Asymptotic solution of SLFM model.

The SLFM model is given by:

$$\tilde{N}(z,t)\frac{\partial^2 Q_F}{\partial z^2} = -AQ_FQ_O$$

$$\tilde{N}(z,t)\frac{\partial^2 Q_O}{\partial z^2} = -rAQ_FQ_O.$$

where $\tilde{N}(n,t) = \langle N | Z = n\rangle_t$.

- Slow chemistry approximation.

As $A \to 0$ the equations become:

$$\frac{\partial^2 Q_F}{\partial z^2} = \frac{\partial^2 Q_O}{\partial z^2} = 0.$$

Since A does not appear in the highest derivative, this is a regular problem $\sim$ the limitting solution $A \to 0$ converges to the solution at $A=0$.
The solution to these equations is:

$$Q_F = a_F z + b_F$$
$$Q_O = a_O z + b_O.$$

Now apply the boundary conditions:

$$Q_F = z$$
$$Q_O = 1 - z.$$

The SLFM model converges to the slow chemistry approximation.

- The fast chemistry case.

First of all, eliminate Q_O. Use $\langle z | z = n\rangle = n$ on

$z = \dfrac{rY_F - Y_O + 1}{r+1}$, for each point in space $\Rightarrow$

$$\Rightarrow \langle z | z = n\rangle = \frac{r\langle Y_F | z = n\rangle - \langle Y_O | z = n\rangle + 1}{r+1} = n \Rightarrow$$

$$\Rightarrow \frac{rQ_F - Q_O + 1}{r+1} = z \Rightarrow \underline{Q_O(z,t) = rQ_F(z,t) + 1 - (r+1)z.}$$

The ODE becomes : $\tilde{N}\dfrac{\partial^2 Q_F}{\partial Z^2} = -A Q_F\left(r Q_F + 1 - (r+1)Z\right).$

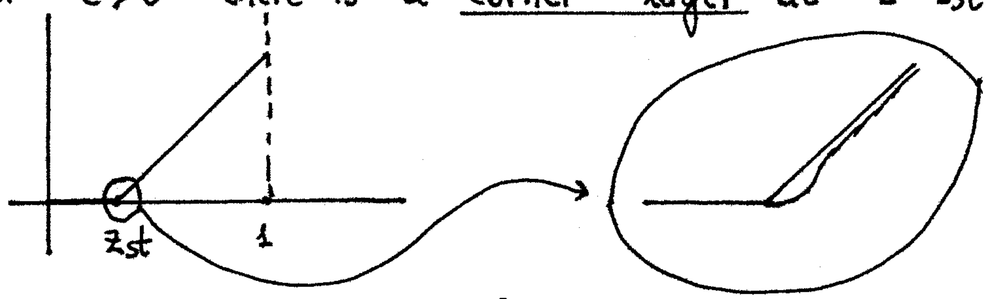
Define $\varepsilon = 1/A$. Then:

$$\varepsilon \tilde{N}\frac{\partial^2 Q_F}{\partial Z^2} = -Q_F\left(r Q_F + 1 - (r+1)Z\right).$$

For $\varepsilon = 0$: $Q_F\left(r Q_F + 1 - (r+1)Z\right) = 0 \rightsquigarrow$ equilibrium chemistry approximation:

$$Q_F(Z) = \frac{Z - Z_{st}}{1 - Z_{st}}\, H(Z - Z_{st}). = Q_F^{eq}(Z)$$

For $\varepsilon > 0$ there is a corner layer at $Z = Z_{st}$



and $$Q_F(Z) = Q_F^{eq}(Z) + \underbrace{\delta(\varepsilon)\, y_1(Z) + \delta^2(\varepsilon)\, y_2(Z) + O(\delta^3)}_{\text{corner layer terms that smooth the corner at } Z = Z_{st}}.$$

Physically, the corner layer corresponds to the thin reaction zone and

$\delta(\varepsilon)$ = thickness of the reaction zone given reaction rate $A = 1/\varepsilon$.

To obtain the behaviour in that zone we must map
$Z_{st} - \delta < Z < Z_{st} + \delta \rightsquigarrow -(\text{big}) < \xi < +(\text{big})$.

