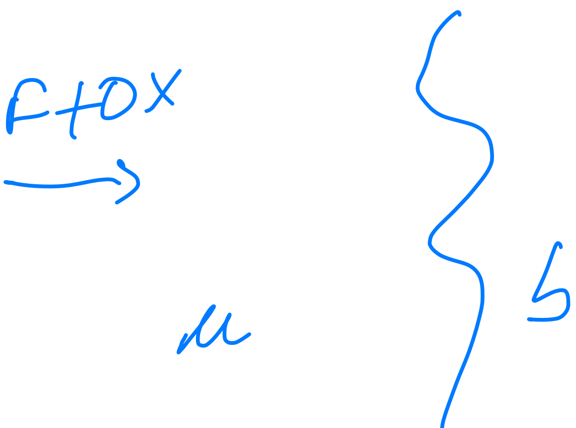
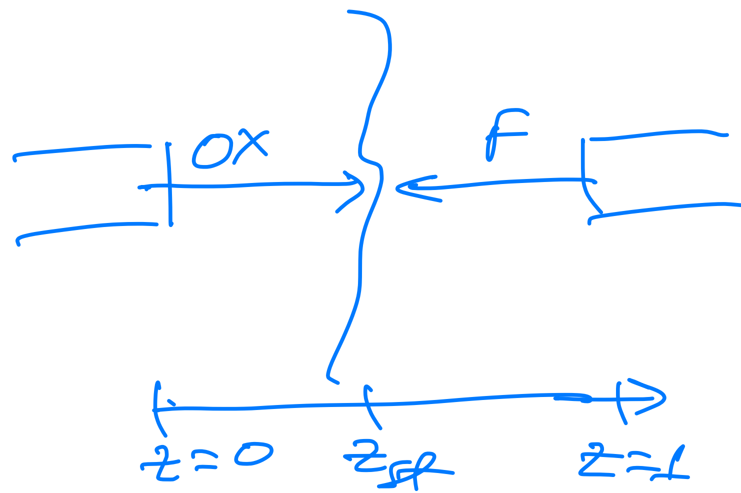
FLAME SURFACE DENSITY MODELS

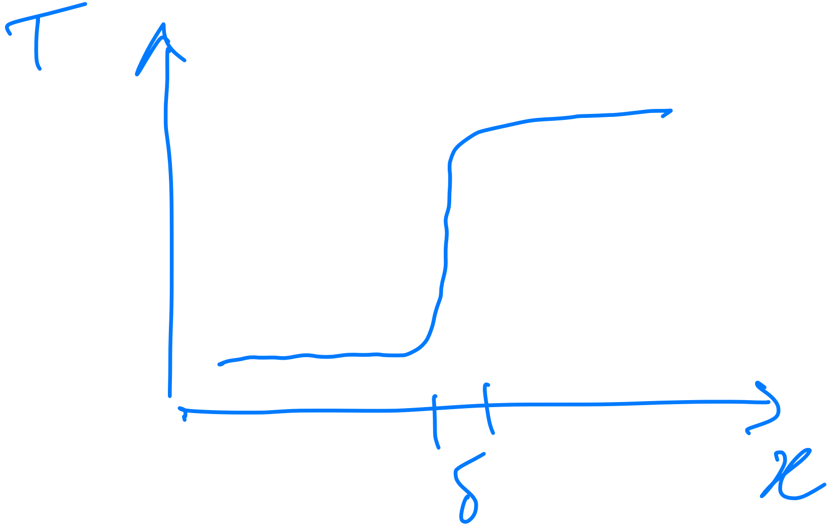
— REVIEW OF BASICS —

PREMIXED



DIFUSION

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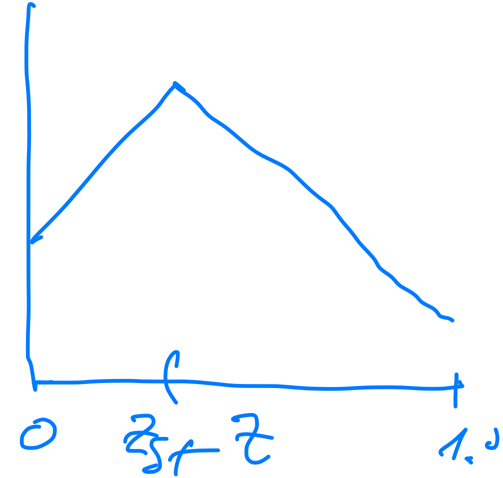
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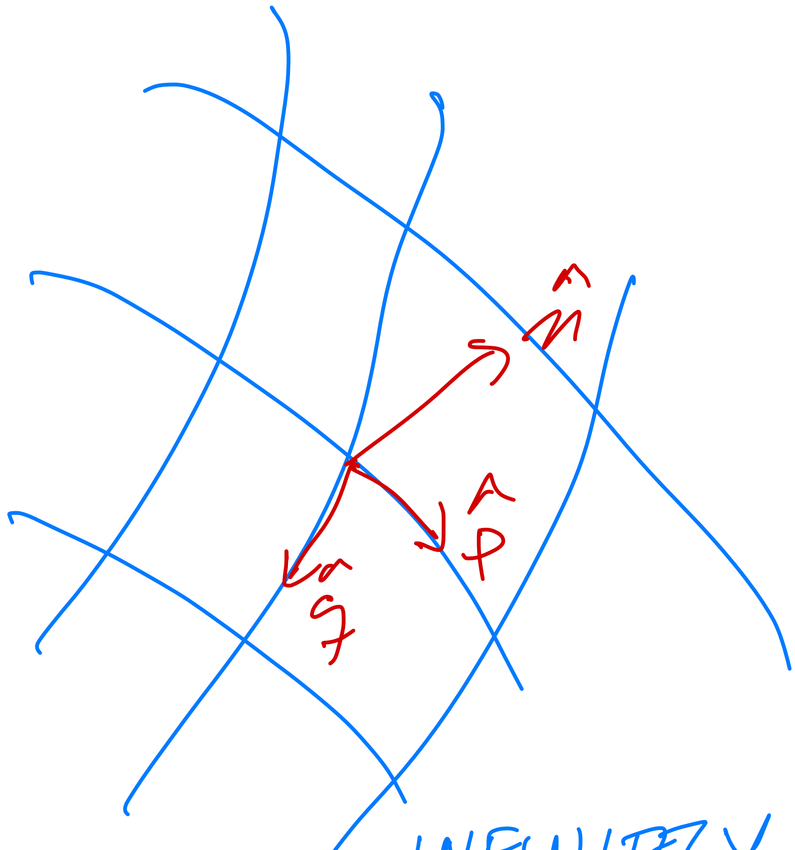
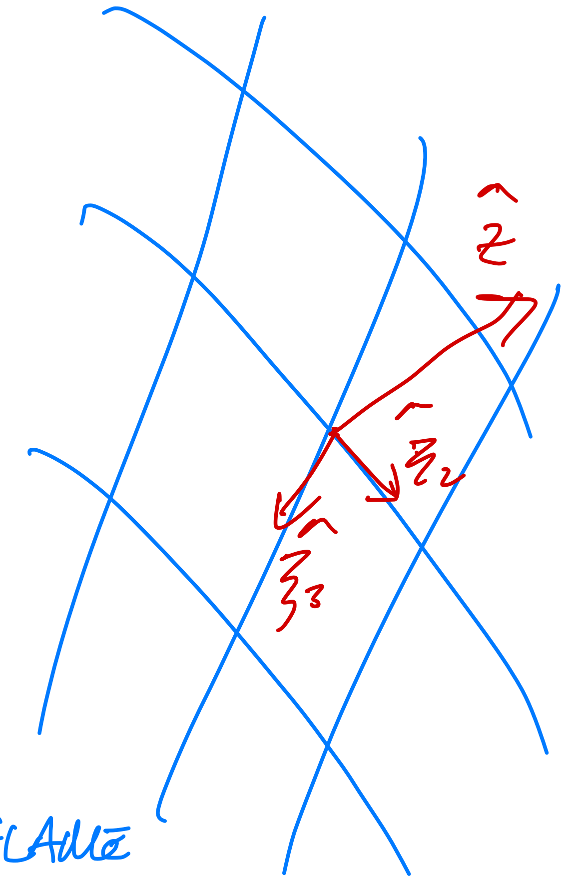




INFINITELY THIN FLAME FRONT LIMIT

INFLUENCE OF TURBULENCE

COHERENT FLAME MODEL

CANDEL & POINSOT, 1990

CST

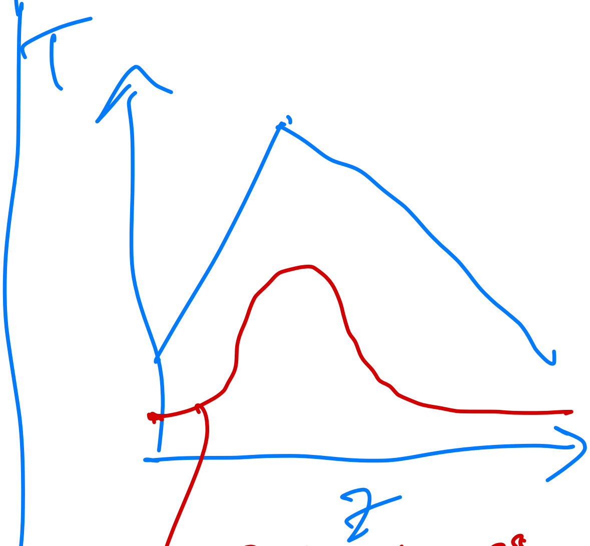
INTERACTION OF STRUCTURES

FLAMELETS

N. PETERS, 2001

TURB. COMB.

"ENSEMBLE OF LAMINAR FLAMES"



PDF (β?)

$$\langle T \rangle = \int_0 T(z)\, P(z)\, dz$$

SEPARATION CHEMISTRY × TURBULENCE

+

−

FLAME STRECH

SIMON C. TAYLOR, PhD LEEDS, 1991

BURNING VELOCITY AND THE INFLUENCE OF FLAME STRETCH

FLAME STRETCH (Γ)

$$\Gamma = \frac{1}{A}\frac{dA}{dt} \qquad (120)$$

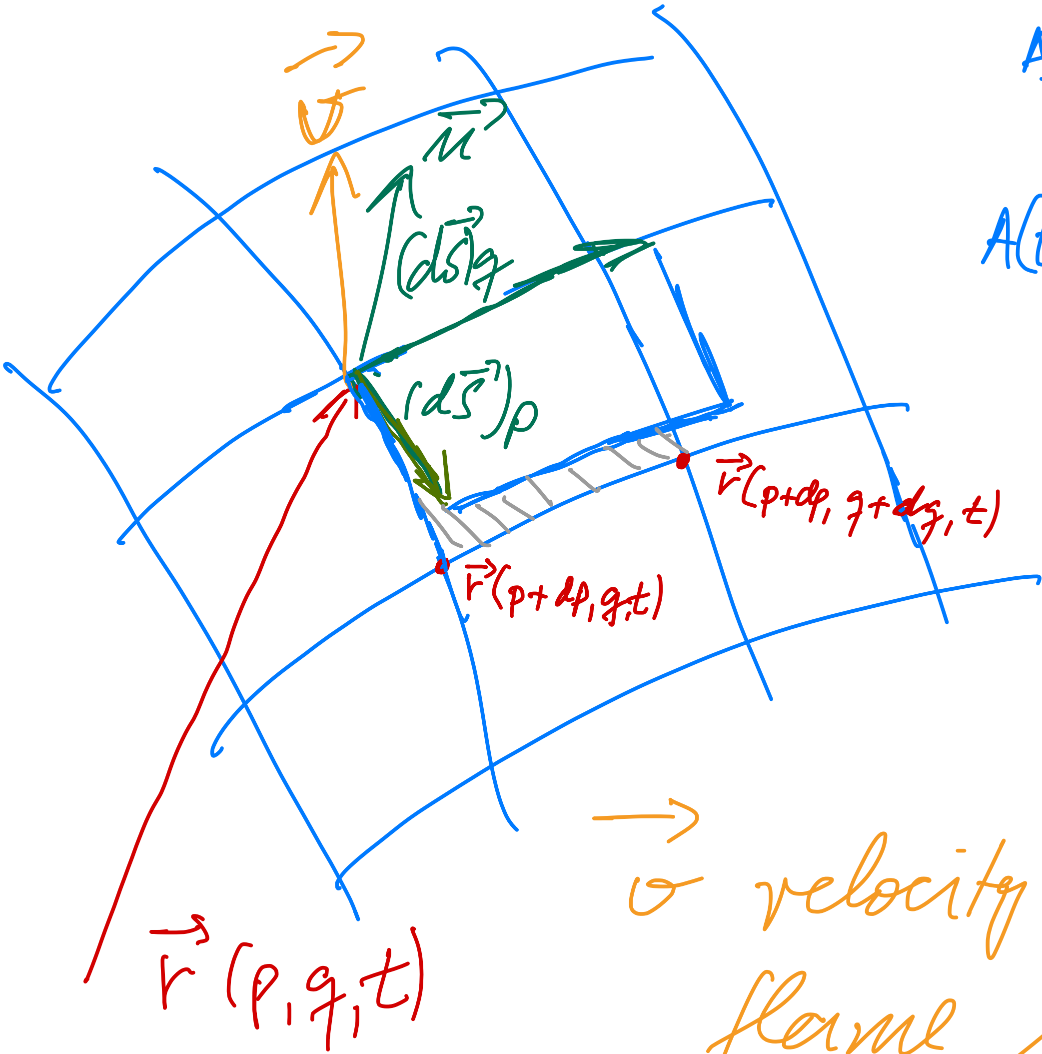
Adimensional

$$K = \frac{\delta}{S_u^0}\Gamma = \frac{\delta}{S_u^0}\frac{1}{A}\frac{dA}{dt} \qquad (121)$$

