AME 514 Applications of Combustion - Fall 2008

Assignment #1

Due Monday 9/22/08, 4:30 pm, at my office (OHE 430J). If you're off campus, you can fax it to 213-740-8071. DEN students should submit through the usual channels.

Part 1: paper review

Read any one of the research papers (not review papers, not textbooks) listed in the reference section of lectures 1 – 3. Some suggested papers and a few others are listed below (along with the reason I think they're important papers). Most of these papers are available on-line or in the Science and Engineering Library. *If you have another paper relevant to the subjects of lectures 1 – 3 that you'd really like to read instead of one of my references because it relates to your research or work, I'll consider it, but you'll have to get my approval in advance.* Notice that most of these papers are somewhat older, but this is partly intentional since these papers have "stood the test of time" at least in my opinion. Papers written by me are off limits, because you need to be free to criticize the paper, which you might not feel comfortable doing to my papers (at least, if you know what's good for you…)

- Spalding, D. B., *Proc. Roy. Soc. (London)* A240, 83 (1957). (Classical theory of flame extinction by heat loss. The mathematical techniques are obsolete but the physical insights are timeless.)
- Levy, A., *Proc. Roy. Soc. (London)* A283, 134 (1965). (Shows $S = 0.3\sqrt{gd}$ at the upward flammability limit.)
- Jarosinsky, J., Strehlow, R. A., Azarbarzin, A., *19th Symp. (International) on Combustion*, Combustion Institute, Pittsburgh, 1982, p. 1549. (Demonstration of limit mechanisms for upward and downward propagating flames in tubes.)
- Giovangligli, V. and Smooke, M. D., *Combust. Sci. Tech.* 87, 241 (1992). (Numerical study of adiabatic flames showing $S_L \rightarrow 0$ and $\delta \rightarrow \infty$ as mixture is made very lean or rich.)
- Krivulin, V. N., Kudryavtsev, E. A., Baratov, A. N., Badalyan, A. M., Babkin, V. S., *Combust. Expl. Shock Waves* 17, 37 (1981). (English translation of Russian article on centrifuge experiments showing $S_{L,lim} \sim g^{1/3}$).
- Kono, M., Kumagai, S., Sakai, T., *16th Symp. (International) on Combustion*, Combustion Institute, 1976, p. 757. (Good experimental study of the effects of spark duration on minimum ignition energy).
- Joulin, G. *Combust. Sci. Tech.* 43, 99 (1985). (Elegant theoretical paper on flame ignition.)
- Champion, M, Deshaies, B., Joulin, G. and Kinoshita, K., *Combust. Flame* 65, 319 (1986). (Very good combined experimental/analytical study of the effects of Lewis number on flame ignition.)
- Bachmeier, F., Eberius, K. H., Just, T. (1973). *Combust. Sci. Technol.* 7, 77 (early characterization of prompt NO formation)
- Puchkarev, V., Gundersen, M. (1997). "Energy efficient plasma processing of gaseous emission using short pulses," Appl. Phys. Lett. 71 (23), 3364 (1997) **or** "Laser-induced fluorescence images of NO distribution after needle-plane pulsed negative corona discharge," G. J. Roth and M. A. Gundersen, IEEE Trans. Plasma Sci. 27, 28 (1999). (Papers on NO_x removal by corona discharges).
- Takahashi, F., Glassman, I. (1984). *Combust. Sci. Technol.* Vol. 37, p. 1. (Paper showing the

effect of temperature and number of C-C bonds on soot formation in premixed flames.)

- Gomez, A., Sidebotham, G., Glassman, I. (1984). "Sooting behavior in temperature-controlled laminar diffusion flames," Combustion and Flame, Vol. 58, 45-57. (Paper characterizing the soot formation processes in non-premixed flames using the smoke height test.)
- Frenklach, M., Wang, H. (1991). Proceedings of the Combustion Institute, Vol. 23, 1559. (The paper introducing the HACA mechanism for aromatic ring formation from flames.)

