AME 513b

Fundamentals and Applications of Combustion II

Lecture 4

Analytical/numerical methods I

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Reminder: structure of deflagration

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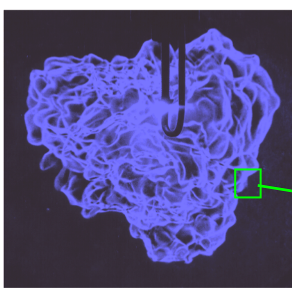
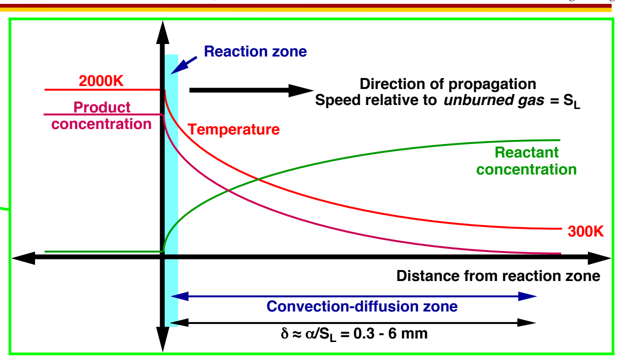


Turbulent premixed flame experiment in a fan-stirred chamber (D. Bradley, Leeds Univ.)



Flame thickness (δ) ~ α/S_L
(α = thermal diffusivity)

- Temperature increases in convection-diffusion zone or preheat zone ahead of reaction zone, even though no heat release occurs there, due to balance between convection & diffusion
- Temperature constant downstream (if adiabatic)
- Reactant concentration decreases in convection-diffusion zone, even though no chemical reaction occurs there, for the same reason

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Structure of deflagration

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- Recall for infinitely thin reaction zone, the temperature profile is an exponential with decay length = flame thickness α/S_L; for flow from left to right (in +x direction):

$$\left.\begin{array}{l} T(x) = T_\infty + \left(T_{ad} - T_\infty\right)e^{x/\delta} \quad (x \le 0) \\ T(x) = T_{ad} = \text{constant} \quad (x \ge 0) \end{array}\right\} \Rightarrow \left.\frac{dT}{dx}\right|_{x=0+} - \left.\frac{dT}{dx}\right|_{x=0-} = -\frac{(T_{ad}-T_\infty)}{\delta}; \delta = \frac{k}{\rho_\infty C_P S_L}$$

- Similarly for fuel mass fraction

$$\left.\begin{array}{l} Y(x) = Y_\infty\left(1 - e^{Le\, x/\delta}\right) \quad (x \le 0) \\ Y(x) = 0 \ (x \ge 0) \end{array}\right\} \Rightarrow \left.\frac{dY}{dx}\right|_{x=0+} - \left.\frac{dY}{dx}\right|_{x=0-} = +\frac{Y_\infty}{\delta}Le$$

- But how to calculate burning velocity? With reaction term:

$$u\frac{dT}{dx} - \frac{k}{\rho C_P}\frac{d^2T}{dx^2} = \frac{\dot{q}'''}{\rho C_P}; \dot{q}''' = \rho Q_R Z Y_F \exp\left(\frac{-E}{\Re T}\right)$$

$$\rho u = \rho_\infty S_L = const. \Rightarrow \rho_\infty S_L C_P \frac{dT}{dx} - k\frac{d^2T}{dx^2} = \rho Q_R Z Y_F \exp\left(\frac{-E}{\Re T}\right)$$

Note that Z is not the usual one based on molar concentrations, but rather based on fuel mass fraction (units of Z = 1/time)

1D laminar premixed flame - formulation

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$$\text{Define } \tilde{T}(x) \equiv \frac{T(x)-T_\infty}{T_{ad}-T_\infty}, \tilde{Y}(x) \equiv \frac{Y_f}{Y_{f,\infty}}, \delta = \frac{k}{\rho_\infty S_L C_P}, \tilde{x} = \frac{x}{\delta}, \beta = \frac{E}{\Re T_{ad}}, \varepsilon = \frac{T_\infty}{T_{ad}}$$

$$\text{Note } C_P\left(T - T_\infty\right) = \left(Y_{F,\infty} - Y_F\right)Q_R \text{ and } C_P\left(T_{ad} - T_\infty\right) = Y_{F,\infty}Q_R \Rightarrow \tilde{T}(x) = 1 - \tilde{Y}(x)$$

$$\Rightarrow \rho_\infty S_L C_P \frac{d\tilde{T}}{dx} - k\frac{d^2\tilde{T}}{dx^2} = \rho\frac{Y_{f,\infty}Q_R}{T_{ad}-T_\infty} Z\frac{Y_F}{Y_{F,\infty}}\exp\left(\frac{-E}{\Re\left(\tilde{T}\left(T_{ad}-T_\infty\right)+T_\infty\right)}\right)$$

$$\Rightarrow \rho_\infty S_L C_P \frac{d\tilde{T}}{dx} - k\frac{d^2\tilde{T}}{dx^2} = \rho C_P Z\tilde{Y}\exp\left(\frac{-E}{\Re\left(\tilde{T}\left(T_{ad}-T_\infty\right)+T_\infty\right)}\right)$$

$$\Rightarrow \frac{d\tilde{T}}{dx} - \frac{k}{\rho_\infty S_L C_P}\frac{d^2\tilde{T}}{dx^2} = \frac{\rho C_P Z}{\rho_\infty S_L C_P}\left(1-\tilde{T}\right)\exp\left(\frac{-E}{\Re T_{ad}\left(\tilde{T}\left(\frac{T_{ad}-T_\infty}{T_{ad}}\right)+\frac{T_\infty}{T_{ad}}\right)}\right)$$

$$\Rightarrow \frac{d\tilde{T}}{d\tilde{x}} - \frac{d^2\tilde{T}}{d\tilde{x}^2} = \Lambda\left(1-\tilde{T}\right)\exp\left(\frac{-\beta}{\tilde{T}\left(1-\varepsilon\right)+\varepsilon}\right); \Lambda \equiv \frac{kZ}{\rho_\infty C_P S_L^2} \text{ - burning rate eigenvalue}$$