$A(t) = (d\vec{s})_p \times (d\vec{s})_q \cdot \vec{n}$

$A(t) = \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right) \cdot \vec{n}\, dp\, dq$

(123)



$\vec{v}$ velocity of the flame surface relative to the laboratory coordinates

at instant $t + dt$:

$$(d\vec{s})_{p'} = \frac{\partial \vec{r}}{\partial p} dp + \frac{\partial \vec{v}}{\partial p} dp\, dt$$

the new area:

$$A(t+dt) = \left\{\left(\frac{\partial \vec{r}}{\partial p} + \frac{\partial \vec{v}}{\partial p}\delta t\right) \times \left(\frac{\partial \vec{r}}{\partial q} + \frac{\partial \vec{v}}{\partial q}\delta t\right)\right\} \cdot \vec{n}\, dp\, dq$$

(126)

Flame stretch, from (120):

$$\Gamma = \frac{1}{\underset{(123)}{A}} \lim_{\delta t \to 0} \frac{\overset{(126)}{A(t+\delta t)} - \overset{(123)}{A(t)}}{\delta t}$$

$$\Gamma = \lim_{\delta t \to 0} \frac{\left\{\left(\frac{\partial \vec{r}}{\partial p} + \frac{\partial \vec{v}}{\partial p}\delta t\right) \times \left(\frac{\partial \vec{r}}{\partial q} + \frac{\partial \vec{v}}{\partial q}\delta t\right) - \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)\right\} \cdot \vec{n}\, dp\, dq}{\left\{\left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)\right\} \cdot \vec{n}\, dp\, dq\, \delta t}$$

$$= \lim_{\delta t \to 0} \frac{\left\{ \cancel{\left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)} + \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{v}}{\partial q}\delta t\right) + \left(\frac{\partial \vec{v}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)\delta t + \left(\frac{\partial \vec{v}}{\partial p} \times \frac{\partial \vec{v}}{\partial q}\right)\delta t^2 - \cancel{\left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)} \right\} \cdot \vec{n}\, dp\, dq}{\left\{\left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)\right\} \cdot \vec{n}\, dp\, dq\, \delta t}$$

$$= \lim_{\delta t \to 0} \frac{\left\{ \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{v}}{\partial q}\right)\cancel{\delta t} + \left(\frac{\partial \vec{v}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)\cancel{\delta t} + \left(\frac{\partial \vec{v}}{\partial p} \times \frac{\partial \vec{v}}{\partial q}\right)\delta t^{\cancel{2}} \right\} \cdot \vec{n}\, \cancel{dp\, dq}}{\left\{\left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right)\right\} \cdot \vec{n}\, \cancel{dp\, dq}\, \cancel{\delta t}}$$

$$
= \lim_{\delta t \to 0} \frac{\left\{ \left(\quad \right) + \left(\quad \right) + \cancel{\left(\frac{\partial \vec{v}}{\partial p} \times \frac{\partial \vec{v}}{\partial q} \right) \delta t} \right\} \cdot \vec{n}}{\left\{ \quad \right\} \cdot \vec{n}}
$$

$$
\Pi = \frac{\left\{ \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{v}}{\partial q} \right) + \left(\frac{\partial \vec{v}}{\partial p} \times \frac{\partial \vec{r}}{\partial q} \right) \right\} \cdot \vec{n}}{\left\{ \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{r}}{\partial q} \right) \right\} \cdot \vec{n}} \qquad (127)
$$

$$\vec{v} = (\vec{v}\cdot\vec{n})\vec{n} + \vec{v}_t \qquad (128)$$

Normal Tangential

Substituind in numeratorul lui (127)

$$\left\{\left(\frac{\partial \vec{v}_t}{\partial p}\times\frac{\partial \vec{r}}{\partial q}\right)+\left(\frac{\partial \vec{r}}{\partial p}\times\frac{\partial \vec{v}_t}{\partial q}\right)\right\}\cdot\vec{n}\ +$$

$$\left\{\underbrace{\left(\frac{\partial(\vec{v}\cdot\vec{n})\vec{n}}{\partial p}\times\frac{\partial \vec{r}}{\partial q}\right)}_{(A)}+\underbrace{\left(\frac{\partial \vec{r}}{\partial p}\times\frac{\partial(\vec{v}\cdot\vec{n})\vec{n}}{\partial q}\right)}_{(B)}\right\}\cdot\vec{n}$$

$(*)$

$$A = (\vec{v}\cdot\vec{n})\left(\frac{\partial \vec{n}}{\partial p}\times\frac{\partial \vec{r}}{\partial q}\right)\cdot\vec{n} + \frac{\partial(\vec{v}\cdot\vec{n})}{\partial p}\underbrace{\left(\vec{n}\times\frac{\partial \vec{r}}{\partial q}\right)\cdot\vec{n}}_{=0}$$

identidade $(\vec{n}\times\vec{a})\cdot\vec{n} = 0$

$$B = (\vec{v}\cdot\vec{n})\left(\frac{\partial\vec{r}}{\partial p}\times\frac{\partial\vec{n}}{\partial q}\right)\cdot\vec{n} + \underbrace{\frac{\partial(\vec{v}\cdot\vec{n})}{\partial q}\left(\frac{\partial\vec{r}}{\partial p}\times\frac{\partial\vec{n}}{\partial p}\right)\cdot\vec{n}}_{=0}$$

enfin $\left\{ A + B \right\}\cdot\vec{n} =$

$$= (\vec{v}\cdot\vec{n})\left\{\left(\frac{\partial\vec{n}}{\partial p}\times\frac{\partial\vec{r}}{\partial q}\right) + \left(\frac{\partial\vec{r}}{\partial p}\times\frac{\partial\vec{n}}{\partial q}\right)\right\}\cdot\vec{n}$$

e o numerador (*) torna-se:

$$\left\{\left(\frac{\partial \vec{\sigma}_t}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right) + \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{\sigma}_t}{\partial q}\right)\right\} \cdot \vec{n} +$$

$$(\vec{\sigma} \cdot \vec{n}) \left\{\left(\frac{\partial \vec{n}}{\partial p} \times \frac{\partial \vec{r}}{\partial q}\right) + \left(\frac{\partial \vec{r}}{\partial p} \times \frac{\partial \vec{n}}{\partial q}\right)\right\} \cdot \vec{n}$$

(129)

fazendo os fatores de escala unitários

$(r, p, q) = 1.0 \quad (??)$

$$\frac{\partial \vec{r}}{\partial p} = \vec{e}_p \quad , \quad \frac{\partial \vec{r}}{\partial q} = \vec{e}_q \, , \; \vec{e}_p \times \vec{e}_q = \vec{u}$$

o denominador de (127) torna-se:

$$\left\{\left(\frac{\partial\vec{r}}{\partial p}\times\frac{\partial\vec{r}}{\partial q}\right)\right\}\circ\vec{n} = \underbrace{\left\{\vec{e}_p\times\vec{e}_q\right\}}_{=\vec{n}}\circ\vec{n} = 1.0$$

enter a sketch: (127)

$$\Gamma = \left\{\left(\frac{\partial\vec{v}_t}{\partial p}\times\underbrace{\frac{\partial\vec{r}}{\partial q}}_{=\vec{e}_q}\right)+\left(\underbrace{\frac{\partial\vec{r}}{\partial p}}_{=\vec{e}_p}\times\frac{\partial\vec{v}_t}{\partial q}\right)\right\}\circ\vec{n}$$

$$+(\vec{v}\cdot\vec{n})\left\{\left(\frac{\partial\vec{n}}{\partial p}\times\underbrace{\frac{\partial\vec{r}}{\partial q}}_{=\vec{e}_q}\right)+\left(\underbrace{\frac{\partial\vec{r}}{\partial p}}_{=\vec{e}_p}\times\frac{\partial\vec{n}}{\partial q}\right)\right\}\cdot\vec{n}$$

usando a identidade

$$\vec{a}\cdot(\vec{b}\times\vec{c}) = (\vec{a}\times\vec{b})\cdot\vec{c} = \det$$

cyclic law for scalar triple products

$$\Gamma = \left\{ \left(\frac{\partial \vec{v}_t}{\partial p} \times \vec{e}_q \right) + \left(\vec{e}_p \times \frac{\partial \vec{v}_t}{\partial q} \right) \right\} \cdot \vec{n}$$

C D

$$+ (\vec{v}\cdot\vec{n}) \left\{ \left(\frac{\partial \vec{n}}{\partial p} \times \vec{e}_q \right) + \left(\vec{e}_p \times \frac{\partial \vec{n}}{\partial q} \right) \right\} \cdot \vec{n}$$

E F

(c): $\left(\frac{\partial \vec{v_t}}{\partial p} \times \vec{e_q}\right)\cdot \vec{n} = \det \begin{vmatrix} \frac{\partial v_t}{\partial p} & 0 & 0 \\ 0 & e_q & 0 \\ 0 & 0 & 1 \end{vmatrix}$

$$= e_q \frac{\partial v_t}{\partial p} = \vec{e_p} \cdot \frac{\partial \vec{v_t}}{\partial p}$$

aqui não é índice repetido

D $\left(\vec{e_p} \times \frac{\partial \vec{v_t}}{\partial q}\right) \cdot \vec{u} = \det \begin{vmatrix} e_p & 0 & 0 \\ 0 & \frac{\partial v_t}{\partial q} & 0 \\ 0 & 0 & 1 \end{vmatrix}$

$$= e_p \frac{\partial v_t}{\partial q} = \vec{e_q} \cdot \frac{\partial \vec{v_t}}{\partial q}$$

Ⓔ: $(\vec{v}\cdot\vec{n})\left(\dfrac{\partial\vec{u}}{\partial p}\times\vec{e}_q\right)\cdot\vec{u}$

$$= (\vec{v}\cdot\vec{n})\left(\frac{\partial u}{\partial p}e_q\right) = (\vec{v}\cdot\vec{n})\left(\vec{e}_p\cdot\frac{\partial\vec{u}}{\partial p}\right)$$

Ⓕ: $(\vec{v}\cdot\vec{u})\left(\vec{e}_p\times\dfrac{\partial\vec{u}}{\partial q}\right) = (\vec{v}\cdot\vec{u})\left(\vec{e}_q\cdot\dfrac{\partial\vec{u}}{\partial q}\right)$

então

$$\Gamma = \left(\vec{e}_\varphi \cdot \frac{\partial \vec{v}_t}{\partial \varphi} + \vec{e}_\eta \cdot \frac{\partial \vec{v}_t}{\partial \eta} \right) + (\vec{v} \cdot \vec{n}) \left(\vec{e}_\varphi \cdot \frac{\partial \vec{n}}{\partial \varphi} + \vec{e}_\eta \cdot \frac{\partial \vec{n}}{\partial \eta} \right) \tag{131}$$

ou

$$\Gamma = \nabla_t \cdot \vec{v}_t + (\vec{v} \cdot \vec{n})(\nabla_t \cdot \vec{n}) \tag{132}$$

Se a velocidade do fluido na chama é $\vec{V}$, a componente tangencial é:

$$\vec{v}_t = \vec{n} \times (\vec{V} \times \vec{n})$$

e o 1º termo na eq (132) é

$$\nabla_t \cdot [\vec{n} \times (\vec{V} \times \vec{n})] \qquad (134)$$

usando a identidade:

$$\nabla \cdot (A \times B) = B \cdot (\nabla \times A) - A \cdot (\nabla \times B)$$

e então,

$$\nabla \cdot (A \times B) = B \cdot (\nabla \times A) - A \cdot (\nabla \times B)$$

$$\nabla \cdot \left[\vec{u} \times (\vec{\nabla} \times \vec{u})\right] = \left(\vec{\nabla} \times \vec{u}\right) \cdot \underbrace{\left(\vec{\nabla} \times \vec{u}\right)} - \vec{u} \cdot \left(\vec{\nabla} \times \left(\vec{\nabla} \times \vec{u}\right)\right)$$

$$\vec{\nabla} \times \vec{u} = \varepsilon_{ijk} \frac{\partial u_k}{\partial x_j}$$

somente $\dfrac{\partial x_j}{\partial x_j} \neq 0$

mas $\varepsilon_{ijj} = 0 \Longrightarrow \left(\vec{\nabla} \times \vec{u}\right) \overset{!}{=} 0$

Finally:

$$\Pi = -\vec{n} \cdot \left(\nabla \times \left(\vec{V} \times \vec{n}\right)\right) + \left(\vec{v} \cdot \vec{n}\right)\left(\nabla \cdot \vec{n}\right) \qquad (138)$$

Velocidade do fluido através da superfície da chama

"displacement speed" with respect to the Lab referential

Este operador ∇ é em relação ao sistema de coordenadas local (Flame Surface) ??

