# Microreactor Engineering

**Goran Jovanovic**
Oregon State University
School of Chemical, Biological, and Environmental Engineering

## Solid Catalyzed Reactions
## Alternative Boundary Conditions

In Affiliation With:

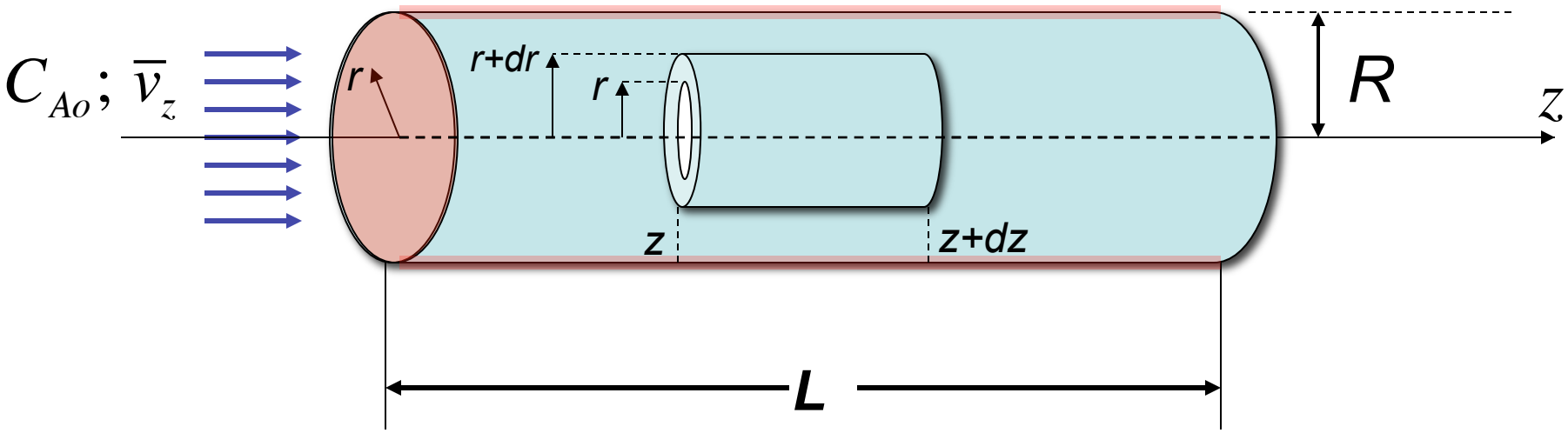
**MBI**
Microproducts Breakthrough Institute

**PTT - LOA**
PTT - Laboratories Of America

# Solid Catalyzed Reactions

Consider a homogenous fluid that enters the microchannel vessel at average velocity $\bar{v}_z$ containing a reactant *A* that undergoes catalytic transformation:

$$A \overset{k''}{\Longrightarrow} B \qquad -r_A'' = -\frac{1}{S_c}\frac{dN_A}{dt} = k'' C_A \left[\frac{moles\ A\ reacted}{m^2 cat - surface \cdot s}\right]$$



# Solid Catalyzed Reactions

Finally, the mathematical model takes the form:

$$-v_z(r)\frac{\partial C_A(z,r)}{\partial z}+D_A\frac{\partial^2 C_A(z,r)}{\partial z^2}+D_A\frac{\partial^2 C_A(z,r)}{\partial r^2}+\frac{D_A}{r}\frac{\partial C_A(z,r)}{\partial r}=0$$

With a choice of two axial boundary conditions (in *z* direction):

$$at\ z=0 \quad \frac{\partial C_A(0,r)}{\partial z}=0$$

$$at\ z=0 \quad C_A(0,r)=C_{Ao}$$

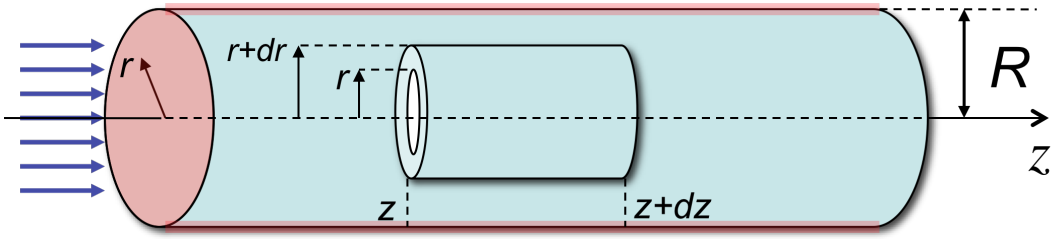
$$at\ z=L \quad \frac{\partial C_A(L,r)}{\partial z}=0$$

