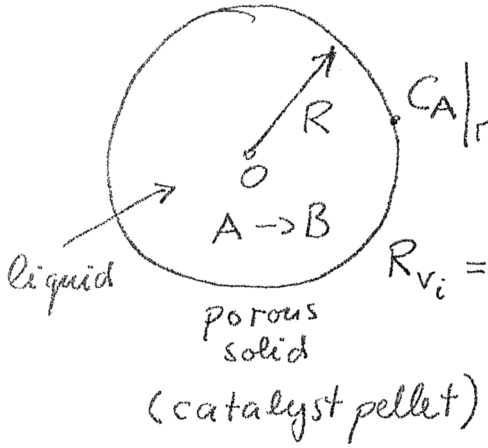
Irreversible

EXAMPLE 3.2-8 Reaction in a Spherical Catalyst Pellet This problem is analogous to the rectangular and cylindrical ones in Examples 3.2-1 and 3.2-7, respectively. The dimensionless variables are as defined in Eq. (3.2-61), with R now being the radius of a spherical catalyst pellet and r the spherical radial coordinate. The differential equation is



$$C_A\big|_{r=R} = C_o$$

$$R_{V_i} = k_{1V} C_A$$

Pseudobinary Conservat. Eq.

$$\frac{DC_i}{Dt} = D_{Ae}\nabla^2 C_i + R_{V_i}$$

D_{Ae} effective diffusivity (accounts for tort. path through pores)

$\Rightarrow$ at steady state and neglecting bulk flow

in sph. coord. $\rightarrow$

$$\boxed{D_{Ae}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dC_A}{dr}\right) = k_{1V} C_A} \quad (*)$$

BC1: $\left.\frac{dC_A}{dr}\right|_{r=0} = 0$; $r=0$ is symm. point

BC2: $C_A = C_{A_0}$ at $r=R$

The differential equation corresponds to the modified spherical Bessel function (B. 4-17 p. 645)

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy}{dx}\right) - m^2 y = 0$$

which has the general solution

$$y(mx) = A\frac{\sinh mx}{mx} + B\frac{\cosh mx}{mx}$$

$$= C\frac{e^{mx}}{mx} + D\frac{e^{-mx}}{mx}$$

We rewrite first our conservation eq. (*) in dimensionless form

$$\boxed{\frac{1}{\eta^2}\frac{d}{d\eta}\left(\eta^2\frac{d\Theta}{d\eta}\right) - Da\,\Theta = 0} \quad (**)$$

with $\eta = \frac{r}{R}$, $\Theta = \frac{C_A}{C_0}$, $Da = \frac{k_V R^2}{D_{Ae}}$ (Damköhler)

cont. Ex 3.2-8

Eq (**) has the general solution

$$\Theta(\eta) = A\,\frac{\sinh(Da^{1/2}\eta)}{\eta} + B\,\frac{\cosh(Da^{1/2}\eta)}{\eta}$$

A, B is determined with BCs

$$\Longrightarrow \boxed{\Theta(\eta) = \frac{\sinh(Da^{1/2}\eta)}{\eta\,\sinh(Da^{1/2})}} \quad (**)$$

concentration at surface

$$\Longrightarrow \boxed{\frac{C_A}{C_0} = \frac{R}{r}\,\frac{\sinh\left(\sqrt{k_V/D_{Ae}}\;r\right)}{\sinh\left(\sqrt{k_V R/D_{Ae}}\;R\right)}} \quad (***)$$

Next we rewrite the solution with the modified Thiele Modulus: $\boxed{\phi \equiv R^* \sqrt{\frac{k_V}{D_{Ae}}}}$

where ϕ^2 measures the relative rates between reaction and diffusion ($\phi \to 0$, very slow reaction, $C_A \to$ uniform)

($\phi \to \infty$, very fast reaction, reaction drives)

$R^* \equiv \frac{V_p}{S_{ex}}$ is the effective radius. For an ideal spherical particle of radius R:

$$\left.\begin{aligned} V_p &= \tfrac{4}{3}\pi R^3 \\ S_{ex} &= 4\pi R^2 \end{aligned}\right\} \Longrightarrow 3R^* = R$$

(***) $\Longrightarrow$ rewrites to: $\boxed{\frac{C_A}{C_0} = \frac{R}{r}\,\frac{\sinh(3\phi r/R)}{\sinh(3\phi)}} \quad (****)$

cont. Ex 3.2-8

Def. Effectiveness Factor

$$\eta^* \equiv \frac{\text{actual consumption of A within particle}}{\text{consumption of A if the entire catalyst was exposed to the exterior concentration}}$$