POINSOT, pg 63 eq (2.79)

$$k = -\vec{n}\vec{n} : \nabla \vec{w} + \nabla \cdot \vec{w} \qquad (2.79)$$

velocity of the flame surface with respect to the Lab. reference

$$k = (\delta_{ij} - n_i n_j) \frac{\partial w_i}{\partial x_j} \qquad (2.80)$$

$$\vec{W} = \vec{u} + S_d \vec{n}$$

Surface (flame) Displacement speed, relative to the flow velocity (as the S_L is)

Unburned gas flow velocity crossing the surface

relative to the Lab.

EQUIVALÊNCIA (138) $\Longleftrightarrow$ (2.80)

by PSH

SIMON	POINSOT
σ	w
v	u

$$\Gamma = \vec{n} \cdot (\vec{\nabla} \times (\vec{v} \times \vec{n})) + (\vec{\sigma} \cdot \vec{n})(\vec{\nabla} \cdot \vec{n}) \quad (138)$$

$$\Gamma = \vec{n} \cdot (\vec{\nabla} \times \underbrace{(\vec{u} \times \vec{n})}_{A}) + (\vec{w} \cdot \vec{n})(\vec{\nabla} \cdot \vec{n})$$

$$A = \vec{u} \times \vec{n} = (\vec{w} - s d \vec{n}) \times \vec{n} = \vec{w} \times \vec{n} - s d \underbrace{\cancel{\vec{n} \times \vec{n}}}_{=0}$$

$$= \vec{w} \times \vec{n}$$

$$\Gamma = -\vec{n} \cdot \underbrace{\left(\vec{\nabla} \times (\vec{w} \times \vec{n})\right)}_{B} + (\vec{w} \cdot \vec{n})(\vec{\nabla} \cdot \vec{n})$$

Sobre o vetor <u>unitário</u> $\vec{n}$:

$$\|\vec{n}\| = 1.0$$

Produto escalar de dois vetores $\vec{a}, \vec{b}$

$$\vec{a} = (a_i) = (a_1, a_2, a_3)$$

$$\vec{b} = (b_j) = (b_1, b_2, b_3)$$

$$\vec{a} \cdot \vec{b} = \|\vec{a}\| \|\vec{b}\| \cos\theta \quad \text{ou}$$

$$= a_1 b_1 + a_2 b_2 + a_3 b_3 = a_i b_i$$

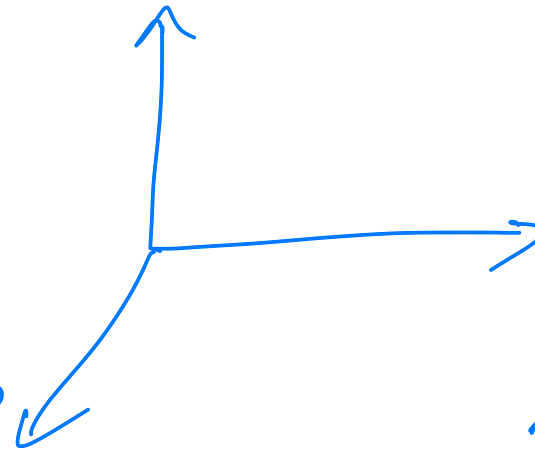
$$\vec{a} \cdot \vec{a} = \|\vec{a}\|^2 = a_1 a_1 + a_2 a_2 + a_3 a_3$$
$$= a_1^2 + a_2^2 + a_3^2$$

Se $\vec{a} = \vec{n} \Rightarrow$ unitário,

$$\vec{n} \cdot \vec{n} = \|\vec{n}\|^2 = 1 = n_1 n_1 + n_2 n_2 + n_3 n_3 = n_i n_i$$

$\therefore$ $\boxed{n_i n_i = 1}$ $\rightarrow$ Vai ser muito útil a seguir

se for numa base ortonormal, $\vec{e}_1, \vec{e}_2, \vec{e}_3$
com $e_i = 1.0$



$$\|\vec{e}_1\|^2 = \vec{e}_1 \cdot \vec{e}_1 = 1.0$$

$$\|\vec{e}_2\|^2 = \|\vec{e}_3\|^2 = 1.0 = \|\vec{e}_1\| = \|\vec{e}_2\| = \|\vec{e}_3\|$$

ou

$$\vec{e}_i \cdot \vec{e}_j = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

$$u_i = \vec{e}_i \cdot \vec{u}$$

$\downarrow$

scalar component of $\vec{u}$ in direction i

& $i = j$, $\vec{e}_i \cdot \vec{e}_i = e_i e_i = \delta_{ii} = 1 + 1 + 1 = \underline{\underline{3}}$

Usando a identidade (Roddy pg 126)

$$\vec{\nabla} \times (\vec{A} \times \vec{B}) = (\vec{B} \cdot \vec{\nabla})\vec{A} - (\vec{A} \cdot \vec{\nabla})\vec{B} + \vec{A}(\vec{\nabla} \cdot \vec{B}) - \vec{B}(\vec{\nabla} \cdot \vec{A})$$

Ⓑ: $$\vec{\nabla} \times (\vec{w} \times \vec{n}) = (\vec{n} \cdot \vec{\nabla})\vec{w} - (\vec{w} \cdot \vec{\nabla})\vec{n} + \vec{w}(\vec{\nabla} \cdot \vec{n}) - \vec{n}(\vec{\nabla} \cdot \vec{w})$$

então:

$$\Gamma = -\vec{n} \cdot \left[(\vec{n} \cdot \vec{\nabla})\vec{w} - (\vec{w} \cdot \vec{\nabla})\vec{n} + \vec{w}(\vec{\nabla} \cdot \vec{n}) - \vec{n}(\vec{\nabla} \cdot \vec{w})\right] + (\vec{w} \cdot \vec{n})(\vec{\nabla} \cdot \vec{n})$$

$$\Gamma = -(\vec{n} \cdot \vec{\nabla})(\vec{w} \cdot \vec{n}) + \underbrace{(\vec{w} \cdot \vec{\nabla})\overset{=1.0}{(\vec{n} \cdot \vec{n})}}_{=0} \underbrace{- (\vec{\nabla} \cdot \vec{n})(\vec{w} \cdot \vec{n}) + (\vec{\nabla} \cdot \vec{w})\overset{=1.0}{(\vec{n} \cdot \vec{n})} + (\vec{\nabla} \cdot \vec{n})(\vec{w} \cdot \vec{n})}_{=0}$$

$$\Gamma = -(\vec{n} \cdot \vec{\nabla})(\vec{w} \cdot \vec{n}) + \vec{\nabla} \cdot \vec{w}$$

Como o produto escalar é comutativo $(\vec{w}\cdot\vec{n}) = (\vec{n}\cdot\vec{w})$,

$$\Gamma = -(\vec{n}\cdot\vec{\nabla})(\vec{n}\cdot\vec{w}) + \vec{\nabla}\cdot\vec{w}$$

usando "double dot product" (Roddy, pg 55):

$$\vec{\vec{M}} : \vec{\vec{N}} = (\vec{A}\cdot\vec{C})(\vec{B}\cdot\vec{D})$$

$\vec{\vec{M}} = \vec{A}\vec{B}$ e $\vec{\vec{N}} = \vec{C}\vec{D}$ ← Diádico

$\vec{A} = \vec{n}$ $\quad$ $\vec{B} = \vec{n}$ $\quad$ $\vec{C} = \vec{\nabla}$ $\quad$ $\vec{D} = \vec{w}$

$\vec{\vec{M}} = \vec{n}\vec{n}$ $\quad$ $\vec{\vec{N}} = \vec{\nabla}\vec{w}$

$$\Gamma = -\vec{\vec{M}} : \vec{\vec{N}} + \vec{\nabla}\cdot\vec{w}$$

$$\boxed{\Gamma = -\vec{n}\vec{n} : \vec{\nabla}\vec{w} + \vec{\nabla}\cdot\vec{w}}$$

POINSOT EQ. (2.79)

SIMON EQ (138)

= cqd

$$K = -\vec{\mu}\vec{\mu} : \nabla\left(\vec{\mu} + s_d\vec{n}\right) + \nabla\cdot\left(\vec{\mu} + s_d\vec{n}\right)$$

$$= -\vec{\mu}\vec{\mu} : \nabla\vec{\mu} + \nabla\cdot\vec{\mu} - \vec{\mu}\vec{\mu} : \nabla\left(s_d\vec{\mu}\right) + \nabla\cdot\left(s_d\vec{n}\right)$$

$$= \underbrace{\left(\delta_{ij} - \mu_i\mu_j\right)\frac{\partial\mu_i}{\partial x_j}}_{A} + \underbrace{\left(\delta_{ij} - n_i n_j\right)\frac{\partial\left(s_d n_i\right)}{\partial x_j}}_{B}$$

(B): $(\delta_{ij} - n_i n_j)\dfrac{\partial(S_d n_i)}{\partial x_j} = \dfrac{\partial S_d n_i}{\partial x_i} - n_i n_j \dfrac{\partial(S_d n_i)}{\partial x_j}$

$$= S_d \frac{\partial n_i}{\partial x_i} + n_i \frac{\partial S_d}{\partial x_i} - \underbrace{n_i n_j \frac{\partial(S_d n_i)}{\partial x_j}}$$

$$n_i n_j \frac{\partial S_d n_i}{\partial x_j} = n_j \frac{\partial(S_d \overbrace{n_i n_i}^{=1.0})}{\partial x_j} - n_j S_d n_i \frac{\partial n_i}{\partial x_j}$$

$$= n_j \frac{\partial S_d}{\partial x_j} - n_j S_d \underbrace{\left[\frac{1}{2}\frac{\partial \overbrace{n_i n_i}^{=1.0}}{\partial x_j}\right]}_{=0}$$

$$u_i n_j \frac{\partial S_d n_i}{\partial x_j} = u_j \frac{\partial S_d}{\partial x_j}$$

então:

$$\text{(B)} : S_d \frac{\partial n_i}{\partial x_i} + \cancel{n_i \frac{\partial S_d}{\partial x_i}} - \cancel{u_j \frac{\partial S_d}{\partial x_j}}$$

finalmente:

$$K = \text{(A)} + \text{(B)}$$

$$\boxed{K = (\delta_{ij} - n_i n_j) \frac{\partial u_i}{\partial x_j} + S_d \frac{\partial n_i}{\partial x_i}}$$

(eq. 2.84)
POINSOT

BALANCE EQUATION FOR PREMIXED LAMINAR FLAME AREA

KUO, 2º Ed., ITEM 4.2

FLAME SURFACE DENSITY (Σ)

$$\Sigma \equiv \frac{\delta A}{\delta V} \qquad (5\text{-}109)$$

From Reynolds Transport Theorem for a moving volume ($V(t)$):

$$\frac{d}{dt}\int_{V(t)} f\, dV = \int_{V(t)} \frac{\partial f}{\partial t}\, dV + \int_{S(t)} f\, \vec{w}\cdot\vec{n}\, dA \qquad (5\text{-}110)$$

$\vec{w}$ — Displacement speed of the (flame) surface

for $f = 1$,

$$\frac{d}{dt}\int_{V(t)} dV = \int_{V(t)} 0 + \int_{S(t)} \vec{w}\cdot\vec{n}\, dA$$

Divergence Theorem

$$\int_{V(t)} \boldsymbol{\nabla}\cdot\vec{w}\, dV$$

entaõ:

$$\frac{d}{dt}\int_{V(t)} dV = \int_{V(t)} \nabla\cdot\vec{w}\, dV \qquad (5\text{-}111)$$

for a Volume element: $\frac{1}{\delta V}\frac{d(\delta V)}{dt} = \nabla\cdot\vec{w}$ (5-112)

we have already,

$$K \equiv \frac{1}{\delta A}\frac{d(\delta A)}{dt} = (\delta_{ij} - n_i n_j)\frac{\partial u_i}{\partial x_j} + S_d \frac{\partial n_i}{\partial x_i} \qquad (2\text{-}84)$$

POINOT

or

$$K = \frac{1}{\delta A}\frac{d(\delta A)}{dt} = \frac{\partial u_i}{\partial x_i} - n_i n_j \frac{\partial u_i}{\partial x_j} + S_d \frac{\partial n_i}{\partial x_i}$$

$$= -\frac{1}{\rho}\frac{\partial \rho}{\partial t} \quad \text{(CONTINUITY)}$$

So

$$K = \frac{1}{\delta A}\frac{d(\delta A)}{dt} = -n_i n_j \frac{\partial u_i}{\partial x_j} - \frac{1}{\rho}\frac{\partial \rho}{\partial t} + S_d \nabla \cdot \vec{n} \quad (*)$$