Prepare a critical review of the article, not to exceed 2 pages, structured as follows:

1. **Motivation**: Why the author(s) conducted the work
2. **Summary of the methods and results**
3. **Summary of the conclusions**
4. **Merits**: Your opinion of the merits of the work
5. **Weaknesses**: Your opinion of the shortcomings of the work

Suggestions:

- Don't repeat text that is in the paper. Summarize in your own words – it shows me that you really do understand the paper.
- Don't use buzz words from the paper without defining them. If you don't understand them and don't feel inclined to learn what they are (which is ok, I don't expect you to understand every detail of the paper) then leave the buzz words out! In other words: "everything you say can and will be used against you…" (Sounds harsh, but that's the way real science is – anything you write in a paper is subject to evaluation and criticism).
- Points 1 and 5 are the most important. Say more than 1 line about item 5, in particular. This really shows what you learned from the paper. It also helps you to generate your own ideas for research.

Here's an example of what I considered to be a really good report from a previous year, though I would prefer the 1 - 5 format as listed above.

Report on "Formation of Nitric Oxide in Premixed Hydrocarbon Flames" by C. P. Fenimore, Proceedings of the Combustion Institute, Vol. 13, p. 373, 1971.

At the time this paper was written, the formation of nitric oxide in premixed hydrocarbon flames had not been completely characterized. Concentrations of NO resulting from simple N2-O2-NO combinations could be calculated but it was still uncertain how fuel-rich flames could produce such high levels of nitric oxide. Fenimore set out to test the known laws of NO formation in relation to hydrocarbon flames in an attempt to find a more accurate explanation for how and where nitric oxide forms.

Experiments were conducted on both nonadiabatic and adiabatic flames. For the nonadiabatic case, flames were generated at atmospheric pressure by using porous plate burners which allowed for variable reactant mixtures. Product gasses were sampled downstream of the flame and analyzed for NO and NO2 concentrations, which were then plotted as a total nitric oxide concentration versus time. As the reaction time increased, the total nitric oxide concentration increased in a linear fashion. Since sampling at the primary reaction zone was not possible due to the proximity of the burner surface, Fenimore extrapolated the NO vs. time plots back to time equal to zero in order to find qualitative observations at the reaction zone. The extrapolated intersections occurred at NO concentrations greater than zero. No nitric oxide was present at time zero which indicated rapid production of NO very close to the flame after which the concentration followed the constant linearly increasing trend obtained by the experiments.

The adiabatic ethylene-air flames were created by using a Meker-type burner which allowed Fenimore to vary the pressure as well as the mixture strength. As with the nonadiabatic flames, data relating NO concentration to time *were plotted and extrapolated back to time zero. The nitric oxide concentrations at time zero (inferred by extrapolation) show a slight increase with pressure for fuel-rich mixtures and an even greater increase for fuel-lean mixtures. With the newly acquired NO concentration intercepts at time zero, a plot of the intercept versus the mixture strength was also created. The higher the pressure cases had intercepts corresponding to higher NO concentrations at the primary reaction zone. The same data set was also plotted as the logarithm of the NO concentration extrapolated intercept divided by the equilibrium NO concentration versus the mixture strength. Quickly formed NO (that at time zero) increased proportionally to pressure raised to the 0.5 power. As the mixtures reached 1.4 to 1.5 times that of a stoichiometric mixture, the NO at the reaction zone sometimes exceeds the equilibrium concentration.*

This work on NO formation in flames accomplished two main tasks. First, it verified the already known mechanisms that describe nitric oxide growth in combustion product gas. The most significant aspect of the research was showing the existence of prompt NO formation in the primary reaction zone. Although it was not possible to sample the gas at the primary reaction zone, Fenimore was able to show that some amount of NO must be forming at the flame front. Without the prompt NO formation, the nitric oxide concentration in the post-flame gas would have to be lower. Since the concentrations of NO vs. time plots are linear, extrapolation to time zero would result in a concentration of zero if no prompt NO formation occurred. This was a major discovery.

At the same time, however, Fenimore does very little to postulate by what mechanisms prompt NO forms. Two reactions are given that could be linked to the formation of nitric oxide in the primary reaction zone, but no experiments are conducted in order to verify or disprove the possibility. It would have been beneficial to attempt to explain the formation of prompt NO rather than just stating that it exists.