1D premixed flame – numerical solution

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- Boundary conditions: x = -∞, T = 0; x = +∞, T = 1
- Cold boundary problem – reactants occurs even at x = -∞, so are already completely reacted by x = 0, so need to assume finite domain with non-zero dT/dx slope at inflow end (equivalent to assuming a small heat loss at cold boundary)
- Can't assume dT/dx = 0 at cold boundary, reaction is too slow at T = 0 and would take enormous domain to reach flame front
- Need to see how different values of dT/dx at cold boundary affect solution

1D premixed flame – Euler method

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- x = 0 is cold boundary (T = 0), assume small but finite dT/dx
- "Guess" eigenvalue Λ

$$\left.\frac{d^2\tilde{T}}{d\tilde{x}^2}\right|_{\tilde{x}=0} = \left.\frac{d\tilde{T}}{d\tilde{x}}\right|_{\tilde{x}=0} - \Lambda(1-0)\exp\left(\frac{-\beta}{0(1-\varepsilon)+\varepsilon}\right)$$

- Fixed grid spacing Δx, at every subsequent grid point use Euler's method (often unstable; may need methods with higher-order accuracy, e.g. Runge-Kutta) to estimate derivatives:

$$\tilde{x}_{i+1} = \tilde{x}_i + \Delta\tilde{x}; \tilde{T}_{i+1} = \tilde{T}_i + \left.\frac{d\tilde{T}}{d\tilde{x}}\right|_i \Delta\tilde{x}$$

$$\left.\frac{d\tilde{T}}{d\tilde{x}}\right|_{i+1} = \left.\frac{d\tilde{T}}{d\tilde{x}}\right|_i + \left.\frac{d^2\tilde{T}}{d\tilde{x}^2}\right|_i \Delta\tilde{x}; \left.\frac{d^2\tilde{T}}{d\tilde{x}^2}\right|_{i+1} = \left.\frac{d\tilde{T}}{d\tilde{x}}\right|_{i+1} - \Lambda(1-\tilde{T}_{i+1})\exp\left(\frac{-\beta}{\tilde{T}_{i+1}(1-\varepsilon)+\varepsilon}\right)$$

- Does T → 1 as x → +∞? If not, adjust guess for Λ

1D premixed flame – results

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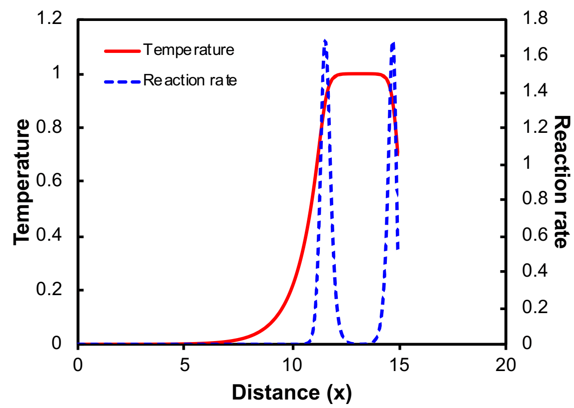
For typical β = 10, ε = 0.2 with Δx = 0.01

dT/dx at x = 0	Λ (Euler)	Λ (Runge)
0.001	896439	868026
0.0001	894518	866203
0.00001	894326	866021



1D premixed flame – numerical solution

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- Why is Λ so big, nearly 10^6?

$$\Lambda \equiv \frac{kZ}{\rho_\infty C_P S_L^2} = \frac{k/\rho_\infty C_P S_L}{S_L} Z = \frac{\delta}{S_L} Z = \left(\text{Flow time across flame zone}\right)\times\left(\text{Chemical rate}\right)$$

- … but chemical rate at flame temperature isn't Z, it's ~ Z exp(-E/RT_{ad}) = $Ze^{-\beta}$
- … and active zone for chemical reaction isn't all of flame thickness δ, it's only the zone near the hot boundary of thickness ~ δ/β
- … and fuel concentration in reaction zone isn't Y_f, it's ~ Y_f/β
- … so we expect $\Lambda e^{-\beta}/\beta^2$ should be an O(1) quantity – let's check for our example (β = 10, ε = 0.2):

$$\frac{\Lambda \exp(-\beta)}{\beta^2} = \frac{866021\exp(-10)}{10^2} = 0.393 \ \text{ OK}$$

