Solid Fuel Combustion

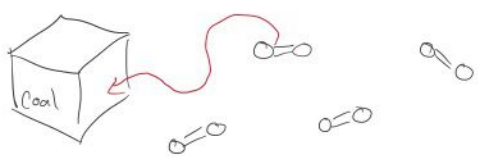
Tuesday, November 14, 2017 3:04 PM

2 rxn mechanisms:

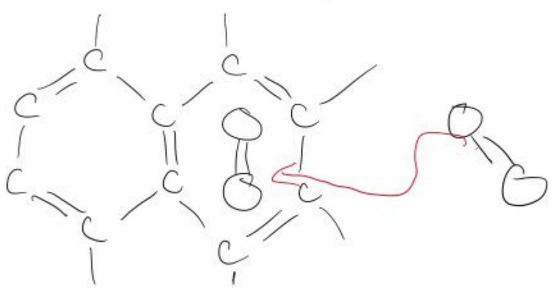
1) <u>Catalysis</u>

<u>homogeneous rxns:</u> rxns that occur in a single phase

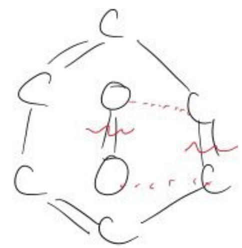
<u>heterogeneous rxn:</u> rxns that occur over 2 physical states. e.g. gas-liquid, gas-solid



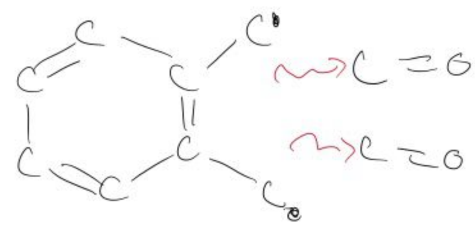
i) transport of rxt molecule to the surface by convection and/or diffusion



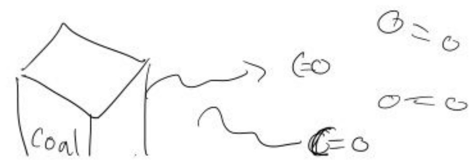
2) adsorption of the rxt molecule on surface



3) elementary rxn steps involving combos of adsorbed molecules, the surface, & gas molecules



4) desorption of product molecules from surface



O=C

5) transport of product molecules from surface by convection and/or diffusion

rate laws:

if rxt A is weakly adsorbed

$$R = k(T)[A]$$

if rxt A is strongly adsorbed

$$R = k(T)$$

if rxt A is weakly adsorbed AND product B is strongly adsorbed

$$R = k(T)\frac{[A]}{[B]}$$

carbon burns via

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

$$CO + \tfrac{1}{2}O_2 \rightarrow CO_2 \quad \text{(global)}$$

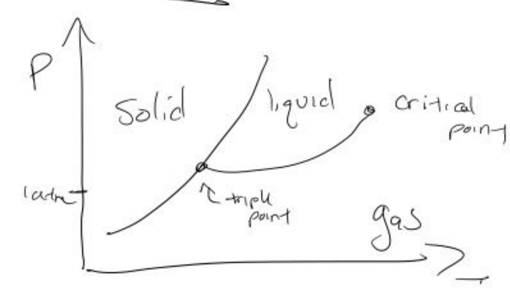
elementary steps

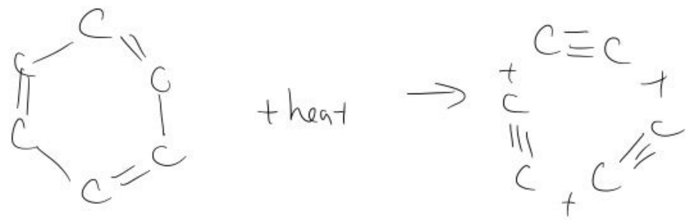
$$H_2 \rightarrow H + H$$
$$O_2 \rightarrow O + O$$
$$O + H_2 \rightarrow OH + H$$
$$H + O_2 \rightarrow OH + O$$
$$CO + O_2 \rightarrow CO_2 + O$$
$$O + H_2O \rightarrow OH + OH$$
$$\boxed{CO + OH \rightarrow CO_2 + H}$$
$$OH + H_2 \rightarrow H_2O + H$$