Associate with strain rate Tensor

Dilatation

Flame curvature

Back to (5-109)

$$\frac{d\Sigma}{dt} = \frac{d}{dt}\left(\frac{\delta A}{\delta V}\right) = \frac{1}{\delta V}\frac{\partial \delta A}{\partial t} - \delta A\, \delta V^{-2} \frac{d}{dt}(\delta V)$$

$$\frac{1}{\Sigma}\frac{d\Sigma}{dt} = \frac{\cancel{\delta V}}{\delta A} \cdot \frac{1}{\cancel{\delta V}} \frac{d}{dt}\delta A - \frac{\cancel{\delta V}}{\cancel{\delta A}} \cancel{\delta A}\, \delta V^{-\cancel{2}} \frac{d}{dt}\delta V$$

$$= \frac{1}{A}\frac{dA}{dt} - \frac{1}{V}\frac{dV}{dt}$$

(*) (5-112)

$$\frac{1}{\Sigma}\frac{d\Sigma}{dt} = -n_i n_j \frac{\partial u_i}{\partial x_j} + \cancel{\frac{\partial u_i}{\partial x_i}} + \cancel{S_d\,\nabla\cdot\vec{n}} - \nabla\cdot\vec{w}$$

$$-\nabla(\vec{u} + S_d\,\vec{n}) = -\cancel{\frac{\partial u_i}{\partial x_i}} - \cancel{S_d\frac{\partial n_i}{\partial x_i}} - n_i\frac{\partial S_d}{\partial x_i}$$

$$\frac{1}{\Sigma}\frac{d\Sigma}{dt} = -n_i n_j \frac{\partial u_i}{\partial x_j} - n_i\frac{\partial S_d}{\partial x_i}$$

ou

$$\times\Sigma \qquad = \left(-\vec{n}\vec{n} : \nabla\vec{u} - \vec{n}\cdot\nabla S_d\right)\times\Sigma \qquad (5-113)$$

$$\frac{d\Sigma}{dt} = -(\vec{n}\vec{n}:\nabla\vec{u})\Sigma - (\vec{n}\cdot\nabla S_d)\Sigma$$

$$\frac{d\Sigma}{dt} = \frac{\partial\Sigma}{\partial t} + \vec{w}\cdot\nabla\Sigma = \frac{\partial\Sigma}{\partial t} + (\vec{u} + S_d\vec{n})\cdot\nabla\Sigma$$

derivada material

então:

$$\frac{\partial\Sigma}{\partial t} + \underbrace{\vec{u}\cdot\nabla\Sigma}_{\nabla\cdot(\vec{u}\Sigma) - \Sigma\nabla\cdot\vec{u}} + S_d\vec{n}\cdot\nabla\Sigma = -(\vec{n}\vec{n}:\nabla\vec{u})\Sigma - (\vec{n}\cdot\nabla S_d)\Sigma$$

$$\frac{\partial \Sigma}{\partial t} + \nabla\cdot(\vec{u}\,\Sigma) = -(\vec{n}\vec{n}:\nabla\vec{u} - \nabla\cdot\vec{u})\,\Sigma \underbrace{- (\vec{n}\cdot\nabla S_d)\,\Sigma - S_d\,\vec{n}\cdot\nabla\Sigma}_{= -\vec{n}\cdot\nabla S_d \Sigma}$$

So :

$$\boxed{\frac{\partial \Sigma}{\partial t} + \nabla\cdot(\vec{u}\,\Sigma) = -(\vec{n}\vec{n}:\nabla\vec{u} - \nabla\cdot\vec{u})\,\Sigma - \vec{n}\cdot\nabla S_d \Sigma} \quad (5\text{-}114)$$

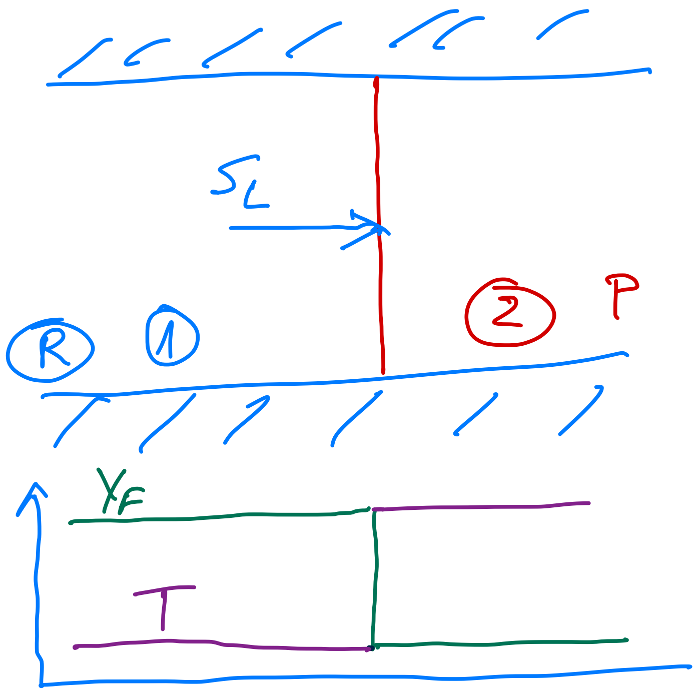
KUO

$$= \nabla\cdot(S_d \Sigma \vec{n}) - S_d \Sigma\, \nabla\cdot\vec{n}$$

So :

$$\underset{1}{\frac{\partial \Sigma}{\partial t}} + \underset{2}{\nabla \cdot (\vec{u}\,\Sigma)} + \underset{3}{\nabla \cdot (S_d \Sigma \vec{n})} = \underset{4}{-(\vec{n}\vec{n} : \nabla \vec{u} - \nabla \cdot \vec{u})\Sigma} + \underset{5}{S_d \Sigma \nabla \cdot \vec{n}}$$

PROGRESS VARIABLE PREMIXED FLAME



ONE STEP CHEMISTRY

$$R \xrightarrow{\nearrow Q} P$$

$$\dot{\omega} = B \rho Y_F \exp\left(T_a / T\right)$$

$$\dot{\omega}_F = -\dot{\omega}$$

CONSERVATION EQ. ON THE FLAME SURFACE

1D, STEADY STATE, ADIABATIC. REFERENTIAL

MASS: $$\rho u = cte = \rho_1 u_1 \equiv \rho_1 S_L \qquad (2.21)$$

MASS FRACTION: $$\rho_1 S_L \frac{dY_F}{dx} = \frac{d}{dx}\left(\rho D \frac{dY_F}{dx}\right) - \dot{\omega} \qquad (2.22)$$

ENERGY: $$\rho_1 c_p S_L \frac{dT}{dx} = \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) + Q\dot{\omega} \qquad (2.23)$$

Integrating from $x = -\infty$ to $x = +\infty$:

$$2.22 \longrightarrow \rho_1 S_L Y_F \Big|_{Y_F^1}^{Y_F^2 = 0} = -\int_{-\infty}^{+\infty} \dot{\omega}\, dx$$

$$-\rho_1 S_L Y_F^1 = -\int_{-\infty}^{+\infty} \dot{\omega}\, dx \qquad (2.24)$$

$$2.23 \longrightarrow \rho_1 c_p S_L (T_2 - T_1) = \lambda \underbrace{\frac{dT}{dx}}_{=0} \Big|_{x = -\infty}^{x_f = 0} + \int_{-\infty}^{+\infty} Q \dot{\omega}\, dx$$

$$\rho_1 c_p S_L (T_2 - T_1) = Q \int \dot{\omega}\, dx \qquad (2.25)$$

$$\frac{(2.25)}{(2.24)} \Rightarrow \frac{\rho_1 c_p S_L (T_2 - T_1)}{\rho_1 S_L Y_F'} = Q$$

$$c_p (T_2 - T_1) = Q Y_F'$$

$$T_2 = T_1 + Q Y_F' / c_p \qquad (2.28)$$

REDUCED VARIABLES

$$Y \equiv Y_F / Y_F'$$

$$\Theta \equiv \frac{T - T_1}{T_2 - T_1} = \frac{T - T_1}{Q Y_F' / c_p} = \frac{c_p (T - T_1)}{Q Y_F'}$$

$x = -\infty$ | $x = +\infty$
$\theta = 0$ | $\theta = 1$
$y = 1$ | $y = 0$

$$\frac{dY_F}{dx} = Y_F' \frac{dy}{dx} \quad ; \quad \frac{d}{dx}\left(\rho D\, Y_F' \frac{dy}{dx}\right)$$

$$\frac{dT}{dx} = (T_2 - T_1)\frac{d\theta}{dx} \quad ; \quad \frac{d}{dx}\left(\lambda (T_2 - T_1)\frac{d\theta}{dx}\right)$$

entaõ 2.22:

$$\rho_1 S_L \cancel{Y_F'} \frac{dY}{dx} = \cancel{Y_F'} \frac{d}{dx}\left(\rho D \frac{dY}{dx}\right) - \dot{\omega} / Y_F'$$

2.23

(2.32)

$$\rho_1 c_p S_L (T_2 - T_1) \frac{d\theta}{dx} = (T_2 - T_1) \frac{d}{dx}\left(\lambda \frac{d\theta}{dx}\right) + Q\dot{\omega}$$

$$\rho_1 S_L \frac{d\theta}{dx} = \frac{\cancel{(T_2 - T_1)}}{c_p \cancel{(T_2 - T_1)}} \frac{d}{dx}\left(\lambda \frac{d\theta}{dx}\right) + \frac{Q\dot{\omega}}{c_p (T_2 - T_1)}$$

$= 1/Y_F'$

using $Le \equiv \dfrac{\lambda}{\rho c_p D} = 1$

$$\rho_1 S_L \frac{d\theta}{dx} = \frac{d}{dx}\left(\rho D \frac{d\theta}{dx}\right) + \frac{\dot{\omega}}{Y_F'} \qquad (2.33)$$

adding (2.32) + (2.33):

$$\rho_1 S_L \frac{d}{dx}(Y+\theta) = \frac{d}{dx}\left(\rho D \frac{d}{dx}(Y+\theta)\right) - \cancel{\frac{\dot{\omega}}{Y_F'}} + \cancel{\frac{\dot{\omega}}{Y_F'}}$$

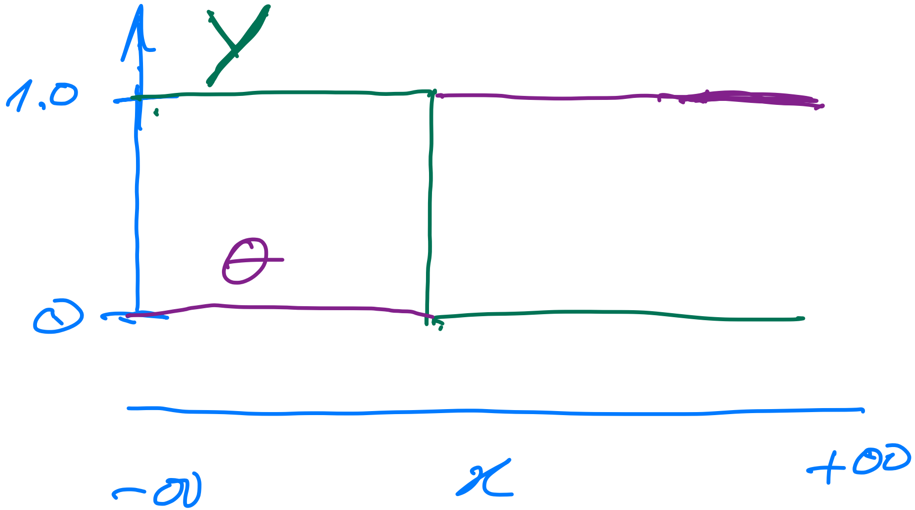
→ CONSERVATIVE TRANSP. EQ!

→ $(Y+\theta)$ IS A CONSERVED SCALAR!

→ em $x = -\infty$ → $Y+\theta = 1$

" $x = +\infty$ → $Y+\theta = 1$

→ ÚNICA SOLUÇÃO $Y+\theta = 1$ (2.35)



θ : Progress Variable (c)

To describe the premixed flame structure it is enough to solve $\boxed{(2.33)}$ and evaluate $\boxed{Y = \theta - 1}$

TURBULENT PREMIXED FLAMES (POINSOT)

RANS: $\phi(\vec{x},t) = \tilde{\phi}(\vec{x}) + \phi''(\vec{x},t)$ ⟵⟶ FAVRE DECOMPOSITION

CONTINUITY : $$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial x_i} = 0 \qquad (5.38)$$

MOMENTUM : $$\frac{\partial \bar{\rho}\tilde{u}_j}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{u}_j) + \frac{\partial \bar{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left(\bar{\tau}_{ij} - \bar{\rho}\widetilde{u_i''u_j''}\right) \qquad (5.39)$$

PROGRESS VARIABLE θ

$$\frac{\partial \bar{\rho}\tilde{\theta}}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{\theta}\tilde{u}_i) = \frac{\partial}{\partial x_i}\left(\bar{\rho}D\frac{\partial \tilde{\theta}}{\partial x_i} - \bar{\rho}\widetilde{u_i''\theta''}\right) + \bar{\dot{\omega}}_\theta \qquad (5.40)$$

- Turbulent fluxes $\widetilde{\bar{\rho} u_i'' u_j''}$ and $\widetilde{\bar{\rho} u_i'' \theta''}$ are modeled are treated using Boussinesq assumption (ν_t, Pr_θ)

- Chemical average source term

$\overline{\dot{\omega}_\theta} \longrightarrow$ CFM

$\longrightarrow$ FLAME SURFACE DENSITY MODEL

$\longrightarrow$ THIN FLAME (FLAMELET) APPROACH

$$\boxed{\overline{\dot{\omega}_\theta} = \rho_0 \langle S_c \rangle_s \Sigma}$$

5-65

ρ_0 : fresh gas density

$\langle S_c \rangle_s$: average flame consumption speed along the iso-surface "s"

$$\frac{kg}{m^3} \times \frac{\cancel{m}}{s} \times \frac{\cancel{m^2}}{\cancel{m^3}}$$

