Our Combustion model

$$\rho\left(\frac{\partial Y_F}{\partial t} + (u\cdot\nabla)Y_F\right) - \nabla\cdot(\rho D \nabla Y_F) = -k\rho^2 Y_F Y_O$$

$$\rho\left(\frac{\partial Y_O}{\partial t} + (u\cdot\nabla)Y_O\right) - \nabla\cdot(\rho D \nabla Y_O) = -r k \rho^2 Y_F Y_O.$$

$$\rho\left(\frac{\partial T}{\partial t} + (u\cdot\nabla)T\right) - \cancel{\frac{1}{\rho}}\,\nabla\cdot(a\rho\nabla T) = +k\rho^2 Y_F Y_O \frac{q}{c_p}$$

$K(T) = A T^{\alpha} \exp\left(\frac{T_a}{T}\right)$. u - fluid model drives combustion.

Define z such that

$$\rho\left(\frac{\partial z}{\partial t} + (u\cdot\nabla)z\right) - \nabla\cdot(\rho D \nabla z) = 0$$

The solution is caught in a center manifold such that $Y_F = Y_F(z,T)$ and $Y_O = Y_O(z,T)$

Center manifold expansion

Expand to 1st order:

$$Y_F = A_1 + A_2 z + A_3 T$$
$$Y_O = B_1 + B_2 z + B_3 T.$$

To give some meaning to z we demand that:

$$\left\{\begin{array}{l} Y_F(1, T_F, \emptyset) = Y_{F,\emptyset} \\ Y_O(1, T_F, \emptyset) = 0. \\ Y_F(0, T_O, \emptyset) = 0 \\ Y_O(0, T_O, \emptyset) = \cancel{1}\, Y_{O,\emptyset} \end{array}\right. \Leftrightarrow \left\{\begin{array}{ll} A_1 + A_2 + A_3 T_F = 1 & (1) \\ B_1 + B_2 + B_3 T_F = 0. & (2) \\ A_1 + A_3 T_O = 0. & (3) \\ B_1 + B_3 T_O = 0. & (4) \end{array}\right.$$

$$A_2 = 1 + A_3(T_O - T_F)$$

$A_1 = -A_3 T_O \Rightarrow -A_3 T_O + A_2 + A_3 T_F = 1 \Rightarrow \cancel{A_2 = A_3(T_O - T_F)}.$

$B_1 = -B_3 T_O \Rightarrow -B_3 T_O + B_2 + B_3 T_F = 0 \Rightarrow B_2 = A_3$

interpretation

$$\begin{cases} Y_F(1, T_{F,\emptyset}) = Y_{F,\emptyset} \\ Y_O(1, T_{F,\emptyset}) = 0 \\ Y_F(0, T_{O,\emptyset}) = 0 \\ Y_O(0, T_O) = Y_{O,\emptyset}. \end{cases} \iff \begin{cases} A_1 + A_2 + A_3 T_F = Y_{F,\emptyset} \\ B_1 + B_2 + B_3 T_F = 0. \\ A_1 + A_3 T_O = 0 \\ B_1 + B_3 T_O = Y_{O,\emptyset}. \end{cases}$$

Write A_1, A_2 in terms of A_3.

$A_1 = -A_3 T_O$.

$A_2 = Y_{F,\emptyset} - A_1 - A_3 T_F = Y_{F,\emptyset} + A_3 T_O - A_3 T_F =$
$= Y_{F,\emptyset} + A_3 (T_O - T_F)$.

Write B_1, B_2 in terms of B_3:

$B_1 = Y_{O,\emptyset} - B_3 T_O$.

$B_2 = -B_1 - B_3 T_F = -(Y_{O,\emptyset} - B_3 T_O) - B_3 T_F =$
$= -Y_{O,\emptyset} + B_3 (T_O - T_F)$.

