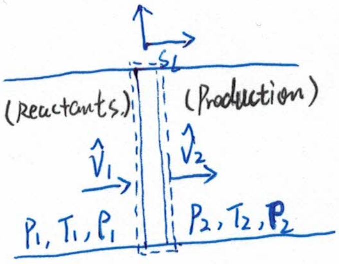
## § Governing Equations for 1D premixed combustion.




① Moving coordinates.

② Consider the tiny control volumn covering the flame zone.

③ 1D Euler equations.

④ Rankine - Hugoniot conditions. $\Delta F = S \cdot \Delta U$

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \quad \xrightarrow[S=0]{\text{R-H condition}} \quad \Delta F = 0: \begin{cases} \rho_1 \hat{u}_1 = \rho_2 \hat{u}_2 \\ \rho_1 \hat{u}_1^2 + P_1 = \rho_2 \hat{u}_2^2 + P_2 \\ \rho_1 \hat{u}_1 (e_1 + \frac{1}{2}\hat{u}_1^2 + \frac{P_1}{\rho_1}) = \rho_2 \hat{u}_2 (e_2 + \frac{1}{2}\hat{u}_2^2 + \frac{P_2}{\rho_2}) \end{cases}$$

where:

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho(e + \frac{1}{2}u^2) \end{bmatrix}, \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ u(\rho(e + \frac{1}{2}u^2) + P) \end{bmatrix}$$

The energy equation can be simplified with the continuity equation, $\Rightarrow h_1 + \frac{1}{2}\hat{u}_1^2 = h_2 + \frac{1}{2}\hat{u}_2^2$

Full equation set:

$$\begin{cases} \rho_1 \hat{u}_1 = \rho_2 \hat{u}_2 & ① \\ \rho_1 \hat{u}_1^2 + P_1 = \rho_2 \hat{u}_2^2 + P_2 & ② \\ h_1 + \frac{1}{2}\hat{u}_1^2 = h_2 + \frac{1}{2}\hat{u}_2^2 & ③ \end{cases} \quad \& \quad \begin{cases} h = h_0 + C_p \Delta T & ④ \\ P_1 = \rho_1 R T & ⑤ \\ P_2 = \rho_2 R T & ⑥ \end{cases}$$

## §. Rayleigh Line & Rankine - Hugoniot Curve.

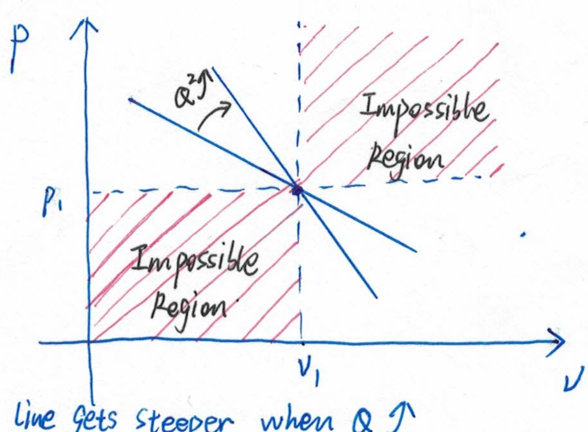
① when the mass flux $Q$ is given, relations between pressure $P$ and density $\rho$ (or $v = \frac{1}{\rho}$) can be described using ① & ②. (The so-called Rayleigh Line)

$$\rho_1 \hat{u}_1 = \rho_2 \hat{u}_2 \triangleq Q \Rightarrow \frac{Q^2}{\rho_1} + P_1 = \frac{Q^2}{\rho_2} + P_2 \Rightarrow \frac{P_2 - P_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} = -Q^2 \text{ or } \left(\frac{P_2 - P_1}{v_2 - v_1} = -Q^2\right)$$

$$\text{or} \left(Q^2 v_1 + P_1 = Q^2 v_2 + P_2\right)$$

namely:

$$P = -Q^2 v + (P_1 + Q^2 v_1)$$




Comments:

