y0
);
T 6 in dh = x(:,7); %K
P 6 in dh = x(:,8); %Pa
P 6 in dh = P 6 in dh./6895; psia
Fa 6 in dh = x(:,1); %mol/s
Xa 6 in dh = (F0-Fa 6 in dh)./F0;
Xa 6 in dh = Xa 6 in dh*100; % (%)
L 6 in dh = 1 * 3.281; %ft
%Plots
figure;
subplot(2,2,1);
plot(L 6 in dh,T 6 in dh);
title ("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
subplot(2,2,2);
plot(L 6 in dh,P 6 in dh);
title("Pressure vs Length");
xlabel("Length (ft)");
ylabel("Pressure (psia)");
subplot (2, 2, [3, 4]);
plot(L 6 in dh, Xa 6 in dh);
title("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
sgtitle ("6 inches diameter pipe (with exan given dH)");
```

```
%comparison between the gaussian and the given value
figure;
subplot(3,1,1);
hold on;
plot(L 6 in, Xa 6 in, "k-");
plot(L 6 in dh, Xa 6 in dh, "k--");
title ("Conversion vs Length (6 in)");
xlabel("Length (ft)");
ylabel("Conversion (%)");
legend("Gaussian", "Given");
hold off;
subplot(3,1,2);
hold on;
plot(L 4 in, Xa 4 in, "k-");
plot(L 4 in dh, Xa 4 in dh, "k--");
title("Conversion vs Length (4 in)");
xlabel("Length (ft)");
ylabel("Conversion (%)");
legend("Gaussian", "Given");
hold off;
subplot(3,1,3);
hold on;
plot(L 2 in, Xa 2 in, "k-");
plot(L 2 in dh, Xa 2 in dh, "k--");
title("Conversion vs Length (2 in)");
xlabel("Length (ft)");
ylabel("Conversion (%)");
legend("Gaussian", "Given");
hold off;
sqtitle ("Comparison of given Heat of reaction vs Gaussian
calculated");
%4 in - DH exam
Tr = 8.664833333333333322; %K
dH ref = 21.96*1000; %cal/mol
%Pipe data:
A = ai 4;
D = di 4;
DO = do 4;
ff = ff 4;
%ODE run
[1,x] =
ode15s(@(L,x)PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0),len span,y0
T 4 in dh = x(:,7); %K
P 4 in dh = x(:,8); %Pa
P 4 in dh = P 4 in dh./6895; psia
Fa 4 in dh = x(:,1); %mol/s
Xa 4 in dh = (F0-Fa 4 in dh)./F0;
```

```
Xa \ 4 \ in \ dh = Xa \ 4 \ in \ dh*100; % (%)
L 4 in dh = 1 * 3.281; % ft
%Plots
figure;
subplot(2,2,1);
plot(L 4 in dh, T 4 in dh);
title("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
subplot(2,2,2);
plot(L 4 in dh,P 4 in dh);
title("Pressure vs Length");
xlabel("Length (ft)");
ylabel("Pressure (psia)");
subplot(2,2,[3,4]);
plot(L 4 in dh, Xa 4 in dh);
title ("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
sqtitle("4 inches diameter pipe (with exam given dH)");
%2 in - DH exam
Tr = 8.6648333333333333322; %K
dH ref = 21.96*1000; %cal/mol
%Pipe data:
A = ai 2;
D = di 2;
DO = do 2;
ff = ff^2;
%ODE run
[1,x] =
ode15s(@(L,x)PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0),len span,y0
T 2 in dh = x(:,7); %K
P 2 in dh = x(:,8); %Pa
P 2 in dh = P 2 in dh./6895; %psia
Fa 2 in dh = x(:,1); %mol/s
Xa 2 in dh = (F0-Fa 2 in dh)./F0;
Xa_2 in_dh = Xa_2 in_dh*100; % (%)
L 2 in dh = 1 * 3.281; % ft
%Plots
figure;
subplot(2,2,1);
plot(L 2 in dh,T 2 in dh);
title("Temperature vs Length");
xlabel("Length (ft)");
ylabel("Temperature (K)");
subplot(2,2,2);
plot(L 2 in dh,P 2 in dh);
