ME 471: Turbulent Combustion, Spring 2012

Stanford University

Homework 3: Non-premixed Turbulent Combustion (I)

Due Tuesday, June 5 in class.

Guidelines: Please turn in a *neat* and *clean* homework that gives all the formulae that you have used as well as details that are required for the grader to understand your solution. Show all work. Required plots should be generated using computer software such as Matlab or similar program. Answers should be written in the blank spaces provided in these homework sheets. Use the back of the page in case you need additional space (not recommended to use more space than provided), for which a clear indication should be written to warn the reader of the presence of text there. Vector quantities are denoted in **bold** letters in what follows.

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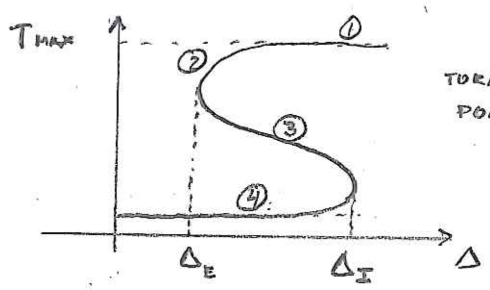
Solve Question 1 and Question 2.

Question 1 (50 pts)

a) Sketch the S-curve obtained by Liñán ("Asymptotic structure of counterflow diffusion flames at large activation energies", 1974) in terms of the reduced Damköhler number Δ versus the maximum temperature $T_{\max}$. Give a brief description of the physical phenomena that take place at both turning points. Locate on the graph the extinction Damköhler number Δ_E and give an explanation of its physical meaning. Finally, give a brief description of each burning regime. (25pts)



TURNING POINTS
- Δ_I : IGNITION DAMKÖHLER NUMBER +2.5
- Δ_E : EXTINCTION DAMKÖHLER NUMBER (DIFFUSION TIME ~ CHEMICAL TIME) +2.5

REGIMES: SEE PAGE 9 (BACK) OF THE INSTRUCTOR NOTES FOR A DESCRIPTION OF EACH REGIME

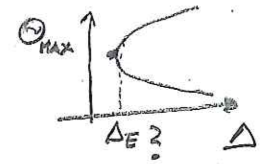
+5 EACH

+25/25

b) In his paper, Liñán ("Asymptotic structure of counterflow diffusion flames at large activation energies", 1974) identified a critical Damköhler number for flame extinction Δ_E in the diffusion-flame regime, which is given by

$$\Delta_E = e^1 \left[(1-|\gamma|) - (1-|\gamma|)^2 + 0.26(1-|\gamma|)^3 + 0.055(1-|\gamma|)^4\right]. \tag{1}$$

In particular, for $\Delta < \Delta_E$ the inner-zone equation



$$\frac{d^2\Theta}{d\eta^2} = (\Theta - \eta)(\Theta + \eta)\exp\left[-\Delta^{-1/3}(\Theta + \gamma\eta)\right] \tag{2}$$

does not have any solution. Equation (2) is subject to $d\Theta/d\eta \to \pm 1$ at $\eta \to \pm\infty$. Equation (2) describes de reactive-diffusive zone in diffusion flames at large activation energies, with $\Theta(\eta)$ being the inner temperature, η a stretched coordinate normal to the flame, and Δ the reduced Damköhler number. Additionally, $1-\gamma$ is twice the ratio between the heat transferred from the flame towards the oxidizer side and the total chemical heat released. Therefore, Δ and γ are external parameters in equation (2) - see class notes or Liñán (1974) paper for a formal derivation of the inner-zone equation (2) if needed -.

Provide a formal derivation of (1) by conveniently manipulating the inner-zone equation (2). (25 pts)

FIRST THING TO NOTICE IS THAT THE SOLUTIONS FOR $\pm\gamma$ ARE TRIVIALLY RELATED, SINCE A CHANGE OF VARIABLES IN (2) $\gamma' = -\gamma$, $\eta' = -\eta$ YIELDS EXACTLY THE SAME PROBLEM. FOR $\gamma > 0$ A PREFERENTIAL LEAKAGE OF OXIDIZER OCCURS, AND FOR $\gamma < 0$ FUEL LEAKAGE IS MORE IMPORTANT. WE WILL FOCUS ON $\gamma > 0$ AND WILL TRY TO FIND AN EXPANSION OF Δ_E IN TERMS OF THE SMALL PARAMETER $m = \frac{1-|\gamma|}{2} \ll 1$, IN SUCH A WAY THAT Δ_E ONLY DEPENDS ON $|\gamma|$ GIVEN THE SYMMETRY DESCRIBED ABOVE.