$$at\ z=L \quad \bar{C}_A(L)=C_A^*$$

# Solid Catalyzed Reactions

And boundary conditions in ***r*** direction:

$$at\ r = 0 \qquad \frac{\partial C_A(z,0)}{\partial r} = 0$$




$$at\ \ r = R$$

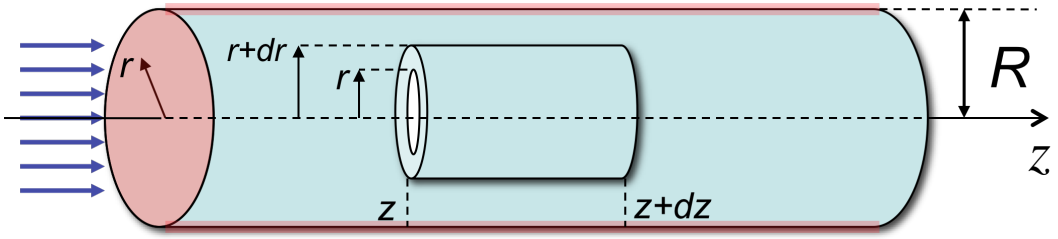
$$-\underbrace{D}_{\frac{m^2}{s}}\ \underbrace{2\pi R \cdot dz}_{m^2 reactor\ surf.}\ \frac{\partial C_A(z,r)}{\partial r}\Bigg|_{\underset{m}{\frac{moles}{m^3 reactor}}} = \underbrace{dA}_{\left(\frac{m^2 of\ reactor\ wall\ surface}{}\right)}\ \underbrace{a}_{\left(\frac{m^2 cat-surface}{m^2\ of\ reactor\ wall\ surface}\right)}\cdot\ \underbrace{k'' C_A}_{\left(\frac{moles\ A\ reacted}{m^2 cat-surface \cdot s}\right)}\Bigg|_R$$

$$-D \cdot 2\pi R \cdot dz \frac{\partial C_A(z,r)}{\partial r}\Bigg|_R = 2\pi R \cdot dz \cdot a\, k'' C_A\Big|_R$$

# Solid Catalyzed Reactions

Similarly we can write for the boundary conditions in ***r*** direction:

$$at\ r = 0 \qquad \frac{\partial C_A(z,0)}{\partial r} = 0$$




$$at\ \ r = R$$

$$-D\ \underbrace{2\pi R \cdot dz}_{m^2}\ \underbrace{\frac{\partial C_A(z,r)}{\partial r}}_{\frac{moles}{m^3 reactor}}\Bigg|_R = \underbrace{dV_r}_{m^3 reactor} \cdot \underbrace{s}_{\frac{m^2 cat-surface}{m^3 reactor}} \cdot \underbrace{k'' C_A}_{\frac{moles\ A\ reacted}{m^2 cat-surface \cdot s}}\Bigg|_R$$

$$-D \cdot 2\pi R \cdot dz \left.\frac{\partial C_A(z,r)}{\partial r}\right|_R = \left(\pi R^2 dz\right) \cdot s \cdot k'' C_A\Big|_R$$

# Solid Catalyzed Reactions: Radial BC's

$$-D\left.\frac{\partial C_A(z,r)}{\partial r}\right|_R = \left(a \cdot k'' C_A\big|_R\right)\left[\frac{mol\ A}{m^2 \cdot s}\right]$$