FLAME SURFACE DENSITY MODEL

$$\overline{\dot{w}_\theta} = \rho_0 \langle S_c \rangle_s \Sigma$$

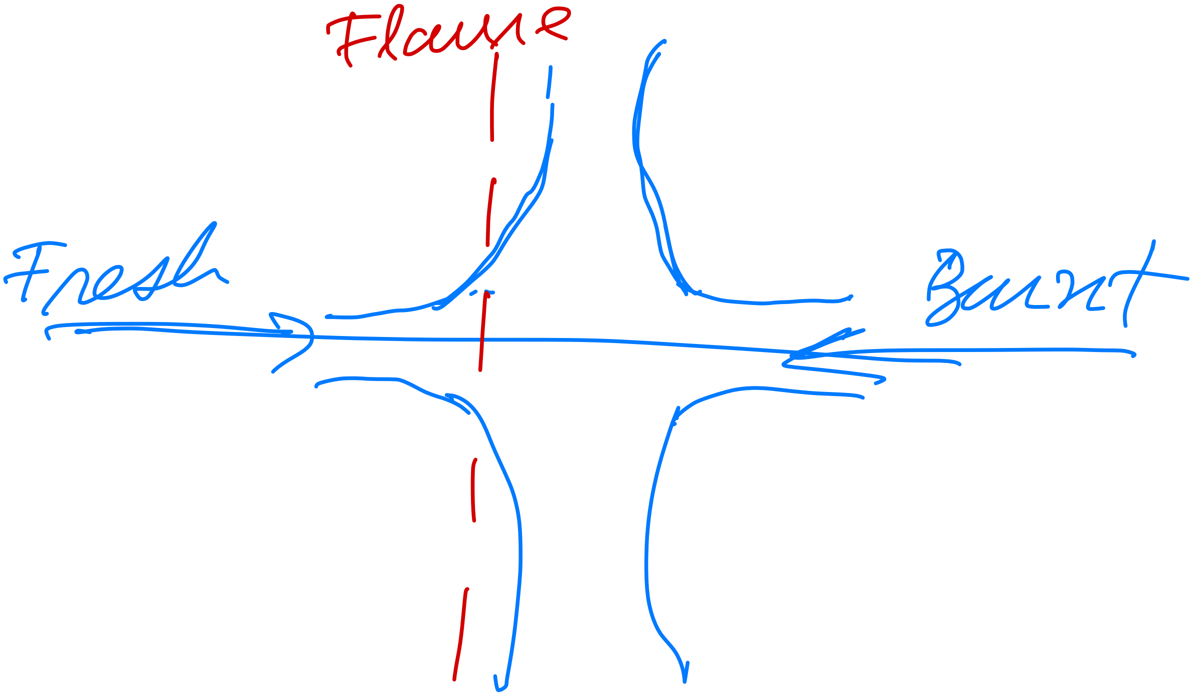
Fresh gas density

average flame consumption speed along the surface

FSD

- LAMINAR STAGNATION POINT FLAME

↳ FLAMELET LIBRARY



$$\langle S_c \rangle_s = \int_0^{+\infty} S_c(k)\, p(k)\, dk \qquad (J.66)$$

mean laminar consumption rate per unit flame surface

sketch values

probability of find the value k

- I_0 → stretch factor to link $\langle S_c \rangle_s$ to S_L^0

→ unstretched laminar flame speed

$$\langle S_c \rangle_s = I_0 S_L^0 \qquad (5.67)$$

and

$$I_0 = \frac{1}{S_L^0} \int_0^{+\infty} S_c(\kappa)\, p(\kappa)\, d\kappa$$

$$P(k) = \delta(k - \bar{k})$$

mean local stretch rate

with (5.66):

$$\langle S_c \rangle_S \approx S_c(\bar{k}) \quad \text{and}$$

$$I_0 \approx \frac{S_c(\bar{k})}{S_L^0} \qquad (5.71)$$

DNS results show $I_0 \approx 1$

$$\Downarrow$$

$$\boxed{\langle S_c \rangle_s = S_L^0}$$

FSD Σ

p/ um ponto sobre a superfície $\theta = \theta_f$,

$$\vec{n} = -\frac{\nabla\theta}{|\nabla\theta|} \qquad (2.96)$$

← The surface density of the iso-temperature θ^* surface is:

$$\Sigma = \overline{|\nabla\theta|\,\delta(\theta - \theta^*)} = \left(\overline{|\nabla\theta|\Big|_{\theta=\theta^*}}\right) P(\theta^*) \qquad (5.77)$$

Surface average operator

$$\langle Q \rangle_s = \frac{\overline{Q\, |\nabla\theta|\, \delta(\theta - \theta^*)}}{\overline{|\nabla\theta|\, \delta(\theta - \theta^*)}} \qquad (5.75)$$

aplicado aos termos da eq 5-114 e seguinte:

① $\rightarrow \dfrac{d\Sigma}{dt}$

$$\langle u_i \rangle_s = \tilde{u}_i + \langle u_i'' \rangle_s$$

② $\nabla \cdot (\vec{u}\Sigma) = \nabla \cdot (\tilde{u}_i \Sigma + \nabla \cdot \langle u_i'' \rangle_s \Sigma$

③ $\nabla \cdot (S_d \Sigma \vec{n}) = \nabla \cdot (\langle S_d \vec{n} \rangle_s \Sigma)$

④ $-(\vec{n}\vec{n} : \nabla \vec{u} - \nabla \vec{u})\Sigma = \left\langle (\delta_{ij} - n_i n_j) \dfrac{\partial u_i}{\partial x_j} \right\rangle_s \Sigma$

⑤ $S_d \Sigma \nabla \cdot \vec{n} = \langle S_d \nabla \cdot \vec{n} \rangle_s \Sigma$

② : $\nabla\cdot(\vec{\tilde{u}}\,\Sigma) + \nabla\cdot(\langle \vec{u}' \rangle_s \Sigma)$

④ : $\langle (\delta_{ij} - n_i n_j) \frac{\partial u_i}{\partial x_j} \rangle_s \Sigma =$

$$\Big(\underbrace{(\delta_{ij} - \langle n_i n_j \rangle_s) \frac{\partial \tilde{u}_i}{\partial x_j}}_{k_m} + \underbrace{\langle (\delta_{ij} - n_i n_j) \frac{\partial u_i'}{\partial x_j} \rangle_s}_{k_t} \Big) \Sigma$$

k_m ↔ mean flow

k_t └ turbulent contribution

FSD Eq.

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_i \Sigma}{\partial x_i} = -\frac{\partial}{\partial x_i}\underbrace{\left(\langle u_i'' \rangle_s \Sigma \right)}_{= \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_c} \frac{\partial \Sigma}{\partial x_i} \right)} + \kappa_m \Sigma + \kappa_t \Sigma + \left\langle s_d \frac{\partial n_i}{\partial x_i} \right\rangle_s \Sigma$$

So:

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial \tilde{u}_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\nu_t}{\sigma_c} \frac{\partial \Sigma}{\partial x_i} \right) + (\kappa_m + \kappa_t)\Sigma + \underbrace{\left\langle s_d \frac{\partial n_i}{\partial x_i} \right\rangle_s \Sigma}_{D}$$

Modelo!

$k_t \Sigma = \alpha_0 \frac{\varepsilon}{k} \Sigma$

$k_m \Sigma \approx 0$ — ou um modelo

D (Destruction term) $= -\beta_0 \langle S_c \rangle_s \frac{\Sigma^2}{1-\tilde{\theta}}$

$\approx S_L^0$

Extended Coherent FLAMELET MODEL

– ECFM –

REF.: Towards the understanding of cyclic variability in SI engine

O. VERMOREL, S. RICHARD, O. COLIN et al.

C&F, 156 (2009)

- SPECIES TRANSP. EQ.

$$\rho_i = \bar{\rho}\,\tilde{Y}_i \longrightarrow O2, N2, CO_2, H_2O, CO, H_2$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\,\tilde{Y}_i\right) = -\nabla\cdot\left(\bar{\rho}\,\tilde{\vec{u}}\,\tilde{Y}_i\right) + \nabla\cdot\left(\sigma_c\,\bar{\rho}\left(\frac{\nu}{S_c}+\frac{\hat{\nu}_t}{S_{ct}}\right)\nabla\tilde{Y}_i\right) + \bar{\rho}\,\tilde{\dot{\omega}}_i \quad (3)$$

$$\bar{\rho}_F = \bar{\rho}_F^{u} + \bar{\rho}_F^{b} \quad (7)$$

$$\bar{\rho}_F^{x} = \bar{\rho}\,\tilde{Y}_F^{x}$$

x – unburned
  – burned

MEAN SENSIBLE ENTHALPY, $\tilde{h}_s$

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{h}_s = -\nabla\cdot\left(\bar{\rho}\,\tilde{\vec{u}}\,\tilde{h}_s\right) + \nabla\cdot\left(\sigma_c\left(\frac{\lambda}{Pr} + \frac{\hat{\lambda}_t}{Pr_t}\right)\nabla\tilde{h}_s\right) + \bar{\rho}\,\tilde{\dot{\omega}}_{hs} \qquad (9)$$

TRACER SPECIES: $\tilde{Y}_{T_i}$ → used for definition of the UNBURNED state

↳ p/ $\tilde{Y}_i = \tilde{Y}_{TF}$, $\tilde{\dot{\omega}}_{TF} = 0$

TF: T = TRACER, F = FUEL

TRACERS : F, O_2, N2, CO_2, H_2O, H_2, CO (7x)

+

O, C, H, N → atomic mass balance eq. (4x)

→ only 3x eq (3), with $\tilde{\dot{\omega}}_i = 0$, are solved

→ não é só elemento químico como no "mixture fraction" model

$\tilde{Y}_{Ti}$ represents the species mass fraction conditional in the fresh (UNBURNED) gases, $\tilde{Y}_i|^u$:

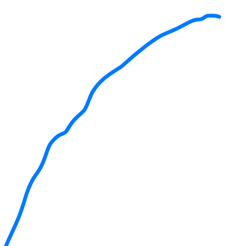
$$\tilde{Y}_{Ti} = \tilde{Y}_i|^u = \frac{\bar{\rho}_i^u}{\bar{\rho}^u} \qquad (10)$$

CFM : - infinitesimal flame thickness

- only two possible thermodynamic states: u / b

$$\tilde{\rho}_i = \tilde{\rho}_i^{u} + \tilde{\rho}_i^{b} \qquad (11)$$

- Assuming all species cross the flame at the same volumetric flow rate:



PROGRESS VARIABLE:

$$\tilde{c}\,\bar{\rho} = \bar{\rho}^{b} \rightarrow \text{burned gases mass fraction}$$

e

$$(1-\tilde{c})\,\bar{\rho} = \bar{\rho}^{u}$$

na prática:

Vem da Eq(3), $\tilde{\dot{\omega}}_F^u \neq 0$

$$\tilde{c} = 1 - \frac{\tilde{Y}_F^u}{\tilde{Y}_{TF}} \qquad (13)$$

Vem da Eq(3), $\tilde{\dot{\omega}}_{TF} = 0$

C é 1) LOCAL, não é transportada

2) como se fosse um "título" para definição de proporção líq-vapor p/ água na linha de líq $(x=0)$ e linha de vapor $(x=1)$. Aqui é usado para ponderar BURNED e UNBURNED

Se $\tilde{y}^{\mu}_{F} = \tilde{y}_{TF} \Longrightarrow$ é regime, $\tilde{c} = 0$

$\bar{\rho} = \bar{\rho}^{\mu}$

$\tilde{y}^{\mu}_{F} = 0 \Longrightarrow$ regime todo, $\tilde{c} = 1$

$\bar{\rho} = \bar{\rho}^{b}$

ainda:

$$\bar{\rho}_i = \bar{\rho}^{\mu}_i + \bar{\rho}^{b}_i$$

$$\bar{\rho}\,\tilde{y}_i = \bar{\rho}^{\mu}\,\tilde{y}_i\Big|^{\mu} + \bar{\rho}^{b}\,\tilde{y}_i\Big|^{b}$$

$$\tilde{Y}_i = \frac{\bar{\rho}^{\mu}}{\bar{\rho}} \tilde{Y}_i\Big|^{\mu} + \frac{\bar{\rho}^{b}}{\bar{\rho}} \tilde{Y}_i\Big|^{b} = (1-\tilde{c})\tilde{Y}_i\Big|^{\mu} + \tilde{c}\,\tilde{Y}_i\Big|^{b} \quad (14)$$

Sai desta Eq.