(1) There're 2 impossible regions as the slope is never positive

(2) when the initial condition is given, the line gets steeper when $Q \uparrow$

② When the energy equation is also considered, relations between pressure $P$ and density $\rho$ (or $\nu = \frac{1}{\rho}$) can be further described. (The so-called Rankine-Hugoniot Curve)

Typically, we re-write the energy equation ③ with ④ as:

$$C_p T_1 + \frac{\hat{u}_1^2}{2} + q = C_p T_2 + \frac{\hat{u}_2^2}{2}$$

where $q = \sum_1 Y_i h^0_{f,i} - \sum_2 Y_i h^0_{f,i}$, indicating the total heat released during the combustion

Combining ①, ② & ⑤, ⑥ yields:

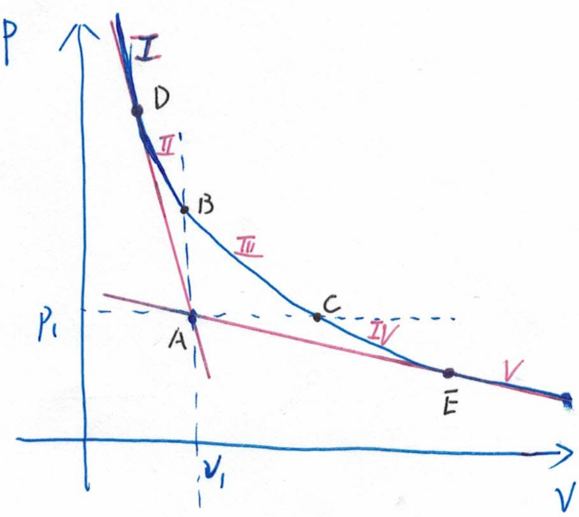
$$\left.\begin{aligned} & C_p(T_2 - T_1) + \frac{1}{2}(\hat{u}_2^2 - \hat{u}_1^2) - q = 0 \\ & T = \frac{P}{\rho R} \\ & \hat{u}_2 - \hat{u}_1 = -\frac{P_2 - P_1}{Q} \\ & \hat{u}_2 + \hat{u}_1 = Q\left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right) \end{aligned}\right\} \Rightarrow \frac{C_p}{R}\left(P_2/\rho_2 - P_1/\rho_1\right) - \frac{1}{2}(P_2 - P_1)\left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right) - q = 0$$

$$\Downarrow \ \gamma \triangleq \frac{C_p}{C_v}, \quad C_p - C_v = R.$$

$$\boxed{\frac{\gamma}{\gamma - 1}(P_2 \nu_2 - P_1 \nu_1) - \frac{1}{2}(P_2 - P_1)(\nu_2 + \nu_1) - q = 0}$$

When $q$, $P_1$, $\nu_1$ are given, relations between $P$ and $\nu$ can be plotted:

D and E are the so-called Chapman-Jouguet points.




The curve is divided into 5 parts:

(1) I: Beyond point D:

Strong detonation

$Ma_2 < 1$, $Ma_1 > 1$

(2) II: Between D and B:

Weak detonation:

$Ma_2 > 1$, $Ma_1 \geq 1$

(3) III: Between B and C: Impossible.

(4) IV: Between C and E:

Weak deflagration.

$Ma_2 < 1$, $Ma_1 \leq 1$

Detonation: a type of combustion involving a supersonic exothermic front accelerating through a medium that eventually drives a shock front propagating in front of it directly.

Deflagration: Subsonic combustion propagating through heat transfer.

(5) V: Below point E:

Strong deflagration.

$Ma_2 > 1 \quad Ma_1 \le 1$

Q: How to determine / understand $Ma_2$ in different regions?