Euler vs 4th-order Runge-Kutta

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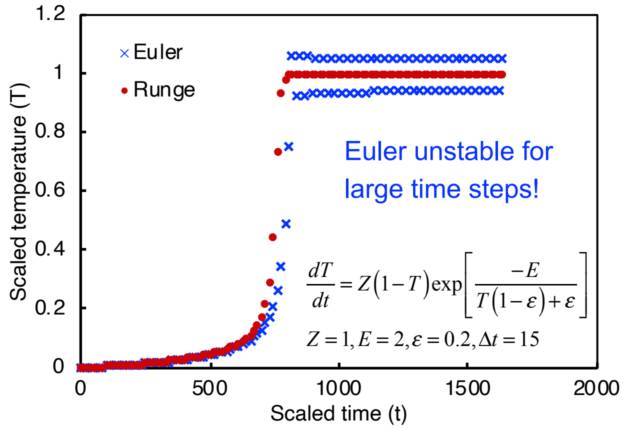
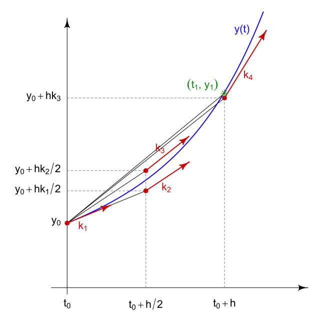
For a 1st order ODE of the form $\frac{d\tilde{T}}{d\tilde{x}} = F\left(\tilde{x},\tilde{T}\right)$, define at location $\tilde{x}$:

$$k_1 = F\left(\tilde{x},\tilde{T}\right)\Delta\tilde{x}; k_2 = F\left(\tilde{x}+\frac{\Delta\tilde{x}}{2},\tilde{T}+\frac{k_1}{2}\right)\Delta\tilde{x}; k_3 = F\left(\tilde{x}+\frac{\Delta\tilde{x}}{2},\tilde{T}+\frac{k_2}{2}\right)\Delta\tilde{x}; k_4 = F\left(\tilde{x}+\Delta\tilde{x},\tilde{T}+k_3\right)\Delta\tilde{x}$$

$$\text{Then } \tilde{T}\Big|_{\tilde{x}+\Delta\tilde{x}} = \tilde{T}\Big|_{\tilde{x}} + \frac{1}{6}\left(k_1+2k_2+2k_3+k_4\right) \text{ vs. } \tilde{T}\Big|_{\tilde{x}+\Delta\tilde{x}} = \tilde{T}\Big|_{\tilde{x}} + k_1 = \tilde{T}\Big|_{\tilde{x}} + \frac{d\tilde{T}}{d\tilde{x}}\Big|_{\tilde{x}}\Delta\tilde{x} \text{ (Euler)}$$





Euler vs 4th-order Runge-Kutta

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For a 2nd order ODE of the form $\frac{d^2\tilde{T}}{d\tilde{x}^2} = F\left(\tilde{x},\tilde{T},\frac{d\tilde{T}}{d\tilde{x}}\right)$, define at location $\tilde{x}$:

$$j_1 = F\left(\tilde{x},\tilde{T},\frac{d\tilde{T}}{d\tilde{x}}\right)\Delta\tilde{x}; k_1 = \frac{d\tilde{T}}{d\tilde{x}}\Delta\tilde{x}$$

$$j_2 = F\left(\tilde{x}+\frac{\Delta\tilde{x}}{2},\tilde{T}+\frac{k_1}{2},\frac{d\tilde{T}}{d\tilde{x}}+\frac{j_1}{2}\right)\Delta\tilde{x}; k_2 = \left(\frac{d\tilde{T}}{d\tilde{x}}+\frac{j_1}{2}\right)\Delta\tilde{x}$$

$$j_3 = F\left(\tilde{x}+\frac{\Delta\tilde{x}}{2},\tilde{T}+\frac{k_2}{2},\frac{d\tilde{T}}{d\tilde{x}}+\frac{j_2}{2}\right)\Delta\tilde{x}; k_3 = \left(\frac{d\tilde{T}}{d\tilde{x}}+\frac{j_2}{2}\right)\Delta\tilde{x}$$

$$j_4 = F\left(\tilde{x}+\Delta\tilde{x},\tilde{T}+k_3,\frac{d\tilde{T}}{d\tilde{x}}+j_3\right)\Delta\tilde{x}; k_4 = \left(\frac{d\tilde{T}}{d\tilde{x}}+j_3\right)\Delta\tilde{x}$$

$$\frac{d\tilde{T}}{d\tilde{x}}\Big|_{\tilde{x}+\Delta\tilde{x}} = \frac{d\tilde{T}}{d\tilde{x}}\Big|_{\tilde{x}} + \frac{1}{6}\left(j_1+2j_2+2j_3+j_4\right) \text{ vs. } \frac{d\tilde{T}}{d\tilde{x}}\Big|_{\tilde{x}+\Delta\tilde{x}} = \frac{d\tilde{T}}{d\tilde{x}}\Big|_{\tilde{x}} + j_1 \text{ (Euler)}$$

$$\tilde{T}\Big|_{\tilde{x}+\Delta\tilde{x}} = \tilde{T}\Big|_{\tilde{x}} + \frac{1}{6}\left(k_1+2k_2+2k_3+k_4\right) \text{ vs. } \tilde{T}\Big|_{\tilde{x}+\Delta\tilde{x}} = \tilde{T}\Big|_{\tilde{x}} + k_1 \text{ (Euler)}$$