Part 2. The usual type of homework questions

Problem #1. Flammability limits

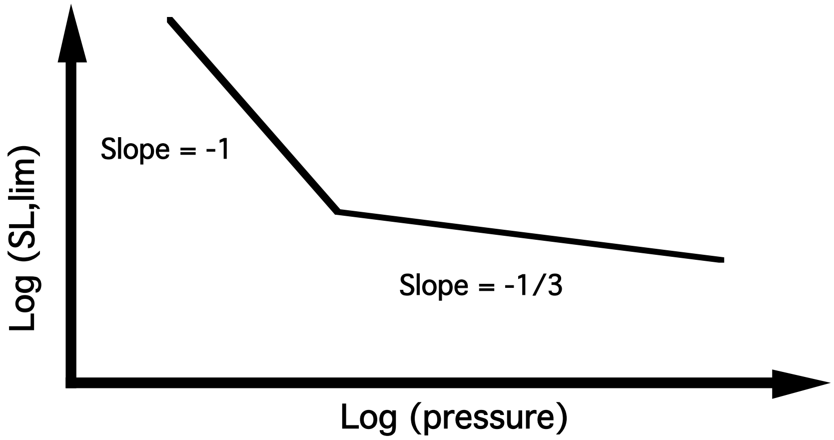
For each of the following extinction limit mechanisms

- Conduction heat losses to a tube wall
- Buoyancy-induced limit for upward propagation in a tube
- Buoyancy-induced limit for downward propagation in a tube
- Radiation heat loss

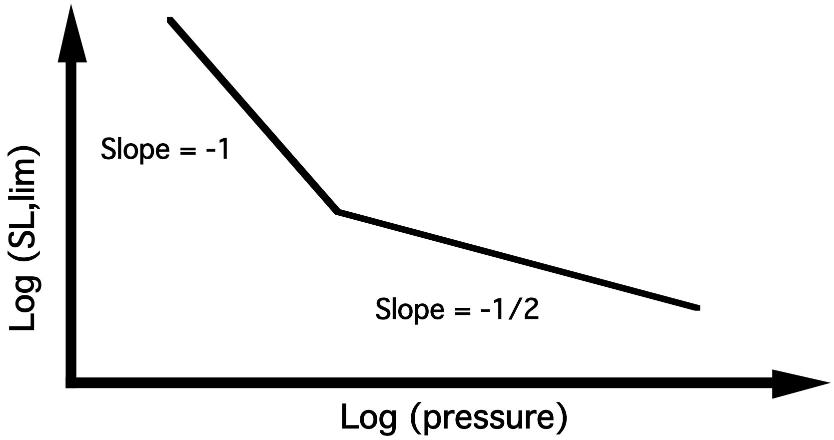
answer the following two questions: (1) Which would extinguish at higher S_L – CO_2 or N_2-diluted stoichiometric CH_4-O_2 mixtures? (2) Which would extinguish at higher adiabatic flame temperature?

Problem #2. Flammability limits

a) Explain the following experimental data taken for **downward** propagating flames in CH_4-air mixtures in a 5 cm diameter tube **at earth gravity**. At approximately what pressure and what $S_{L,lim}$ would the "knee" of this curve occur?



b) Explain the following experimental data taken for downward propagating flames in CH_4-air mixtures in a 5 cm diameter tube **at zero-gravity**. At approximately what pressure and what $S_{L,lim}$ would the "knee" of this curve occur?



Possibly useful information: $g = 980$ cm/sec^2; $T_{ad} \approx 1500$K; $T_o \approx 300$K; α (air, 1 atm) = 0.2 cm^2/sec; $\alpha \sim P^{-1}$; k(air, 1 atm) = 0.026 W/mK; $k \sim P^0$; $\beta \approx 14$ = constant; Λ of CH_4-air combustion products, 1 atm) = 10^6 W/m^3; $\Lambda \sim P^1$.

Problem #3. Ignition

For H_2-air mixtures with initial temperature 300K and pressure 1 atm, heating value $Q_R = 1.2 \times 10^8$ J/kg for hydrogen (note on the rich side that not all of the hydrogen is consumed!!), with mixture C_P = 8 cal/mole K,

a) Calculate and plot the adiabatic flame temperature as a function of equivalence ratio (ϕ), assuming constant C_P and no dissociation, according to the relation $Q_R Y_F = C_P(T_{ad} - T_\infty)$, where Y_f is the fuel mass fraction (which in turn is a function of the equivalence ratio ϕ).

b) Using the simple relation $S_L \sim (\alpha\Omega)^{1/2}$ with $\Omega \sim \exp(-E/RT_{ad})$, determine the proportionality constant needed to obtain S_L = 200 cm/sec at $\phi = 1$. Assume $\alpha \approx 1$ cm^2/sec and E = 27 kcal/mole.

c) From this information, calculate and plot S_L and $\delta = \alpha/S_L$ as a function of ϕ.

d) Assuming $Le_{H2} = 0.3$, $Le_{O2} = 1.1$, and using a weighted-average Le given by

$$Le = [1/(1+\phi)]\, Le_{H2} + [\phi/(1+\phi)]\, Le_{O2}$$

calculate and plot the equilibrium radius of the stationary spherical flame as a function of ϕ.

e) From this information calculate and plot the minimum ignition energy as a function of ϕ.

f) Compare this to the experimental results of Lewis and von Elbe. To what do you attribute the differences?