We obtain:

$$Y_F = -A_3 T_O + (Y_{F,\emptyset} + A_3 (T_O - T_F)) Z + A_3 T$$
$$Y_O = (Y_{O,\emptyset} - B_3 T_O) + (-Y_{O,\emptyset} + B_3 (T_O - T_F)) Z + B_3 T.$$

To obtain A_3 and B_3:

Define $\mathcal{L} \xi = \rho \left(\dfrac{\partial \xi}{\partial t} + (u \cdot \nabla) \xi \right) - \nabla \cdot (\rho D \nabla \xi)$

Then we know that

$$\mathcal{L} Y_F = -k\rho^2 Y_F Y_O.$$
$$\mathcal{L} Y_O = -rk\rho^2 Y_F Y_O \qquad \mathcal{L} Z = 0$$
$$\mathcal{L} T = +k\rho^2 Y_F Y_O \frac{q}{c_p}.$$

Write:

$\mathcal{L} Y_F = \mathcal{L}\left(-A_3 T_O + (Y_{F,\emptyset} + A_3 (T_O - T_F)) Z + A_3 T\right) =$
$= (Y_{F,\emptyset} + A_3 (T_O - T_F)) \mathcal{L} Z + A_3 \mathcal{L} T. =$
$= A_3 \mathcal{L} T = +k\rho^2 Y_F Y_O \dfrac{q}{c_p} A_3$

then: $\dfrac{q}{c_p} A_3 = -1 \Rightarrow A_3 = -\dfrac{c_p}{q}.$

Also $\mathcal{L} Y_O = k\rho^2 Y_F Y_O \dfrac{q}{c_p} B_3 = -rk\rho^2 Y_F Y_O \Rightarrow B_3 = -\dfrac{r c_p}{q}$.

Define ~~$\tau = c_p/q$.~~ $\tau_0 = q/c_p$.

Then our equations become:

Define non-dimensionalized temperature:

$$\tau = \frac{c_p T}{q} \quad , \quad \tau_F = \frac{c_p T_F}{q} \quad , \quad \tau_O = \frac{c_p T_O}{q}.$$

Our equations become:

$$Y_F = \tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))\, Z - \tau$$

$$Y_O = (Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))\, Z - r\tau$$

Another remarkable property of this manifold is that Z can be written as an affine function of Y_F and Y_O: $Z = \lambda_1 Y_F + \lambda_2 Y_O + \lambda_3$.

Abbreviate: $Y_F = A_1 + A_2 Z - \tau$

$Y_O = B_1 + B_2 Z - r\tau$.

Then: $Z = \lambda_1 (A_1 + A_2 Z - \tau) + \lambda_2 (B_1 + B_2 Z - r\tau) + \lambda_3 =$

$= (A_1\lambda_1 + B_1\lambda_2 + \lambda_3) + (A_2\lambda_1 + B_2\lambda_2) Z - (\lambda_1 + r\lambda_2)\tau$

It follows that

$$\begin{cases} A_1\lambda_1 + B_1\lambda_2 + \lambda_3 = 0 \\ A_2\lambda_1 + B_2\lambda_2 = 1 \\ \lambda_1 + r\lambda_2 = 0 \end{cases} \Leftrightarrow \begin{bmatrix} A_1 & B_1 & 1 \\ A_2 & B_2 & 0 \\ 1 & r & 0 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \Leftrightarrow$$

$$\Leftrightarrow \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \frac{1}{rA_2 - B_2} \begin{bmatrix} 0 & r & -B_2 \\ \cancel{0} & \cancel{-1} & \cancel{A_2} \\ (rA_2 - B_2) & -(aA_1 r - B_1) & -(\end{bmatrix}$$

$$\cancel{\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix}}$$

The solution is:

$$\lambda_1 = \frac{r}{rA_2 - B_2} \quad , \quad \lambda_2 = \frac{-1}{rA_2 - B_2} \quad , \quad \lambda_3 = \frac{B_1 - rA_1}{rA_2 - B_2}$$

Therefore:

$$Z = \lambda_1 Y_F + \lambda_2 Y_O + \lambda_3 = \frac{rY_F - Y_O + (B_1 - rA_1)}{rA_2 - B_2} = \frac{rY_F - Y_O - (rA_1 - B_1)}{rA_2 - B_2}.$$

Substitute

$rA_1 - B_1 = r(\tau_O) - (Y_{O,\emptyset} + r\tau_O) = r(\tau_O - \tau) - Y_{O,\emptyset}$.