ADDITIONALLY, NOTE THAT $Y_{O_2} \sim \Delta^{-1/3}/\beta\,(\Theta - \eta)$ AND $Y_F \sim \Delta^{-1/3}/\beta\,(\Theta + \eta)$ AS OBSERVED BY USING THE INNER ASYMPTOTIC EXPANSION OF THE TEMPERATURE (EQ 70 IN LIÑÁN'S PAPER) TOGETHER WITH THE ALGEBRAIC RELATIONS (3) AND (4) FROM LIÑÁN'S PAPER.

A SMALL PARAMETER $m = \frac{1-|\gamma|}{2} \ll 1$ IS DEFINED HERE, NOTICE THAT AS $\gamma \to 1$ THE OXIDIZER LEAKAGE THROUGH THE FLAME INCREASES FOR A FIXED Δ AND BECOMES INFINITE FOR $\Delta < \Delta_E$. FOR $\gamma > 1$ THERE EXISTS A PREMIXED STRUCTURE ON THE FUEL SIDE WITH A LARGE EXCESS OF OXIDIZER.

TO OBTAIN THE EXPANSION (1), ONE FIRST NEEDS TO SHIFT THE INNER COORDINATE η TO REGIONS WHERE THE OXIDIZER MASS FRACTION BECOMES OF ORDER UNITY: $\xi = 2\eta + b/m$, WITH b AN ORDER-UNITY PARAMETER (NOTICE THAT THIS REGION GOES TO INCREASINGLY POSITIVE VALUES - I.E. TO THE FUEL SIDE - AS $\gamma \to 1$). ALSO, A NEW VARIABLE $\varphi = \Theta + \eta$ IS DEFINED TO DENOTE THE INNER FUEL MASS FRACTION. IN THESE VARIABLES, EQ (2) BECOMES

$$\frac{d^2\varphi}{d\xi^2} = \frac{b}{4m} e^{-\Delta^{-1/3} b}\, \varphi \left[1 + (\varphi - \xi)\frac{m}{b}\right] e^{-\Delta^{-1/3}\left[\varphi - m\xi\right]}$$

SUBJECT TO $\begin{cases} \dfrac{d\varphi}{d\xi} \to 1 & \text{AS } \xi \to +\infty \\ \dfrac{d\varphi}{d\xi} \to 0 & \text{AS } \xi \to -\infty. \end{cases}$

IT IS MORE EXPEDIENT TO RESCALE φ AND ξ AS $\tilde{\varphi} = \varphi\Delta^{-1/3}$ AND $\tilde{\xi} = \xi\Delta^{-1/3}$, WITH $\tilde{b} = b\Delta^{-1/3}$, IN SUCH A WAY THAT THE DAMKÖLER NUMBER IS DROPPED FROM THE EXPONENTIAL:

$$\frac{d^2\varphi}{d\xi^2} = \delta\varphi\left[1+(\varphi-\xi)\frac{m}{b}\right]e^{-(\varphi-m\xi)}, \quad \text{SUBJECT TO} \begin{cases} \frac{d\varphi}{d\xi}\to 1 \text{ AS } \xi\to+\infty \\ \frac{d\varphi}{d\xi}\to 0 \text{ AS } \xi\to-\infty \end{cases}$$

WHERE THE TILDES HAVE BEEN DROPPED. EXPANDING φ AND $\delta = \frac{b\Delta}{4m}e^{-b}$ IN POWERS OF m:

$$\left.\begin{aligned}\varphi &= \varphi_0 + m\varphi_1 + O(m^2)\\ \delta &= \delta_0 + m\delta_1 + O(m^2)\end{aligned}\right\}$$ ONE OBTAINS, TO LEADING ORDER:

$$\frac{d^2\varphi_0}{d\xi^2} = \delta_0\varphi_0 e^{-\varphi_0}$$ SUBJECT TO $\frac{d\varphi_0}{d\xi}\to 1$ AS $\xi\to+\infty$ ($\varphi_0\sim\xi+\cancel{\varphi}^{\,0}$ FROM OUTER SOL.), AND $\frac{d\varphi_0}{d\xi}\to 0$ AS $\xi\to-\infty$ ($\varphi\to\cancel{\varphi}^{\,0}$ FROM OUTER SOL.).

