HW 4 – FIT EQN TO DATA

e.g., $r_{MODEL} = f(a_1, a_2, P_1, P_2)$ WHERE a_1 & a_2 ARE UNKNOWN SCALARS (ONE VALUE)

P_1 & P_2 ARE KNOWN ARRAYS OF EXP'L VALUES

GOAL FIND VALUES OF a_1 & a_2 THAT

→ MINIMIZE $\sum (r_{EXP} - r_{MODEL})^2$ = SUM OF SQUARED ERRORS ⟹ USE SOFTWARE THAT DOES THIS

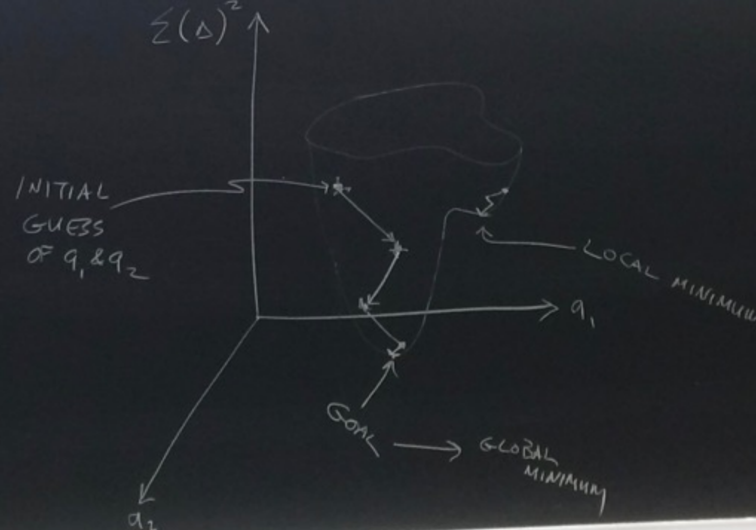
OR OTHER "OBJECTIVE FUNCTION" ↗

e.g. $\sum \left(\frac{r_{exp} - r_{MODEL}}{r_{exp}} \right)^2$

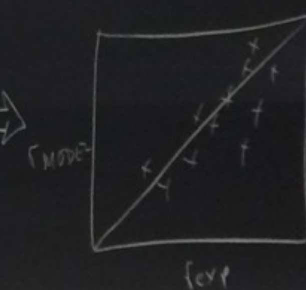
fminsearch IN MATLAB

Solver IN EXCEL

OR YOUR CHOICE



⟹

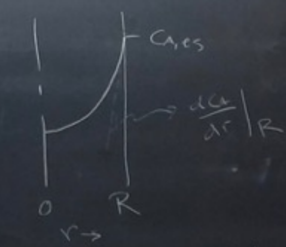


LAST TIME – 1^{st} ORDER, "IRREV" RXN IN POROUS SLAB CATALYST $\Rightarrow$ e.g., $r_A = \frac{-k C_A}{1 + K_A C_A}$ @ RELATIVELY LOW C SUCH THAT $r \to -k C_A$

$$\frac{d^2\Psi}{d\lambda^2} - \phi^2 \Psi = 0$$

B.C. 1) @ $\lambda = 0$ $\frac{d\Psi}{d\lambda} = 0$

@ $\lambda = 1$ $\Psi = 1$



ϕ = THIELE MODULUS = $R(m)\sqrt{\frac{k_r(1/s)}{D_{eff}(m^2/s)}}$

$$\phi^2 = \frac{R\, k_r C_{A,cs}}{D_{eff}\left(\frac{C_{A,cs} - 0}{R}\right)} = \frac{\text{RATE IF ALL SITES SEE } C_{A,cs} \text{ (NEG'L DIFF RESIST)}}{\text{DIFF. RATE WITH NO RXN \& CENTER CONC} = 0}$$

(MAX DIFF. RATE WITH NO RXN)

NET RATE "A" DIFFUSES INTO LAYER

$$= A_r(m^2)\, D_{eff}\left(\frac{m^2}{s}\right) \frac{dC_A}{dr}\left(\frac{mol}{m^3\, m}\right)$$

$\frac{mol}{s}$

$$\Psi(\lambda) = \frac{\cosh(\phi\lambda)}{\cosh\phi} \quad \text{where } \cosh x = \frac{e^x + e^{-x}}{2}$$

$\Psi(\lambda) \downarrow C_A(r)$

$\cosh$ ← HYPERBOLIC COSINE

WANT AVE RATE OVER CATALYST LAYER → (1) INTEGRATE $k_r C_A(r)$ OVER r & AVERAGE

(2) GET $\frac{dC_A}{dr}\Big|_{r=R}$ OR $\frac{d\Psi}{d\lambda}\Big|_{\lambda=1}$ & GET AVE. RATE FROM THIS

HYPERBOLIC TANGENT. ⟶ $\tanh x = \dfrac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$

$$\left.\frac{d\Psi}{d\lambda}\right|_{\lambda=1} = \phi^2\left(\frac{\tanh\phi}{\phi}\right) = \phi\tanh\phi$$

WE KNOW $-r_{A,TRUE} = k_T C_A$

WE WANT ⟶ $-r_{A,OBS} = k_{OBS} C_{A,es}$

$k_{OBS} = k$ OBSERVED WITH DIFFUSION RESISTANCE $\neq k_{TRUE}$ WHEN SIGNIFICANT DIFFUSION RESISTANCE IS PRESENT

$$-r_{A,OBS} = \eta\, k_{TRUE} C_{A,es}$$

$-r_{A,OBS}$: RATE WITH SIGNIFIC DIFF. RESIST.