$\cancel{rA_2 - B_2 = r(Y_{O,\emptyset} + r\tau) + (Y_{O,\emptyset} + r(\tau_O - \tau_F))}$

$\cancel{= (r+1) Y_{O,\emptyset} + r}$

$rA_2 - B_2 = r(Y_{F,\emptyset} - (\cancel{\tau_O} - \tau_F)) + (Y_{O,\emptyset} + r(\cancel{\tau_O} - \tau_F))$ WOW!

$= r Y_{F,\emptyset} + Y_{O,\emptyset}$.

and we find that:

$$Z = \frac{rY_F - Y_O + Y_{O,\emptyset}}{rY_{F,\emptyset} - Y_{O,\emptyset}}.$$

Note that there is no dependence on τ, τ_F or τ_O !!

To summarize:

The center-manifold approximation to our model is:

$$\rho\left(\frac{\partial Z}{\partial t} + (u\cdot\nabla) Z\right) - \nabla\cdot(\rho D \nabla Z) = 0.$$

$$\rho\left(\frac{\partial \tau}{\partial t} + (u\cdot\nabla)\tau\right) - \nabla\cdot(\rho D\nabla\tau) = k\rho^2 Y_F Y_O.$$

$$Y_F = \tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z - \tau = Y_F(Z,\tau).$$

$$Y_O = (Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))Z - r\tau$$

$$\cancel{K = AT^a \exp(T_a/T) = A\tau^a}$$

and $$Z = \frac{rY_F - Y_O + Y_{O,\emptyset}}{rY_{F,\emptyset} - Y_{O,\emptyset}}$$

If we take this as a definition of Z, then the equations relating Y_F, Y_O with Z, t can be used to obtain τ up to 1st order.

Recall $\tau = \dfrac{c_p T}{q}$, $\tau_F = \dfrac{c_p T_F}{q}$, $\tau_O = \dfrac{c_p T_O}{q}$.

Fast chemistry limit

Assumption : $Y_F Y_O = 0$.

(F and O can not coexist be they react immediately)

Consider also $\dfrac{rY_F - Y_O + Y_{O,0}}{rY_{F,0} + Y_{O,0}} = Z$.

or $rY_F - Y_O + Y_{O,0} = Z\,(rY_{F,0} + Y_{O,0})$

To solve, two cases:

Case 1 : $Y_F \neq 0$.

Then $Y_O = 0 \Leftrightarrow$

$$rY_F + Y_{O,0} - Z\,(rY_{F,0} + Y_{O,0}) = 0 \Leftrightarrow$$

$$rY_F = Z\,(rY_{F,0} + Y_{O,0}) - Y_{O,0}$$

Requires : $rY_F > 0 \Leftrightarrow Z > \dfrac{Y_{O,0}}{rY_{F,0} + Y_{O,0}}$

Define : $Z_{st} = \dfrac{Y_{O,0}}{rY_{F,0} + Y_{O,0}}$

Then : $rY_F = (rY_{F,0} + Y_{O,0})(Z - Z_{st})\,H(Z - Z_{st})$ for all $0 \leq Z \leq 1$