title ("Pressure vs Length");
xlabel("Length (ft)");
ylabel("Pressure (psia)");
```

```
subplot (2, 2, [3, 4]);
plot(L 2 in dh, Xa 2 in dh);
title ("Conversion vs Length");
xlabel("Length (ft)");
ylabel("Conversion (%)");
sgtitle("2 inches diameter pipe (with exam given dH)");
%PFR Function
function f=PFR(L,x,T0,P0,F0,M0,v0,Q,Tr,dH ref,A,ff,D,D0)
%variables
Fa = x(1);
Fb = x(2);
Fc = x(3);
Fd = x(4);
Fe = x(5);
Ff = x(6);
T = x(7);
P = x(8);
%R gas constant
R = 1.98720425864083; %cal/(mol*K)
%rate constant (s-1)
k = 3.98e12*exp(-59100/(R*T));
%conversion
Xa = (F0-Fa)/F0;
%total molar flow
Ft = Fa+Fb+Fc+Fd+Fe+Ff; %mol/s
%volumetric flow
v = v0*(Ft/F0)*(T/T0)*(P0/P); %m3/s
%concentrations
Ca = (F0-F0*Xa)/v; %mo1/m3
Cb = (0.3*F0*Xa) / v; %mo1/m3
Cc = (0.065*F0*Xa) / v; %mol/m3
Cd = (0.6675*F0*Xa) / v; %mol/m3
Ce = (0.635*F0*Xa) / v; %mol/m3
Cf = (0.3*F0*Xa) / v; %mo1/m3
%reaction rate
ra = -k*Ca; %mol/s*m3
rb = k*Cb; %mol/s*m3
rc = k*Cc; %mol/s*m3
rd = k*Cd; %mol/s*m3
re = k*Ce; %mol/s*m3
rf = k*Cf; %mol/s*m3
%Density
rho = M0/v; %Kg/m3
%heat of reaction
dH = dH ref + integral(@dCP,Tr,T);
%Heat capacities (cal/molK)
cpA = 21.14 + 0.02056*T;
cpB = 17.88 + 0.01645*T;
cpC = 13.34 + 0.01589*T;
cpD = 12.29 + 0.01022*T;
cpE = 6.98 + 0.01012*T;
```

```
cpF = 6.42 + 0.00082*T;
%Temperature along the length of the reactor
FiCpi = Fa*cpA + Fb*cpB + Fc*cpC + Fd*cpD + Fe*cpE + Fd*cpD + Ff*cpF;
dTdl = (ra*dH - Q*(1/(2*pi*(DO/2))))/(FiCpi) * A;
%Molar flow of A along the length of the reactor
dFadl = ra * A;
%Molar flow of B along the length of the reactor
dFbdl = rb * A;
%Molar flow of C along the length of the reactor
dFcdl = rc * A;
%Molar flow of D along the length of the reactor
dFddl = rd * A;
%Molar flow of E along the length of the reactor
dFedl = re * A;
%Molar flow of F along the length of the reactor
dFfdl = rf * A;
%pressure drop along the length of the reactor
G = M0 / A;
dPdl = -(2*ff*(G^2))/(rho*D);
f = [dFadl;dFbdl;dFcdl;dFddl;dFedl;dFfdl;dTdl;dPdl];
end
function x=dCP(T)
    %heat Capacities (cal/mol*K)
    cpA = 21.14 + 0.02056*T;
    cpB = 17.88 + 0.01645*T;
    cpC = 13.34 + 0.01589*T;
    cpD = 12.29 + 0.01022*T;
    cpE = 6.98 + 0.01012*T;
    cpF = 6.42 + 0.00082*T;
    dCp = -cpA + 0.3*cpB + 0.065*cpC + 0.6675*cpD + 0.653*cpE +
0.3*cpF;
    x = dCp;
end
```

# Plots and Results:

## Temperature plots

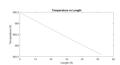


Figure 1 – Temperature vs Length plot of 2 inches diameter pipe (gaussian calculated enthalpy)

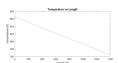


Figure 2 - Temperature vs Length plot of 4 inches diameter pipe (gaussian calculated enthalpy)

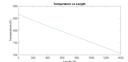


Figure 3 - Temperature vs Length plot of 6 inches diameter pipe (gaussian calculated enthalpy)

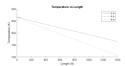


Figure 4 – Grouped Temp vs Len plot (gaussian calculated enthalpy)

