

AME 436	Assigned: 2/15/08
Problem Set #2	Due: 2/22/08 at 4:30 pm in my office mailbox (OHE 430J) (email or fax to me at 213-740-8071 if you're off campus, DEN students can also fax to the usual number)

**Note:** some of the special symbols on this page seem to show up properly only with Internet Explorer and not other web browsers – gotta luv Microsoft...

### **Problem #1**

Using the Zeldovich equation for burning velocity ( $S_L$ ), and typical “baseline” values of ambient temperature ( $T_\infty$ ), adiabatic flame temperature ( $T_{ad}$ ), order of reaction ( $n$ ) and activation energy ( $E$ ), answer the following questions:

- How does the reactant temperature  $T_\infty$  affect  $S_L$ , everything else (including the product temperature  $T_{ad}$ ) held constant? That is, will a 10% increase in  $T_\infty$  cause a more or less than 10% increase/decrease in  $S_L$ ?
- How does  $T_{ad}$  affect  $S_L$ , everything else (including  $T_\infty$ ) held constant? That is, will a 10% increase in  $T_{ad}$  cause a more or less than 10% increase/decrease in  $S_L$ ?
- How does the activation energy ( $E$ ) affect  $S_L$ , everything else (including  $T_\infty$  and  $T_{ad}$ ) held constant? That is, will a 10% increase in  $E$  cause a more or less than 10% increase/decrease in  $S_L$ ?
- How does the concentration of fuel in the reactants affect  $S_L$ , everything else (including  $T_\infty$  and  $T_{ad}$ ) held constant? That is, will a 10% increase in the concentration of fuel in the reactants cause a more or less than 10% increase/decrease in  $S_L$ ?
- How does the pressure of the reactants affect  $S_L$ ? That is, will a 10% increase in pressure cause a more or less than 10% increase/decrease in  $S_L$ ?

### **Problem #2**

For the homogeneous reaction/ignition problem discussed in class, write a short computer program to solve the differential equation that results. You can use the [simple Excel sheet](#) I created (or you build your own in Excel, Matlab, etc.) Using your program, and taking into account the definitions of the dimensionless input parameters  $\phi$  (phi),  $\beta$  (beta) and  $H$  answer the following:

- How does the reactant temperature  $T_\infty$  affect the dimensional time for ignition to occur (arbitrarily defined as 90% completion of reaction), everything else (including the product temperature  $T_{ad}$ ) held constant? That is, will a 10% increase in  $T_\infty$  cause

a more or less than 10% increase/decrease in the dimensional time for ignition to occur? How does the activation energy affect your conclusion, that is, will a 10% increase in  $E$  change the sensitivity of ignition time to  $T_\infty$ ?

b) How does  $T_{ad}$  affect the dimensional time for ignition to occur, everything else (including  $T_\infty$ ) held constant? How does the activation energy affect your conclusion? How does the activation energy affect your conclusion, that is, will a 10% increase in  $E$  change the sensitivity of ignition time to  $T_{ad}$ ?

c) How does the concentration of fuel in the reactants affect the dimensional time for ignition to occur?

d) How does the pressure of the reactants affect the dimensional time for ignition to occur?

### **Problem #3**

a) Calculate and plot the homogeneous ignition time (default definition is time to reach initial temperature + 400K) at constant pressure as a function of temperature for a stoichiometric  $H_2 - O_2$  mixture at 1 atm over the initial temperature range 800K - 1500K using the on-line chemical kinetics calculator at <http://navier.engr.colostate.edu/tools/homkin.html>. Use for 800K the following parameters: integration time 10 seconds, time interval 0.1 seconds, HydrogenOxygen mechanism. For higher initial temperatures the time to ignition will decrease and you'll have to decrease the integration time and time interval.

b) From this information, estimate the effective activation energy of  $H_2 - O_2$  combustion from a plot of  $\ln(\text{ignition time})$  vs.  $1/T_\infty$  (the slope of this plot is  $E/R$ ). (Note: the slope won't be very constant; there will be a "kink" near 1000K because of a change in the dominant chemical reactions at that temperature.)

c) Calculate and plot the ignition time at constant pressure as a function of pressure for a stoichiometric  $H_2 - O_2$  mixture at 800K over the pressure range 1 atm - 10 atm using the on-line chemical kinetics calculator.

d) From this information, estimate the effective order of reaction ( $n$ ) of  $H_2 - O_2$  combustion from a plot of ignition time vs. pressure (the slope of this plot on a log-log scale is  $1-n$ )

### **Problem #4**

Using the  $d^2$  law for droplet burning, explain

a) How does the reactant temperature  $T_\infty$  affect the total droplet burning time, everything else (including the product temperature  $T_{ad}$ ) held constant? How does the activation energy affect your conclusion, that is, will a 10% increase in  $E$  change the sensitivity of droplet burning time to  $T_\infty$ ?

- b) How does  $T_{ad}$  affect the total droplet burning time, everything else (including  $T_{\infty}$ ) held constant? How does the activation energy affect your conclusion, that is, will a 10% increase in  $E$  change the sensitivity of droplet burning time to  $T_{ad}$ ?
- c) How does the concentration of oxygen in the atmosphere affect the total droplet burning time?
- d) How does the pressure of the reactants affect the total droplet burning time?

Problem #5 (from a previous midterm exam)

**Problem #5**

Ronney Oil & Gas Company claims to have developed a fuel, called PDR<sup>®</sup>, whose chemical formula is  $C_8H_{18}$  (octane) and has all the same thermodynamic properties, transport properties, etc. as  $C_8H_{18}$ . The **only** difference between  $C_8H_{18}$  and PDR<sup>®</sup> is that using PDR<sup>®</sup> leads to **10% lower activation energy (E) for all chemical reactions**. If PDR<sup>®</sup> fuel were used instead of  $C_8H_{18}$ , how would each of the following be affected? In particular, state whether the property would increase, decrease or remain the same, and if there is a change, would it be by more than, less than, or equal to 10%. (Notice the operative words: LOWER ACTIVATION ENERGY.) **No credit without explanation!**

- a) Fuel heating value  
b) Constant-volume adiabatic flame temperature  
c) Burning velocity of a stoichiometric premixed octane-air flame  
d) Burning time of a liquid octane fuel droplet

Note: Ronney Oil & Gas Company frequently appears on exams!