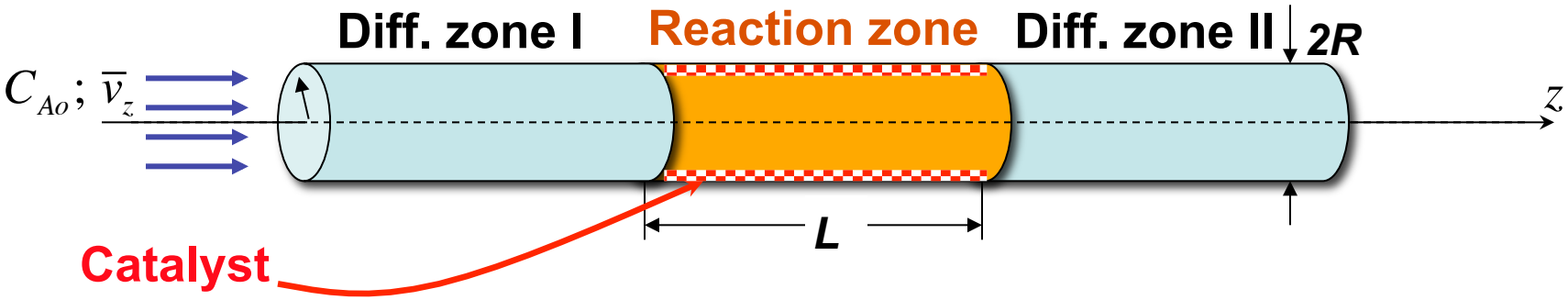
$$\boxed{-\left.\frac{\partial C_A(z,r)}{\partial r}\right|_R = \frac{a}{D} \cdot k'' C_A\big|_R}$$

$$-D \cdot 2\pi R \cdot dz \left.\frac{\partial C_A(z,r)}{\partial r}\right|_R = \left(\pi R^2 dz\right) \cdot s \cdot k'' C_A\big|_R$$

$$\boxed{-\left.\frac{\partial C_A(z,r)}{\partial r}\right|_R = \frac{R \cdot s}{2D} \cdot k'' C_A\big|_R}$$

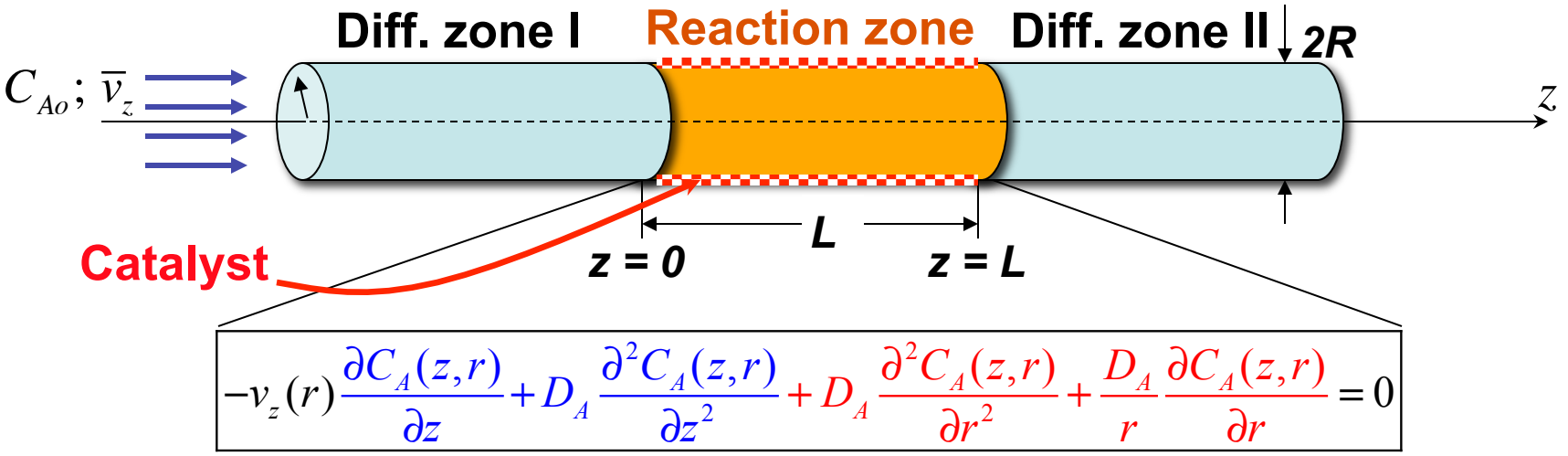
# Solid Catalyzed Reactions

Consider a microchannel vessel with characteristic dimension of approximately ***R* ≈100** μm, and length ***L***; where ***L*>>>*R***. In addition consider that a solid catalyzed chemical reaction of known kinetics takes place at the walls of the microreactor vessel. This microreactor consists of three segments, out of which only the middle segment contains catalyst.