1D laminar premixed flame – Runge-Kutta

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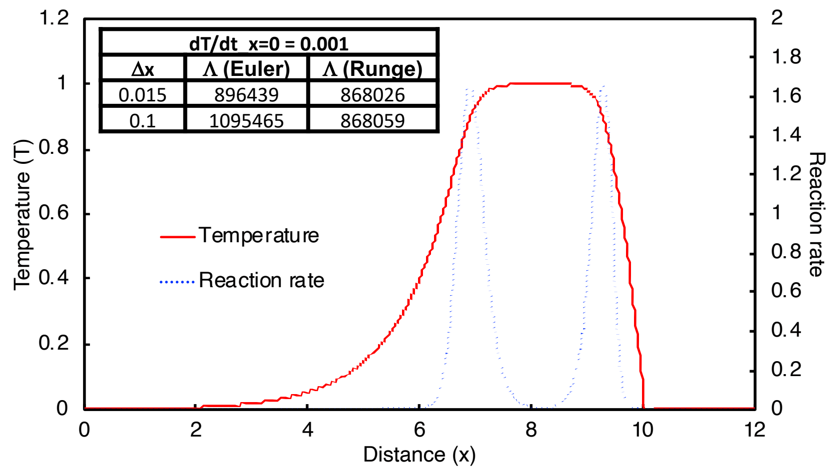
$$\frac{d^2\tilde{T}}{d\tilde{x}^2} = F\left(\tilde{x},\tilde{T},\frac{d\tilde{T}}{d\tilde{x}}\right) = \frac{d\tilde{T}}{d\tilde{x}} - \Lambda\left(1-\tilde{T}\right)\exp\left(\frac{-\beta}{\tilde{T}\left(1-\varepsilon\right)+\varepsilon}\right)$$

- Similar to Euler for small Δx but VERY different for larger Δx



Δx	Λ (Euler)	Λ (Runge)
0.015	896439	868026
0.1	1095465	868059

Deflagrations - burning velocity

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- Approximate closed-form analytical solution for 1st-order reaction (Zeldovich, 1940)

$$S_L = \frac{\sqrt{2Le\ \alpha Z\exp(-\beta)}}{\beta(1-\varepsilon)};\beta \equiv \frac{E}{\Re T_{ad}},\varepsilon \equiv \frac{T_\infty}{T_{ad}}$$

T_{ad} = adiabatic flame temperature; T_∞ = ambient temperature

- Note still in the form $S_L \sim (\alpha\omega)^{1/2}$, where $\omega \sim Ze^{-\beta}$ is an overall reaction rate (units 1/time)
- Note also that we can treat the reaction zone as source of thermal energy and sink of reactants according to

$$\left.\frac{dT}{dx}\right|_{x=0+} - \left.\frac{dT}{dx}\right|_{x=0-} = -\frac{(T_{ad}-T_\infty)}{\delta} = -\frac{(T_{ad}-T_\infty)}{\alpha/S_L} = -\frac{(T_{ad}-T_\infty)}{\alpha}\frac{\sqrt{2Le\alpha Ze^{-\beta}}}{\beta(1-\varepsilon)} = -\frac{T_{ad}}{\beta}\sqrt{\frac{2LeZe^{-\beta}}{\alpha}}$$

$$\text{and } \left.\frac{dY}{dx}\right|_{x=0+} - \left.\frac{dY}{dx}\right|_{x=0-} = +\frac{Y_\infty}{\delta}Le = +\frac{Y_\infty}{\alpha/S_L}Le = +\frac{Y_\infty}{\alpha}\frac{\sqrt{2Le\alpha Ze^{-\beta}}}{\beta(1-\varepsilon)}Le = +\frac{Y_\infty Le}{\beta(1-\varepsilon)}\sqrt{\frac{2LeZe^{-\beta}}{\alpha}}$$

Deflagrations - burning velocity

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- More rigorous analysis (Bush & Fendell, 1970) using Matched Asymptotic Expansions
  - Convective-diffusive (CD) zone (no reaction) of thickness δ
  - Reactive-diffusive (RD) zone (no convection) of thickness $\delta/\beta(1-\varepsilon)$ where $1/[\beta(1-\varepsilon)]$ is a small parameter
  - $T(x) = T_0(x) + T_1(x)/[\beta(1-\varepsilon)] + T_2(x)/[\beta(1-\varepsilon)]^2 + \ldots$
  - Collect terms of same order in small parameter
  - Match T & dT/dx at all orders of $\beta(1-\varepsilon)$ where CD & RD zones meet

$$S_L = \frac{\sqrt{2Le\,\alpha Ze^{-\beta}}}{\beta(1-\varepsilon)}\left(1+\frac{1.344-3(1-\varepsilon)}{\beta(1-\varepsilon)}\right); \beta \equiv \frac{E}{\Re T_{ad}}, \varepsilon \equiv \frac{T_\infty}{T_{ad}}$$

- Still same form as simple estimate ($S_L \sim (\alpha\omega)^{1/2}$, where $\omega \sim Ze^{-\beta}$ is an overall reaction rate, units 1/s), with additional constants
- Again β^{-2} term on reaction rate
  - Reaction doesn't occur over whole flame thickness δ, only in thin zone of thickness δ/β
  - Reactant concentration isn't at ambient value $Y_{i,\infty}$, it's at $1/\beta$ of this since temperature is within $1/\beta$ of T_{ad}