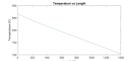


Figure 5 - Temperature vs Length plot of 6 inches diameter pipe (given delta H)

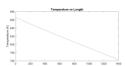


Figure 6 - Temperature vs Length plot of 4 inches diameter pipe (given delta H)

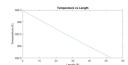


Figure 7 - Temperature vs Length plot of 2 inches diameter pipe (given delta H)

# Pressure plots

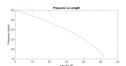


Figure 8 – Pressure vs Length plot for 2 inches diameter pipe (gaussian calculated enthalpy)

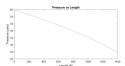


Figure 9 - Pressure vs Length plot for 4 inches diameter pipe (gaussian calculated enthalpy)

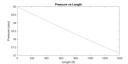


Figure 10 - Pressure vs Length plot for 6 inches diameter pipe (gaussian calculated enthalpy)

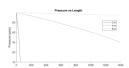


Figure 11 – Grouped Pressure vs Length plot (gaussian calculated enthalpy)

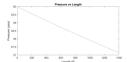


Figure 12 - Pressure vs Length plot for 6 inches diameter pipe (given delta H)

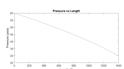


Figure 13 - Pressure vs Length plot for 4 inches diameter pipe (given delta H)

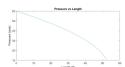


Figure 14 - Pressure vs Length plot for 2 inches diameter pipe (given delta H)

# Conversion plots

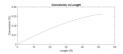


Figure 15 – Conversion vs Length plot for the 2 inches diameter pipe (gaussian calculated enthalpy)

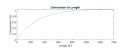


Figure 16 – Conversion vs Length plot for the 4 inches diameter pipe (gaussian calculated enthalpy)

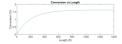


Figure 17 - Conversion vs Length plot for the 6 inches diameter pipe (gaussian calculated enthalpy)

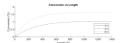


Figure 18 – Grouped Conversion vs Length plot (gaussian calculated enthalpy)

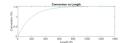


Figure 19 – Conversion vs Length plot for the 6 inches diameter pipe (given delta H)

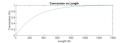


Figure 20 - Conversion vs Length plot for the 4 inches diameter pipe (given delta H)

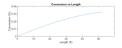


Figure 21 - Conversion vs Length plot for the 4 inches diameter pipe (given delta H)

## Comparison of given Heat of reaction vs Gaussian calculated

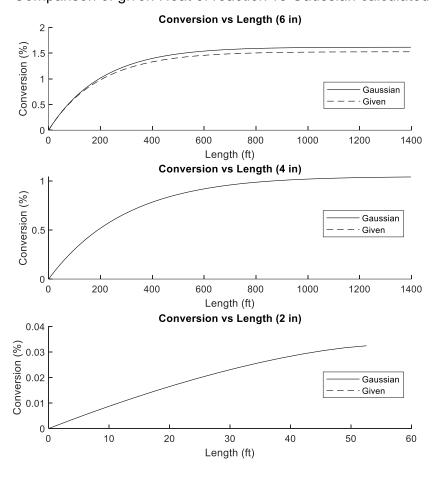


Figure 22 – Comparison of given Heat of Reaction vs Gaussian calculated per each diameter

### Optimal pipe

Since there is some error in my conversion model, I can't calculate the optimal pipe to be used, but method to find which one is the better option is as follows:

- 1. Find the length required for the pipe to reach a conversion of 80%.
- 2. Discard the pipe in which the pressure at that length is lower than 25 psia.
- 3. Multiply the pipe length by its corresponding weight per ft (found in the engineering toolbox).
- 4. Select the lightest pipe.