AME 514 Applications of Combustion – Spring 2017

Assignment #1

Due Friday 2/17/17, 4:00 pm, in the drop box in OHE 430N (Xerox room in the OHE 430 suite of offices.) While hard copies are preferred, if you're off campus you can email your assignment to ronney@usc.edu. 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 below (along with the reason I think they're important papers). Most of these papers are available in the "papers" folder in the lecture note folders on the course website. Also look on the course home page, towards the bottom of the page under "Getting copies of articles cited in the lecture notes" for information about getting the papers through the USC library online journals system. *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 mostly 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…)

- Giovangigli, V. and Smooke, M. (1992). Application of Continuation Methods to Plane Premixed Laminar Flames, *Combust. Sci. Tech.* 87, 241-256. (Excellent computational work showing the non-existence of flammability limits in the absence of losses.)
- Levy, A. (1965). An optical study of flammability limits, *Proc. Roy. Soc. (London)* A283, 134. (The original paper showing the relationship between buoyancy and flammability limits.)
- 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.)
- Kono, M., Kumagai, S., Sakai, T., *16th Symposium (International) on Combustion*, Combustion Institute, 1976, p. 757. (Good experimental study of the effects of spark duration on minimum ignition energy).
- Ballal, D. R., Lefebvre, A. H., "The influence of flow parameters on minimum ignition energy and quenching distance," *15th Symposium (International) on Combustion*, Combustion Institute, 1975, pp. 1473-1481. (Classic study of the effects of flow and turbulence 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)
- 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. PLEASE IDENTIFY EACH SECTION WITH A HEADING.

1) Why the author(s) conducted the work – what did they intend to do that was **<u>new</u>** at the time?
2) Summary of the methods used (is the work experimental, computational, analytical or some combination?)
3) Summary of the most important results
4) Summary of the conclusions – this is not just a restatement of the results, but how the authors **interpreted** the results to create a **new piece of knowledge** that didn't exist before the work was done.
5) Your opinion of the merits of the work
6) Your opinion of the shortcomings of the work
7) **<u>ONE sentence</u>** summary of the **most important message** the authors were trying to convey. Again this is not a restatement of the results but a summary of the new knowledge created by the work.

In discussing the importance of the paper that you're reviewing, you may find it useful to look at how many times it has been cited and what others have done with the information. To do this:

1. Go to http://www.usc.edu/libraries/
2. Above the search box, click on "Database quicklinks" then enter "Web of Science" in the search box
3. Type in some information about the paper in the search fields - author(s), journal, key words in the title, etc. (Some papers, notably older Combustion Symposium papers, are not included in the Web of Science, but you can use Google Scholar instead … not as respected a source by academics because it includes non-peer-reviewed sources, but it's useful nonetheless).
4. When you find the paper, click on the number next to "Times cited"

That will show you what articles have cited this paper and how recently the paper has been considered important by others. I'm particularly interested in having you review "classic" papers, i.e. ones that are older but continue to be cited often - which is an indication that it represented a breakthrough in the field at the time it was published.

Suggestions:

- Put the paper in its proper historical context. That is, don't say, "in the past few years some researchers have proposed that the earth is round…" Say, "at the time this paper was written, most scientists believed that the earth was flat but Prof. Columbus proposed the revolutionary idea that the earth was spherical in shape and set out to prove this by reaching India (which was known to be east of Spain) by sailing west across the Atlantic Ocean."

- Make it clear what is a **new result** from the current paper vs. previously known facts vs. facts reconfirmed in the current paper.
- Don't repeat text that is in the paper, and don't copy/paste from Wikipedia. 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 potentially to criticism).
- Points 1 and 7 are the most important. This really shows what you learned from the paper. It also helps you to generate your own ideas for research.
- If you state specific numbers (e.g., "The authors found that the engine used 6.3886 grams of fuel per minute to produce 1567.83 watts of power and 9.47982 grams of fuel per minute to produce 22.4857 watts of power") then you need to indicate why you mentioned these numbers, and are they good numbers or bad numbers? What did they prove or disprove? (In general, for any technical paper, if you state a fact you need to put it in context, i.e. why did you consider that fact important enough to state it?)