A: Take derivative of the Rankine-Hugoniot curve:

$$\frac{d}{dv}\left[\frac{\gamma}{\gamma-1}(pv - p_1 v_1) - \frac{1}{2}(p-p_1)(v+v_1) - q\right] = 0$$

$$\Leftrightarrow \frac{\gamma}{\gamma-1}\left(\frac{dp}{dv}\cdot v + p\right) = \frac{1}{2}\frac{dp}{dv}(v+v_1) + (p-p_1)$$

at CJ points: $\frac{dp}{dv} = \frac{p_2 - p_1}{v_2 - v_1}$.

$$\Rightarrow \frac{\gamma}{\gamma-1}\left(\frac{p_2-p_1}{v_2-v_1} v_2 + p_2\right) = \frac{1}{2}\frac{p_2-p_1}{v_2-v_1}(v_2+v_1) + (p_2-p_1)$$

$$\Leftrightarrow \frac{p_2-p_1}{v_2-v_1} = -\frac{\gamma p_2}{v_2} = -\gamma p_2 \rho_2$$

$$\Rightarrow Ma_2^2 \triangleq \frac{\hat{u}_2^2}{a_2^2} = \frac{(\rho_2 \hat{u}_2)^2}{(\rho_2 a_2)^2} = \frac{Q^2}{\gamma p_2 \rho_2} = -\frac{p_2-p_1}{v_2-v_1}\frac{1}{\gamma p_2 \rho_2} = 1 \quad (\text{at } D \text{ and } E)$$

Some comments on $Ma_2^2$:

$$Ma_2^2 = \frac{Q^2}{\gamma p_2 \rho_2} = \frac{Q^2 v_2}{\gamma p_2}$$

In Region I: $Q^2$ and $v_2$ varies slower than $p_2$, thus $Ma_2^2 < 1$

In Region II: $Q^2$ increase rapidly towards $+\infty$, while $p_2$ and $v_2$ varies little, $\Rightarrow Ma_2^2 > 1$

In Region IV: $Q^2$ tends to 0, while $p_2$ and $v_2$ holds nearly constant, $\Rightarrow Ma_2^2 < 1$

In Region V: $Q^2$ changes little, $p_2$ is confined, but $v_2 \to +\infty$, $\Rightarrow Ma_2^2 > 1$

It should be noted that: (in reality) weak detonation (II) and strong deflagration (V) hardly occur!

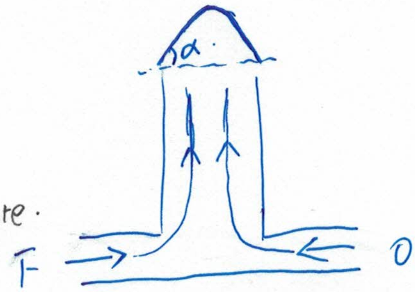
## §. Laminor Premixed Flame Structure:

Take the Bunsen burner for example.

$\phi < 1$ : deep-violet, CH dominate

$\phi > 1$ : green, $C_2H_x$ dominate

$\phi >> 1$ : intense-yellow, Carbon particle dominate.




The high temperature zone lies in the front of the flame, but the reaction rate is small as the reaction process is ending.

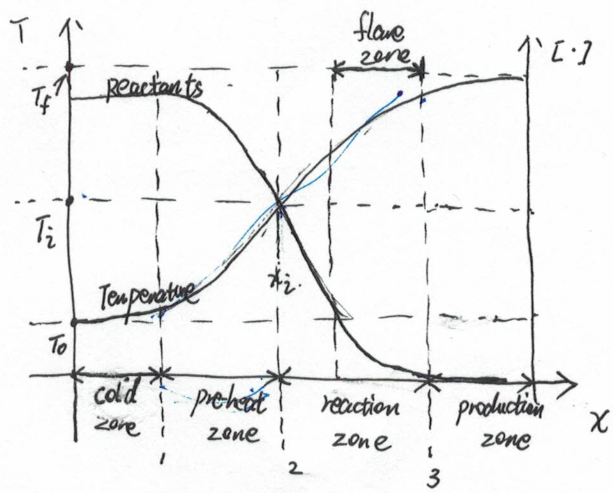
For burned gas, $T\uparrow$ results in $\rho\downarrow$, due to continuity, the normal velocity $V_n\uparrow$.

## § Flame Speed & Remarks on Q2-HW3

* General Structure (1D, laminar, premixed)

Governing Equation for energy:

$$\rho_u S_L C_p \frac{dT}{dx} - \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) = -\sum h_i w_i$$




① Consider the pre-heat zone:

It's assumed that there's no reaction!

Hence the chemical source term vanished!