Vem da Eq(3)

$(1-\tilde{c})$

$\tilde{c}$

Vem da Eq(3) com $\tilde{\dot{\omega}}_i = 0$, pois $\tilde{Y}_i\Big|^{\mu} = \tilde{Y}_{T_i}$

Lembre que no CFM

$$\bar{\rho}\tilde{\dot{\omega}}_i = \bar{\rho}\Big|^{\mu} \tilde{Y}_{T_i} S_L \bar{\Sigma}$$

(Veja OBS p/ $\bar{\rho}\tilde{\dot{\omega}}_F^{b}$ ao final do texto)

SENSIBLE
- ENTHALPY, $\bar{h}_s$

sai dest Eq 7

$$\tilde{h}_s = (1-\tilde{c})\,\tilde{h}_s\Big|^u + \tilde{c}\,\tilde{h}_s\Big|^b \qquad (15)$$

Eq (9)

Eq (9) with $\bar{\rho}\tilde{\dot{\omega}}h_s\Big|^u = \bar{\rho}\sum h_i^\circ \underbrace{\tilde{\dot{\omega}}_i\Big|^u}_{=0} = 0$

mas também $\tilde{h}_s = c_p T \longrightarrow \sum \tilde{Y}_i \tilde{h}_{s,i}\Big|^u = c_p T^u$

$$\longrightarrow \sum \tilde{Y}_i \tilde{h}_{s,i}\Big|^b = c_p T^b$$

enter:
$$\bar\rho\big|^u = \frac{\bar p W^u}{R T^u} \quad ; \quad \bar\rho\big|^b = \frac{\bar p W^b}{R T^b}$$

- REACTION RATES (CFM)

$$\bar\rho\,\tilde{\dot\omega}_i = \rho_i^u S_L \bar\Sigma \overset{eq(16)}{=} \bar\rho\big|^u \tilde Y_{T_i} S_L \bar\Sigma \qquad (18a)$$

$$\bar\rho\,\tilde{\dot\omega}_F^u = \bar\rho^u \tilde Y_{TF} S_L \bar\Sigma \qquad (18b)$$

$$\bar\rho\,\tilde{\dot\omega}_{h_s} = \sum h_i^0 \bar\rho\,\tilde{\dot\omega}_i$$

$\tilde{\dot\omega}_F^b \rightarrow$ post-oxidation in the burned gas

$\rightarrow$ if $\tilde\phi < 1.0 \rightarrow$ negligible

OBS: 1) Qualquer quantidade condicionada ao estado da mistura fresca (UNBURNED) não tem termo fonte das reações de chama pré-misturada (PF). Por isso, a Eq(3) dá $\tilde{Y}_i\Big|^u = \tilde{Y}_{T_i}$ se for feito $\tilde{\dot{w}}_i = 0$. O mesmo vale para a entalpia sensível condicionada ao estado UNBURNED $h_s\Big|^u$, que é calculada com Eq(4) fazendo-se $\bar{\rho}\tilde{\dot{w}}_{h_s} = 0$

2) Veja que a Eq(3) pode ser usada p/ $\tilde{Y}_F^u$ e $\tilde{Y}_F^b$, com os respectivos termos

fontes $\bar{\rho}\,\tilde{\dot{\omega}}_F^{u}$ e $\bar{\rho}\,\tilde{\dot{\omega}}_F^{b}$. Mas $\tilde{Y}_F^{u} \neq \tilde{Y}_F\Big|^{u} = \tilde{Y}_{TF}$

pois e

$$\bar{\rho}\,\tilde{\dot{\omega}}_F^{u} = \bar{\rho}^{u}\,\tilde{Y}_{TF}\,S_L\,\Sigma \qquad \rho\tilde{\dot{w}}_{TF} = 0$$

3) Veja que não faz sentido $\bar{\rho}\,\tilde{\dot{\omega}}_F^{b} = \bar{\rho}^{u}\,\tilde{Y}_{TF}\,S_L\,\Sigma$.

S_L é definido como a velocidade que a mistura fresca (UNBURNED) chega à frente de chama.

Assim, na Eq (3), p/ $\tilde{Y}_F^{b}$, $\bar{\rho}\,\tilde{\dot{\omega}}_F^{b}$ só pode representar reações de pós oxidação na frente de chama (PF)

4) a eq (3) p/ $\tilde{Y}_F^u$ ou $\tilde{Y}_F^b$ avalia o balanço destas espécies, com seus respectivos termos fonte e transporte convectivo e difusivo.

$\tilde{Y}_F^u$ e $\tilde{Y}_F^b$ não são usados p/ definir (diretamente) os estados termodinâmicos UN/BURNED.

ECFM

REF : A new LES model coupling flame surface density and tabulated ...

G. LECOCQ, ..., VERVISCH...

COMB. SYMP. 2011

- TKI : "Stores the reaction rate of "c" and a characteristic delay of auto-ignition, the only quantities required to predict KNOCK occurrence"

- $\tilde{\tau}_c^*$ → physical time required to reach a value of "c" (e.g. 1e-3)

- $\tilde{Y}_{IR}$ → intermediate species, an auto-ignition precursor

$$\frac{\partial \bar{\rho} \tilde{Y}_{IR}}{\partial t} + \nabla \cdot (\quad) = \nabla \cdot (\nabla (\quad)) + \bar{\rho}\, \tilde{Y}_{T_{fuel}}\, f(\tilde{\tau}_c^*)$$

Function to account for the non-linear precursor production

ECFM SOURCE TERM

$$\bar{\rho}\,\tilde{\dot{\omega}}_c = \underbrace{\rho^u S_L \bar{\Sigma}_{\tilde{c}}}_{\text{Taxa de reação da Pré-Mistura (PF)}} + \underbrace{(1-\tilde{c})}\,\bar{\rho}\,\tilde{\dot{\omega}}_c^{TKI}$$

auto-ignition contribution, with the fresh (unburned) gases mass fraction $(1-\tilde{c})$

Só esta fração da massa pode passar pelo processo de AI

- Massa de combustível que pode reagir:

$$\tilde{Y}_{fuel} = \tilde{Y}_{T_{fuel}} - \tilde{Y}^{TKI}_{fuel} - \tilde{Y}^{PF}_{fuel}$$

máximo valor que pode ser atingido:

$$0 = \tilde{Y}_{T_{fuel}} - \tilde{Y}^{TKI,MAX}_{fuel} - \tilde{Y}^{PF}_{fuel}$$

$$\tilde{Y}^{TKI,MAX}_{fuel} = \tilde{Y}_{T_{fuel}} - \tilde{Y}^{PF}_{fuel}$$

ou também: $\tilde{Y}^{TKI,max}_{fuel} = \tilde{Y}_{fuel} + \tilde{Y}^{TKI}_{fuel}$

Isto é a massa de fuel que pode ser examinada pela reação de AI

Isto é o que vai de fato "reagir"

AI – PROGRESS VARIABLE c^{TKI}

$$c^{TKI} = \tilde{Y}^{TKI}_{fuel} / \left(\tilde{Y}_{fuel} + \tilde{Y}^{TKI}_{fuel} \right) \qquad (6)$$

Se $\tilde{Y}_{fuel} = 0 \implies c^{TKI} = \tilde{Y}^{TKI}_{fuel} / \tilde{Y}^{TKI}_{fuel} = 1.0$ //

$\tilde{Y}^{TKI}_{fuel} = 0 \implies c^{TKI} = 0$ //

$\tilde{Y}_{fuel}^{TKI}$ TRANSP. EQ.

$$\frac{\partial \bar{\rho} \tilde{Y}_{fuel}^{TKI}}{\partial t} + \nabla \cdot (\ \ ) = \nabla \cdot (\nabla (\ )) + \underbrace{(1-\tilde{C})}\, \bar{\rho}\, \tilde{\dot{\omega}}_c^{TKI} (C^{TKI})\, \tilde{Y}_{T fuel}$$

unburned mass fraction undergoing AI

avanço da reacção de AI

para transferir source term de

$\bar{\rho}\tilde{\dot{w}}_c = \rho|^{u} S_L \bar{\Sigma} \quad P|$

$\bar{\rho}\tilde{\dot{w}}_i = \rho|^{u} \tilde{Y}_{T_i} S_L \Sigma$

SPECIES BASED ECFM (SB-ECFM)

REF. DEVELOPMENT OF A SPECIES BASED EXTENDED COHERENT FLAMELET MODEL
ASME, 2018

INTRODUCTION

1) Previous REFERENCE BASED ECFM computed the UNBURNED state

from REAL and TRACERS species.

Limitations:

a) small discrepancies between real and tracers transport leads to inaccurate or even negative Y_i^M

b) it is assumed, implicitly, the unburned states correspond to the same mixture fraction

→ é explicado sobre as perturbações numéricas (discretização). Não vi quais outros problemas poderiam levar ao problema a)

2) In the SB-ECFM, the UNBURNED states are defined entirely by the transported species in each zone

3) Complete decoupling $\dot{\tilde{\omega}}_i^{PF} \times \dot{\tilde{\omega}}_i^{TKI}$

??

4) Not restricted to UPWIND scheme

COMBUSTION MODELING

FSD EQ.

$$\frac{\partial \bar{\Sigma}}{\partial t} + \nabla\cdot(\tilde{\vec{u}}\,\bar{\Sigma}) = \nabla\cdot\left(\mu_t \bar{\Sigma}\right) + \alpha \overset{\text{ITNFS}}{k_t}\,\bar{\Sigma} + \frac{2}{3}\,\overset{K_t\ (\text{CFM})}{\tilde{\nabla}\cdot\vec{u}}\,\bar{\Sigma} +$$

$$+ \underbrace{\frac{2}{3} S_L \frac{(1-\tilde{c}_\Sigma)}{\tilde{c}_\Sigma}\,\bar{\Sigma}^2}_{\text{CURVATURE (??)}} - \underbrace{S_L \frac{1}{(1-\bar{c})}\,\bar{\Sigma}^2}_{D\ (\text{CFM})} + \tilde{\dot{\omega}}_\Sigma^{TKI} + \tilde{\dot{\omega}}_\Sigma^{ISSIM}$$

Simula a influência da vela na $\bar{\Sigma}$ eq.

$$S_L = f\left(p, T_u, EGR\,(Vol), X_{EGR}, \phi_u\right); \quad \bar{c} = \frac{\bar{\rho}}{\rho_b}\tilde{c}$$

- COMBUSTION MODEL

Transport eqs. for $\tilde{Y}_i^u$ and $\tilde{Y}_i^b$

Unburned Species :

$$\underbrace{F, O2, CO, CO2, H2, H_2O, N2}$$

Burned :

$+\ O, H, OH, N, NO$

$$\frac{\partial \bar\rho \tilde{Y}_i^{x}}{\partial t} + \nabla\cdot\left(\bar\rho \tilde{u}\, \tilde{Y}_i^{x}\right) = \nabla\left(\mu_t \nabla \tilde{Y}_i^{x}\right) + \bar\rho \tilde{\dot\omega}_i^{x} + \bar\rho \tilde{S}_i^{x}$$

Evaporation gaseous source term

$$\tilde{S}_i^{x} = 0 \quad , \quad i \neq F$$

$$\tilde{S}_F^{u} = (1 - \tilde{c})\tilde{S}_F \quad , \quad \tilde{S}_F^{b} = \tilde{c}\,\tilde{S}_F$$

Mean species mass fraction:

$$\tilde{Y}_i = \tilde{Y}_i^{u} + \tilde{Y}_i^{b} \longrightarrow \sum \tilde{Y}_i = \sum \tilde{Y}_i^{u} + \sum \tilde{Y}_i^{b}$$

, 1.0

MASS PROGRESS VARIABLE, from species only,

$$\tilde{C} = \frac{\sum_i \tilde{Y}_i^b}{\sum_i \tilde{Y}_i^u + \sum_i \tilde{Y}_i^b} \qquad (4)$$

→ compare with eq (13), CFM

TKI PROGRESS VARIABLE

consistent with (6) CFM

$$\tilde{C}_{ai} = \frac{\tilde{Y}_{N_2}^{b,ai}}{\tilde{Y}_{N_2}^{b,ai} + \tilde{Y}_{N_2}^{b,\Sigma}} \qquad \tilde{C} \quad (5)$$

$\tilde{C}$ → $\dfrac{\text{mass of burned gases}}{\text{total mass of gases (u+b)}}$

Transp. Eq.

→ it is the burned gases fraction coming from AI

Desconfio que a escolha por N_2 é por ser a espécie de maior fração mássica e menos reativa.