<u>Example report</u>

"On the Western Boundary of the Hydrodynamic Medium" by C. Columbus (*Journal of Modern Exploration and Exploitation*, Volume 1, p. 1, 1493).

1) Why the author(s) conducted the work – what did they intend to do that was **<u>new</u>** at the time?

   At the time this paper was written, most scientists believed that the earth was flat but Prof. Columbus proposed the revolutionary idea that the earth was spherical in shape and set out to prove this by reaching Asia (which was known to be east of Spain) by traveling west across a high Reynolds number hydrodynamic medium colloquially known as the "Atlantic Ocean." The idea of reaching an eastern destination by travelling west was considered absurd by most scientists at the time. Prof. Columbus knew that if such a route proved feasible, it would provide significant gains in efficiency for transporting valuable materials such as silk and spices from Asia back to Spain.

2) Summary of the methods used (is the work experimental, computational, analytical or some combination?)

   With a research grant from the Crown of Castile, Prof. Columbus procured 3 large experimental apparatuses operated by about 90 students and postdocs for his experiments. They used well-established aerodynamic methods to propel their apparatuses westward through the hydrodynamic medium despite considerable resistance to motion. They also used established geometric theory to monitor their progress although they were unsure of the western boundary condition.

3) Summary of the most important results

After nearly 2 months in the hydrodynamic media (punctuated by a visit to the Canary Islands for repairs to his apparatuses) and numerous experimental difficulties his team reached the western boundary condition of the hydrodynamic medium. He found that the western boundary was not a contiguous one but was comprised of numerous individual subdomains, each one surrounded by the hydrodynamic media. This was consistent with previous descriptions of parts of Asia, particularly the region now known as Indonesia. Many of these subdomains were inhabited and he studied the habits of their indigenous populations. On the other hand, there were discrepancies between the descriptions of the structure of these subdomains and their inhabitants and those of Asia. Moreover, Prof. Columbus's team did not find the silk and spices they were expecting to find in Asia. After 3 months of investigation he and his research team returned eastward to his home institution using the same propulsion methods used on the westward voyage.

4) Summary of the conclusions – this is not just a restatement of the results, but how the authors **interpreted** the results to create a **new piece of knowledge** that didn't exist before the work was done.

   Prof. Columbus's concluded that his hypothesis was verified, i.e. that there was indeed a westward route across the hydrodynamic medium to inhabited subdomains, however, there were discrepancies between his observations and published reports about Asia.

5) Your opinion of the merits of the work

   This work led to additional investigations on the characteristics of the western boundary condition, three by the original author and further investigations many by others. Prof. Columbus's investigations are among the most widely known and highly cited in the field, appearing in many later publications and eventually in textbooks read by almost every student in Europe and the Americas.

6) Your opinion of the shortcomings of the work

   Prof. Columbus concluded that he had reached Asia whereas (as later research proved) he had in fact reached a continent not widely known to or accepted by Europeans at the time. He did not seem to accept that neither the indigenous people he encountered nor the lands he observed matched known, established descriptions of the people and lands of eastern Asia, and thus had not in fact reached Asia. Another problem was that by interacting with the indigenous peoples, Prof. Columbus and his students introduced new microorganisms into the local environment which had a devastating impact on the local population, though at the time of Prof. Columbus's investigation the existence of these microorganisms and their link to diseases was not known.

7) **ONE sentence** summary of the **most important message** the authors were trying to convey. Again this is not a restatement of the results but a summary of the new knowledge created by the work.

   A western boundary condition of the hydrodynamic media exists, and this boundary does not possess a singularity that would result in one falling off the edge of the earth.

[By the way, I know that some of the historical facts in my paper report are not accurate, but I use them for illustrative purposes.]