	ΔH_f (kJ/kmol)
CO_2	-393546
CO	-110541
OH	38985
H	217977

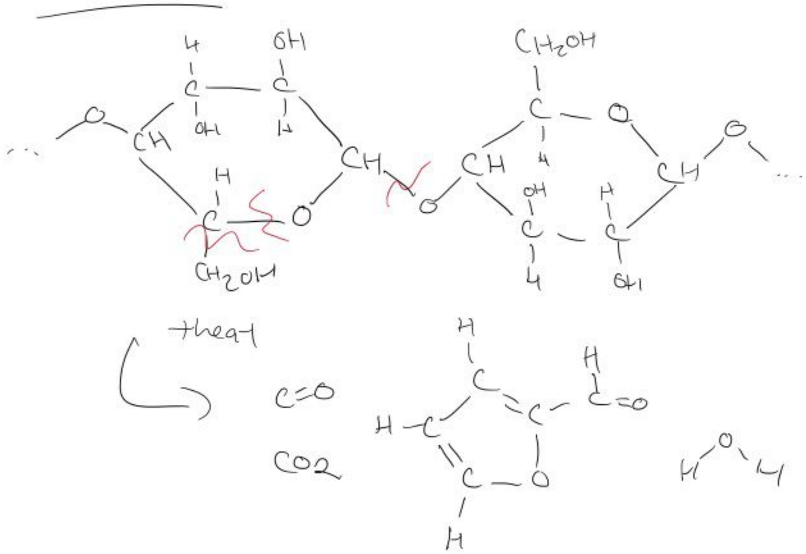
$\Delta H_{rxn} = -104013$ kJ/kmol

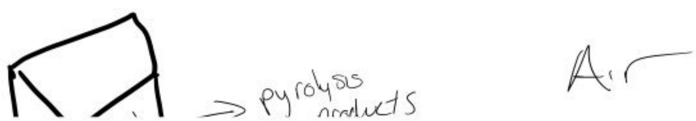
2) pyrolysis

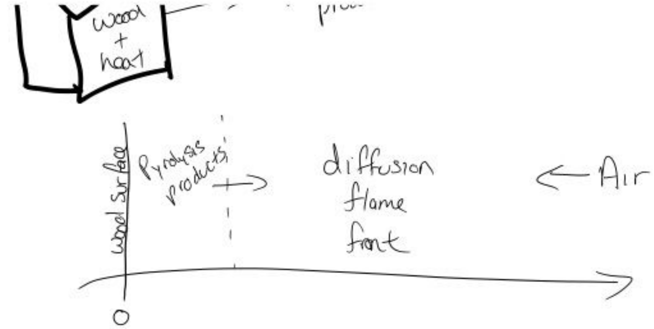




for wood:







One-film model

Assumptions

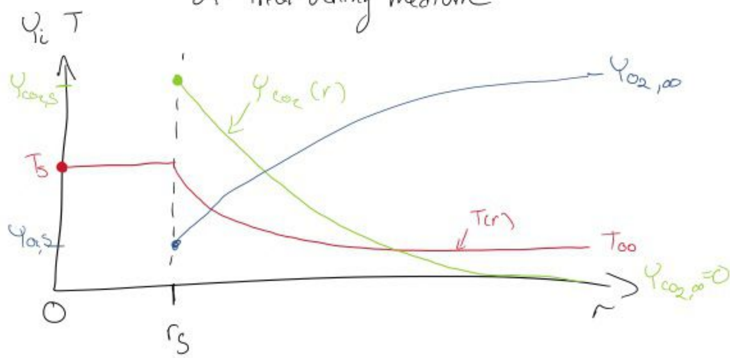
1) burning process is quasi-steady
2) Spherical carbon particles burning in a quiescent, infinite ambient medium that only contains O_2 & inert gas. No interactions w/ other particles. no convection
3) Carbon reacts w/ O_2 to produce CO_2 ($C + O_2 \rightarrow CO_2$).
4) gas phase only has O_2, CO_2 & inerts. O_2 diffuses inward. CO_2 diffuses outward. inerts form stagnant layer (Stefan problem)

5) k, c_p, ρ, D_{AB} all constant

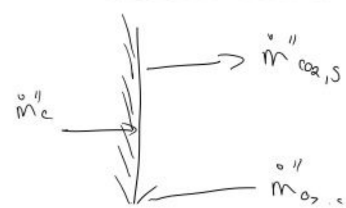
$$Le = k/(\rho c_p D) = 1$$

6) carbon particle impervious to gas

7) particle has uniform T & radiates as a grey body to surroundings w/o participation of intervening medium