~~Also~~ Moreover

$$1 - Z_{st} = \frac{rY_{F,0} + Y_{O,0} - Y_{O,0}}{rY_{F,0} + Y_{O,0}} = \frac{rY_{F,0}}{rY_{F,0} + Y_{O,0}} \Rightarrow$$

$$\Rightarrow rY_{F,0} + Y_{O,0} = \frac{rY_{F,0}}{1 - Z_{st}}$$

Then : $rY_F = rY_{F,0}\,\dfrac{Z - Z_{st}}{1 - Z_{st}}\,H(Z - Z_{st}) \Rightarrow$

$$\Rightarrow \boxed{Y_F = Y_{F,0}\,\frac{Z - Z_{st}}{1 - Z_{st}}\,H(Z - Z_{st})}$$

Case 2 : $Y_O \neq 0$

Then $Y_F = 0 \Leftrightarrow$

$$Y_O - Y_{O,0} + Z\,(rY_{F,0} + Y_{O,0}) = 0 \Leftrightarrow$$

$$Y_O = Y_{O,0} - Z\,(rY_{F,0} + Y_{O,0}) =$$

$$= (rY_{F,0} + Y_{O,0})(Z_{st} - Z) =$$

$$= Y_{O,0}\,\frac{Z_{st} - Z}{Z_{st}}$$

$Y_O > 0 \Rightarrow$ require $Z < Z_{st}$, therefore

$$\boxed{Y_O = Y_{O,\emptyset}\,\frac{Z_{st}-Z}{Z_{st}}\,H(Z_{st}-Z).}$$

Now we can relate the temperature τ as a function of Z:
Use: $Y_F = Y_F(Z,\tau) = \tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z - \tau \Rightarrow$

$$\Rightarrow \tau = \tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z - Y_F =$$

$$= \tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z - Y_{F,\emptyset}\,\frac{Z - Z_{st}}{1 - Z_{st}}\,H(Z - Z_{st}).$$

- For $Z < Z_{st}$: $\tau = \tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z.$

Use: $Y_O = Y_O(Z,\tau) = (Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))Z - r\tau \Rightarrow$

$$\Rightarrow r\tau = (Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))Z - Y_O$$

- For $Z > Z_{st}$: $r\tau = (Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))Z$

In general:

$$\tau = [\tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z]\,H(Z - Z_{st}) + [(Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))Z]\,H(Z_{st} - Z) =$$

Putting this all-together, in the fast chemistry limit, Z is the leading equation and Y_F, Y_O and τ are slaves to Z.

$$\tau = [\tau_O + (Y_{F,\emptyset} - (\tau_O - \tau_F))Z]\,H(Z - Z_{st}) + [(Y_{O,\emptyset} + r\tau_O) - (Y_{O,\emptyset} + r(\tau_O - \tau_F))Z]\,\frac{H(Z_{st} - Z)}{r}.$$

Averaging $\dot{w}_F$ on the fast chemistry limit

Note that $\dot{w}_O = r\dot{w}_F$. Want $\dot{w}_F$.

$$\dot{w}_F = \rho\left(\frac{\partial Y_F}{\partial t} + (u\cdot\nabla)Y_F\right) - \nabla\cdot(\rho D\nabla Y_F) =$$
$$= \rho\left(\frac{\partial Y_F}{\partial t} + (u\cdot\nabla)Y_F\right) - D\,\nabla\cdot(\rho\nabla Y_F)$$

where $\quad Y_F = Y_{F,\emptyset}\,\dfrac{Z - Z_{st}}{1 - Z_{st}}\,H(Z - Z_{st})$.

Define $\quad L(A) = \rho\left(\dfrac{\partial A}{\partial t} + (u\cdot\nabla)A\right) - D\nabla\cdot(\rho\nabla A)$.

Then $\quad \dot{w}_F = L\left(Y_{F,\emptyset}\,\dfrac{Z - Z_{st}}{1 - Z_{st}}\,H(Z - Z_{st})\right)$

To compute this, note that L is linear operator, therefore:

$$L(A+B) = L(A) + L(B)$$
$$L(\lambda A) = \lambda L(A) \qquad \text{for } \lambda = \text{const}.$$

Want to find $L(AB)$ and $L(A(B))$.