In other words, gas entering the pre-heat zone is heated by the conduction through interface 2.

$$\Rightarrow \rho_u S_L \cdot C_p \cdot \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) \xrightarrow{\int_{-\infty}^{x_i}} \rho_u S_L C_p (T_i - T_0) = \lambda \frac{dT}{dx}\Big|_{-\infty}^{x_i} = \lambda \frac{dT}{dx}\Big|_{x=x_i}.$$

$$\left( \frac{dT}{dx}\Big|_{x=-\infty} = 0 \right)$$

Suppose the width of flame $\delta$ is known, then flame speed can be approximated by the $\boxed{\text{Thermal Theory}}$ as the gradient of $T$ can be approximated by $\frac{T_f - T_i}{\delta}$.

$$\Rightarrow \rho S_L C_p (T_i - T_0) = \lambda \frac{T_f - T_i}{\delta} \Rightarrow S_L = \frac{\lambda (T_f - T_i)}{\rho C_p (T_i - T_0)} \frac{1}{\delta} = \underbrace{\alpha}_{\text{Thermal Diffusivity.}} \frac{T_f - T_i}{T_i - T_0} \frac{1}{\delta}$$

Only related to the properties o[f] mixture, indepe[ndent] of flow configurati[on]

② Consider the reaction zone.

Energy from convection (due to the temperature difference) is much smaller compared to the diffusion term. Hence can be neglected!

Indicating that the conduction through interface 2 is sustained by reaction!

$$\Rightarrow -\frac{d}{dx}\left(\lambda\frac{dT}{dx}\right) = -\bar{z}h_i w_i \xRightarrow{\int_{x_i}^{+\infty}} \lambda\frac{dT}{dx}\Big|_{x=x_i} = \int_{x_i}^{+\infty} -\bar{z}h_i w_i\, dx$$ (not convinient to solve!)

With some mathematical manipulation by multiply $\frac{dT}{dx}$ to both sides!

$$-\frac{d}{dx}\left(\lambda\frac{dT}{dx}\right)\cdot\frac{dT}{dx} = -\bar{z}h_i w_i\cdot\frac{dT}{dx} \xRightarrow[\text{Integrate by parts}]{\int_{x_i}^{+\infty}} \left(\lambda\frac{dT}{dx}\right)^2\Big|_{x=x_i} = -\int_{T_i}^{T_f} 2\lambda\,\bar{z}h_i w_i\, dT$$

$$\left( LHS = -\frac{1}{2\lambda}\frac{d}{dx}\left(\lambda\frac{dT}{dx}\right)^2,\quad \frac{dT}{dx}\Big|_{x=+\infty} = 0 \right)$$

$$\Rightarrow \lambda\frac{dT}{dx}\Big|_{x=x_i} = \sqrt{-2\lambda\int_{T_i}^{T_f}\bar{z}h_i w_i\, dT}$$

Combined with previous expression of $\lambda\frac{dT}{dx}\big|_{x=x_i}$ yields:

$$\rho S_L C_p (T_i - T_0) = \sqrt{-2\lambda\int_{T_i}^{T_f}\bar{z}h_i w_i\, dT} \quad\Rightarrow\quad S_L = \sqrt{\underbrace{\frac{\lambda}{\rho C_p}}_{\alpha}\cdot\frac{-2}{\rho C_p(T_f - T_0)}\cdot\frac{1}{T_i - T_0}\int_{T_i}^{T_f}\bar{z}h_i w_i\, dT}$$

This is the so-called $\boxed{\text{ZFK Theory}}$!

Q: What's the dependence of $S_L$ to $\phi$?

A: As $\phi$ is related to $Z$ by: $\phi = \frac{Z}{1-Z}\left(\frac{1-Z_{st}}{Z_{st}}\right)$ : monotonic!

Recall that the Adiabatic Flame temperature $T_{ad}$ is related to $Z$. (HW2)

Hence, $S_L$ follows the same shape as $T_{ad}$!