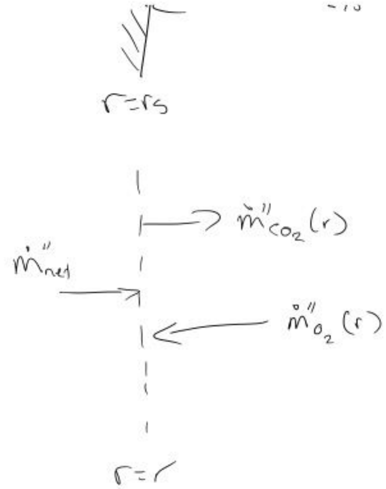


Mass & Species conservation



@ surface

$$\dot{m}''_C = \dot{m}''_{CO_2} - \dot{m}''_{O_2}$$



@ $r > r_s$

$$\dot{m}''_{net}(r) = \dot{m}''_{CO_2} - \dot{m}''_{O_2}$$

mass flow is const.

$$\dot{m}''_{C,s} = \frac{\dot{m}_C}{4\pi r_s^2} = \frac{\dot{m}_{CO_2}}{4\pi r_s^2} - \frac{\dot{m}_{O_2}}{4\pi r_s^2}$$

$$\dot{m}_C = \dot{m}_{CO_2} - \dot{m}_{O_2}$$

$$\dot{m}''_{net}(r) = \frac{\dot{m}_{net}}{\cancel{4\pi r^2}} = \frac{\dot{m}_{CO_2}}{\cancel{4\pi r^2}} - \frac{\dot{m}_{O_2}}{\cancel{4\pi r^2}}$$

$$\dot{m}_{net} = \dot{m}_{CO_2} - \dot{m}_{O_2}$$

$$\dot{m}''_C = \dot{m}''_{net} = \dot{m}''_{CO_2} - \dot{m}''_{O_2}$$

just carbon surface:

$$1C + 1O_2 \rightarrow 1CO_2$$

$$12.01\ kg\ C + 31.999\ kg\ O_2 \rightarrow 44.01\ kg\ CO_2$$

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

$$\nu = \frac{31.999\ kg\ O_2}{12.01\ kg\ C} = 2.664 = \nu_I$$

$$\dot{m}_{O_2} = \nu_I \dot{m}_c$$

$$\dot{m}_{CO_2} = (1+\nu_I)\dot{m}_c$$

Fick Law:

$$\dot{m}''_{O_2} = Y_{O_2}\left(\dot{m}''_{O_2} + \dot{m}''_{CO_2}\right) - \rho D \frac{dY_{O_2}}{dr}$$

$$\dot{m}''_{O_2} = \frac{\dot{m}_{O_2}}{4\pi r^2} = \frac{-\nu_I \dot{m}_c}{4\pi r^2}$$

$$\dot{m}''_{CO_2} = \frac{\dot{m}_{CO_2}}{4\pi r^2} = \frac{\dot{m}_c(\nu_I+1)}{4\pi r^2}$$

$$\frac{-\nu_I \dot{m}_c}{4\pi r^2} = Y_{O_2}\left(\frac{\cancel{-\nu_I \dot{m}_c}}{4\pi r^2} + \frac{(\cancel{\nu_I}+1)\dot{m}_c}{4\pi r^2}\right) - \rho D \frac{dY_{O_2}}{dr}$$

$$-\nu_I \dot{m}_c = \dot{m}_c Y_{O_2} - 4\pi r^2 \rho D \frac{dY_{O_2}}{dr}$$

$$-\dot{m}_c = \dot{m}_c\left(\frac{Y_{O_2}}{\nu_I}\right) - 4\pi r^2 \rho D \frac{d(Y_{O_2}/\nu_I)}{dr}$$

$$\dot{m}_c = \frac{4\pi r^2 \rho D}{1+(Y_{O_2}/\nu_I)} \frac{d(Y_{O_2}/\nu_I)}{dr}$$

B.C.'s:

$$Y_{O_2}(r_s) = Y_{O_2,s}$$

$$Y_{O_2}(r\to\infty) = Y_{O_2,\infty}$$

$$\dot{m}_c = 4\pi r_s \rho D \ln\left[\frac{1 + Y_{O_2,\infty}/\nu_I}{1 + Y_{O_2,s}/\nu_I}\right]$$