Decompose: $\quad L = L_1 - D\nabla\cdot(\rho\nabla)$.

L_1 respects the product rule and the chain rule:

$$L_1(AB) = AL_1(B) + BL_1(A)$$
$$L_1(A(B)) = \frac{\partial A}{\partial B}L_1(B).$$

Now consider:

$$\nabla\cdot(\rho\nabla(AB)) = \nabla\cdot(\rho A\nabla B + \rho B\nabla A) = \nabla\cdot(\rho A\nabla B) + \nabla\cdot(\rho B\nabla A) =$$
$$\left(\begin{aligned} &= \rho A\nabla^2 B + \nabla(\rho A)\cdot\nabla B + \rho B\nabla^2 A + \nabla(\rho B)\cdot\nabla A = \\ &= \rho A\nabla^2 B + \rho B\nabla^2 A + (\rho\nabla A + A\nabla\rho)\cdot\nabla B + (\rho\nabla B + B\nabla\rho)\cdot\nabla A \end{aligned}\right)$$

$$= A\nabla\cdot(\rho\nabla B) + B\nabla\cdot(\rho\nabla A) + \rho\nabla B\cdot\nabla A + \rho\nabla A\cdot\nabla B =$$
$$= A\nabla\cdot(\rho\nabla B) + B\nabla\cdot(\rho\nabla A) + 2\rho\nabla A\cdot\nabla B.$$

It follows that

$$L(AB) = L_1(AB) - D\nabla\cdot(\rho\nabla(AB)) =$$
$$= AL_1(B) + BL_1(A) - D\left(A\nabla\cdot(\rho\nabla B) + B\nabla\cdot(\rho\nabla A) + 2\rho\nabla A\cdot\nabla B\right) =$$
$$= A\left(L_1(B) - D\nabla\cdot(\rho\nabla B)\right) + B\left(L_1(A) - D\nabla\cdot(\rho\nabla A)\right) - 2\rho D\nabla A\cdot\nabla B =$$
$$= AL(B) + BL(A) - 2\rho D\nabla A\cdot\nabla B.$$

Also

$$\nabla\cdot(\rho\nabla A(B)) = \nabla\cdot\left(\rho\frac{\partial A}{\partial B}\nabla B\right) = \frac{\partial A}{\partial B}\nabla\cdot(\rho\nabla B) + \rho\nabla B\cdot\nabla\left(\frac{\partial A}{\partial B}\right)$$

therefore

$$\begin{aligned} L(A(B)) &= L_1(A(B)) - D\,\nabla\cdot(\rho\nabla A(B)) = \\ &= \frac{\partial A}{\partial B}L_1(B) - D\left(\frac{\partial A}{\partial B}\nabla\cdot(\rho\nabla B) + \rho\nabla B\cdot\nabla\left(\frac{\partial A}{\partial B}\right)\right) = \\ &= \frac{\partial A}{\partial B}\left(L_1(B) - D\,\nabla\cdot(\rho\nabla B)\right) - \rho D\,\nabla\left(\frac{\partial A}{\partial B}\right)\cdot\nabla B \\ &= \frac{\partial A}{\partial B}L(B) - \rho D\,\nabla\left(\frac{\partial A}{\partial B}\right)\cdot\nabla B. \end{aligned}$$

We have then:

$$L(AB) = A\,L(B) + B\,L(A) - 2\rho D\,(\nabla A\cdot\nabla B).$$

$$L(A(B)) = \frac{\partial A}{\partial B}L(B) - \rho D\,\nabla\left(\frac{\partial A}{\partial B}\right)\cdot\nabla B$$

