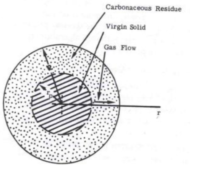
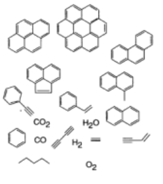
Chapitre VI

Combustion des Matériaux Solides

Applications industrielles

Transition du gaz en particules des suies





Phase hétérogène

$$C + O_2 \rightarrow CO_2$$
$$C + 0.5O_2 \rightarrow CO$$
$$C + CO_2 \rightarrow 2CO$$
$$C + H_2O \rightarrow CO + H_2$$

Phase homogène

$$CO + 0.5O_2 \rightarrow CO_2$$
$$CO + H_2O \rightarrow CO_2 + H_2$$
$$CO_2 + H_2 \rightarrow CO + H_2O$$

Modèle à un film

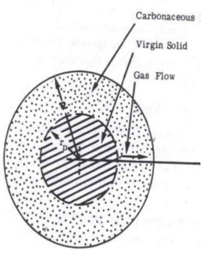
Hypothèses :

1) Flamme de diffusion sphérique symétrique

2) Le nombre de Lewis : $Le = \frac{\alpha}{D_{ox}} = \frac{k_g / \rho C_{pg}}{D_{ox}} = 1$

3) Propriétés constantes : k_g, C_{pg} et ρD_{ox} (diffusivité d'oxydant)

4) Phénomène stationnaire



Position du problème

Vitesse de la combustion de carbone: $\dot{m}_c \,(kg/s)$

3

Combustion de carbone

Réaction chimique infiniment rapide et flamme mince à la surface

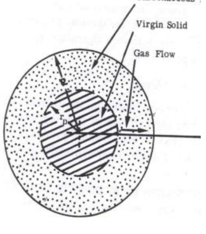
Compétition entre le transport et la cinétique chimique

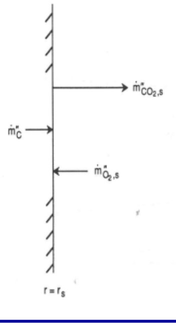
$C + \nu O_2 \rightarrow (1+\nu) CO_2$

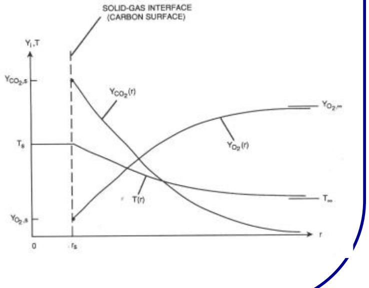
$\nu = \frac{MW_{O2}}{MW_C} = \frac{32}{12} = 2.664$

$\dot{m}_{O2} = \nu \dot{m}_C$

$\dot{m}_{CO2} = (1+\nu)\dot{m}_C$





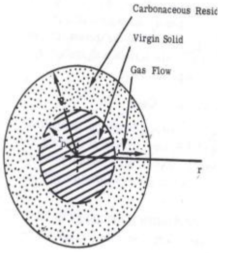


4

1) Vitesse de la combustion de carbone contrôlée par le transport

Conservation de la masse

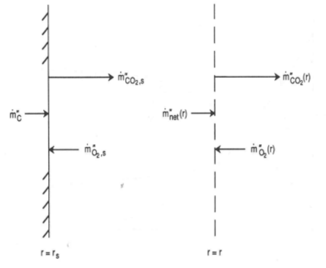
$$\dot{m}'' r^2 = \dot{m}''_c r_s^2 = \text{cons tan t}$$



Conservation de l'oxygène (opposé à r)

$$\frac{d}{dr} r^2 \rho_g D_{ox} \frac{dY_{O2}}{dr} - [\dot{m}'' r^2] \frac{dY_{O2}}{dr} = 0$$

$$r^2 \rho_g D_{ox} \frac{dY_{O2}}{dr} - [\dot{m}'' r^2] Y_{O2} = C$$

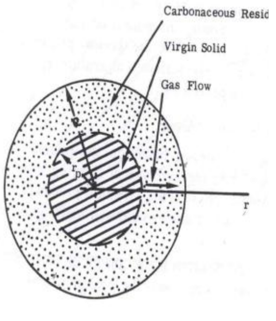


Conditions aux limites : $r \rightarrow r_s$

$$C = r_s^2 \rho_g D_{ox} \left.\frac{dY_{O2}}{dr}\right|_s - \dot{m}''_C r_s^2 Y_{O2,s}$$