Deflagrations - burning velocity

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- What if not a single reactant, or not 1st order reaction, or Le ≠ 1? Mitani (1980) extended Bush & Fendell for reaction of the form
  $\nu_A A + \nu_B B \rightarrow products; \dot{\omega} = ZY_A^{\nu_A} Y_B^{\nu_B} \exp(-E_a/\Re T)$
  where A is the deficient reactant, e.g. fuel in a lean mixture, resulting in

$$S_L = \left(2\alpha Ze^{-\beta} Y_{A,\infty}^{\nu_A+\nu_B-1} \frac{\nu_A(\nu_B/\nu_A)^{\nu_B}}{(\beta(1-\varepsilon))^{\nu_A+\nu_B+1}} \frac{1}{Le_A^{-\nu_A}} \frac{1}{Le_B^{-\nu_B}} G\right)^{1/2}$$

$$G \equiv \int_0^\infty y^{\nu_A}(y+a)^{\nu_B} e^{-y}\,dy\ ;\ \ a \equiv \beta(1-\varepsilon)(\phi-1)/Le_B; \phi = \text{equivalence ratio}$$

- Recall order of reaction (n) = $\nu_A + \nu_B$
- Still same form as simple estimate, but now $\beta^{-(n+1)}$ term since n may be something other than 1 (as Bush & Fendell assumed)
- Also have $Le_A^{-\nu A}$ and $Le_B^{-\nu B}$ terms – why? For fixed thermal diffusivity (α), for higher Le_A, D_A is smaller, gradient of Y_A must be larger to match with T profile, so concentration of A is higher in reaction zone

Sidebar: calculating Lewis numbers

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- Lewis number (Le) is the ratio of the thermal diffusivity of the entire mixture (since heat is conducted through the entire mixture) to the mass diffusivity of the reactant of interest into the entire mixture
- Example: lean (ϕ = 0.5) CH_4-air mixture: 0.25 CH_4 / 1 O_2 / 3.77 N_2.
  - From CSU website: at 1 atm, 300K, D_{CH4} = 0.23068 cm^2/s (called "Mixture Diffusivity")
  - Thermal diffusivity of the entire mixture (α) = 0.22438 cm^2/s) (called "Mixture Thermal Diffusivity")
  - Le_{CH4} = 0.22438/0.23068 = 0.9727
- For non-premixed flames, if you have pure fuel or O_2 on one side, you can't calculate Le since you need ≥ 2 species to have a D, but there are products (CO_2 and H_2O) diffusing towards the reactant boundaries, so include a small amount of stoichiometric products (e.g. 1% CO_2 and 2% H_2O if CH_4 is the fuel) with the reactants to obtain a D

1D premixed flame - stretched

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- Mass + momentum conservation, 2D, const. density (ρ)

$$\frac{\partial u_x}{\partial t}+u_x\frac{\partial u_x}{\partial x}+u_y\frac{\partial u_x}{\partial y}=-\frac{1}{\rho}\frac{\partial P}{\partial x}+\mu\left(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2}\right) \quad \text{(x momentum)}$$

$$\frac{\partial u_y}{\partial t}+u_x\frac{\partial u_y}{\partial x}+u_y\frac{\partial u_y}{\partial y}=-\frac{1}{\rho}\frac{\partial P}{\partial y}+\mu\left(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2}\right) \quad \text{(y momentum)}$$

$$\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}=0 \quad \text{(mass conservation)}$$

(u_x, u_y = velocity components in x, y directions)

admit an exact, steady ($\partial/\partial t$ = 0) solution which is the same with or without viscosity (!!!):

$$u_x=\Sigma x,\ u_y=-\Sigma y, P=-\frac{\rho\Sigma^2}{2}\left(x^2+y^2\right)$$

Σ = rate of strain (units s^{-1})

- Similar result in 2D axisymmetric (r, z) geometry:

$$u_r=-\Sigma r/2,\ u_z=\Sigma z$$

Very simple flow characterized by a single parameter Σ, easily implemented experimentally using counter-flowing round jets…

1D premixed flame - stretched

- Instead of ρu = constant as in plane flame, u = $-\Sigma x$

$$u\frac{dT}{dx}-\frac{k}{\rho C_P}\frac{d^2T}{dx^2}=\frac{\dot{q}'''}{\rho C_P}; u=-\Sigma x \Rightarrow -\rho\Sigma x C_P\frac{dT}{dx}-k\frac{d^2T}{dx^2}=\rho Q_R Z Y_F \exp\left(\frac{-E}{\Re T}\right)$$

$$\Rightarrow \frac{\Sigma x}{\alpha}\frac{dT}{dx}+\frac{d^2T}{dx^2}=-\frac{\rho Q_R Z Y_F}{k}\exp\left(\frac{-E}{\Re T}\right);$$

$$\text{Let } \tilde{x}=\frac{x}{\sqrt{2\alpha/\Sigma}} \Rightarrow \frac{\Sigma x}{2\alpha}\frac{\sqrt{2\alpha/\Sigma}}{\sqrt{2\alpha/\Sigma}}\frac{dT}{dx}+\frac{1}{2}\frac{2\alpha/\Sigma}{2\alpha/\Sigma}\frac{d^2T}{dx^2}=-\frac{\rho Q_R Z Y_F}{2k}\exp\left(\frac{-E}{\Re T}\right)$$

$$\Rightarrow \tilde{x}\frac{dT}{d\tilde{x}}+\frac{1}{2}\frac{d^2T}{d\tilde{x}^2}=-\frac{\alpha\rho Q_R Z Y_F}{k\Sigma}\exp\left(\frac{-E}{\Re T}\right)=-\frac{Q_R Z Y_F}{C_p\Sigma}\exp\left(\frac{-E}{\Re T}\right)$$

