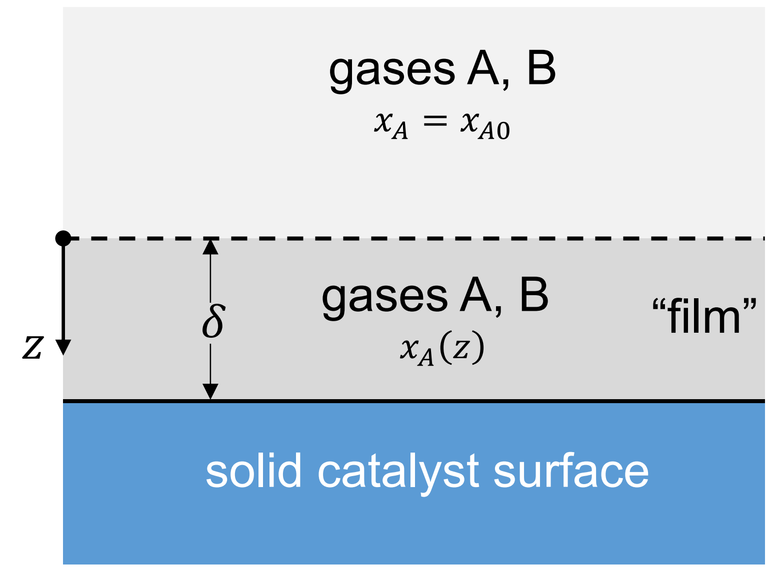
# EXAMPLE 3: 26FEB2020

## Film model of mass transfer (more complex)

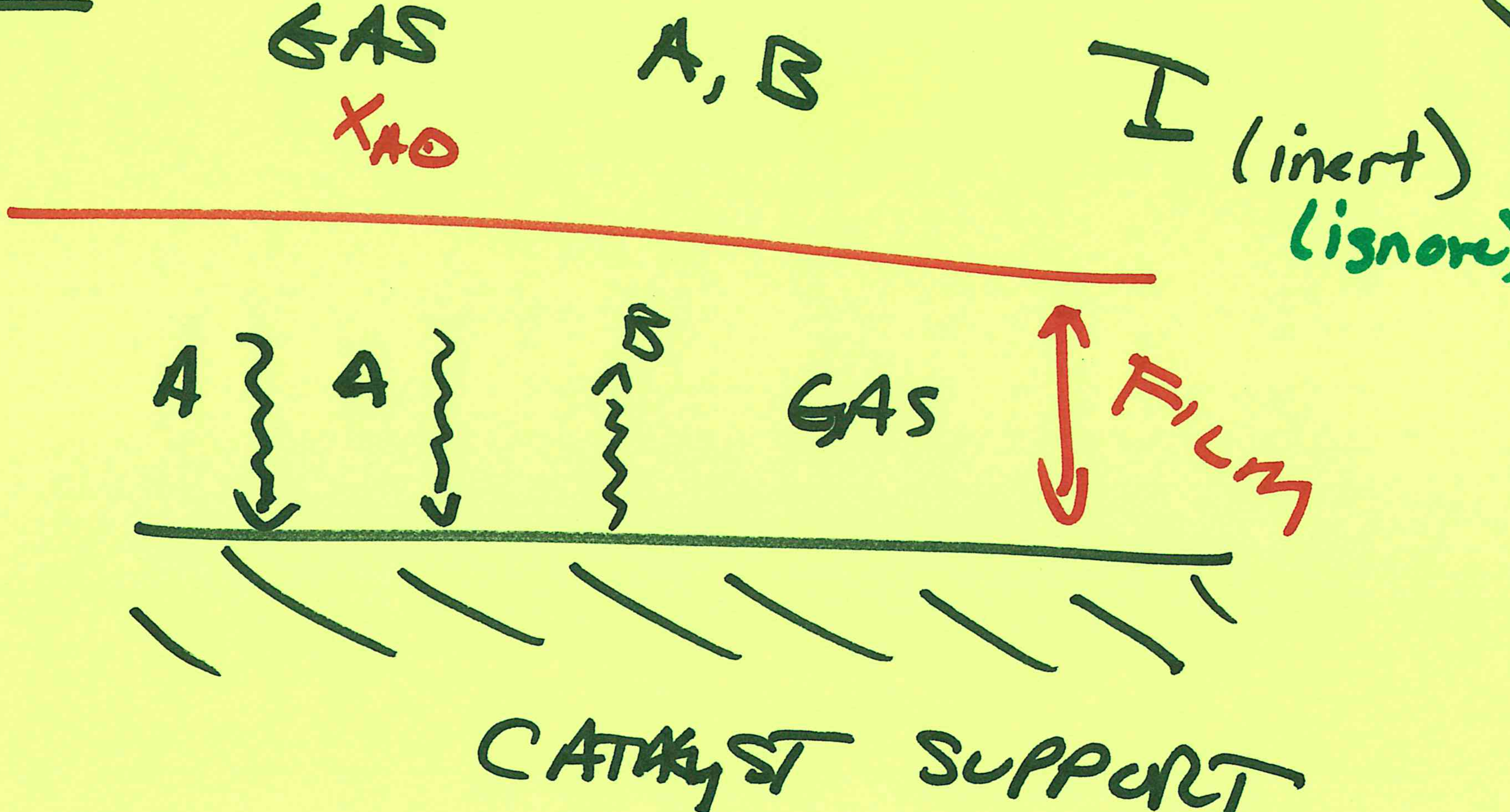
**QUICK START**

**<u>Example 3</u>:** Heterogeneous catalysis
An irreversible, instantaneous chemical reaction $(2A \rightarrow B)$ takes place at a catalyst surface, as shown. The reaction is "diffusion-limited," however, because the rate of completion of the reaction is determined by the rate of diffusion through the "film" near the catalyst surface. Calculate the steady state composition distribution in the film $x_A(z)$ and the flux of product $B$ away from the surface.




- Deploy the "film model"
- It has become *a way of thinking about* diffusion in some circumstances

## MODEL




How can we model this reactor?
(reflect!)

$2A \rightarrow B$

- at surface
- fast
- irreversible
- assuming diffn limited

★ $\boxed{\text{Use micro, species A mass bal}}$

The **Equation of Species Mass Balance in Terms of Combined Molar quantities** in Cartesian, cylindrical, and spherical coordinates for binary mixtures of A and B.

The general case, where the combined molar flux with respect to molar velocity ($\underline{N}_A$), is given on page 1.

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## In terms of total molar flux, $\underline{N}_A$

**Microscopic species mass balance**, in terms of molar flux; Gibbs notation

$$\frac{\partial c_A}{\partial t} = -\nabla \cdot \underline{N}_A + R_A$$

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**Microscopic species mass balance**, in terms of combined molar flux; Cartesian coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{\partial N_{A,x}}{\partial x} + \frac{\partial N_{A,y}}{\partial y} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

**Microscopic species mass balance**, in terms of combined molar flux; cylindrical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{A,r})}{\partial r} + \frac{1}{r}\frac{\partial N_{A,\theta}}{\partial \theta} + \frac{\partial N_{A,z}}{\partial z}\right) + R_A$$

**Microscopic species mass balance**, in terms of combined molar flux; spherical coordinates

$$\frac{\partial c_A}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{A,r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{A,\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{A,\phi}}{\partial \phi}\right) + R_A$$