Loi de Fick (à la surface de carbone)

$$\dot{m}''_{O2,s} r_s^2 = r_s^2 \rho_g D_{ox} \left.\frac{dY_{O2}}{dr}\right|_s - \dot{m}''_C r_s^2 Y_{O2,s}$$



Réaction chimique infiniment rapide

$$\dot{m}''_{O2,s} = \nu \dot{m}''_C$$

$$\nu \dot{m}''_c r_s^2 = r_s^2 \rho_g D_{ox} \left.\frac{dY_{O2}}{dr}\right|_s - \dot{m}''_C r_s^2 Y_{O2,s}$$

$$C = \nu \dot{m}''_c r_s^2$$

$$r^2 \rho_g D_{ox} \frac{dY_{O2}}{dr} - [\dot{m}''_C r_s^2] Y_{O2} = \nu \dot{m}''_C r_s^2$$

$$r^2\rho_g D_{ox}\frac{dY_{O2}}{dr}-\left[\dot m_C'' r_s^2\right](Y_{O2}+\nu)=0$$

$$\ln(Y_{O2}+\nu)=-\frac{\left[\dot m_C'' r_s^2\right]}{\rho_g D_{ox}}\cdot\frac{1}{r}+C$$

Conditions aux limites : $\left.\begin{array}{l} r\to\infty \\ Y_{O2}\to Y_{O2,\infty}\end{array}\right\} \Rightarrow \quad C$

$$\ln\left(\frac{Y_{O2}+\nu}{Y_{O2,\infty}+\nu}\right)=-\frac{\left[\dot m_C'' r_s^2\right]}{\rho_g D_{ox}}\cdot\frac{1}{r}$$

Conditions aux limites : $r\to r_s, \quad Y_{O2}\to Y_{O2,s}$

$$\frac{\dot m_C'' r_s}{\rho_g D_{ox}}=\ln\left(\frac{Y_{O2,\infty}+\nu}{Y_{O2,s}+\nu}\right) \quad\Rightarrow\quad \dot m_C''=\frac{\rho_g D_{ox}}{r_s}\ln\left(\frac{Y_{O2,\infty}+\nu}{Y_{O2,s}+\nu}\right) \qquad (kg/m^2 s)$$

$$\dot m_C=4\pi r_s\rho D_{ox}\ln\left(\frac{1+Y_{O2,\infty}/\nu}{1+Y_{O2,s}/\nu}\right) \qquad (kg/s)$$

7

$$\dot m_C=4\pi r_s\rho D_{ox}\ln\left(1+\frac{Y_{O2,\infty}-Y_{O2,s}}{\nu+Y_{O2,s}}\right)$$

$$B_{O,m}\equiv\frac{Y_{O2,\infty}-Y_{O2,s}}{\nu+Y_{O2,s}} \qquad\qquad \dot m_C=4\pi r_s\rho D_{ox}\ln\left(1+B_{O,m}\right)$$

Terme du logarithme

$$\ln\left(1+B_{O,m}\right)=B_{O,m}-\frac{1}{2}B_{O,m}^2+\frac{1}{3}B_{O,m}^2-\ldots$$

$$\ln\left(1+B_{O,m}\right)\approx B_{O,m} \qquad (\text{si } B_{0,m} \text{ est petit})$$

$$\dot m_C=4\pi r_s\rho D_{ox}\left(\frac{Y_{O2,\infty}-Y_{O2,s}}{\nu+Y_{O2,s}}\right)=\frac{(Y_{O2,\infty}-Y_{O2,s})}{\left(\dfrac{\nu+Y_{O2,s}}{4\pi r_s\rho D_{ox}}\right)}\equiv\frac{\Delta Y}{R_{diff}}$$