Part 2. The usual type of homework questions

Note: If you're looking for a convenient source of data on thermal conductivity, thermal diffusivity, heat capacity, etc., of gas mixtures, either download GASEQ (a free, Windows-based program):

http://www.gaseq.co.uk/

GASEQ works fine for me on every version of Windows I've tried including Windows 8, but if it won't install for you I don't have any insight as to how to make it work on your computer. Alternatively you can use the equilibrium calculator on this website: http://navier.engr.colostate.edu/tools/

Problem #1. Rankine-Hugoniot relations

For a stoichiometric methane-air mixture at 1 atm and 298K, determine:

(a) The Chapman-Jouget detonation velocity (u_1) in units of m/s.
(b) The pressure change across the deflagration in units of Pascals (N/m^2).

Note that I have intentionally not given you any property data, not because I'm too lazy to do so but because I want to you to get used to looking up property data yourselves. For part (b), use any published value for S_L you wish, but state your reference.

Problem #2. Temperatures of non-premixed flames

a) Calculate and plot the temperature profile (T vs. x) for a planar 1D methane-air non-premixed flame with both reactants at 298K for no flow and L = 1 cm. You can get the thermal and mass diffusivities (and thus calculate Lewis numbers) from the Colorado State website mentioned above.
b) Repeat (a) for a flow u(L) = -1 m/s (that is, flow from right to left)
c) Calculate and plot the temperature profile (T vs. x) for a counterflow methane-air non-premixed flame with both reactants at 298K and a stretch rate $\Sigma = 100\ s^{-1}$. (Notice the similarity to part (b) where you had $u/L = (1\ m/s)/(0.01\ m) = 100\ s^{-1}$).
d) Calculate the temperature profile in the heptane droplet example in Lecture 1, from $r = r_d$ to $r = \infty$.

Problem #3. Premixed flames

a) Using the method for estimating the burning rate eigenvalue given in Lecture 1, calculate and plot the burning velocity as a function of the strength of the (fictitious) heat sink $(dT/dx)_{x=0}$. (I started this for you, just continue it. The Excel spreadsheet I used for the calculations is in the Lecture 1 folder … you can use it if you wish or write your own Excel sheet, Matlab code, etc.) Does the burning velocity $S_L \sim 1/\Lambda^{1/2}$ go to zero at some large value of $(dT/dx)_{x=0}$, i.e. when the strength of the heat sink is large? (Hint: your answer should be NO.) Why doesn't it, i.e. what's wrong with the approach I used when $(dT/dx)_{x=0}$ is not extremely small?

b) For very small $(dT/dx)_{x=0}$, calculate and plot S_L/S_L^o as a function of β for ε = 0.2, where S_L^o is a reference value of S_L taken for β = 10, ε = 0.2. Compare your results to the prediction of Bush and Fendell (1970).

c) For very small $(dT/dx)_{x=0}$, calculate and plot S_L/S_L^o as a function of ε for β = 10. Compare your results to the prediction of Bush and Fendell (1970).

d) If instead of a uniform flow, the flame is in a strained counterflow with u(x) = -Σx, show that the governing equation becomes

$$\tilde{x}\frac{d\tilde{T}}{d\tilde{x}}+\frac{1}{2}\frac{d^2\tilde{T}}{d\tilde{x}^2}=-Da\left(1-\tilde{T}\right)\exp\left(\frac{-\beta}{\tilde{T}\left(1-\varepsilon\right)+\varepsilon}\right)$$

where $\tilde{T}=\dfrac{T-T_\infty}{Y_{i,\infty}Q_R/C_P}=\dfrac{T-T_\infty}{T_{ad}-T_\infty}$ (as before), $\tilde{x}\equiv\dfrac{x}{\sqrt{2\alpha/\Sigma}}, Da\equiv\dfrac{Z}{\Sigma}$

e) Using a method similar to that used for the planar unstretched flame discussed in class, solve this equation for the stretched flame. In this case the goal is to determine the peak flame temperature (at $\tilde{x}$ = 0) as a function of Da. So start with an initial condition for T (starting with some value slightly less than 1) at $\tilde{x}$ = 0 and $d\tilde{T}/d\tilde{x}=0$ at $\tilde{x}$ = 0 (required by symmetry), then find the value of Da that leads to $\tilde{T}\rightarrow 0$ as $\tilde{x}\rightarrow\infty$. I put the spreadsheet for the planar case in the AME 514 lecture 1 folder so you can use that as a template if you want.