* Special Case : $Le \triangleq \frac{\lambda}{\rho C_p D} = \frac{\alpha}{D} = 1.$

Governing Equation:

$$\dot{m}\cdot C_p\frac{dT}{dx} - \lambda\frac{d^2T}{dx^2} = q_c\cdot\dot{\omega} \qquad \text{(energy)}$$

$$\dot{m}\frac{dY}{dx} - \rho D\frac{d^2Y}{dx^2} = -\dot{\omega} \qquad \text{(specise)}.$$

Q: How to Eliminate $\dot{\omega}$?

A: multiply the specise equation by $q_c$ and adding them up!

$$\Rightarrow \dot{m} C_p \frac{dT}{dx} + \dot{m} q_c \frac{dY_i}{dx} = \lambda \frac{d^2 T}{dx^2} + \rho D q_c \frac{d^2 Y_i}{dx^2}$$

With proper non-dimensionlized:

$$\tilde{T} = \frac{C_p}{q_c \cdot Y_u} T, \quad \tilde{Y}_i = Y_i / Y_u, \quad \tilde{x} = \frac{C_p \cdot \dot{m}}{\lambda} x$$

$$\Rightarrow \frac{d\tilde{T}}{d\tilde{x}} + \frac{d\tilde{Y}}{d\tilde{x}} = \frac{d^2\tilde{T}}{d\tilde{x}^2} + \frac{1}{Le} \cdot \frac{d^2\tilde{Y}_i}{d\tilde{x}^2} \xrightarrow{\int_{-\infty}} (\tilde{T} + \tilde{Y}_i)\Big|_{-\infty} = \frac{d\tilde{T}}{d\tilde{x}} + \frac{1}{Le}\frac{d\tilde{Y}}{d\tilde{x}}$$

$$\left( \frac{d\tilde{T}}{d\tilde{x}}\Big|_{x=-\infty} = 0, \quad \frac{d\tilde{Y}_i}{d\tilde{x}}\Big|_{x=-\infty} = 0, \quad \tilde{T}|_{x=-\infty} = \tilde{T}_u, \quad \tilde{Y}_i|_{x=-\infty} = Y_u / Y_u = 1. \right)$$

$$\Rightarrow (\tilde{T} + \tilde{Y}) - (\tilde{T}_u + 1) = \frac{d\tilde{T}}{d\tilde{x}} + \frac{1}{Le}\frac{d\tilde{Y}}{d\tilde{x}} \quad \text{( no simplifation ! )}$$

Suppose $Le = 1$, and denote $\tilde{W} = \tilde{T} + \tilde{Y}$, then it become a simple ODE:

$$\frac{d\tilde{W}}{d\tilde{x}} = \tilde{W} + C_0 \qquad (C_0 = \text{const}).$$

$$\Rightarrow \quad \tilde{W} = C' e^{\tilde{x}} - C_0 \Rightarrow C' = 0, \text{ otherwise } \tilde{W} \text{ diverges!} \Rightarrow \tilde{W} = \text{const!}$$

( Theoritical Solution!)

§ Flame Thickness & Remarks on Q1-HW3

Directly follows from the thermal theory, with $\frac{dT}{dx}\Big|_{x_i}$ being approximated as:

$$\frac{dT}{dx}\Big|_{x=x_i} \doteq \frac{T_f - T_0}{\delta_f}$$

$$\rho S_L C_p (T_i - T_0) = \lambda \frac{dT}{dx}\Big|_{x=x_i} \Rightarrow \delta_F \doteq \frac{\lambda}{\rho C_p} \frac{T_f - T_0}{T_i - T_0} \frac{1}{S_L}$$

$\rightarrow \sim O(1)$ as $T_f \sim T_i$

if $S_L$ is given / mesured from experiments, then $\delta_F$ can be estimated provided that the thermal and transport properties are given!

Typically, for $CH_4 - O_2$, $P = 1atm$, $T \approx 1500k$. $\delta_F \sim 1mm$.

for $H_2 - O_2$, $P = 1atm$, $T \approx 1500k$ $\delta_F \sim 0.3mm$.

§ Thermal Explosion.

Chemical reactions promotes the temperature! , Constant Volumn!