Résistance diffusive : $R_{diff}=\dfrac{\nu+Y_{O2,s}}{4\pi r_s\rho D_{ox}}$

8

2) Vitesse de la combustion de carbone contrôlée par la cinétique chimique

$$C + O_2 \rightarrow CO_2$$

Taux de réaction chimique: $\dot{m}''_C = k_c MW_C [O_{2,s}]$

Constante de vitesse sous forme d'Arrhenius : $k_c = A \exp[-E_A / R_u T_s]$

$$[O_{2,s}] = \frac{\rho}{MW_{O2}} Y_{O2,s} = \frac{MW_{mix}}{MW_{O2}} \frac{P}{R_u T_s} Y_{O2,s} \qquad (kmol/m^3)$$

$$\dot{m}_C = 4\pi r_s^2 k_c \frac{MW_C MW_{mix}}{MW_{O2}} \frac{P}{R_u T_s} Y_{O2,s}$$

$$\dot{m}_C = K_{kin} Y_{O2,s} \qquad \Rightarrow \qquad \dot{m}_C = \frac{Y_{O2,s} - 0}{1/K_{kin}} \equiv \frac{\Delta Y}{R_{kin}}$$

$$R_{kin}\ (\text{résistance}) = \frac{1}{K_{kin}\ (\text{cinétique})} = \frac{\nu R_u T_s}{4\pi r_s^2 MW_{mix} k_c P} \qquad \nu = \frac{MW_{O2}}{MW_C}$$

Analogie électrique

$$R_{diff} = \frac{\nu + Y_{O2,s}}{4\pi r_s \rho D_{ox}} \qquad R_{kin} = \frac{\nu R_u T_s}{4\pi r_s^2 MW_{mix} k_c P}$$

$$\dot{m}_C = \frac{(Y_{O2,\infty} - Y_{O2,s})}{R_{diff}} \qquad \dot{m}_C = \frac{Y_{O2,s} - 0}{R_{kin}}$$

$$\dot{m}_C = \frac{Y_{O2,\infty} - 0}{R_{diff} + R_{kin}}$$

Compétition entre le transport et la cinétique chimique

$$\frac{R_{kin}}{R_{diff}} = \left(\frac{\nu}{\nu + Y_{O2,s}}\right)\left(\frac{R_u T_s}{MW_{mix} P}\right)\left(\frac{\rho D_{ox}}{k_c}\right)\left(\frac{1}{r_s}\right)$$

$$\frac{R_{kin}}{R_{diff}} << 1 \quad \Rightarrow \quad \dot{m}_C = \frac{Y_{O2,\infty}}{R_{diff}} \qquad (T_s \uparrow \Rightarrow k_c \uparrow,\ r_s \uparrow,\ P \uparrow)$$

$$\frac{R_{kin}}{R_{diff}} \approx 1 \quad \Rightarrow \quad \dot{m}_C = \frac{Y_{O2,\infty}}{R_{diff} + R_{kin}}$$

$$\frac{R_{kin}}{R_{diff}} >> 1 \quad \Rightarrow \quad \dot{m}_C = \frac{Y_{O2,\infty}}{R_{kin}} \qquad (T_s \downarrow \Rightarrow k_c \downarrow,\ r_s \downarrow, P \downarrow)$$

11

Méthode itérative

1) En supposant $Y_{O2,s}$=0

$$R_{diff} = \frac{\nu + Y_{O2,s}}{4\pi r_s \rho D_{ox}}$$

$$R_{kin} = \frac{\nu R_u T_s}{4\pi r_s^2 MW_{mix} k_c P}$$

$$\dot{m}_C = \frac{Y_{O2,\infty} - 0}{R_{diff} + R_{kin}}$$

2) Combustion contrôlée par la cinétique $\Rightarrow \quad Y_{O2,s} = \dot{m}_C R_{kin}$

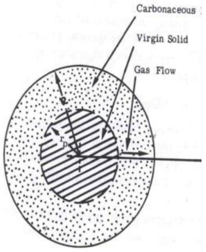
$$R_{diff,\,n+1} = \frac{(\nu+Y_{O2,s})_{n+1}}{(\nu+Y_{O2,s})_n}\frac{(\nu+Y_{O2,s})_n}{4\pi r_s \rho D_{ox}} = \frac{(\nu+Y_{O2,s})_{n+1}}{(\nu+Y_{O2,s})_n} R_{diff,\,n}$$

$$\frac{\dot{m}_{C,n+1} - \dot{m}_{C,n}}{\dot{m}_{C,n}} \le \varepsilon\% \ (\varepsilon \approx 1) \qquad \Rightarrow \quad \text{solution finale}$$