Now we can compute $\dot{w}_F$:

$$\dot{w}_F = L\left(Y_{F,\emptyset}\frac{Z-Z_{st}}{1-Z_{st}}\,H(Z-Z_{st})\right) = Y_{F,\emptyset}\,L\left(\frac{Z-Z_{st}}{1-Z_{st}}H(Z-Z_{st})\right) =$$

$$= Y_{F,\emptyset}\,L\left(\frac{Z-Z_{st}}{1-Z_{st}}\right)H(Z-Z_{st}) + Y_{F,\emptyset}\frac{Z-Z_{st}}{1-Z_{st}}L\left(H(Z-Z_{st})\right) - 2\rho D\left[\nabla\left(\frac{Z-Z_{st}}{1-Z_{st}}\right)\cdot\nabla\left(H(Z-Z_{st})\right)\right]Y_{F,\emptyset}$$

Take the terms individually:

1st term:

$$L\left(\frac{Z-Z_{st}}{1-Z_{st}}\right) = \frac{1}{1-Z_{st}}L(Z) = 0.$$

2nd term

$$\begin{aligned} L\left(H(Z-Z_{st})\right) &= \delta(Z-Z_{st})\,L(Z-Z_{st}) - \rho D\,\nabla\left(\delta(Z-Z_{st})\right)\cdot\nabla(Z-Z_{st}) = \\ &= \delta(Z-Z_{st})L(Z) - \rho D\,\delta'(Z-Z_{st})\,\nabla Z\cdot\nabla Z = \\ &= -\rho N\,\delta'(Z-Z_{st}) \end{aligned}$$

where we defined

$$N = D(\nabla Z\cdot\nabla Z) \longleftarrow \text{scalar dissipation}$$

3rd term:

$$\nabla\left(\frac{Z-Z_{st}}{1-Z_{st}}\right)\cdot\nabla\left(H(Z-Z_{st})\right) = \frac{1}{1-Z_{st}}\nabla Z\cdot\left[\delta(Z-Z_{st})\nabla Z\right] = \frac{\delta(Z-Z_{st})}{1-Z_{st}}(\nabla Z\cdot\nabla Z)$$

Putting it all together:

$$\dot{w}_F = Y_{F,\emptyset} \frac{Z - Z_{st}}{1 - Z_{st}} \left[-\rho N \delta'(Z - Z_{st}) \right] + 2\rho D \frac{\delta(Z - Z_{st})}{1 - Z_{st}} (\nabla Z \cdot \nabla Z) \, Y_{F,\emptyset} =$$

$$= \frac{Y_{F,\emptyset} \rho N}{1 - Z_{st}} \left[-(Z - Z_{st}) \delta'(Z - Z_{st}) + 2\delta(Z - Z_{st}) \right] =$$

$$= Y_{F,\emptyset} \rho N \frac{1}{1 - Z_{st}} \left[-\delta(Z - Z_{st}) + 2\delta(Z - Z_{st}) \right] =$$

$$= \rho N Y_{F,\emptyset} \frac{\delta(Z - Z_{st})}{1 - Z_{st}}.$$

therefore we obtained: $\boxed{\dot{w}_F = \rho N Y_{F,\emptyset} \frac{\delta(Z - Z_{st})}{1 - Z_{st}}}$

<u>Remark</u>: reaction takes place at regions where $Z = Z_{st}$. thus is then the physical meaning of Z_{st}

Hydrogen / air = 0.028.
Methane / air = 0.05
DNS = 0.5 !

↳ experimentalists also increase Z_{st} in their experiments in order to see more detail.
We do this only for calculation purposes.

<u>Remark</u> : If we assume that $p = \text{const}$ (ex. open jet) then $p = \frac{\rho R T}{W}$, $W = \left(\sum \frac{Y_i}{W_i} \right)^{-1} = W(Z)$, $T = T(Z)$.