Define $\xi = \dfrac{1}{\delta}(Z - Z_{st})$.

Then : $\dfrac{\partial Q_F}{\partial Z} = \dfrac{\partial Q_F}{\partial \xi}\dfrac{\partial \xi}{\partial Z} = \dfrac{1}{\delta}\dfrac{\partial Q_F}{\partial \xi} \Longrightarrow \dfrac{\partial^2 Q_F}{\partial Z^2} = \dfrac{1}{\delta^2}\dfrac{\partial^2 Q_F}{\partial \xi^2}$

and $Z = Z_{st} + \delta\xi$. Substitute to the ODE :

$$\frac{\varepsilon \tilde{N}}{\delta^2(\varepsilon)}\frac{\partial^2 Q_F}{\partial \xi^2} = -Q_F\left[r Q_F + 1 - (r+1)\left(Z_{st} + \delta(\varepsilon)\xi\right)\right] \quad \text{as} \quad \varepsilon \to 0^+$$

Note that

$$1-(r+1)Z_{st} = 1-(r+1)\frac{1}{r+1} = 1-1=0.$$

so the ODE simplifies to:

$$\frac{\varepsilon\tilde{N}}{\delta^2(\varepsilon)}\frac{\partial^2 Q_F}{\partial \xi^2} = -Q_F\left[rQ_F-(r+1)\delta(\varepsilon)\xi\right]$$

The solution is:

$$Q_F(\xi;\varepsilon) = y_0(\xi) + \delta(\varepsilon)y_1(\xi) + O(\delta^2).$$

For $\varepsilon = 0 \Rightarrow \delta(\varepsilon)=0 \Rightarrow Q_F(\xi;0) = y_0(\xi)$
also $Q_F(\xi,0) = Q_F^{eq}(Z_{st}+\delta(\varepsilon)\xi) = Q_F^{eq}(Z_{st}) = 0$ $\Big\}\Rightarrow$

$\Rightarrow y_0(\xi) = 0. \Rightarrow Q_F(\xi;\varepsilon) = \delta(\varepsilon)y_1(\xi) + O(\delta^2).$

Substitute to the ODE:

$$\cancel{\frac{\varepsilon\tilde{N}}{\delta^2}\frac{\partial^2 Q_F}{\partial\xi^2}} =$$

$$\frac{\varepsilon N}{\delta^2}\frac{\partial^2(\delta y_1)}{\partial\xi^2} = -\delta y_1\left[r\delta y_1-(r+1)\delta\xi\right] + O(\delta^3) \Leftrightarrow$$

$$\Leftrightarrow \frac{\varepsilon N}{\delta^2}\frac{\partial^2 y_1}{\partial\xi^2} = -y_1\left[r\delta y_1-(r+1)\delta\xi\right] + O(\delta^2) \Leftrightarrow$$

$$\Leftrightarrow \frac{\varepsilon N}{\delta^3}\frac{\partial^2 y_1}{\partial\xi^2} = -ry_1^2 + (r+1)\xi y_1$$

The RHS has finite value as $\varepsilon\to 0$ therefore so must the LHS:

$$\frac{\partial^2 y_1}{\partial\xi^2} \sim \frac{\delta^3}{\varepsilon N}$$

Recall that δ is the thickness of reaction zone $\Rightarrow \partial^2 y_1/\partial\xi^2$ has order 1 values and:

$$\frac{\delta^3}{\varepsilon N} \sim 1 \Leftrightarrow \delta^3 \sim \varepsilon N \Leftrightarrow \delta \sim (\varepsilon N)^{1/3}.$$

It follows from this result that
at $\xi = 0$ $(Z=Z_{st})$: $Q_F \sim \delta(\varepsilon)y_1(0) \sim (\varepsilon N_{st})^{1/3} \sim (N_{st}/A)^{1/3}$.

