

AME 436	Assigned: Friday 2/12/2016
Problem Set #2	<ul style="list-style-type: none"> • Due Friday 2/19/2016 at 4:30 pm in drop-off box in OHE 430N (back room of the OHE 430 suite of offices, where the Xerox machine is located) • Hard copies are preferred but you can email your assignment to the graders at ame436usc@gmail.com if you're off campus. Emailed files must be a single .pdf file, not 10 or 20 .jpg images! • DEN students submit through the usual channels.

Problem #1 (20 points) (from a previous midterm exam)

Ronney Oil and Gas Co. has invented a new fuel, called PDR™, that has the same chemical formula as octane (C_8H_{18}) and all the same chemical, thermodynamic and transport properties as octane. The **only** difference between octane and PDR™ is that PDR™ has **10% lower activation energy for all chemical reactions involving the fuel molecule**. PDR™ does not affect the rate of any chemical reaction not involving the fuel molecule. If PDR™ were used instead of octane fuel, how would each of the following combustion properties change? In particular, would the property increase, decrease or remain the same and if it changes, is the change less than, more than, or exactly 10%?

- Constant-pressure adiabatic flame temperature of a stoichiometric mixture
- Laminar burning velocity of a stoichiometric mixture
- Time for homogeneous explosion in a stoichiometric mixture
- Burning rate of a fuel droplet burning in air
- Rate of thermal NO formation immediately downstream of a stoichiometric premixed flame
- Amount of unburned hydrocarbon emission from a premixed-charge engine.
- Amount of soot formation in a rich premixed flame
- Amount of soot emission from a non-premixed flame.

Problem #2 (15 points)

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

- How does the reactant temperature T_∞ affect S_L , everything else (including the product temperature T_{ad}) held constant? That is, will a 10% increase in T_∞ cause a more or less than 10% increase/decrease in S_L ?
- How does adiabatic flame temperature T_{ad} affect S_L , everything else (including T_∞) 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 concentration of fuel in the reactants affect S_L , everything else (including T_∞ 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 #3 (15 points)

For the homogeneous reaction/ignition problem discussed in class, and taking into account the definitions of the dimensionless input parameters ϕ , β and H in the equation on page 35 of the Lecture 4 notes, answer the following questions about homogeneous ignition. You can use the simple Excel sheet (<http://ronney.usc.edu/AME436/autoignition.xls>) (also embedded in that Lecture 4 slide) I created or you build your own program in Excel, Matlab, wolframalpha.com, etc.)

- How does the reactant temperature T_∞ 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_∞ cause a more or less than 10% increase/decrease in the dimensional time for ignition to occur?
- How does T_{ad} affect the **dimensional** time for ignition to occur, everything else (including T_∞) held constant?
- How does the concentration of fuel in the reactants affect the **dimensional** time for ignition to occur?
- How does the pressure of the reactants affect the **dimensional** time for ignition to occur?

Problem #4 (20 points)

- Calculate and plot the homogeneous ignition time at constant pressure as a function of temperature for a stoichiometric ($\phi = 1$) C_3H_8 - air mixture at 1 atm over the initial temperature range 1000K - 2000K using the on-line chemical kinetics calculator at

<http://navier.engr.colostate.edu/~dandy/code/code-5/index.html>.

Use for 1000K the following parameters: integration time 1 seconds, time interval 0.05 seconds, MethaneOxygenNitrogen mechanism (note that the “MethaneOxygenNitrogen” mechanism includes many other hydrocarbon molecules including C_3H_8). For higher initial temperatures the time to ignition will decrease and you should decrease the integration time. Note that if you click on the question marks you’ll find out what the calculation parameters mean:

- **Integration time:** The integration proceeds from time zero until this final time.
- **Time interval:** The time interval for solution printouts to the text output file.
- **Ignition time:** For calculations at constant pressure or constant volume, the program computes an ignition time, which is denoted as the time when the temperature first reaches a value equal to the specified ignition temperature. The default value for this quantity is the initial temperature plus 400 K.

(None of these three calculation parameters have any effect on the calculation itself, just how the data is presented.)

- From this information, estimate the effective activation energy of C_3H_8 - air combustion from a plot of $\ln(\text{ignition time})$ vs. $1/T_\infty$ (the slope of this plot is E/R). (Note: the slope may not be very constant due to change in the dominant chemical reactions above a certain temperature. If this happens, determine separately the effective activation energies for these two regions, above and below the kink.)

- c) Calculate and plot the ignition time at constant pressure as a function of pressure for a stoichiometric C_3H_8 – air mixture at 1000K 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 C_3H_8 - air combustion from a plot of ignition time vs. pressure (the slope of this plot on a log-log scale is $1-n$)
- e) For initial temperature 1000K and pressure 1 atm, how different is the ignition time change for $\phi = 0.5$ or $\phi = 2$ compared to $\phi = 1$?
- f) For initial temperature 1000K, pressure 1 atm and $\phi = 1$, how different is the ignition time for H_2 – air and CH_4 – air mixtures compared to the C_3H_8 -air mixture?

Problem #5 (15 points)

Using the d^2 law for droplet burning, explain following.

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

Problem #6 (15 points)

Is Heywood's formula for the time constant for NO formation (τ_{NO}) reasonable? Let's check.

- (a) For a stoichiometric C_3H_8 -air mixture at initial temperature 298K and initial pressure 1 atm, calculate the constant-pressure adiabatic temperature using GASEQ.
- (b) Put this temperature and pressure into Heywood's formula and calculate τ_{NO} .
- (c) Using the Colorado State chemical kinetics calculator, input this temperature and pressure, plus the mole fractions of all species other than NO into the online form. Select "MethaneOxygenNitrogen" mechanism (note that the "MethaneOxygenNitrogen" mechanism includes many other hydrocarbon molecules including C_3H_8) and select "Constant Temperature and Pressure" for the process. Use an integration time similar to your calculated τ_{NO} .
- (d) From the results of this calculation, plot the mole fraction of NO vs. time and find the slope (units are mole fraction NO per second) for the first part where it's nearly linear.
- (e) The time constant is the equilibrium NO mole fraction (calculated from GASEQ) divided this slope [which will have units of (mole fraction NO)/(mole fraction NO per second) = seconds]. Compare this to Heywood's prediction. I found that Heywood's τ_{NO} is 67% higher than the "true" value obtained using the detailed CSU chemical kinetics calculator.