It can be shown that

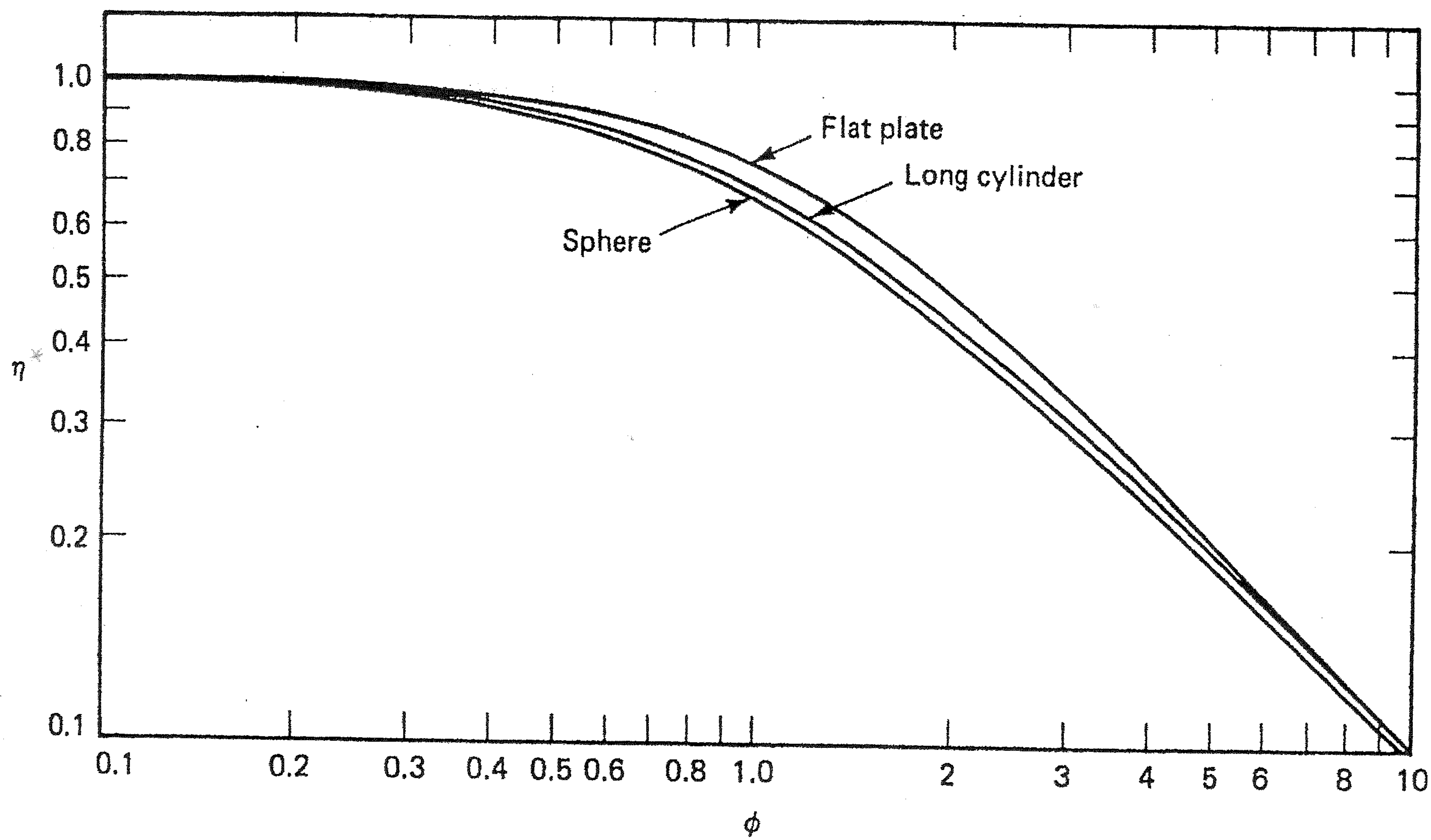
$$\eta^* = \frac{4\pi R^2 D_{Ae}\left(\frac{dC_A}{dr}\right)_{r=R}}{\frac{4}{3}\pi R^3 k_v C_0} \Longleftarrow \boxed{\eta^* = \frac{k_v \int_0^R S(r)\, C_A(r)\, dr}{k_v\, C_0 \int_0^R S(r)\, dr}}$$

for spherical particle: $S(r) = 4\pi r^2$

Subst. the solution ($\ast\ast\ast\ast$) of $C_A(r)$ into η^* above, yields

$$\coth x = \frac{e^x + e^{-x}}{e^x - e^{-x}} \qquad \boxed{\eta^* = \frac{1}{3\phi^2}\left(3\phi \coth 3\phi - 1\right)}$$

The effectiveness factor is used to describe mass transfer and chemical reaction in porous catalyst. The figure (below) shows an effectiveness $\eta^* \approx 1$ for ($\phi \to 0$) very slow reaction rates compared to diffusion rate. The entire particle takes part in the reaction. Low effectiveness ($\eta^* \to 0$) is obtained for ($\phi \to \infty$) very fast reaction rates. The reaction becomes limited to the surface.



Effectiveness factors for porous catalysts (from Aris, 1957)