At steady state

no homogeneous rxn

**Fick's law of diffusion**, Gibbs notation: $\underline{N}_A = x_A(\underline{N}_A + \underline{N}_B) - cD_{AB}\nabla x_A$

$$= c_A\underline{v}^* - cD_{AB}\nabla x_A$$

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Rxn:

**Fick's law of diffusion**, Cartesian coordinates:

$$\begin{pmatrix} \cancel{N_{A,x}} \\ \cancel{N_{A,y}} \\ N_{A,z} \end{pmatrix}_{xyz} = \begin{pmatrix} x_A(N_{A,x} + N_{B,x}) - cD_{AB}\frac{\partial x_A}{\partial x} \\ x_A(N_{A,y} + N_{B,y}) - cD_{AB}\frac{\partial x_A}{\partial y} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{xyz}$$

$N_{A_z} = -2N_{B_z}$

stoichiometry

**Fick's law of diffusion**, cylindrical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,z} \end{pmatrix}_{r\theta z} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,z} + N_{B,z}) - cD_{AB}\frac{\partial x_A}{\partial z} \end{pmatrix}_{r\theta z}$$

**Fick's law of diffusion**, spherical coordinates:

$$\begin{pmatrix} N_{A,r} \\ N_{A,\theta} \\ N_{A,\phi} \end{pmatrix}_{r\theta\phi} = \begin{pmatrix} x_A(N_{A,r} + N_{B,r}) - cD_{AB}\frac{\partial x_A}{\partial r} \\ x_A(N_{A,\theta} + N_{B,\theta}) - \frac{cD_{AB}}{r}\frac{\partial x_A}{\partial \theta} \\ x_A(N_{A,\phi} + N_{B,\phi}) - \frac{cD_{AB}}{r\sin\theta}\frac{\partial x_A}{\partial \phi} \end{pmatrix}_{r\theta\phi}$$

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## Micro Species A mass balance:

$$\frac{dN_{A,z}}{dz} = 0$$

integrate: $\boxed{N_{A,z} = C_1}$

## Fick's Law of Diffusion:

assume T, P constant ⟹ $cD_{AB}$ const.

$$N_{A,z} = x_A(N_{Az} + N_{Bz}) - cD_{AB}\frac{dx_A}{dz}$$

$N_{Bz} = -\frac{1}{2}N_{A,z}$

(from stoichiometry)

$$N_{Az} = x_A \left(\frac{1}{2}\right) N_{Az} - cD_{AB} \frac{dx_A}{dz}$$

$$\left(1 - \frac{x_A}{2}\right) N_{Az} = - cD_{AB} \frac{dx_A}{dz}$$

$$\vdots$$

solve for $x_A$ w/ 2 Boundary conditions

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Boundary conditions: $z = 0 \quad x_A = x_{A0}$

$z = \delta \quad x_A = 0 \leftarrow$ it all reacts!

(See HW4 solns) //