$$Let\ \tilde{T}=\frac{T-T_\infty}{Y_{i,\infty}Q_R/C_P}=\frac{T-T_\infty}{T_{ad}-T_\infty} \Rightarrow \tilde{x}\frac{d\tilde{T}}{d\tilde{x}}+\frac{1}{2}\frac{d^2\tilde{T}}{d\tilde{x}^2}=-\frac{ZY_{F,\infty}Q_R}{C_P\left(T_{ad}-T_\infty\right)\Sigma}\frac{Y_F}{Y_{F,\infty}}\exp\left(\frac{-E}{\Re T}\right)$$

$$\Rightarrow \tilde{x}\frac{d\tilde{T}}{d\tilde{x}}+\frac{1}{2}\frac{d^2\tilde{T}}{d\tilde{x}^2}=-\frac{Z}{\Sigma}\tilde{Y}_F\exp\left(\frac{-E}{\Re T}\right)=-\frac{Z}{\Sigma}\left(1-\tilde{T}\right)\exp\left(\frac{-E}{\Re T}\right)=-\frac{Z}{\Sigma}\left(1-\tilde{T}\right)\exp\left(\frac{-E}{\Re T}\right)$$

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

1D premixed flame - stretched

- In addition to the unstretched flame parameters β and ε, there is a stretch rate parameter Da = Z/Σ
- Need to determine Da at extinction and effect of Da on burning velocity S_L relative to unstretched value $S_{L,o}$ up to extinction limit:

$$\text{Recall } \tilde{x}\equiv\frac{x}{\sqrt{2\alpha/\Sigma}}, Da\equiv\frac{Z}{\Sigma}$$

$$\text{At flame location: } S_L=-u=-\left(-\Sigma x_f\right)=\Sigma\tilde{x}_f\sqrt{\frac{2\alpha}{\Sigma}}=\tilde{x}_f\sqrt{2\alpha\Sigma}=\sqrt{2\alpha Z}\frac{\tilde{x}_f}{\sqrt{Da}}$$

$$\Rightarrow S_L=\sqrt{2\alpha Z}\frac{\tilde{x}}{\sqrt{Da}}$$

$$\text{Also } \Lambda\equiv\frac{kZ}{\rho_\infty C_P S_{L,o}^2}=\frac{\alpha_\infty Z}{S_{L,o}^2}\Rightarrow S_{L,o}=\sqrt{\alpha_\infty Z}\sqrt{\frac{1}{\Lambda}}\Rightarrow\frac{S_L}{S_{L,o}}=\sqrt{2\Lambda}\frac{\tilde{x}}{\sqrt{Da}}$$

- Hot boundary condition: by symmetry, dT/dx = 0 at x = 0
- Solution method: pick Da, find T at x = 0 that satisfies cold boundary condition: T → 0 as x → ∞ (in practice reverse is easier!)

1D premixed flame - stretched

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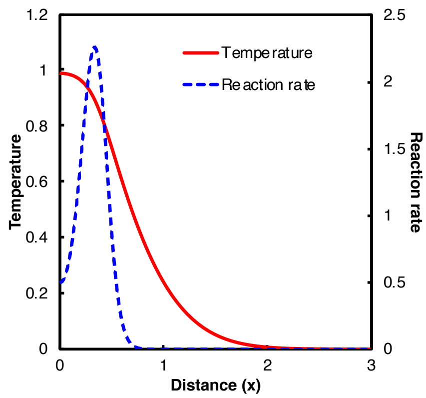
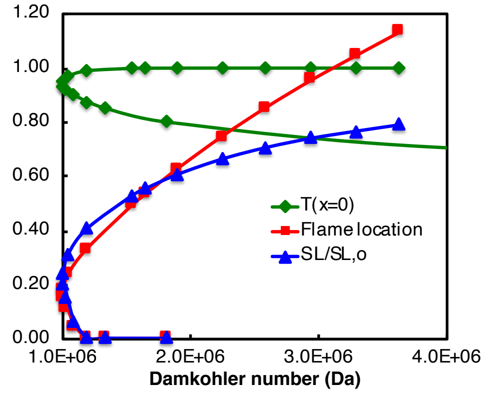
- Determine Da at extinction and effect of Da on burning velocity up to extinction limit
- Why doesn't $S_L/S_{L,o}$ → 1 as Da → ∞? Flame location defined as location of maximum reaction rate, which can't be at T = 1 since there's no fuel there! {max. rate near (1 – 1/β)}





$\beta = 10,\ \varepsilon = 0.2$

1D premixed flame - stretched

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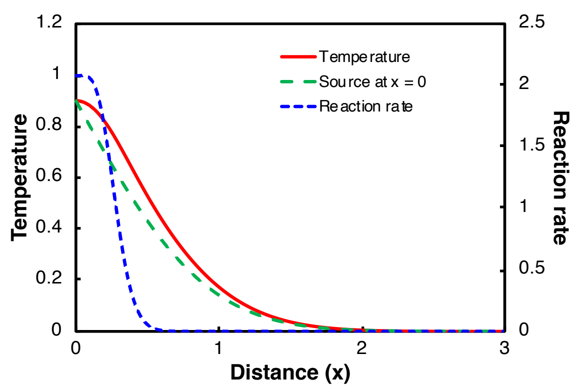
- Recall stretched non premixed flame –outside of reaction zone

$$\tilde{x}\frac{d\tilde{T}}{d\tilde{x}}+\frac{1}{2}\frac{d^2\tilde{T}}{d\tilde{x}^2}=0 \Rightarrow \tilde{T}(\tilde{x})=C_1 erf(\tilde{x})+C_2$$