SINCE $\frac{d^2\varphi_0}{d\xi^2} = \frac{1}{2}\frac{d}{d\varphi_0}\left(\frac{d\varphi_0}{d\xi}\right)^2 = \delta_0\varphi_0 e^{-\varphi_0}$, INTEGRATING THIS EQUATION BETWEEN $\varphi_0 = 0$ AND $\varphi_0 \to +\infty$, ONE OBTAINS THAT $\underline{\underline{\delta_0 = 1/2}}$, WHERE USE OF THE RESULT $\int_0^{+\infty}\varphi_0 e^{-\varphi_0}d\varphi_0 = 1$ HAS BEEN MADE. +15

SIMILARLY, IN THE SECOND APPROXIMATION, THE PROBLEM

$$\frac{d^2\varphi_1}{d\xi^2} - \delta_0\varphi_1(1-\varphi_0)e^{-\varphi_0} = \delta_0\varphi_0 e^{-\varphi_0}\left[\xi + k + \frac{\varphi_0-\xi}{b}\right] \quad (*)$$

SUBJECT TO $\frac{d\varphi_1}{d\xi}\to 0$ AT $\xi\to\pm\infty$ IS FOUND, WITH $k = \delta_1/\delta_0$. THE HOMOGENEOUS SOLUTION OF THIS EQUATION IS SIMPLY $\varphi_{1h} = \frac{d\varphi_0}{d\xi}$ SINCE $\frac{d\varphi_1}{d\xi} = \frac{d^2\varphi_0}{d\xi^2} = \varphi_0\delta_0 e^{-\varphi_0}$ AND $\frac{d^2\varphi_1}{d\xi^2} = \delta_0\varphi_0' e^{-\varphi_0} - \varphi_0\delta_0\varphi_0' e^{-\varphi_0} = \delta_0\varphi_1 e^{-\varphi_0}(1-\varphi_0)$. MULTIPLYING $(*)$ BY φ_{1h} AND USING THAT $\varphi_{1h}'' - \delta_0\varphi_{1h}(1-\varphi_0)e^{-\varphi_0} =$ ONE OBTAINS

$$\underbrace{\varphi_{1h}\varphi_1'' - \varphi_{1h}''\varphi_1}_{(\varphi_{1h}\varphi_1' - \varphi_{1h}'\varphi_1)'} + \cancel{\varphi_{1h}''\varphi_1} - \cancel{\delta_0\varphi_1(1-\varphi_0)e^{-\varphi_0}\varphi_{1h}} = \delta_0\varphi_0\varphi_{1h}e^{-\varphi_0}\left[\xi+k+\frac{\varphi_0-\xi}{b}\right]$$

$$(\varphi_{1h}\varphi_1' - \varphi_{1h}'\varphi_1)' = \delta_0\varphi_0\varphi_{1h}e^{-\varphi_0}\left[\xi+k+\frac{\varphi_0-\xi}{b}\right],$$ THEREFORE:

$$\frac{d}{d\xi}\left(\frac{d\varphi_1}{d\xi}\frac{d\varphi_0}{d\xi} - \frac{d^2\varphi_0}{d\xi^2}\varphi_1\right) = \delta_0\varphi_0\frac{d\varphi_0}{d\xi}e^{-\varphi_0}\left[\xi+k+\frac{\varphi_0-\xi}{b}\right].$$

INTEGRATING FROM $\xi = -\infty$ TO $+\infty$, AND APPLYING BOUNDARY CONDITIONS ONE OBTAINS

$$\int_{-\infty}^{+\infty}\delta_0\varphi_0\frac{d\varphi_0}{d\xi}e^{-\varphi_0}\left[\xi+k+\frac{\varphi_0-\xi}{b}\right]d\xi = 0$$ AS A SOLVABILITY CONDITION,

WHICH CAN BE SPLIT INTO THE FOLLOWING INTEGRALS:

$$\underbrace{\int_0^{+\infty}\varphi_0 k e^{-\varphi_0}d\varphi_0}_{1} + \underbrace{\int_0^{+\infty}\frac{\varphi_0^2}{b}e^{-\varphi_0}d\varphi_0}_{2} + \underbrace{\left(1-\frac{1}{b}\right)\int_{-\infty}^{+\infty}\varphi_0 e^{-\varphi_0}\frac{d\varphi_0}{d\xi}\xi d\xi}_{3} = 0$$

WITH ① $= k$, ② $= 2/b$, ③ $= \varsigma(1-1/b)$ WITH $\varsigma = \int_{-\infty}^{+\infty}\varphi_0 e^{-\varphi_0}\frac{d\varphi_0}{d\xi}\xi d\xi$ A CONSTANT THAT NEEDS TO BE OBTAINED NUMERICALLY. THE SOLVABILITY CONDITION FOR THE SECOND ORDER THEN REDUCES TO:

$$k + \varsigma + (2-\varsigma)/b = 0 \Rightarrow k = (\varsigma-2)/b - \varsigma = \delta_1/\delta_0 \Rightarrow \delta_1 = \frac{(\varsigma-2)}{2b} - \varsigma/2$$

