FLAMELET EQUATIONS

- Croco's transformation

$$x_1, x_2, x_3, t \longrightarrow \xi, \xi_2, \xi_3, \tau$$

$$\frac{\partial}{\partial t} = \cancelto{1}{\frac{\partial \tau}{\partial t}} \frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} + \frac{\partial \xi_k}{\partial t}\frac{\partial}{\partial \xi_k} \qquad k = 2, 3$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} + \frac{\partial \xi_k}{\partial t}\frac{\partial}{\partial \xi_k} \qquad (1a)$$

$$\frac{\partial}{\partial x_i} = \cancelto{0}{\frac{\partial \tau}{\partial x_i}} \frac{\partial}{\partial \tau} + \frac{\partial \xi}{\partial x_i}\frac{\partial}{\partial \xi} + \frac{\partial \xi_k}{\partial x_i}\frac{\partial}{\partial \xi_k}$$

$$\frac{\partial}{\partial x_i} = \frac{\partial \xi}{\partial x_i}\frac{\partial}{\partial \xi} + \frac{\partial \xi_k}{\partial x_i}\frac{\partial}{\partial \xi_k} \qquad (1b)$$

Hypotesis : 1c) Gradients are only relevant in the direction normal to the plane tangent to the $\xi_{STOICHOMETRIC}$ surface. So $\frac{\partial}{\partial \xi_k} \approx 0$

1b) - ξ is based on the mixture fraction definition

1a) - flame reaction zone is infinitesimally thin

Let us consider the general transport equation for the specie Ψ_α

$$\underbrace{\rho \frac{\partial \Psi_\alpha}{\partial t}}_{(a)} + \underbrace{\rho u_i \frac{\partial \Psi_\alpha}{\partial x_i}}_{(b)} = \underbrace{\frac{\partial}{\partial x_i}\left[\rho D \frac{\partial \Psi_\alpha}{\partial x_i}\right]}_{(c)} + \underbrace{\dot{\omega}_\alpha}_{(d)} \qquad (2)$$

Since ξ is based on the mixture fraction, one has:

$$\rho \frac{\partial \xi}{\partial t} + \rho u_i \frac{\partial \xi}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\rho D \frac{\partial \xi}{\partial x_i}\right] \qquad (3)$$

Let us now introduce the transformation rules (eq 1a and 1b) in the eq (2), term by term:

$$(a): \rho \frac{\partial \Psi_\alpha}{\partial t} = \rho \left[\frac{\partial \Psi_\alpha}{\partial \tau} + \frac{\partial \xi}{\partial t}\frac{\partial \Psi_\alpha}{\partial \xi} + \frac{\partial \xi_k}{\partial t}\frac{\partial \Psi_\alpha}{\partial \xi_k}\right]$$

$$(b): \rho u_i \frac{\partial \Psi_\alpha}{\partial x_i} = \rho u_i \left[\frac{\partial \xi}{\partial x_i}\frac{\partial \Psi_\alpha}{\partial \xi} + \frac{\partial \xi_k}{\partial x_i}\frac{\partial \Psi_\alpha}{\partial \xi_k}\right]$$

(a) +(b) :

$$\rho \frac{\partial \Psi_\alpha}{\partial \tau} + \left(\rho \frac{\partial \xi}{\partial t} + \rho u_i \frac{\partial \xi}{\partial x_i}\right)\frac{\partial \Psi_\alpha}{\partial \xi} + \left(\rho \frac{\partial \xi_k}{\partial t} + \rho u_i \frac{\partial \xi_k}{\partial x_i}\right)\frac{\partial \Psi_\alpha}{\partial \xi_k} \qquad (4)$$

term (c) written on the LHS of (2):

$$-(c): -\frac{\partial}{\partial x_i}\left[\rho D \frac{\partial \Psi_\alpha}{\partial x_i}\right] = -\frac{\partial}{\partial x_i}\left[\rho D \left(\underbrace{\frac{\partial \xi}{\partial x_i}\frac{\partial \Psi_\alpha}{\partial \xi}}_{(e)} + \underbrace{\frac{\partial \xi_k}{\partial x_i}\frac{\partial \Psi_\alpha}{\partial \xi_k}}_{(f)}\right)\right] \qquad (5)$$