12

Equation de l’énergie (Shvab-Zeldovich)

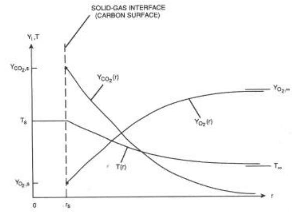
$$\frac{d}{dr} r^2 k_g \frac{dT}{dr} - [\dot{m}'' r^2] C_{pg} \frac{dT}{dr} = 0$$



$$\frac{d\left(r^2 \frac{dT}{dr}\right)}{dr} = Z\dot{m} \frac{dT}{dr} \qquad Z \equiv \frac{C_{pg}}{4\pi k_g}$$

Conditions aux limites

$$\left.\begin{aligned} r = r_s, \quad T = T_s \\ r \rightarrow \infty, \ T = T_\infty \end{aligned}\right\} \Rightarrow \qquad T(r)$$



$$\left.\frac{dT}{dr}\right|_{r=r_s} = \frac{Z\dot{m}_C}{r_s^2}\left[\frac{(T_\infty - T_s)\exp\left(-Z\dot{m}_C / r_s\right)}{1 - \exp\left(-Z\dot{m}_C / r_s\right)}\right]$$

13

Bilan d’énergie à la surface d’une particule

$$\dot{m}_C h_C + \dot{m}_{O2} h_{O2} - \dot{m}_{CO2} h_{CO2} = \dot{Q}_{s-i} + \dot{Q}_{s-f} + \dot{Q}_{rad}$$

$$\dot{m}_{O2} = \nu \dot{m}_C$$

$$\dot{m}_{CO2} = (1+\nu)\dot{m}_C$$

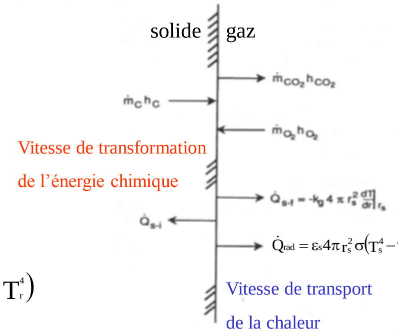
$$h = h_f^0 + C_p \Delta T$$

$$\dot{m}_C h_C + \dot{m}_{O2} h_{O2} - \dot{m}_{CO2} h_{CO2} = \dot{m}_C\left[h_{f,C}^0 + \nu\, h_{f,O2}^0 - (1+\nu)\, h_{f,CO2}^0\right]$$

$$\dot{Q}_{s-i} = 0 \text{ (inertie thermique)}$$

$$\dot{Q}_{s-f} = -k_g 4\pi r_s^2 \left.\frac{dT}{dr}\right|_{r=r_s}$$

$$\dot{Q}_{rad} = \varepsilon_s 4\pi r_s^2 \sigma\left(T_s^4 - T_r^4\right)$$



$$\dot{m}_C \Delta h_C = -k_g 4\pi r_s^2 \left.\frac{dT}{dr}\right|_{r=r_s} + \varepsilon_s 4\pi r_s^2 \sigma\left(T_s^4 - T_r^4\right)$$

14

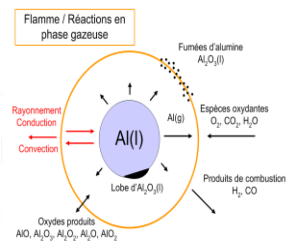
$$\dot{m}_C \Delta h_C = \dot{m}_C C_{pg}\left[\frac{\exp\left(\frac{-\dot{m}_C C_{pg}}{4\pi k_g r_s}\right)}{1-\exp\left(\frac{-\dot{m}_C C_{pg}}{4\pi k_g r_s}\right)}\right](T_s - T_\infty) + \varepsilon_s 4\pi r_s^2 \sigma\left(T_s^4 - T_r^4\right)$$

Application à la combustion d'une particule des métaux (Aluminium, etc.)