FSD and AI PROGRESS VARIABLES

→ The PF separates "fresh" AI gases and burned gases

→ The cell mass fraction is given by

$$\tilde{Y}_i = (1 - \tilde{c}_\Sigma) Y_i \big|^{ai} + \tilde{c}_\Sigma Y_i \big|^{b} \quad (1261)$$

CONVERGE

→ The fresh AI gas $Y_i|^{ai}$ is treated as bimodal (in reality, a homogeneous zone):

$$Y_i|^{ai} = \underbrace{(1 - \tilde{c}_{ai})}_{\Downarrow \text{FIG 1} \atop = (1-\tilde{c})} Y_i|^{u} + \tilde{c}_{ai} Y_i|^{b} \quad (12.62)$$

conditioned State $|^{ai}$

↳ calculado a partir de Eq. Transp- condicionada a AI

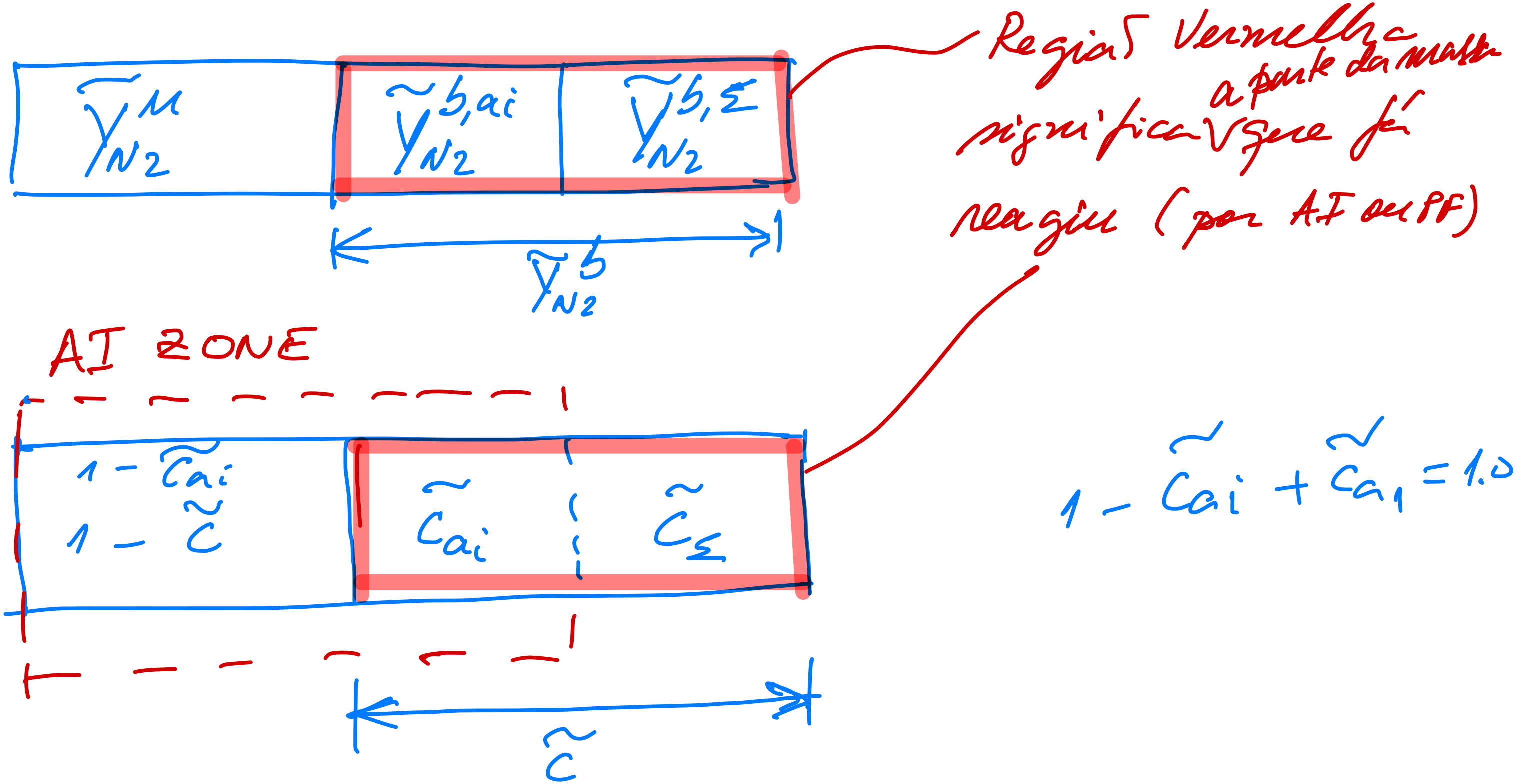

Região Vermelha a parte da matriz significante que faz reagir (por AI ou PF)
AI ZONE
1 - c̃ai
1 - c̃
c̃ai
c̃Σ
c̃
1 - c̃ai + c̃a1 = 1.0

FIG. 1

AUTO IGNITION PROGRESS VARIABLE

da FIG 1:

$$C_{ai} = \frac{\tilde{C}_{ai}}{(1-\tilde{C}) + \tilde{C}_{ai}} \quad (6) \quad = \frac{\tilde{C}_{ai}}{(1-\tilde{C}_{ai}) + \tilde{C}_{ai}} = \tilde{C}_{ai}$$

dá a proporção da massa nos estados "u" e "b" da região AI

$(1-\tilde{C})$ $\quad$ $(\tilde{C}_{ai})$

$C_{ai} = 0$, nada passou p/ AI de "u" p/ "b"

$C_{ai} = 1$, toda massa "u" passou p/ AI p/ "b"

FSD PROGRESS VARIABLE ($\tilde{c}_\Sigma$)

from FIG. 1 $\quad 1-\tilde{c}+\tilde{c}=1.0$

$$1-\tilde{c}+(\tilde{c}_{ai}+\tilde{c}_\Sigma)=1.0$$

$$\boxed{\tilde{c}_\Sigma = \tilde{c}-\tilde{c}_{ai}}$$

CHEMICAL SOURCE TERMS

$$\widetilde{\dot{\omega}}_{\tilde{Y}_i^u} = -Y_i^u \Big[\underbrace{(1-\tilde{C}_\Sigma)}_{= \underbrace{(1-\tilde{c}) + \tilde{C}_{ai}}_{A}} \widetilde{\dot{\omega}}_c^{TKI} + (1 - C_{ai}) \left(\widetilde{\dot{\omega}}_c^{\Sigma} + \widetilde{\dot{\omega}}_c^{ISSIM} \right) \Big]$$

B

conditional mass fraction of i in the "UNBURNED" gases

$$Y_i^u = \frac{\tilde{Y}_i^u}{(1-\tilde{c})}$$

AI source term

$$\widetilde{\dot{\omega}}_c^{TKI} = (T_u, P, Y_{EGR}, \phi_u, C_{ai})$$

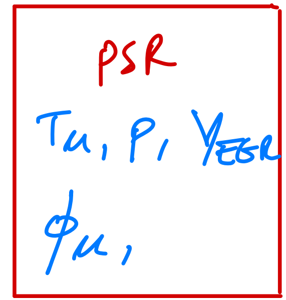
eq(6)

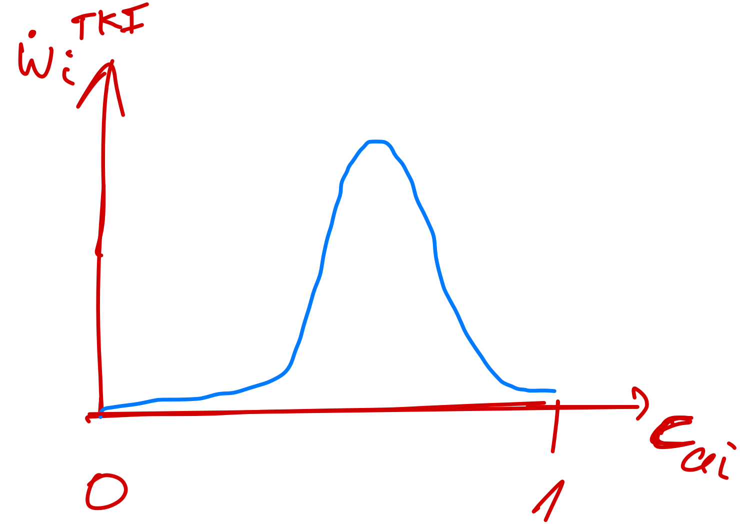
como???

eu imagino:

$$\phi_u = \alpha_F \frac{Y_F^u}{Y_{O_2}^u}$$

coef. esteq.





ainda $\tilde{\dot{w}}_c^{\Sigma} = \frac{\rho^u}{\bar{\rho}} S_L \bar{\Sigma} \Rightarrow \tilde{\dot{w}}_{Y_i^u}^{\Sigma} = Y_i^u \frac{\rho^u}{\bar{\rho}} S_L \bar{\Sigma}$

$\tilde{\dot{w}}_c^{ISSIM}$ → simula a influência da vela na $\bar{\Sigma}$ eq.

(A) parte da massa que pode passar pelo processo de AI

(B) parte da massa da região AI que pode passar pela PF

$$Y_i^{ai} = \underbrace{Y_i^{u,ai}\left(1 - c_{ai}\right)} + Y_i^{b,ai}\, c_{ai}$$

For the BURNED gases species:

$$\tilde{\dot{\omega}}_{\tilde{Y}_i^b} = Y_i^{b*}\left[(1-\tilde{c}_\Sigma)\,\tilde{\dot{\omega}}_c^{TKI} + (1-c_{ai})\left(\tilde{\dot{\omega}}_c^{\Sigma} + \tilde{\dot{\omega}}_c^{ISSIM}\right)\right]$$

$$+ \underbrace{(1-\tilde{c})}_{???}\,\tilde{\dot{\omega}}_i^{bg}$$

post-combustion oxidation

burned gas composition, two steps ECFM chemistry para N_2 temos que diferenciar PF de AI:

$$\tilde{\dot{\omega}}_{\tilde{Y}^{b,ai}_{N_2}} = Y^{b*}_{N_2}\left(1-\tilde{C}_{\Sigma}\right)\tilde{\dot{\omega}}_c^{TKI} + \left(1-\tilde{c}\right)\frac{\tilde{Y}^{b,ai}_{N_2}}{\tilde{Y}^{b,ai}_{N_2}+\tilde{Y}^{b,\Sigma}_{N_2}}\tilde{\dot{\omega}}^{bg}_{N_2}$$

e

$$\tilde{\dot{\omega}}_{\tilde{Y}^{b,\Sigma}_{N_2}} = Y^{b*}_{N_2}\left(1-c_{ai}\right)\left(\tilde{\dot{\omega}}_c^{\Sigma} + \tilde{\dot{\omega}}_c^{ISSIM}\right) + \left(1-\tilde{c}\right)\frac{\tilde{Y}^{b,\Sigma}_{N_2}}{\tilde{Y}^{b,ai}_{N_2}+\tilde{Y}^{b,\Sigma}_{N_2}}\tilde{\dot{\omega}}^{bg}_{N_2}$$

conditional N_2
in burned gases

3 - ZONE ECFM

→ cria um estado de MISTURA

air (+ exaust gas recirc.) + fuel

ECFM 3Z

COLIN, BENKENIDA, 2004

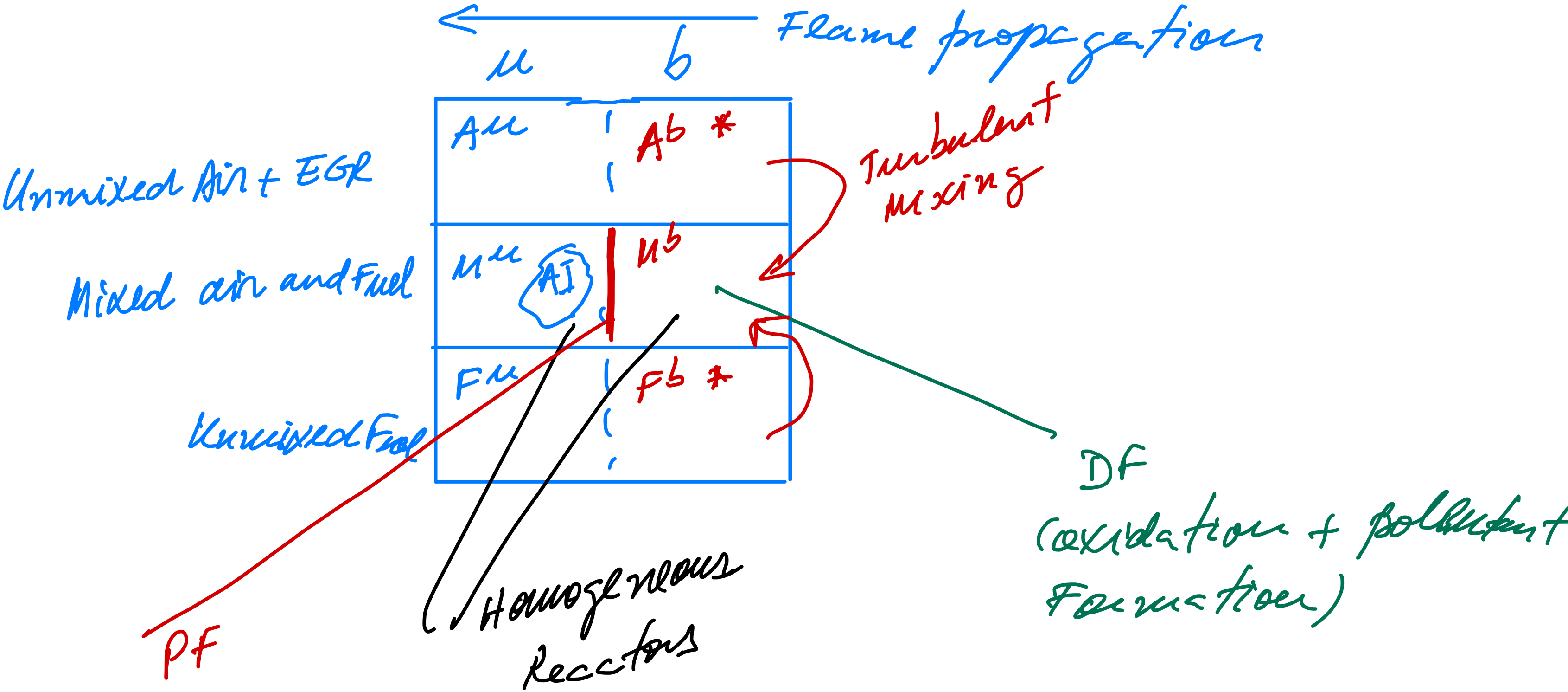
3Z : 1) a pure fuel zone

2) a " air + EGR zone

3) a mixed zone ⟷ diffusion flame

→ the mixture fraction space is discretized by only three points

→ na forma dos traços



$$PDF(z) = a\,\delta(z) + b\,\delta(z-\bar{z}^u) + c\,\delta(z-1)$$

MIXTURE FRACTION (FUEL TRACER)

average value of z in the mixed zone

A^b e F^b não significa Air + EGR e Fuel queimados, mas sim que eles vão se misturar com os gases queimados da zona de mistura M^b.