(e): $$-\frac{\partial}{\partial x_i}\left[\rho D \frac{\partial \xi}{\partial x_i}\frac{\partial \psi_\alpha}{\partial \xi}\right] = -\frac{\partial}{\partial x_i}\left[\rho D\frac{\partial\xi}{\partial x_i}\right]\frac{\partial\psi_\alpha}{\partial\xi} - \rho D \frac{\partial \xi}{\partial x_i}\frac{\partial}{\partial x_i}\left(\frac{\partial\psi_\alpha}{\partial\xi}\right)$$

$$= -\frac{\partial}{\partial x_i}\left[\rho D\frac{\partial\xi}{\partial x_i}\right]\frac{\partial\psi_\alpha}{\partial\xi} - \rho D \frac{\partial \xi}{\partial x_i}\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi} \qquad (6)$$

(f): $$-\frac{\partial}{\partial x_i}\left[\rho D \frac{\partial \xi_k}{\partial x_i}\frac{\partial \psi_\alpha}{\partial \xi_k}\right] = -\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\xi_k}{\partial x_i}\right)\frac{\partial\psi_\alpha}{\partial\xi_k} - \rho D \frac{\partial \xi_k}{\partial x_i}\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi_k} \qquad (7)$$

Substituting (4), (6) and (7) in (2), one has:

$$\rho\frac{\partial\psi_\alpha}{\partial\tau} + \left(\rho\frac{\partial\xi}{\partial t} + \rho u_i\frac{\partial\xi}{\partial x_i}\right)\frac{\partial\psi_\alpha}{\partial\xi} + \left(\rho\frac{\partial\xi_k}{\partial t} + \rho u_i\frac{\partial\xi_k}{\partial x_i}\right)\frac{\partial\psi_\alpha}{\partial\xi_k}$$

$$-\frac{\partial}{\partial x_i}\left[\rho D\frac{\partial\xi}{\partial x_i}\right]\frac{\partial\psi_\alpha}{\partial\xi} - \rho D\frac{\partial\xi}{\partial x_i}\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi}$$

$$-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\xi_k}{\partial x_i}\right)\frac{\partial\psi_\alpha}{\partial\xi_k} - \rho D\frac{\partial\xi_k}{\partial x_i}\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi_k} = \dot{\omega}_\alpha \qquad (8)$$

or

$$\rho\frac{\partial\psi_\alpha}{\partial\tau} + \overbrace{\left[\rho\frac{\partial\xi}{\partial t} + \rho u_i\frac{\partial\xi}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\xi}{\partial x_i}\right)\right]}^{=0 \text{ (see eq. (3))}}\frac{\partial\psi_\alpha}{\partial\xi} +$$

$$\left[\rho\frac{\partial\xi_k}{\partial t} + \rho u_i\frac{\partial\xi_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\xi_k}{\partial x_i}\right)\right]\overbrace{\frac{\partial\psi_\alpha}{\partial\xi_k}}^{\approx 0 \text{ hypothesis (1c)}}$$

$$-\rho D\frac{\partial\xi}{\partial x_i}\left(\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi}\right) - \rho D\frac{\partial\xi_k}{\partial x_i}\left(\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi_k}\right) = \dot{\omega}_\alpha$$

So that:

$$\rho\frac{\partial\psi_\alpha}{\partial\tau} - \rho D\frac{\partial\xi}{\partial x_i}\left(\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi}\right) - \rho D\frac{\partial\xi_k}{\partial x_i}\left(\frac{\partial^2\psi_\alpha}{\partial x_i\partial\xi_k}\right) = \dot{\omega}_\alpha$$

$$\frac{\partial}{\partial x_i}\left(\cancel{\frac{\partial\psi_\alpha}{\partial\xi_k}}^{=0}\right) \quad (1c)$$

$$\rho\frac{\partial\psi_\alpha}{\partial\tau}\underbrace{-\rho D\frac{\partial\xi}{\partial x_i}\left(\frac{\partial^2\psi_\alpha}{\partial x_i\,\partial\xi}\right)} = \dot\omega_\alpha$$

$$\longrightarrow -\rho D\frac{\partial\xi}{\partial x_i}\left[\frac{\partial\xi}{\partial x_i}\frac{\partial}{\partial\xi}\left(\frac{\partial\psi_\alpha}{\partial\xi}\right)+\frac{\partial\xi_k}{\partial x_i}\cancelto{0}{\frac{\partial}{\partial\xi_k}\left(\frac{\partial\psi_\alpha}{\partial\xi}\right)}\right] \quad (1c)$$