Réaction chimique à une étape

$$Al + \frac{3}{4}O_2 \rightarrow \frac{1}{2}Al_2O_3$$

$$\left.\begin{matrix}\dot{m}_c \\ T_s \\ T_r\end{matrix}\right\} \text{connus} \quad \Rightarrow \quad T_\infty \text{ (milieu réactif)}$$



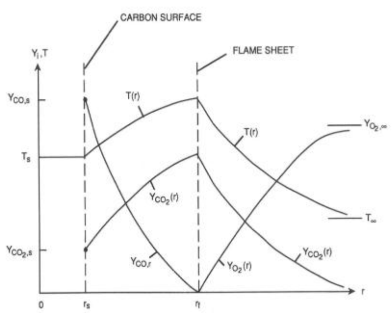
15

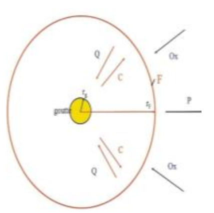
Modèle à deux films

Zone 1) à la surface de particule (CO)

Zone 2) à la flamme (CO_2)

On doit disposer d'autant d'équations que d'inconnues $\left\{\begin{matrix}\dot{m}_C \\ r_f \\ Y_{CO2,s} \\ Y_{CO2,f} \\ Y_{I,f}\end{matrix}\right. \quad \Rightarrow \quad D^2(t)$





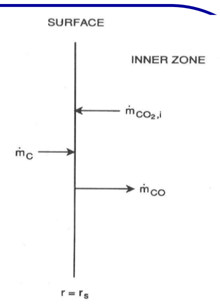
16

Zone 1) à la surface de particule $(C + CO_2 \rightarrow 2CO)$

$$1\_kg\,C + \nu_s\_kg\,CO_2 \rightarrow (\nu_s + 1)\_kg\,CO$$

$$\nu_s = 44/12 = 3.664$$

$$\dot{m}_C = \dot{m}_{CO} - \dot{m}_{CO2,\,i}$$



Zone 2) à la flamme $\begin{pmatrix} C + 0.5O_2 \rightarrow CO \\ CO + 0.5O_2 \rightarrow CO_2 \end{pmatrix}$

$$1\_kg\,C + \nu_f\_kg\,O_2 \rightarrow (\nu_f + 1)\_kg\,CO_2$$

$$\nu_f = \nu_s - 1$$

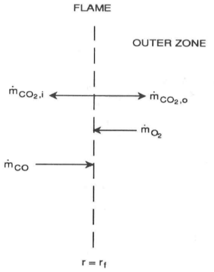
$$\dot{m}_{CO} - \dot{m}_{CO2,\,i} = \dot{m}_{CO2,\,o} - \dot{m}_{O2}$$

ou $\quad \dot{m}_C = \dot{m}_{CO2,\,o} - \dot{m}_{O2}$

$$\dot{m}_{CO2,\,i} = \nu_s \dot{m}_C$$

$$\dot{m}_{O2} = \nu_f \dot{m}_C = (\nu_s - 1)\dot{m}_C$$

$$\dot{m}_{CO2,\,o} = (\nu_f + 1)\dot{m}_C = \nu_s \dot{m}_C$$



17

Conservation de l'espèce chimique, CO_2 (Loi de Fick)

Equation 1) Zone interne de CO_2

$$-\dot{m}_{CO2,\,i} = Y_{CO2}(-\dot{m}_{CO2,\,i} + \dot{m}_{CO}) - 4\pi r^2 \rho D_{ox} \frac{d(Y_{CO2})}{dr}$$

$$\dot{m}_{CO2,\,i} = \nu_s \dot{m}_C$$

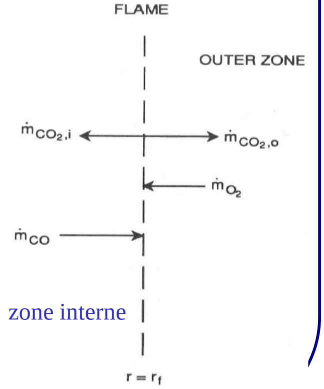
$$\dot{m}_{CO} = (1 + \nu_s)\dot{m}_C \qquad \Leftarrow \dot{m}_{CO} = \dot{m}_{CO2,\,i} + \dot{m}_{CO2,\,o} - \dot{m}_{O2}$$

$$\dot{m}_C = \frac{4\pi r^2 \rho D_{ox}}{(1 + Y_{CO2}/\nu_s)} \frac{d(Y_{CO2}/\nu_s)}{dr}$$