f) Using your results from part (e), find the value of $\tilde{x}$ at the location of maximum reaction rate (right side of the equation). Define this as the flame location $\tilde{x}_f$. At this point, the burning velocity S_L must oppose the local flow velocity u = -Σx. Also define $S_{L,o}$ as the planar (unstrained) burning velocity obtained in part (a). Using these facts, show that

$$\frac{S_L}{S_{L,o}}=\sqrt{2\Lambda}\frac{\tilde{x}}{\sqrt{Da}}$$

and plot $S_L/S_{L,o}$ as a function of Da. You should find that this plot is C-shaped with a minimum value of Da (≈ 10^6) at which combustion can be sustained in this strained counterflow.

Problem #4. Flammability limits

a) For lean CH_4-air mixtures at 1 atm pressure and zero gravity, calculate and plot the burning velocity at the flammability limit ($S_{L,lim}$) as a function of tube diameter over the range 0.05 cm < d < 50 cm. Note that the mechanism of extinction will change as d changes, so the relevant formula for $S_{L,lim}$ will change. The mechanism yielding the largest value of $S_{L,lim}$ will determine the extinction mechanism for that condition.
b) Repeat part (a) for a fixed tube diameter of 5 cm but with pressure varying over the range 0.01 atm < P < 10 atm.

c) Repeat part (a) for a fixed tube diameter of 5 cm but with gravity (g) varying over the range 100g downward to 100 g upward.
d) Repeat part (a) for a fixed tube diameter of 5 cm but with the mixture thermal diffusivity (α) varying by a factor of 100 higher or lower than the nominal value for air.

Problem #5. Ignition

For H_2-air mixtures with initial temperature 300K and pressure 1 atm

a) Calculate and plot the adiabatic flame temperature T_{ad} and burned-gas thermal diffusivity α as a function of equivalence ratio (ϕ) using GASEQ or another chemical equilibrium calculator
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 E = 27 kcal/mole.
c) From this information, calculate and plot S_L and $\delta = \alpha/S_L$ as a function of ϕ.
d) From the Colorado State website, find the cold-gas Lewis numbers of H_2 and O_2 as a function of ϕ, then determine the effective Le as a function of ϕ using a weighted-average:

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

e) From this information calculate and plot the equilibrium radius (R_Z) of the stationary spherical flame as a function of ϕ.
f) From this information calculate and plot the minimum ignition energy (as predicted by Joulin's (1985) model) as a function of ϕ.
g) Compare this to the experimental results of Lewis and von Elbe. To what do you attribute the differences?

Problem #6. Miscellaneous (similar to a problem from a previous year's final exam)

Ronney Chemicals, Inc., has invented a new fuel additive, called PDR®, which **increases the activation energy for ALL chemical reactions by 10%** but has **no effect on any other chemical, thermodynamic or transport property.** Note this is **activation energy (E) not heating value (Q_R)**. 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. **No credit without explanation!**

a) Adiabatic flame temperature (T_{ad}) of a stoichiometric premixed C_3H_8-air mixture
b) The adiabatic flame ball radius (R_Z) of a stoichiometric C_3H_8-air mixture
c) The minimum ignition energy (E_{min}) of a stoichiometric C_3H_8-air mixture
d) Burning velocity (S_L) of a stoichiometric premixed C_3H_8-air flame
e) Chapman-Jouget detonation velocity of a stoichiometric premixed C_3H_8-air flame
f) Extinction stretch rate (Σ_{ext}) of a premixed C_3H_8-air flame
g) Peak temperature of a nonpremixed C_3H_8-air stretched counterflow flame