THE TWO-TERM EXPANSION OF δ BECOMES:

$$\delta = \frac{b\Delta}{4m}e^{-b} = \frac{1}{2}\left[1 - \left(\varsigma - \frac{(\varsigma-2)}{b}\right)m + O(m^2)\right]$$

BY PERFORMING $\frac{d\Delta}{db} = 0$, A VALUE $b = 1 + O(m)$ IS OBTAINED, WHICH MAKES Δ TO BE MINIMUM: $\Delta = \Delta_E$. IN THIS WAY, THE TWO-TERM EXPANSION OF Δ_E CAN BE WRITTEN AS

$$\Delta_E = 2em(1-2m) = e\left\{(1-|\gamma|) - (1-|\gamma|)^2\right\}.$$

FROM A NUMERICAL INTEGRATION OF (2) (SEE FIG 8 OF LIÑÁN'S PAPER), ONE CAN OBTAIN THAT $\Delta_E = 0.856$ FOR $\gamma = 0$. USING THIS CONDITION AND THE SYMMETRY OF Δ_E AT $\gamma = 0$ ($d\Delta_E/d\gamma = 0$ AT $\gamma = 0$, SEE FIG 12 OF LIÑÁN'S PAPER), THE THIRD AND FOURTH ORDERS OF THE EXPANSION OF Δ_E CAN BE OBTAINED, WHICH YIELDS $\underline{\underline{\Delta_E = e\left\{(1-|\gamma|) - (1-|\gamma|)^2 + 0.26(1-|\gamma|)^3 + 0.055(1-|\gamma|\right.}}$ +10

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Question 2 (50 pts)

For a steady laminar counterflow diffusion flame with constant density and equal diffusivities of fuel and oxidizer,

a) Prove that the scalar dissipation rate $\chi = D|\nabla Z|^2$ can be written as

$$\chi = \frac{a}{2\pi} \exp\left[-2(\mathrm{erfc}^{-1}(2Z))^2\right] \tag{3}$$

where Z is the mixture fraction, a is the strain rate, and $\mathrm{erfc}(p) = (2/\sqrt{\pi}) \int_p^\infty \mathrm{e}^{-t} dt$ is the complementary error function.

SOL: LOOK AT PAGE 9 OF THE INSTRUCTOR NOTES FOR DERIVATION OF (3).

+30

b) What is the physical meaning of the scalar dissipation rate at stoichiometry $\chi_{st} = \chi(Z = Z_{st})$? In this formulation, Z_{st} is the stoichiometric mixture fraction.

IT REPRESENTS THE INVERSE OF THE DIFFUSION TIME THROUGH THE STOICHIOMETRIC SURFACE.

+5

c) Using (3), prove that χ_{st} is of order aZ_{st}^2 when $Z_{st} \ll 1$. This result is valid for hydrocarbon-air flames, in which Z_{st} is typically a small number. According to this result, is the diffusion time through the stoichiometric surface much larger or much smaller than the characteristic strain time?

SINCE $Z = \frac{1}{2} \mathrm{erfc}\left(\frac{z}{\sqrt{2}}\right) \sim \frac{1}{\sqrt{2\pi}} \frac{e^{-z^2/2}}{z}$ FOR LARGE z, AND $\chi = a\left(\frac{dZ}{dz}\right)^2 \sim \frac{a}{2\pi}\left(-e^{-\frac{z^2}{2}}\right)^2$

DIMENSIONLESS !

THEN $\chi \sim a Z^2 z^2 = 2a Z^2 \underbrace{\mathrm{erfc}^{-1}(2Z)^2}_{O(1) \text{ WHEN } Z \to Z_{st}} \Longrightarrow \chi_{st} \sim 2a Z_{st}^2$ +10

ALSO, SINCE $\chi_{st} \sim \frac{1}{t_{d_{st}}} \sim a Z_{st}^2$, THEN $t_{d_{st}} \gg \frac{1}{a} \Rightarrow$ THE DIFFUSION TIME THROUGH THE STOICHIOMETRIC SURFACE IS MUCH LARGER THAN THE STRAIN TIME FOR $Z_{st} \ll 1$ SINCE $Z = Z_{st}$ IS LOCATED DEEP INSIDE THE AIR SIDE.

+5