Conditions aux limites :

$$Y_{CO2}(r \rightarrow r_s) = Y_{CO2,\,s}$$

$$Y_{CO2}(r \rightarrow r_f) = Y_{CO2,\,f}$$



18

Equation 2) Zone externe de CO_2

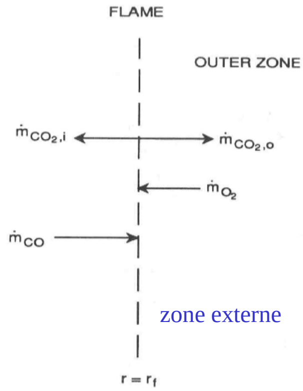
$$\dot{m}_{CO2,o} = Y_{CO2}(\dot{m}_{CO2,o} - \dot{m}_{O2}) - 4\pi r^2 \rho D_{ox} \frac{d(Y_{CO2})}{dr}$$

$$\dot{m}_{O2} = \nu_f \dot{m}_C = (\nu_s - 1)\dot{m}_C$$
$$\dot{m}_{CO2,o} = (\nu_f + 1)\dot{m}_C = \nu_s \dot{m}_C$$

$$\dot{m}_C = \frac{-4\pi r^2 \rho D_{ox}}{(1 - Y_{CO2}/\nu_s)} \frac{d(Y_{CO2}/\nu_s)}{dr}$$

Conditions aux limites :

$$Y_{CO2}(r \to r_f) = Y_{CO2,f}$$
$$Y_{CO2}(r \to \infty) = 0$$



Equation 3) Conservation de l'espèce inerte, N_2

$$\left.\begin{aligned}
\dot{m}_C &= \frac{4\pi r^2 \rho D_{ox}}{(1 + Y_{CO2,i}/\nu_s)} \frac{d(Y_{CO2,i}/\nu_s)}{dr} \\
\dot{m}_C &= \frac{-4\pi r^2 \rho D_{ox}}{(1 - Y_{CO2,o}/\nu_s)} \frac{d(Y_{CO2,o}/\nu_s)}{dr} \\
Y_{CO2,i} + Y_{CO2,o} &= 1 - Y_{CO2,f} = Y_I
\end{aligned}\right\} \Rightarrow \dot{m}_C = \frac{4\pi r^2 \rho D_{ox}}{Y_I} \frac{d(Y_I)}{dr}$$

Conditions aux limites

$$Y_I(r \to r_f) = Y_{I,f}$$
$$Y_I(r \to \infty) = Y_{I,\infty}$$

Equation 4) $\quad Y_{CO2,f} = 1 - Y_{I,f}$

Equation 5) Cinétique chimique à la surface pour la clôture

$$C + CO_2 \rightarrow 2CO$$

$$\dot{m}_C'' = k_c MW_C [CO_{2,s}]$$

$$[CO_{2,s}] = \frac{\rho}{MW_{CO2}} Y_{CO2,s} = \frac{MW_{mix}}{MW_{CO2}} \frac{P}{R_u T_s} Y_{CO2,s} \quad (kmol/m^3)$$

Constante de vitesse sous forme d'Arrhenius

$$k_c(m/s) = 4.016 \times 10^8 \exp\left[\frac{-29790}{T_s(K)}\right]$$

$$\dot{m}_C = 4\pi r_s^2 k_c \frac{MW_C MW_{mix}}{MW_{CO2}} \frac{P}{R_u T_s} Y_{CO2,s} \quad \Rightarrow \quad \dot{m}_c = f(Y_{CO2,s})$$

Expression compacte

$$\dot{m}_C = K_{kin} Y_{CO2,s} \quad \text{avec} \quad K_{kin} = 4\pi r_s^2 k_c \frac{MW_C MW_{mix}}{MW_{CO2}} \frac{P}{R_u T_s}$$