Problem #4. NO formation

a) For a stoichiometric premixed laminar methane-air flame, plot the log of NO concentration as a function of distance from the flame front. (Make it a big plot since you will be drawing several other curves on the same plot.) Explain the shape of this plot briefly.
b) On the same plot, draw the NO concentration as a function of distance from the flame front for a very lean methane-air flame. Explain the shape of this plot briefly.
c) Repeat b) for a stoichiometric methane-air flame with just enough exhaust gas recirculation to have the same adiabatic flame temperature as the flame of part b)
d) Repeat b) for a very rich methane-air flame.
e) Repeat b) for a very rich CO-air flame.

(Consider both thermal and prompt NO formation, and the relative magnitudes of both types of NO for each of these flames).

f) In terms of **maximum NO concentration**, how would a nonpremixed methane-air flame with no fuel or air dilution compare to the premixed flames in a) – e), i.e. which premixed flames would have a higher maximum NO, and which would have a lower maximum NO?

Problem #5. Soot formation.

Rank each member of the following groups (rank the members of each group separately, don't try to rank across groups) in terms of their propensity to form soot, and explain why. For example group 1: d, a, c, b; group 2: a, d, c, b.

Group 1:

a. Stoichiometric premixed methane-air flame
b. Non-premixed methane-air flame with no fuel or air dilution
c. Non-premixed methane-air flame with synthetic air having 30% O_2 rather than the usual 21%
d. Non-premixed ethane-air flame with no fuel or air dilution

Group 2 (all with N_2 dilution adjusted to obtain same peak temperature):

a. Slightly rich premixed propane-air flame (propane: $H_3C\text{-}CH_2\text{-}CH_3$)
b. Slightly rich premixed butane-air flame (butane: $H_3C\text{-}CH_2\text{-}CH_2\text{-}CH_3$)
c. Slightly rich premixed propylene-air flame (propylene: $H_3C{=}CH\text{-}CH_3$)
d. Non-premixed propane-air flame

Group 3

a. Slightly rich premixed propane-air flame with no heat losses
b. Same flame as 3a but with substantial heat losses in burned gas
c. Non-premixed propane-air flame with same peak temperature as in 3a and no heat losses

d. Same flame as in 3c but with substantial heat losses

Problem #6. Miscellaneous

Ronney Oil and Gas Co. claims to have invented a new fuel additive, called PDR®, which **increases the fuel heating value (Q_R) by 10%** but has **no effect on any other chemical, thermodynamic or transport property.** Estimate by what percent each of the following combustion properties would increase or decrease by adding PDR® to propane (C_3H_8) in each of the following cases (i.e. is there less than 10% change, exactly 10% change, or more than 10% change). In some cases there may be no change at all. **(Again, 3 points per part, 1 part free, but do all parts in this case.)**

a) Flame-front temperature of a non-premixed C_3H_8-air flame under diffusion-controlled burning conditions
b) Extinction stretch rate of a premixed C_3H_8-air flame
c) The burning velocity **at the downward flammability limit** ($S_{L,lim}$) of a lean premixed C_3H_8-air flame in a large diameter tube.
d) The burning velocity **at the radiation-induced flammability limit** ($S_{L,lim}$) of a lean premixed C_3H_8-air flame with negligible buoyancy effects
e) The adiabatic flame ball radius in a stoichiometric premixed C_3H_8-air mixture
f) The amount of soot production in a rich premixed C_3H_8-air flame at equivalence ratio 1.4
g) The amount of soot production in a nonpremixed laminar C_3H_8 jet flame
h) Amount of prompt NO in the products of a rich premixed C_3H_8-air flame at equivalence ratio 1.4, far downstream of the flame where chemical equilibrium is reached, with N_2 added to obtain the same adiabatic flame temperature as a C_3H_8-air mixture without PDR® additive