$\rho = \rho^{eq}(Z)$ density is also a function of Z.

we may then write:

$$\langle \dot{w}_F \rangle = \int_0^{+\infty} \int_0^1 \rho(Z) N Y_{F,\emptyset} \frac{\delta(Z - Z_{st})}{1 - Z_{st}} P(Z, N; x) \, dZ \, dN =$$

$$= \int_0^{+\infty} \rho(Z_{st}) N Y_{F,\emptyset} \frac{P(Z_{st}, N; x)}{1 - Z_{st}} \, dN.$$

Frozen chemistry limit

No interaction between chemistry and mixing. Mixing takes place first. Chemistry follows.

$T = T_0$: $Y_F = Y_{F,\emptyset} Z$

$Y_O = Y_{O,\emptyset}(1-Z)$.

The time it takes for mixing to complete is:

$T_{mix} \sim \frac{l}{u}$ (due to turbulance

The time it take for the chemistry.

$T_{ch} \sim \frac{1}{k\rho}$.

Damköhler number : $Da = \frac{T_{mix}}{T_{ch}}$

Frozen chemistry limit : $Da \ll 1$.

Fast chemistry limit

F + O can not mix. They immediately react into product.
Therefore $Y_F Y_O = 0$.

Also : $\frac{r Y_F - Y_O + Y_{O,\emptyset}}{r Y_{F,\emptyset} + Y_{O,\emptyset}} = Z$.

Solve fore Y_F, Y_O the following perturbed equations:

$$Y_F Y_O = \varepsilon$$

$$r Y_F - Y_O + Y_{O,\emptyset} = Z(r Y_{F,\emptyset} + Y_{O,\emptyset}).$$

Write $Y_O = r Y_F + Y_{O,\emptyset} - Z(r Y_{F,\emptyset} + Y_{O,\emptyset})$

$Y_F Y_O = 0 \Leftrightarrow$

$Y_F (r Y_F + Y_{O,\emptyset} - Z(r Y_{F,\emptyset} + Y_{O,\emptyset})) = 0$.

If $Y_F \neq 0$.

$r Y_F + Y_{O,\emptyset} - Z(r Y_{F,\emptyset} + Y_{O,\emptyset}) = 0$

$$Y_F = \frac{Z(r Y_{F,\emptyset} + Y_{O,\emptyset}) - Y_{O,\emptyset}}{r}$$

requires : $Z \geqslant \frac{Y_{O,\emptyset}}{r Y_{F,\emptyset} + Y_{O,\emptyset}}$.

Write $rY_F = Y_O - Y_{O,\emptyset} + Z\,(rY_{F,\emptyset} + Y_{O,\emptyset})$ $\qquad Y_O > 0.$

$Y_O\, rY_F = 0 \Leftrightarrow$

$Y_O - Y_{O,\emptyset} + Z\,(rY_{F,\emptyset} + Y_{O,\emptyset}) = 0. \Leftrightarrow$

$Y_O = Y_{O,\emptyset} - Z\,(rY_{F,\emptyset} + Y_{O,\emptyset}). > 0.$

But $Z < \dfrac{Y_{O,\emptyset}}{rY_{F,\emptyset} + Y_{O,\emptyset}}.$

Define: $\underline{Z_{st} = \dfrac{Y_{O,\emptyset}}{rY_{F,\emptyset} + Y_{O,\emptyset}}}$, $H(z) = \begin{cases} 1, & z > 0 \\ 0, & z < 0. \end{cases}$

Heaviside function.