21

Eq.(1) $\dot{m}_C = 4\pi \left(\frac{r_s r_f}{r_f - r_s}\right) \rho D_{ox} \ln\left(\frac{1 + Y_{CO2,f}/\nu_s}{1 + Y_{CO2,s}/\nu_s}\right)$

Eq.(2) $\dot{m}_C = -4\pi r_f \rho D_{ox} \ln(1 - Y_{CO2,f}/\nu_s)$

Eq.(3) $\dot{m}_C = K_{kin} Y_{CO2,s}$

Eq.(4) $Y_{I,f} = Y_{I,\infty} \exp(-\dot{m}_C / 4\pi r_f \rho D_{ox}) = (1 - Y_{O2,\infty}) \exp(-\dot{m}_C / 4\pi r_f \rho D_{ox})$

Eq.(5) $Y_{CO2,f} = 1 - Y_{I,f}$

$$\left\{ \begin{array}{l} \dot{m}_C \\ r_f \\ Y_{CO2,s} \\ Y_{CO2,f} \\ Y_{I,f} \end{array} \right.$$

Solution du problème ($Y_{CO2,s}$ connue)

Vitesse de combustion : $\dot{m}_C = 4\pi r_s \rho D_{ox} \ln(1 + B_{CO2,m})$

Nombre de transfert de masse : $B_{CO2,m} = \frac{2Y_{O2,\infty} - [(\nu_s - 1)/\nu_s] Y_{CO2,s}}{\nu_s - 1 + [(\nu_s - 1)/\nu_s] Y_{CO2,s}}$

22

Méthode itérative

1) Vitesse de combustion contrôlée par la diffusion

$Y_{CO2,s}=0$

2) Potentiel du transfert

$$B_{CO2,\,m}=\frac{2Y_{O2,\,\infty}-[(\nu_s-1)/\nu_s]Y_{CO2,\,s}}{\nu_s-1+[(\nu_s-1)/\nu_s]Y_{CO2,\,s}}$$

3) Conservation de l'espèce chimique

$$\dot{m}_C=4\pi r_s\rho D_{ox}\ln(1+B_{CO2,\,m})$$

4) Cinétique chimique

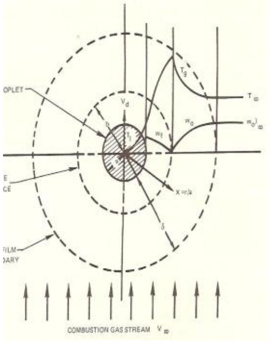
$$Y_{CO2,\,s}=\frac{\dot{m}_C}{K_{kin}}$$

$$\frac{\dot{m}_{C,n+1}-\dot{m}_{C,n}}{\dot{m}_{C,n}}\le\varepsilon\%\ (\varepsilon\approx1)\qquad\Rightarrow\quad \text{solution finale}$$

23

Cas des environnements convectifs

$$\begin{cases} Nu=2+0.6\,Re^{1/2}\,Pr^{1/3} \\ Re=\dfrac{\rho|u_s-u_g|2r_s}{\mu} \end{cases}$$



Cas du milieu au repos : Nu=2

$$\dot{m}_{C,\,conv}=\frac{Nu}{2}\dot{m}_C$$

24

Temps de vie des particules solides

$$D^2(t) = D_0^2 - K_B t$$

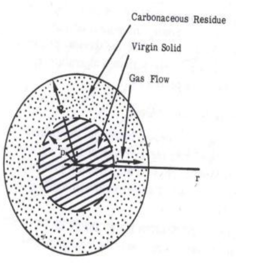
Constante de gazéification

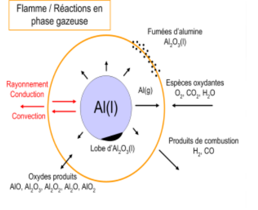
$$K_B = \frac{8\rho D_{ox}}{\rho_s} \ln(1 + B)$$

$B = B_{o,m}$ ou $B_{CO2,m}$

$$t_{gazéif} = \frac{D_0^2}{K_B}$$

$$t_{tot} = t_{gazéif} + t_{pré} \approx \frac{D_0^2}{K_B} + \left[\frac{\rho_s C_{ps}}{12 k_g} \ln\left(\frac{T_f - T_0}{T_f - T_s}\right)\right] D_0^2$$





25