$$M^b \longrightarrow T^b$$

$$A^b, F^b, A^u, M^u, F^u \longrightarrow T^u$$

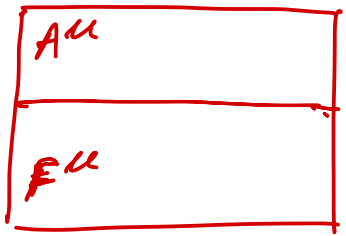
- Probability to find a droplet in the burned gases : $\tilde{c}$

u/ " " : $1 - \tilde{c}$

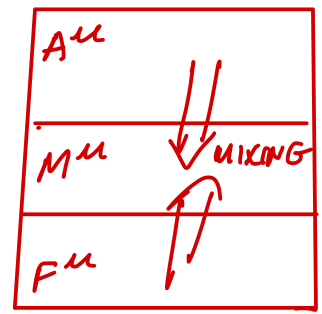
→ $\tilde{c}$ is the local burned mass fraction in mixed zone (M)

- combustão só pode ocorrer na ZONA DE MISTURA (M^u)

Processo Idealizado de Combustão no modelo de zonas (DI ENGINE)

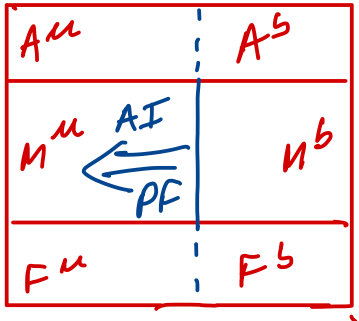


(a) (injeção de fuel alimenta a região F^u)



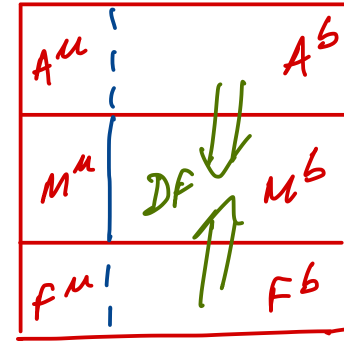
(b) Formação de mistura

$A^u + F^u \rightarrow M^u$



(c) Combustão Pré-misturada

- Auto Ignição (TEI)
- PF (Σ)
- gases queimados produzidos são transferidos p/ M^b



(d) Combustão NÃO PRÉ MISTURADA (DIFFUSION FLAME)

- THE GLOBAL SPECIES EQUATIONS

FUEL, O2, N2, NO, CO_2, CO, H_2, H_2O, O, H, N, OH,

SOOT

"burned gases" include: M^b, F^b, A^b UNMIXED ZONES

$$\frac{\partial \bar{\rho}\tilde{Y}_x}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{Y}_x}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial \tilde{Y}_x}{\partial x_i}\right) + \bar{\dot{\omega}}_x \qquad (2)$$

$$\tilde{Y}_x = \frac{\bar{m}_x}{\bar{m}} = \frac{\bar{m}_x/V}{\bar{m}/\underbrace{V}_{\text{cell Volume}}} = \frac{\bar{\rho}_x}{\underbrace{\bar{\rho}}_{\text{mean density}}} \qquad (3)$$

Fuel is divided in two parts: Y^{u}_{Fu} e Y^{b}_{Fu}

will be consumed by AI and PF

DF

$$\frac{\partial \bar{\rho}\,\tilde{Y}^{\mu}_{F\mu}}{\partial t} + \frac{\partial \bar{\rho}\,\tilde{u}_i\,\tilde{Y}^{\mu}_{F\mu}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma}\frac{\partial \tilde{Y}^{\mu}_{F\mu}}{\partial x_i}\right) + \bar{\rho}\,\tilde{S}^{\mu}_{F\mu} + \tilde{\dot{\omega}}^{\mu}_{F\mu}$$

$$- \tilde{\dot{\omega}}^{\mu\to b}_{F\mu}$$

consumo de $\tilde{Y}^{\mu}_{F\mu}$ por PF ou ΔI

→ Transferência de $\tilde{Y}^{\mu}_{F\mu}$ (ñ queimado) de F^{μ} p/ F^{b}

e ainda

$$\frac{\partial \bar{\rho}\,\tilde{Y}^{b}_{F\mu}}{\partial t} + \left(\quad \right) = \left(\quad \right) + \bar{\rho}\,\tilde{S}^{b}_{F\mu} + \tilde{\dot{\omega}}^{b}_{F\mu} + \tilde{\dot{\omega}}^{\mu\to b}_{F\mu}$$

consumido por DF

$\tilde{\dot{S}}_{Fu} \longrightarrow$ liquid droplets evaporation rate

$\tilde{\dot{S}}^{b}_{Fu} = \tilde{\dot{S}}_{Fu} \, \tilde{c}$ probabilidade de encontrar uma gota na região burned (5)

$\tilde{\dot{S}}^{u}_{Fu} = \tilde{\dot{S}}_{Fu} (1 - \tilde{c})$

– Multi-Fuel : $\tilde{Y}^{u}_{Fu,i}$ and $\tilde{Y}^{b}_{Fu,i}$ $\quad i = 1 - N_{FUELS}$

TRACER EQS.

$$\frac{\partial \bar{\rho}\tilde{Y}_{TX}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{Y}_{TX}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\left(\frac{\mu}{Sc} + \frac{\mu_t}{Sc_t}\right)\frac{\partial \tilde{Y}_{TX}}{\partial x_i}\right) + \bar{\rho}\tilde{\dot{S}}_X \quad (7)$$

$\tilde{Y}_{TFM} \Leftrightarrow$ mean mixture fraction in other combustion models.

– THE MIXING MODEL

FICTIOUS SPECIES

- Unmixed fuel ($\tilde{Y}^F_{Fu}$), fuel contained in regions F^u and F^b
- Unmixed oxygen ($\tilde{Y}^A_{O_2}$), O_2 contained in regions A^u and A^b

$\bar{\rho}\,\tilde{Y}^F_{Fu}$ é uma fração da massa total de fuel ($\bar{\rho}\,\tilde{Y}^u_{Fu} + \bar{\rho}\,\tilde{Y}^b_{Fu}$). Por isso n entra no balanço de massa global

$\bar{\rho}\,\tilde{Y}^A_{O_2}$ idem

$$\frac{\partial \bar{\rho} \tilde{Y}^{F}_{Fu}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{Y}^{F}_{Fu}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}^{F}_{Fu}}{\partial x_i} \right) + \bar{\rho} \tilde{\dot{S}}_{Fu} + \bar{\rho} \tilde{\dot{E}}^{F \to M}_{Fu} \quad (8)$$

$$\frac{\partial \bar{\rho} \tilde{Y}^{A}_{O_2}}{\partial t} + \left(\qquad \right) = \left(\qquad \right) + \bar{\rho} \tilde{\dot{E}}^{A \to M}_{O_2} \quad (9)$$

MIXING SOURCE TERMS:

$$\tilde{\dot{E}}^{F \to M}_{Fu} = - \frac{1}{\tilde{\tau}_{mi}} \tilde{X}^{F}_{Fu} \left(1 - \tilde{X}^{F}_{Fu} \right) \quad (10)$$

$$= - \frac{1}{\tilde{\tau}_{mi}} \tilde{Y}^{F}_{Fu} \left(1 - \tilde{Y}^{F}_{Fu} \frac{\bar{\rho} M^{M}}{\bar{\rho}^{M}/_{M} \, M_{Fu}} \right) \quad (11)$$

$$\dot{\tilde{E}}_{O_2}^{A \to M} = -\frac{1}{\tilde{\tau}_m} \tilde{Y}_{O_2}^{A} \left(1 - \frac{\tilde{Y}_{O_2}^{A}}{\tilde{Y}_{O_2}^{\infty}} \frac{\bar{\rho}\, M^M}{\bar{\rho}^M \big|_M M_{air+EGR}} \right) \qquad (12)$$

└ oxygen mass fraction in the unmixed air.

MIXING TIME SCALE

$$\tilde{\tau}_m^{-1} = \beta_m\, \varepsilon / k \qquad (13)$$

└ $= 1.0$

- CONDITIONAL COMPOSITIONS IN THE MIXED ZONE

  - GLOBAL AND UNMIXED SPECIES IN A CELL:

$$\bar{\rho}_X^{M} = \bar{\rho}\,\tilde{Y}_X^{M} = \bar{\rho}_X - \bar{\rho}_X^{A} = \bar{\rho}\,\tilde{Y}_X - \bar{\rho}\,\tilde{Y}_X^{A} \qquad (20)$$

  - TRACERS IN THE MIXED ZONE

$$\bar{\rho}_{TX}^{M} = \bar{\rho}\,\tilde{Y}_{TX}^{M} = \bar{\rho}_{TX} - \bar{\rho}_X^{A} = \bar{\rho}\,\tilde{Y}_{TX} - \bar{\rho}\,\tilde{Y}_X^{A} \qquad (21)$$

  - BURNED/UNBURNED DENSITIES

$$\bar{\rho}_{Fu}^{u,M} = \bar{\rho}\,\tilde{Y}_{Fu}^{u,M} = \bar{\rho}_{Fu}^{u} - \bar{\rho}_{Fu}^{u,F} = \bar{\rho}\,\tilde{Y}_{Fu}^{u} - \bar{\rho}\,\tilde{Y}_{Fu}^{u,F}$$

$$\bar{\rho}_{Fu}^{b,M} = \bar{\rho}\,\tilde{Y}_{Fu}^{b,M} = \bar{\rho}_{Fu}^{b} - \bar{\rho}_{Fu}^{b,F} = \bar{\rho}\,\tilde{Y}_{Fu}^{b} - \bar{\rho}\,\tilde{Y}_{Fu}^{b,F}$$

UNMIXED UNBURNED/BURNED FUEL MASS FRACTIONS:

$$\overline{\rho}_{Fu}^{u,F} = \overline{\rho}\,\widetilde{Y}_{Fu}^{u,F} = (1-\widetilde{c})\,\overline{\rho}_{Fu}^{F}$$

$$\overline{\rho}_{Fu}^{b,F} = \overline{\rho}\,\widetilde{Y}_{Fu}^{b,F} = \widetilde{c}\,\overline{\rho}_{Fu}^{F} \qquad (23)$$

FUEL OXIDATION MODELS

- AI, PF $\longrightarrow \tilde{\dot{\omega}}^{u}_{FM}$

- DIFUSION FLAME (DF)

$$\begin{matrix} F^{S} \xrightarrow{\text{MIXING}} \\ A^{S} \xrightarrow[\text{MIXING}]{} \end{matrix} M^{b} \longrightarrow \underline{\underline{DF}}, \; \tilde{\dot{\omega}}^{S}_{FM}$$

- POST-FLAME KINETICS
  - $CO \rightarrow CO_2$
  - NO

UNBURNED FUEL OXIDATION

- partial oxidation of fuel into CO, CO_2

$$\alpha(1 - r_{CO})\left[C_xH_y + \left(x + \frac{y}{4}\right)O_2 \longrightarrow x\,CO_2 + \frac{y}{2}H_2O\right]$$

$$\alpha\, r_{CO}\left[C_xH_y + \left(\frac{x}{2} + \frac{y}{4}\right)O_2 \longrightarrow x\,CO + \frac{y}{2}H_2O\right]$$

$$(1 - \alpha)\left[C_xH_y + \frac{x}{2}O_2 \longrightarrow x\,CO + \frac{y}{2}H_2\right]$$

if $\Phi \geq 1 \qquad \alpha = 1$

if $1 \leq \Phi \leq \phi_{CRIT} \rightarrow \alpha \quad \dfrac{\dfrac{4(x + y/4)}{\Phi} - 2x}{2x + y}$

if $\phi_{CRIT} \leq \Phi \longrightarrow \alpha = 0$

$$\phi_{CRIT} = \frac{2}{x}\left(x + y/4\right)$$

$$r_{CO} = \frac{CO}{CO_2} \approx 0.9$$

if $\bar{\Phi} > \phi_{CRIT}$, ñ tem O_2 nem para oxidar o fuel p/ CO

→ a part of the unburned fuel is transported as "burned" fuel (F^b) in zone M^b

$$\tilde{\dot{\omega}}^{u \to b}_{Fu}\Big|_M = -\tilde{\dot{\omega}}^{u,M}_{Fu}\Big|_M \left(1 - \frac{\phi_{CRIT}}{\bar{\Phi}}\right)$$

FUEL POST-OXIDATION IN BURNED GASES

↳ Fuel resulting from TRANSFER MECHANISM

M^b — perfectly mixed

→ chemistry controlled ($\tilde{\tau}_c$)

$$\tilde{\dot{\omega}}^{b,M}_{Fu}\Big|_{b,M} = -\frac{\bar{\rho}\,\tilde{Y}^{b,M}_{Fu}\big|_{b,M}}{\tilde{\tau}_c}$$

$$\tilde{\tau} = A e^{T_a/\tilde{T}_b}$$

$A = 2 \times 10^{-6}$
$T_a = 6000\,K$

$\Big\}$ from engine parameters

POST-FLAME KINETICS

Equilibrium

$$N_2 \rightleftarrows 2N$$

$$O_2 \rightleftarrows 2O$$

$$H_2 \rightleftarrows 2H$$

$$2OH \rightleftarrows O_2 + H_2$$

$$2H_2O \rightleftarrows O_2 + 2H_2$$

CO oxidation:

$$CO + OH \leftrightarrow CO_2 + H$$

NO MECHANISM