Then we obtained:

$$rY_F = [Z\,(rY_{F,\emptyset} + Y_{O,\emptyset}) - Y_{O,\emptyset}]\, H(Z - Z_{st})$$

$$= (rY_{F,\emptyset} + Y_{O,\emptyset})\,(Z - Z_{st})\, H(Z - Z_{st}) =$$

$$= \frac{Y_{O,\emptyset}\,(Z - Z_{st})}{Z_{st}}\, H(Z - Z_{st}).$$

$$1 - Z_{st} = \frac{rY_{F,0} + Y_{O,\emptyset} - Y_{O,\emptyset}}{rY_{F,\emptyset} + Y_{O,\emptyset}} = \frac{rY_{F,\emptyset}}{rY_{F,\emptyset} + Y_{O,\emptyset}}. \Rightarrow rY_{F,\emptyset} + Y_{O,\emptyset} = \frac{rY_{F,\emptyset}}{1 - Z_{st}}.$$

then

$$\boxed{Y_F = Y_{F,\emptyset}\, \frac{Z - Z_{st}}{1 - Z_{st}}\, H(Z - Z_{st})}$$

$$Y_O = Y_{O,\emptyset} - Z\,(rY_{F,\emptyset} + Y_{O,\emptyset}) = (rY_{F,\emptyset} + Y_{O,\emptyset})\,(Z_{st} - Z) =$$

$$= \frac{Y_{O,\emptyset}\,(Z - Z_{st})}{Z_{st}}\, H(Z_{st} - Z).$$

so

$$\boxed{Y_O = Y_{O,\emptyset}\, \frac{Z - Z_{st}}{Z_{st}}\, H(Z_{st} - Z)}$$

What about the temperature?

Take

$$\frac{c_p}{q}(T-T_0) = Y_{F,\emptyset} Z - Y_F = Y_{F,\emptyset} Z - Y_{F,\emptyset}\frac{Z-Z_{st}}{1-Z_{st}} H(Z-Z_{st}) =$$

$$= Y_{F,\emptyset}\left(Z - \frac{Z-Z_{st}}{1-Z_{st}} H(Z-Z_{st})\right)$$

$$\cancel{\frac{c_p}{q}(T-T_0) = Y_{O,\emptyset}(1-Z) - Y_{O,\emptyset}\frac{Z-Z_{st}}{Z_{st}} H(Z-Z_{st})}$$

For $Z < Z_{st}$ we obtain:

$$\frac{c_p}{q}(T-T_0) = Y_{F,\emptyset} Z$$

For $Z > Z_{st}$

$$\frac{c_p}{q}(T-T_0) = Y_{O,\emptyset}(1-Z) - Y_O = Y_{O,\emptyset}(1-Z).$$

Putting these together we get.

$$\frac{c_p}{q}(T-T_0) = Y_{F,\emptyset} Z\, H(Z_{st}-Z) + Y_{O,\emptyset}(1-Z) H(Z-Z_{st}) =$$

$$= Y_{F,\emptyset} Z\,(1 - H(Z_{st}-Z)) + Y_{O,\emptyset}(1-Z) H(Z-Z_{st}) =$$

$$= Y_{F,\emptyset} Z + [Y_{O,\emptyset}(1-Z) - Y_{F,\emptyset} Z] H(Z-Z_{st})$$

Thus:

$$T = T_0 + \frac{q\, Y_{F,\emptyset}}{c_p} Z + \frac{q}{c_p}\left[Y_{O,\emptyset}(1-Z) - Y_{F,\emptyset} Z\right] H(Z-Z_{st})$$

Putting this all-together, in the fast-chemistry limit:

$$\frac{\partial Z}{\partial t} + (u\cdot\nabla) Z - \nabla\cdot(\rho D \nabla Z) = 0$$

$$Y_F = Y_{F,\emptyset}\frac{Z-Z_{st}}{1-Z_{st}} H(Z-Z_{st})$$

$$Y_O = Y_{O,\emptyset}\frac{Z-Z_{st}}{Z_{st}} H(Z_{st}-Z).$$

$$T = T_0 + \frac{q}{c_p}\left\{Y_{F,\emptyset} Z + \left[Y_{O,\emptyset}(1-Z) - Y_{F,\emptyset} Z\right] H(Z-Z_{st})\right\}.$$

where: $Z_{st} = \dfrac{Y_{O,\emptyset}}{r Y_{F,\emptyset} + Y_{O,\emptyset}}$