Boundary conditions for source at $\tilde{x}=0$ are $\tilde{x}=0:\tilde{T}=\tilde{T}_o;\tilde{x}\to\infty:\tilde{T}=0$

$$\Rightarrow C_1=-\tilde{T}_o, C_2=\tilde{T}_o \Rightarrow \tilde{T}(\tilde{x})=\tilde{T}_o\left[1-erf(\tilde{x})\right]$$



Flames in spherical geometry

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- Assumptions: 1D spherical; ideal gases; adiabatic (except for possible ignition source Q(r,t) to be employed later); 1 limiting reactant (call it "fuel"); 1-step overall reaction; ρD, k, C_P, etc. constant; low Mach #; no body forces
- Governing equations for mass, energy & species conservations (Y_F = limiting reactant mass fraction; Q_R = its heating value)

$$\frac{\partial \rho}{\partial t}+\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\rho u\right)=0;\ \text{ideal gas with P = constant} \Rightarrow \rho T=\rho_\infty T_\infty=\text{constant}$$

$$\rho C_p\frac{\partial T}{\partial t}+\rho C_p\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 uT\right)=\frac{k}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)+\rho Q_R Y_F Z\exp\left(\frac{E}{\Re T}\right)$$

$$\rho\frac{\partial Y_F}{\partial t}+\rho u\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 Y_F\right)=\frac{\rho D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial y}{\partial r}\right)-\rho Y_F Z\exp\left(\frac{E}{\Re T}\right)$$

Flames in spherical geometry

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- Non-dimensionalize (recall $T_{ad} = T_\infty + Y_\infty Q_R/C_P$)

$$\tilde{T}\equiv\frac{T}{T_{ad}};\tau\equiv te^{-\beta}Z;R\equiv r\sqrt{\frac{e^{-\beta}Z}{\alpha}};U\equiv\frac{u}{\sqrt{Z\alpha e^{-\beta}}};\beta\equiv\frac{E}{\Re T_{ad}}$$

$$\varepsilon\equiv\frac{T_\infty}{T_{ad}};\tilde{Y}\equiv\frac{Y_F}{Y_{F,\infty}};Le\equiv\frac{k}{\rho C_p D};\Omega\equiv\frac{Q(r,t)}{\rho_\infty C_p T_\infty e^{-\beta}Z}$$

leads to, for mass, energy and species conservation

$$\frac{\partial(1/\tilde{T})}{\partial\tau}+\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{1}{\tilde{T}}U\right)=0$$

$$\frac{\partial\tilde{T}}{\partial\tau}+U\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\tilde{T}\right)=\frac{\tilde{T}}{\varepsilon}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial\tilde{T}}{\partial R}\right)+(1-\varepsilon)\tilde{Y}\exp\left[-\beta\left(\frac{1}{\tilde{T}}-1\right)\right]+\Omega(R,\tau)\tilde{T}$$

$$\frac{\partial\tilde{Y}}{\partial\tau}+U\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\tilde{Y}\right)=\frac{1}{Le}\frac{\tilde{T}}{\varepsilon}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial\tilde{Y}}{\partial R}\right)-\tilde{Y}\exp\left[-\beta\left(\frac{1}{\tilde{T}}-1\right)\right]$$

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- Initial & boundary conditions
  - Initial condition: T = T_∞, $Y_F = Y_{F,\infty}$, U = 0 everywhere)

$$\tilde{T}(R,0)=\varepsilon;\tilde{Y}(R,0)=1;U(R,0)=0 \text{ for all R}$$

  - At infinite radius, T = T_∞, y = y_∞,U = 0 for all times)

$$\tilde{T}(R,\tau)=\varepsilon;\tilde{Y}(R,\tau)=1;U(R,\tau)=0 \text{ as } R\to\infty$$

  - Symmetry condition at r = 0 for all times

$$\frac{\partial\tilde{T}}{\partial R}=\frac{\partial\tilde{Y}}{\partial R}=\frac{\partial U}{\partial R}=0 \text{ at R=0 and as } R\to\infty$$

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- Special case: steady (?) solutions with reaction confined to a thin zone (large β) at (unknown) R = R* with (unknown) temperature T*

$$\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{1}{\tilde{T}}U\right)=0\Rightarrow U=0 \text{ (zero convection velocity everywhere)}$$

$$\Rightarrow 0=\frac{\tilde{T}}{\varepsilon}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial\tilde{T}}{\partial R}\right)+(1-\varepsilon)\tilde{Y}\exp\left[-\beta\left(\frac{1}{\tilde{T}}-1\right)\right] \text{ (energy eqn.; steady, } U=0)$$

$$\text{Outside reaction zone: } \frac{\tilde{T}}{\varepsilon}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial\tilde{T}}{\partial R}\right)=0\Rightarrow\tilde{T}(R)=\frac{C_1}{R}+C_2$$

