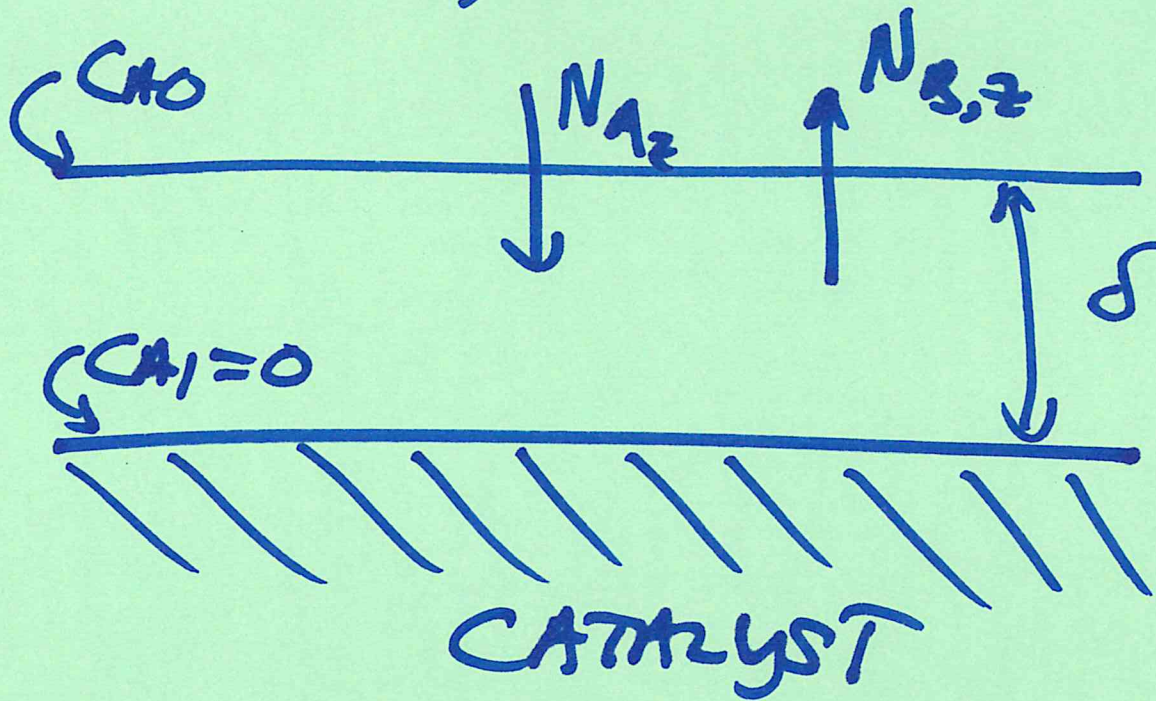
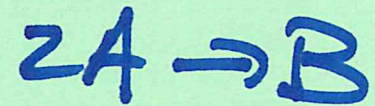


Catalytic converter  
A, B

FAMM 20 Mar 19 (1)



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

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

$$N_{A,z} = C_1$$

2

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

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

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

Steady

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

no homogeneous rxn

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

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

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

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

$\frac{dN_A}{dz} = -c$   
 $N_A z = c_1$

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

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

Fick's law of diffusion, Cartesian coordinates:

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



Fick's law of diffusion, cylindrical coordinates:

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

Fick's law of diffusion, spherical coordinates:

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



# Fick's Law

(3)

$$N_{Az} = X_A (N_{Az} + N_{Bz}) - c D_{AB} \frac{dx_A}{dz}$$

$$N_{Az} = -z N_{Bz}$$

at steady state

∴  
Solve

BC:

$$z = 0$$

$$z = \delta$$

$$X_A = X_{A0}$$

$$X_A = 0$$

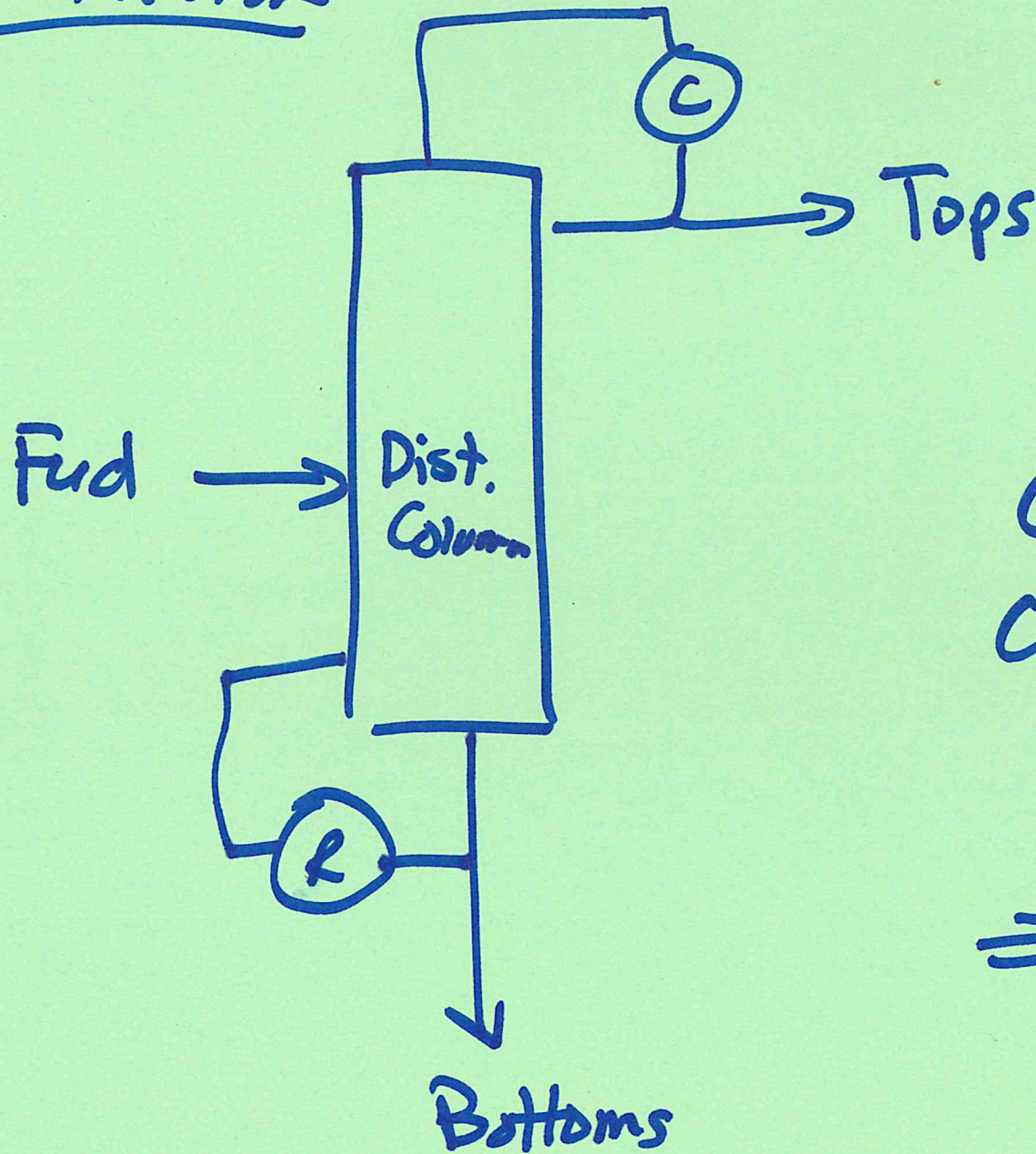
(fast heterogeneous rxn)



# Distillation

FAM  
20 Mar 19

①



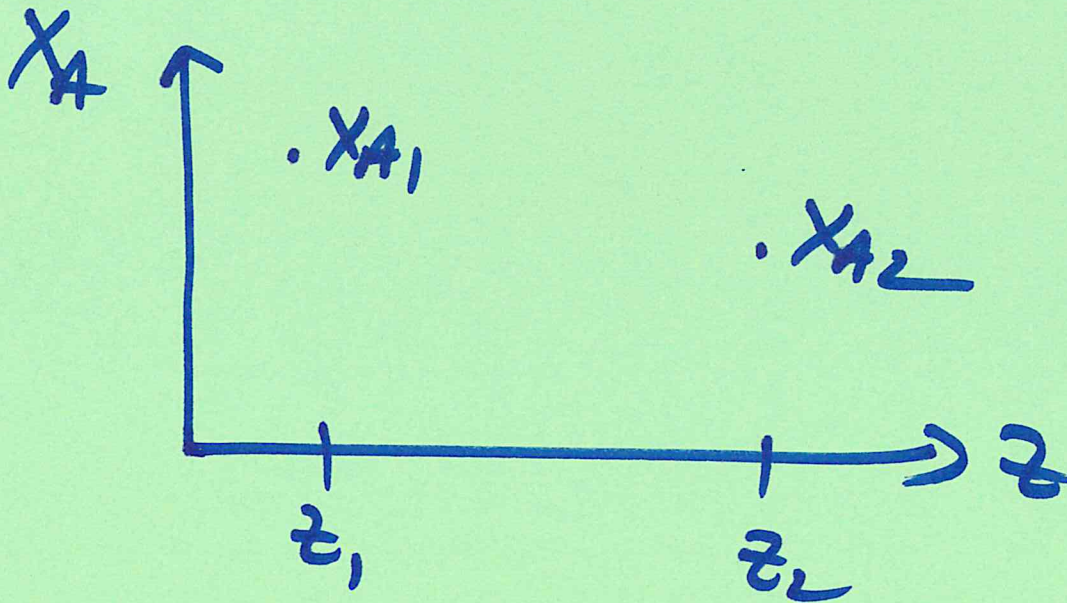
CMO:  
Constant  
molar  
overflow  
⇒ equimolar  
counter diffn  
in gas  $\phi$



Equimolar counter diffusion (2)

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

$$\underline{V}^* = 0$$



# Equivolar counter diff

(3)

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

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

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

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

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

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

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

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

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

Fick's law of diffusion, Cartesian coordinates:

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

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:

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

SOLVE