We define the local Damköhler number from this result:

$$Da_s(t) = \frac{1-Z_{st}}{Z_{st}}\frac{A}{N_{st}(t)}.$$

Purely for convenience we write:

$$Q_F(Z_{st}) \sim \left[\frac{Z_{st}}{1-Z_{st}}\,\frac{N_{st}}{A}\right]^{1/3}.$$

We define the local Damköhler number to be:

$$Da_s(t) = \frac{1-Z_{st}}{Z_{st}}\,\frac{A}{N_{st}(t)}$$

Then it follows that

$$\cancel{Q_F(Z_{st}) \sim Da_s(t)}$$
$$\cancel{Q_F(Z_{st},t) \sim Da_s(t)}^{-1/3}.$$

$$\boxed{Q_F(Z_{st},t) \sim Da_s(t)^{-1/3}}$$

~~We also obtain~~

The Quasi-steady state condition.

$$a = \frac{1}{A Q_F Q_0} \frac{\partial Q_F}{\partial t} \ll 1.$$

Local Damköhler number $Da_s(t) = \frac{1-Z_{st}}{Z_{st}} \frac{A}{N_{st}(t)}$ where $N_{st}(t) = \tilde{N}(Z_{st}, t)$.

(derivation ?).

Check consistency with asymptotic approximation of the quasi-state solution. (dominant balance).

This is given by: $Q_F(Z_{st}, t) = Da_s(t)^{-1/3}$. (derivation ?).

$$\frac{\partial Da_s}{\partial t} = \frac{1-Z_{st}}{Z_{st}} A \frac{\partial}{\partial t}\left(\frac{1}{N_{st}}\right) = \frac{1-Z_{st}}{Z_{st}} A \left(\frac{-1}{N_{st}^2}\right) \frac{\partial N_{st}}{\partial t} =$$
$$= -\frac{Da_s(t)}{N_{st}(t)} \frac{\partial N_{st}}{\partial t}$$

therefore,

$$\left.\frac{\partial Q_F}{\partial t}\right|_{Z=Z_{st}} = (-1/3)\, Da_s^{-4/3}(t) \frac{\partial Da_s}{\partial t} =$$
$$= (-1/3)\, Da_s^{-4/3}(t) \left[-\frac{Da_s(t)}{N_{st}(t)} \frac{\partial N_{st}}{\partial t}\right]$$
$$= \frac{1}{3} \frac{Da_s^{-1/3}}{N_{st}} \frac{\partial N_{st}}{\partial t}$$

Also $A Q_F Q_0 = rA\, Da_s^{-2/3}(t)$. , so we obtain:

$$a = \frac{1}{A Q_F Q_0} \frac{\partial Q_F}{\partial t} = \frac{1}{rA\, Da_s^{-2/3}(t)} \frac{Da_s^{-1/3}}{N_{st}} \frac{\partial N_{st}}{\partial t} =$$
$$= \frac{1}{rA\, Da_s^{-1/3}(t)} \frac{1}{N_{st}} \frac{\partial N_{st}}{\partial t} =$$
$$= \frac{1}{r\, Da_s^{-1/3}(t)} \frac{N_{st}}{A} \frac{1}{N_{st}^2} \frac{\partial N_{st}}{\partial t} = \qquad Da_s(t) = \frac{1-Z_{st}}{Z_{st}} \frac{A}{N_{st}(t)}$$
$$= \frac{1}{r\, Da_s^{-1/3}(t)} \frac{1-Z_{st}}{Z_{st}} \frac{1}{Da_s(t)} \frac{1}{N_{st}^2} \frac{\partial N_{st}}{\partial t} =$$
$$= \frac{1-Z_{st}}{r Z_{st}} \frac{1}{Da_s^{2/3}(t)} \frac{1}{N_{st}^2} \frac{\partial N_{st}}{\partial t}$$

and $Z_{st} = \frac{1}{r+1} \Rightarrow \frac{1-Z_{st}}{r Z_{st}} = 1$ (wow!).

therefore: $$a = \frac{1}{Da_s^{2/3}(t)} \frac{1}{N_{st}^2} \frac{\partial N_{st}}{\partial t} \ll 1$$
must be true in order for the quasi-steady equation to be a dominant balance.

Under this condition:

$$\boxed{\begin{aligned} \tilde{N}(z,t)\frac{\partial^2 Q_F}{\partial z^2} &= -A Q_F Q_0 \\ \tilde{N}(z,t)\frac{\partial^2 Q_0}{\partial z^2} &= -rA Q_F Q_0 . \end{aligned}}$$