So finally:

$$\boxed{\rho\frac{\partial\psi_\alpha}{\partial\tau}-\rho D\left(\frac{\partial\xi}{\partial x_i}\frac{\partial\xi}{\partial x_i}\right)\frac{\partial^2\psi_\alpha}{\partial\xi^2}=\dot\omega_\alpha} \qquad (9)$$

with the definition of the SCALAR DISSIPATION RATE (χ)

$$\chi \equiv 2D\sum_{i=1}^{3}\left(\frac{\partial\xi}{\partial x_i}\right)^2 = 2D\left[\left(\frac{\partial\xi}{\partial x_1}\right)^2+\left(\frac{\partial\xi}{\partial x_2}\right)^2+\left(\frac{\partial\xi}{\partial x_3}\right)^2\right] \qquad (10)$$

physical space

eq (9) becomes:

$$\boxed{\frac{\partial\psi_\alpha}{\partial\tau}-\frac{\chi}{2}\frac{\partial^2\psi_\alpha}{\partial\xi^2}=\frac{\dot\omega_\alpha}{\rho}} \qquad (11)$$

$$\left[\frac{1}{s}\right] \qquad \left[\frac{1}{s}\right]\left[-\right] \qquad \left[\frac{\frac{kg}{m^3\,s}}{\frac{kg}{m^3}}\right]$$

transformed space

for STEADY STATE FLAMELET:

$$\underbrace{-\frac{\chi}{2}\frac{\partial^2\psi_\alpha}{\partial\xi^2}}_{\tau_{flow}} = \underbrace{\frac{\dot\omega_\alpha}{\rho}}_{\tau_{CHEM}}$$

, balance between τ_{flow} and τ_{CHEM}

$$Da = \frac{\tau_{FLOW}}{\tau_{CHEM}}$$

$$\frac{\partial}{\partial t}\rho\left(\int_{T_0}^{T} c_p\, dT\right) = -\nabla\cdot\left[\rho\vec{v}\int_{T_0}^{T} c_p\, dT - \rho D\nabla\int_{T_0}^{T} c_p\, dT\right] = \sum_{\alpha=1}^{N} h_{f,\alpha}^{o}\dot{\omega}_{\alpha} \qquad (12)$$

defining, for sake of simplicity,

$$\theta \equiv \int_{T_0}^{T} c_p\, dT \qquad (13)$$

and

$$\dot{\omega}_{\theta} \equiv \sum_{\alpha=1}^{N} h_{f,\alpha}^{o}\dot{\omega}_{\alpha} \qquad (14)$$

one has:

$$\frac{\partial}{\partial t}(\rho\theta) + \nabla\cdot(\rho\vec{v}\theta) - \nabla\cdot\left[\rho D\nabla\theta\right] = \dot{\omega}_{\theta} \qquad (15a)$$

or in indicial notation:

$$\underbrace{\frac{\partial}{\partial t}(\rho\theta)}_{(a)} + \underbrace{\rho u_i\frac{\partial}{\partial x_i}(\theta)}_{(b)} - \underbrace{\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial(\theta)}{\partial x_i}\right)}_{(c)} = \underbrace{\dot{\omega}_{\theta}}_{(d)} \qquad (15b)$$

Applying the same procedure done for eq (2), one gets:

$$\frac{\partial\theta}{\partial\tau} - \frac{\chi}{2}\frac{\partial^2\theta}{\partial\xi^2} = \frac{\dot{\omega}_{\theta}}{\rho}$$

or, defining $\int_{T_0}^{T} c_p\, dT \equiv \bar{c}_p T$,

$$\boxed{\frac{\partial T}{\partial\tau} - \frac{\chi}{2}\frac{\partial^2 T}{\partial\xi^2} = \frac{\sum_{\alpha=1}^{N} h_{f,\alpha}^{o}\dot{\omega}_{\alpha}}{\rho\bar{c}_p}} \qquad (16)$$