1. Explain the following by presenting an argument.

   (a) Systems with non-premixed combustion and simpler to design and safe to operate.

   (b) Non-premixed flames are typically mixing controlled.

   (c) Non-premixed flames exhibit no reference thickness.

   (d) Non-premixed flames have no reference speed.

   (e) A non-premixed flame usually lies along the points where mixing produces a stoichiometric flame.

   (f) An unstrained non-premixed flame shuts out with time.

   (g) With increasing strain rates, the maximum flame temperature decreases.

   (h) Upon reaching a critical strain rate, a non-premixed flame extinguishes abruptly.

2. We have learnt that non-premixed flames are mixing (diffusion) controlled. Therefore, several global parameters of interest (such as flame location, flame temperature) can be arrived at without paying attention to the rate of reaction (which typically proceeds at a much faster rate compared to diffusion).

   In this problem, we consider a laminar non-premixed flame: gaseous fuel issues out of a nozzle, quiescent air from the ambient serves as the oxidizer, establishing a conical flame. Follow the steps below to arrive at the height of the flame.

   (a) Oxidizer arrives at the flame by diffusion. For a nozzle diameter d and diffusion coefficient D, write down an expression for the time taken for diffusion of oxidizer to the flame tip, t_D.

   (b) During the time t_D, the fuel issuing at a mass flow rate $\dot{m}_F$, reaches the flame tip, whose height is h. Write a relation for h in terms of these variables.

   (c) If this flame is established at an ambient pressure of $1\,\mathrm{atm}$ versus $0.1\,\mathrm{atm}$, how does the height of the flame vary?

   (d) Given that $D \sim T^{1.75}$, if the ambient temperature is $250\,\mathrm{K}$ versus $300\,\mathrm{K}$, how does the height of the flame vary?

3. If Z_1, Z_2, Z_3 are all conserved scalars, is any linear combination of these scalars also a conserved scalar? Comment on the uniqueness of the mixture fraction definition.

4. A conserved scalar (Z) was defined in the lecture based on mass fractions of fuel, oxidizer, and temperature, for the case of a single step reaction chemistry. For a real flame, multi-step kinetics is involved, and therefore, that quantity is not a passive conserved scalar anymore.

   One candidate suggested for the passive scalar for the case of real flames is,

   $$Z_p = \sum_{k=1}^{N} a_{kp} \frac{W_p}{W_k} Y_k, \tag{1}$$

   where a_{kp} is the number of elements of type p in species k. Typically, $p = \{\mathrm{C, H, O, N}\}$ for most hydrocarbon flames. For example, $a_{\mathrm{CH_4,C}} = 1, a_{\mathrm{CH_4,H}} = 4$.

   This suggestion is based on the idea that species may be consumed or produced in a reaction, but the amounts of elements are always conserved. Mathematically, if the jth chemical reaction is represented as

   $$\sum_{k=1}^{N} \nu'_{kj} M_k \rightleftharpoons \sum_{k=1}^{N} \nu''_{kj} M_k, \text{ for } j = 1 \ldots M, \text{ then}$$

   $$\sum_{k=1}^{N} a_{kp}(\nu'_{kj} - \nu''_{kj}) = 0$$

   If all molecular diffusivities are assumed to be equal $(D_{ij} = D)$, show that Z_p defined by (1) is a conserved scalar (Hint: Start with the species mass balance equation). Define a normalized mixture fraction, z_p, based on Z_p. What values does z_p take on the fuel side and the oxidizer side? Is $z_C = z_H = z_O = z_N$? Why or why not?

5. Identify the regions where NO and OH are produced and consumed from the plots of Y_{NO} and Y_{OH} vs z provided here. Read up on NO formation mechanisms (for instance, CKL $3.9) and explain the kinetics behind the production of NO in the regions identified. What are some strategies to mitigate NO formation? Elaborate on some of them.
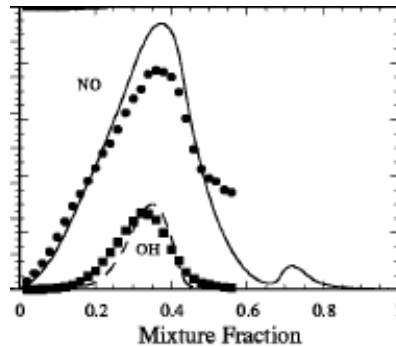
Courtesy: Sandia D flame. Prof. Pitsch's lectures at the CEFRC summer school, 2014

6. Burke-Schumann solution:

   (a) Starting with the steady flamelet equations, obtain solutions of flame structure: $Y_F(z), Y_O(z)$ in terms of the stoichiometric mixture fraction (z_{st}, where the flame is positioned)

   (b) Draw the structure of the flame (Y_F, Y_O) in the z-space.

   (c) Calculate the point in z space where a pure CH_4-air non-premixed flame will be located (z_{st}), under the infinitely fast irreversible chemistry assumption.

7. Starting with the steady flamelet equations, derive an expression for the flame temperature in a Burke-Schumann flame (infinitely fast irreversible chemistry) as a function of z, in terms of the stoichiometric mixture fraction, z_{st} (Hint: solve for temperature profile on fuel side and oxidizer side separately). Consider the following cases:

   (a) Counter-flowing stream of methane against air

   (b) Counter-flowing stream of 5% methane, 95% Nitrogen (fuel mixture is diluted) against air.