* Adiabatic.

$$\rho_0 C_v \cdot \frac{dT}{dt} = \underbrace{B \cdot Q_c C_F e^{-T_a/T}} = -Q_c \frac{dC_F}{dt}$$

Simplify with non-dimension variables:

$$\tilde{T} = \frac{C_v \rho_0}{Q_c \cdot C_{F,0}} T \ , \ \tilde{C}_F = \frac{C_F}{C_{F,0}} \Rightarrow \frac{d\tilde{T}}{dt} = -\frac{d\tilde{C}_F}{dt} = B\tilde{C}_F e^{(-\frac{\tilde{T}_a}{\tilde{T}})}$$

$$\Rightarrow \frac{d}{dt}(\tilde{T} + \tilde{C}_F) = 0 \Rightarrow \tilde{T} + \tilde{C}_F = \text{const} \Rightarrow \tilde{T} - \tilde{T}_0 = 1 - \tilde{C}_F$$

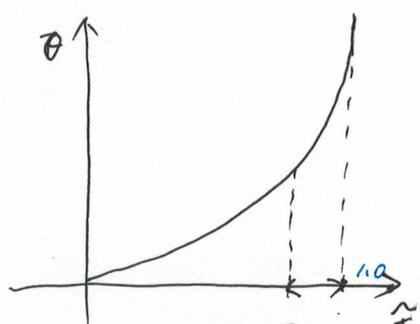
At initial $(t \to 0)$. $\tilde{T} \approx \tilde{T}_0$ , $\tilde{C}_F \sim 1$

perturbation: $\tilde{T}$ as : $\tilde{T} = T_0 + \varepsilon\theta(t) + O(\varepsilon^2)$ , $\varepsilon = \frac{\tilde{T}_0^2}{\tilde{T}_a} \ll 1$.

$$\text{with } \hat{t} = \frac{B e^{-\tilde{T}_a/\tilde{T}_0}}{\varepsilon} t \ , \Rightarrow \frac{d\theta}{d\hat{t}} = e^{(-\frac{\tilde{T}_a}{\tilde{T}} + \frac{\tilde{T}_a}{\tilde{T}_0})} = e^{\frac{\tilde{T}_a}{\tilde{T}\tilde{T}_0}(\tilde{T} - \tilde{T}_0)}$$

$$= e^{\frac{\tilde{T}_a \varepsilon}{\tilde{T}\tilde{T}_0}\theta} \xrightarrow{t \to 0} e^{\theta}$$

$$\Rightarrow \theta = -\ln(1 - \hat{t}) \Rightarrow \tilde{T} \text{ diverges when } \hat{t} \to 1 \Rightarrow t_I = c_v \frac{T_0^2}{T_a} \frac{e^{T_a/T_0}}{Q_c Y_{F,0} B}$$




* Non-Adiabatic

Difference; Heat loss through boundary!

Employ the notion learnt in heat transfer course:

$$-Sh(T - T_0)$$

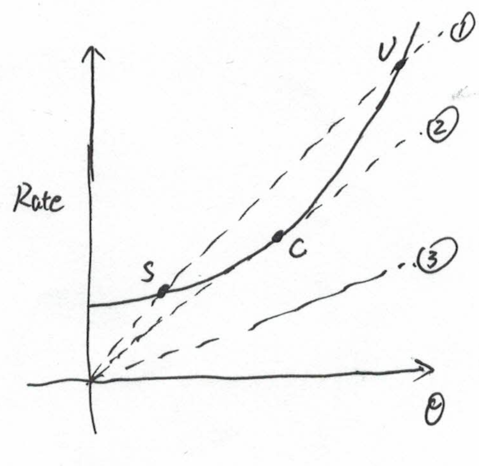
Governing Equation:

$$V\rho_0 \cdot C_v = V \cdot Q_c B C_F e^{-T_a/T} - Sh(T - T_0)$$

Again: $\tilde{T} = \frac{C_v \rho_0}{Q_c \cdot C_{F,0}} T$ $\quad \tilde{C}_F = C_F / C_{F,0}$ , $\hat{t} = t/\tau_c$

New: $\tau_c = \frac{\varepsilon}{B e^{-T_a/T_0}}$ $\quad \tau_L = \frac{C_v \rho_0}{(S/V)h}$ $\quad \hat{h} = \frac{\tau_c}{\tau_L}$

$$\Rightarrow \frac{d\theta}{d\hat{t}} = e^{\theta} - \hat{h}\theta$$



## § Ignition and Distinction (well-stirred Reactor Analogy) & Remarks on Q4-HW3

Governing Equation: (Energy Balance)

$$\dot{V} \rho_0 C_p (T_f - T_0) = V \cdot Q_c \cdot B \cdot C_F \cdot e^{-T_a/T_f}$$

Use $C_p$ instead of $C_v$! Open system, flow exists!