Surface kinetics

$$R_c = \dot{m}'''_{c,s} = k_c MW_c [O_{2,s}]$$

$$[O_{2,s}] = \frac{MW_{mix} P}{R_u T_s}\left(\frac{Y_{O_2,s}}{MW_{O_2}}\right)$$

$$\dot{m}'''_{c,s} = k_c \frac{MW_c MW_{mix}}{MW_{O_2}} \frac{P}{R_u T_s} Y_{O_2,s}$$

$$\dot{m}_{c,s} = 4\pi r_s^2 \underbrace{k_c \frac{MW_c MW_{mix}}{MW_{O_2}} \frac{P}{R_u T_s}}_{K_{kin}} Y_{O_2,S}$$

Circuit Analogy

Ohm's law $\quad I = \frac{\Delta V}{R}$

by analogy $\dot{m}_c = K_{kin} Y_{O_2,s} = \dfrac{(Y_{O_2,s} - 0)}{1/K_{kin}} = \dfrac{\Delta Y}{R_{kin}}$

$$\dot{m}_c = 4\pi r_s \rho D \ln\left[1 + \frac{Y_{O_2,\infty} - Y_{O_2,s}}{Y_{O_2,s} + \nu_1}\right]$$

$$B_{O_2,\infty} = \text{transfer \#} = \frac{Y_{O_2,\infty} - Y_{O_2,s}}{Y_{O_2,s} + \nu_1}$$

$$\dot{m}_c = 4\pi r_s \rho D \ln\left[1 + B_{O_2,\infty}\right]$$

B_{O_2} is small:

$$\ln(1 + B_{O_2,\infty}) = B_{O_2,\infty} - \tfrac{1}{2} B_{O_2,\infty}^2 + \tfrac{1}{3} B_{O_2,\infty}^3 \cdots \cong B_{O_2,\infty}$$

$\nu_1 = 2.664$

$Y_{O_2,\infty} = 0.233$ (air)

$Y_{O_2,s} = 0 - 0.233$ (range)

$Y_{O_2,s} = 0$: $\ln(1 + B_{O_2,\infty}) = 0.0838$

$B_{O_2,\infty} = 0.0875$

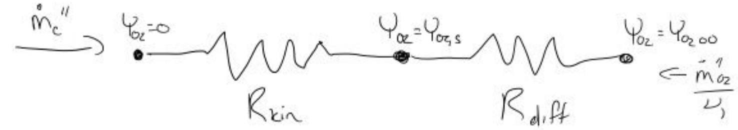
$Y_{O_2,s} = 0.233$: $\ln(1 + B_{O_2,\infty}) = 0$

$B_{O_2,\infty} = 0$

$\dot{m}_c = 4\pi r_s \rho D \left[Y_{O_2,\infty} - Y_{O_2,s}\right.$

$\left. \dots (\nu_1 + Y_{O_2,s}) \right]$

$$= \underbrace{\frac{4\pi r_s \rho D}{\nu_1 + Y_{O_2,s}}}_{1/R_{diff}} \underbrace{\left(Y_{O_2,\infty} - Y_{O_2,s}\right)}_{\Delta Y}$$



$$\dot{m}_c = \frac{(Y_{O_2,\infty} - 0)}{R_{kin} + R_{diff}}$$

$$R_{kin} = 1/K_{kin} = \frac{\nu_1 R_u T_s (MW_{O_2}/MW_c)}{4\pi r_s^2 MW_{mix} k_c \rho}$$

$$R_{diff} = \frac{\nu_1 + Y_{O_2,s}}{\rho D 4\pi r_s}$$

limiting cases:

$R_{kin} << R_{diff}$ → diffusion controlled

$R_{diff} << R_{kin}$ → kinetically controlled

regime	R_{kin}/R_{diff}	Burning Rate law	
diffusive controlled	<< 1	$\dot{m}_c = Y_{O_2,\infty}/R_{diff}$	$r_s \uparrow$ $T_s \uparrow$ $P \uparrow$
kinetics controlled	>> 1	$\dot{m}_c = Y_{O_2,\infty}/R_{kin}$	$r_s \downarrow$ $T \downarrow$ $P \downarrow$

in between ~ 1 $m_c = T_{a,\infty}/(R_{kin} + R_{diff})$