$$\tilde{T}=\tilde{T}^* \text{ at } R=R^* \text{ and } \tilde{T}=\varepsilon \text{ at } R=\infty\Rightarrow\tilde{T}(R)=\varepsilon+\left(\tilde{T}^*-\varepsilon\right)\frac{R^*}{R};\left.\frac{d\tilde{T}}{dR}\right|_{R=R^*}=-\frac{\tilde{T}^*-\varepsilon}{R^*}$$

$$\text{and } 0=\frac{1}{Le}\frac{\tilde{T}}{\varepsilon}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial\tilde{Y}}{\partial R}\right)-\tilde{Y}\exp\left[-\beta\left(\frac{1}{\tilde{T}}-1\right)\right] \text{ (reactant eqn.)}$$

$$\text{Outside reaction zone: } \frac{1}{Le}\frac{\tilde{T}}{\varepsilon}\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial\tilde{Y}}{\partial R}\right)=0\Rightarrow\tilde{Y}(R)=\frac{C_1}{R}+C_2$$

$$\tilde{Y}=0 \text{ at } R=R^* \text{ and } \tilde{Y}=1 \text{ at } R=\infty\Rightarrow\tilde{Y}(R)=1-\frac{R^*}{R};\left.\frac{d\tilde{Y}}{dR}\right|_{R=R^*}=\frac{1}{R^*}$$

Flames in spherical geometry

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- Matching at R = R*

$$-kA\frac{dT}{dr}\bigg|_{R=R^*} = Q_R\,\rho DA\frac{dY}{dr}\bigg|_{R=R^*} = \frac{C_P\left(T_{ad}-T_\infty\right)}{Y_\infty}\rho DA\frac{dY}{dr}\bigg|_{R=R^*}$$

$$-\frac{d\tilde{T}}{dR}\bigg|_{R=R^*} = \frac{\left(T_{ad}-T_\infty\right)}{T_{ad}}\frac{\rho C_P D}{k}\frac{d\tilde{Y}}{dR}\bigg|_{R=R^*} = \frac{1-\varepsilon}{Le}\frac{d\tilde{Y}}{dR}\bigg|_{R=R^*}$$

$$-\left(-\frac{\tilde{T}^*-\varepsilon}{R^*}\right) = \frac{1-\varepsilon}{Le}\frac{1}{R^*} \Rightarrow \tilde{T}^* = \varepsilon + \frac{1-\varepsilon}{Le} \text{ or } T^* = T_\infty + \frac{T_{ad}-T_\infty}{Le}$$

- This is a *flame ball* solution - note for Le < > 1, T^* > < T_{ad}; for Le = 1, $T^* = T_{ad}$
- For adiabatic flames (as here) R* = R_Z is called the *Zeldovich radius*
- Generally unstable
  - R < R_Z: shrinks and extinguishes
  - R > R_Z: expands and develops into steady flame
  - R_Z related to requirement for initiation of steady flame - expect $E_{min} \sim R_Z^3$
- … but stable for a few carefully (or accidentally) chosen mixtures

Steady spherical flames (?!?)

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$$\frac{d\tilde{T}}{dR}\bigg|_{R=R^*+} = -\frac{\tilde{T}^*-\varepsilon}{R^*};\frac{d\tilde{T}}{dR}\bigg|_{R=R^*-} = 0;\text{ recall }\frac{dT}{dx}\bigg|_{x=0+} - \frac{dT}{dx}\bigg|_{x=0-} = -\frac{T_{ad}}{\beta}\sqrt{\frac{2LeZe^{-\beta}}{\alpha}}$$

$$\Rightarrow R_Z = \frac{\beta^*(1-\varepsilon)}{Le}\sqrt{\frac{\alpha e^{\beta^*}}{2LeZ}};\beta^* \equiv \frac{E}{\Re T^*}$$

$$\text{or } R_z = \frac{\delta}{Le}exp\left(\frac{\beta}{2}\left(\frac{1}{\tilde{T}^*}-1\right)\right);\text{ recall }\delta = \frac{\alpha}{S_L};S_L = \frac{\sqrt{2Le\,\alpha Z}}{\beta(1-\varepsilon)}\exp\left(\frac{-\beta}{2}\right)$$

Steady spherical flames (?!?)

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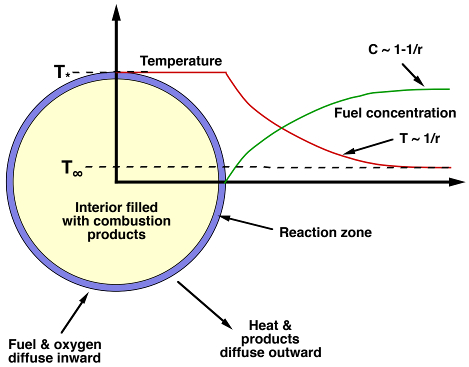
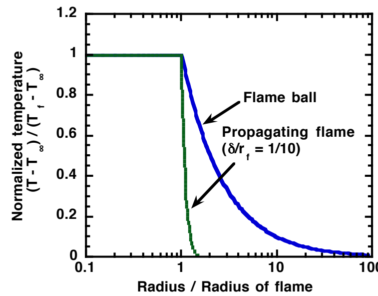
- How can a spherical flame not propagate???





Space experiments show ~ 1 cm diameter flame balls possible
Movie: 500 sec elapsed time
6.75% H_2 – 13.5% O_2 – 79.75% SF_6, 1 atm
$Le_F \approx 0.06$
Field of view 30 cm x 22 cm

References

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