V: reactor volumn. $T_0$: initial temperature of mixture.

$T_f$: Reaction temperature. $C_F$: Reactant concentration in the burner.

Similar non-dimensional form: (with $\tilde{T} - \tilde{T}_0 = 1 - \tilde{C}_F$)

$$\tilde{T}_f - \tilde{T}_0 = Da \cdot (\tilde{T}_{ad} - \tilde{T}_f) e^{-\tilde{T}_a/\tilde{T}_f}$$

where:

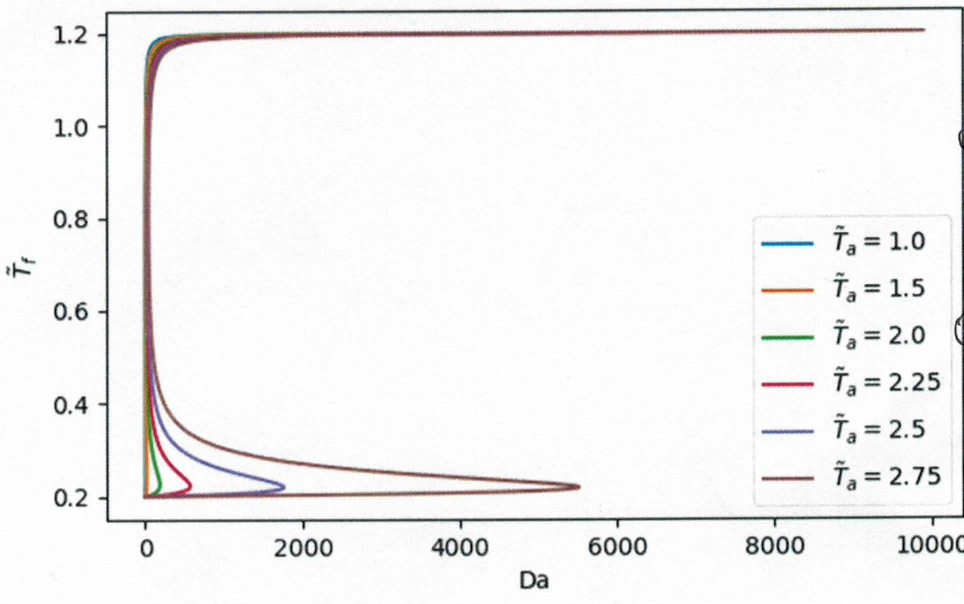
$$\tilde{T} = \frac{C_p}{q_c \cdot Y_{F,0}} T, \quad \tilde{T}_{ad} - \tilde{T}_f = \tilde{C}_F, \quad \tilde{T}_{ad} = 1 + \tilde{T}_0$$

and

$$Da = \frac{B}{\dot{V}/V} = \frac{\dot{V}/V}{1/B} = \frac{\text{Flow time}}{\text{Reaction time}}.$$

In numerical calculation, $\tilde{T}_0$ is pre-defined, and Da is calculated with given $\tilde{T}_f$.

For example, take $\tilde{T}_0 = 0.2$, then $\tilde{T}_{ad} = 1.2$, $\tilde{T}_f \in (\tilde{T}_0, \tilde{T}_{ad})$, the plot of $\tilde{T}_f$ - Da is shown as:




Understanding:

① Da ↑ ⇒ Flow time ↑ ⇒ Enough time of reaction! ⇒ Ignition!

② Da ↓ ⇒ Flow time ↓ ⇒ Insufficient reaction ⇒ Extinction!