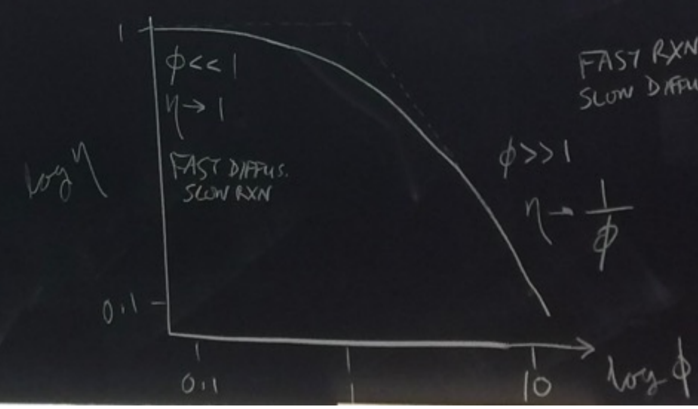
$k_{TRUE} C_{A,es}$ ⟶ RATE WITH NEGLIGIBLE DIFF RESIST.

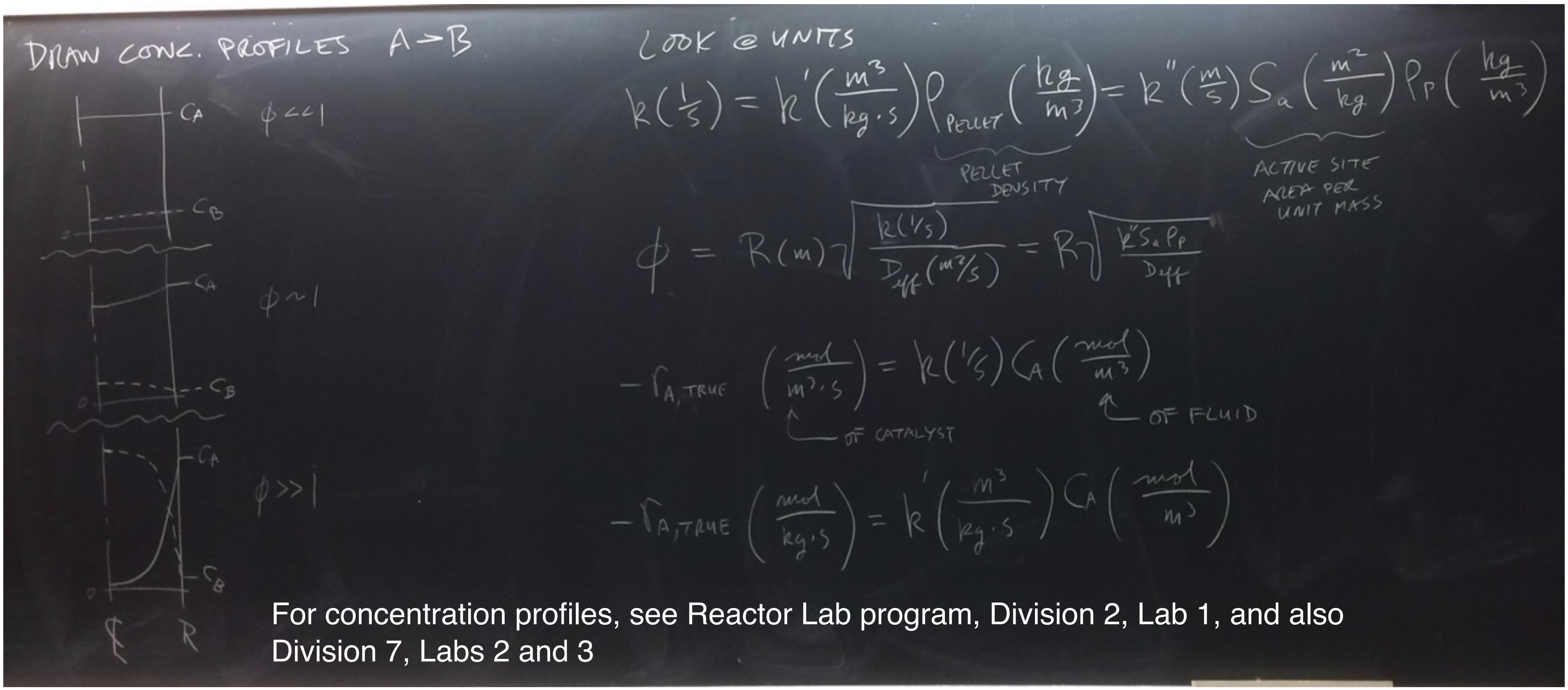
$$\therefore \eta = \frac{\text{RATE WITH DIFFUSION RESISTANCE}}{\text{RATE WITH NO DIFF. RESIST.}}$$

= "INTERNAL EFFECTIVENESS FACTOR" (GREEK "ETA")

FOR THIS CASE ⟶ "IRREV" 1st ORDER, A → B, ISOTHERMAL

$$\eta = \frac{\tanh\phi}{\phi}$$





For concentration profiles, see Reactor Lab program, Division 2, Lab 1, and also Division 7, Labs 2 and 3