   What are the maximum flame temperatures attained in the two cases? Which one results in higher temperature? Explain why. Take a value of $q = 50100\,\text{kJ/kg}, c_P = 1400\,\text{J/kg} \cdot \text{K}, T_F^\circ = 400\,\text{K}, T_O^\circ = 300\,\text{K}$. (Ans: 2237 K, 1310 K)

8. It is interesting to compare the maximum temperature reached in a non-premixed flame with the adiabatic flame temperature achieved in a premixed flame.

   (a) Simplify the expression for the maximum flame temperature in a Burke Schumann flame derived in Problem 7 above for the case, $T_F^\circ = T_O^\circ = T_\circ$, and denote it as $T_{\text{diff}}^{\max}$.

   (b) Next, let us obtain the maximum temperature in a premixed where the same amount of fuel is mixed with oxidizer in stoichiometric proportions:

       (i) Let Y_F^{mix} and Y_O^{mix} denote the amounts of fuel and oxidizer present at the non-premixed flame location, but in a non-burning situation (pure mixing). Obtain Y_F^{mix} in terms of z_{st}. Note: oxidizer (Y_O^{mix}) is already in stoichiometric proportion.

       (ii) For a premixed flame with this amount of fuel, write down an expression for the maximum flame temperature, and denote it as $T_{\max}^{\text{prem}}$. We know that $T_{\text{prem}}^{\max}$ is the adiabatic flame temperature for the aforesaid mixture of fuel and oxidizer.

   (c) Are $T_{\text{diff}}^{\max}$ and $T_{\text{prem}}^{\max}$ equal? Comment on your observation.

9. An analytical solution for $z(x_1)$ can be derived for the steady strained flame case, with additional assumptions of constant density and diffusion coefficients (x_1: axial direction).

   (a) (Class exercise) Let us get to this solution in steps:

(i) Verify that the governing equation for z for the 1D steady stagnation point flow case with additional assumptions of constant density and diffusion coefficients is given by $-\rho a x_1 \dfrac{dz}{dx_1} = \dfrac{d}{dx_1}\left(\rho D \dfrac{dz}{dx_1}\right)$

(ii) Do a variable transformation using $\xi = x_1\sqrt{\dfrac{a}{2D}}$ and verify that the resulting equation becomes

$$\xi\frac{dz}{d\xi} = \frac{-1}{2}\frac{d^2 z}{d\xi^2}$$

(iii) Taking $f(\xi) = dz/d\xi$, integrate once to obtain that $f = k\exp(-\xi^2)$, where k is a constant of integration.

(iv) Integrate the above expression again to obtain z

(v) Employ suitable boundary conditions for fuel $(x_1 \to -\infty)$ and oxidizer $(x_1 \to \infty)$ and verify that the solution is given by $z = \dfrac{1}{2}[1 - \mathrm{erf}(\xi)]$,

(b) Derive an expression for χ in terms of z, and thereby, an expression for χ_{st} in terms of z_{st}. What is the value of χ_{st} for the cases 7a and 7b above, given $a = 30\,\mathrm{s}^{-1}$? (Ans: $0.74s^{-1}, 9.47s^{-1}$)

10. (Refer section TP $3.4) One way to monitor the reactivity of a non-premixed flame system is by evaluating the fuel consumption rate per unit flame area, $\dot{\Omega}_F$, expressed as

$$\dot{\Omega}_F = \int_{x_f^-}^{x_f^+} \dot{\omega}_F dx,$$
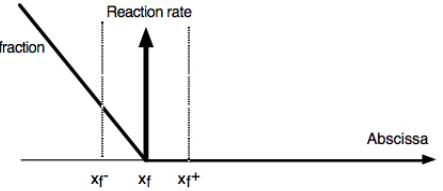
where x_f^- and x_f^+ are points located behind and after the flame front respectively, yet infinitely close to the flame front (see Fig. above). Consider the case of a 1D steady strained non-premixed flame, with infinitely fast chemistry.

(a) Starting with the species equation for a steady problem, assuming that the convection of species mass is negligible compared to diffusion, rewrite $\dot{\Omega}_F$ in terms of gradients of Y_F in the physical space, and further, in terms of gradients in mixture fraction space.

(b) Using $z = \dfrac{1}{2}[1 - \mathrm{erf}(\xi)]$, where $\xi = x_1\sqrt{\dfrac{a}{2D}}$, obtain an expression for $\dot{\Omega}_F$ as function of strain rate, a, Y_F°, and z_{st}.

(c) Comment on how $\dot{\Omega}_F$ varies with a. Can extinction be predicted for large a as observed experimentally? Support your answer with arguments.

11. The adiabatic flame speeds of a stoichiometric methane/air mixture and ethylene/air mixture are given as: 40 cm/s and 72 cm/s respectively. Obtain an estimate for the scalar dissipation rates at extinction for their non-premixed flame counterparts with the respective fuel and air counter-flowing against each other. Recall that asymptotic analysis provides an estimate for scalar dissipation rates at extinction, $\chi_{st,q} \sim \dfrac{z_{st}^2 (1 - z_{st})^2}{\delta/S_u^0}$.

Take a typical value for thermal diffusivity, $\alpha = 1.5 \times 10^{-5}\mathrm{m}^2/\mathrm{s}$. Calculate the corresponding values of strain rate at extinction a_q using this estimate of $\chi_{st,q}$ in a 1D stagnation point flame. (Ans: $28.8s^{-1}, 93.36s^{-1}$)