$$\text{Geometric aspect ratio: } \frac{R}{L} <<< 1$$

# Solid Catalyzed Reactions – Open-Open BC




$$-v_z(r)\frac{\partial C_A(z,r)}{\partial z}+D_A\frac{\partial^2 C_A(z,r)}{\partial z^2}+D_A\frac{\partial^2 C_A(z,r)}{\partial r^2}+\frac{D_A}{r}\frac{\partial C_A(z,r)}{\partial r}=0$$

$$@z=0 \quad \frac{\partial C_A^I(l,r)}{\partial \xi}=\frac{\partial C_A(0,r)}{\partial z};\; C_A^I(l,r)=C_A(0,r)$$

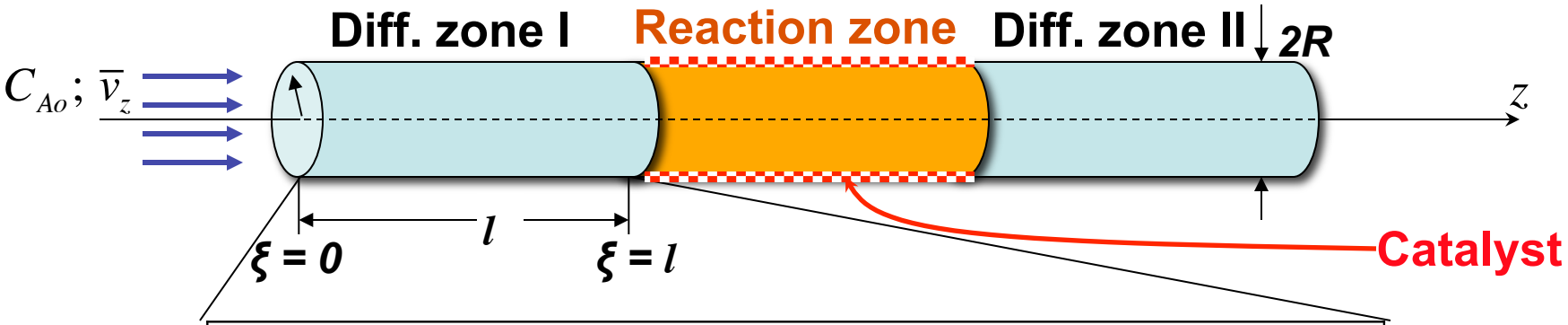
$$@z=L \quad \frac{\partial C_A(L,r)}{\partial z}=\frac{\partial C_A^{II}(0,r)}{\partial \eta};\; C_A(L,r)=C_A^{II}(0,r)$$

$$\left.\frac{\partial C_A(z,0)}{\partial r}\right|_{r=0}=0;$$

$$-\left.\frac{\partial C_A(z,r)}{\partial r}\right|_R=\left.\frac{a}{D}\cdot k''C_A\right|_R$$

$$-\left.\frac{\partial C_A(z,r)}{\partial r}\right|_R=\left.\frac{R\cdot s}{2D}\cdot k''C_A\right|_R$$

# Solid Catalyzed Reactions – Open-Open BC




$$-v_\xi(r)\frac{\partial C_A^I(\xi,r)}{\partial \xi}+D_A\frac{\partial^2 C_A^I(\xi,r)}{\partial \xi^2}+D_A\frac{\partial^2 C_A^I(\xi,r)}{\partial r^2}+\frac{D_A}{r}\frac{\partial C_A^I(\xi,r)}{\partial r}=0$$

$$@\xi=0 \quad \frac{\partial C_A^I(0,r)}{\partial \xi}=0;\ C_A^I(0,r)=C_{Ao}$$

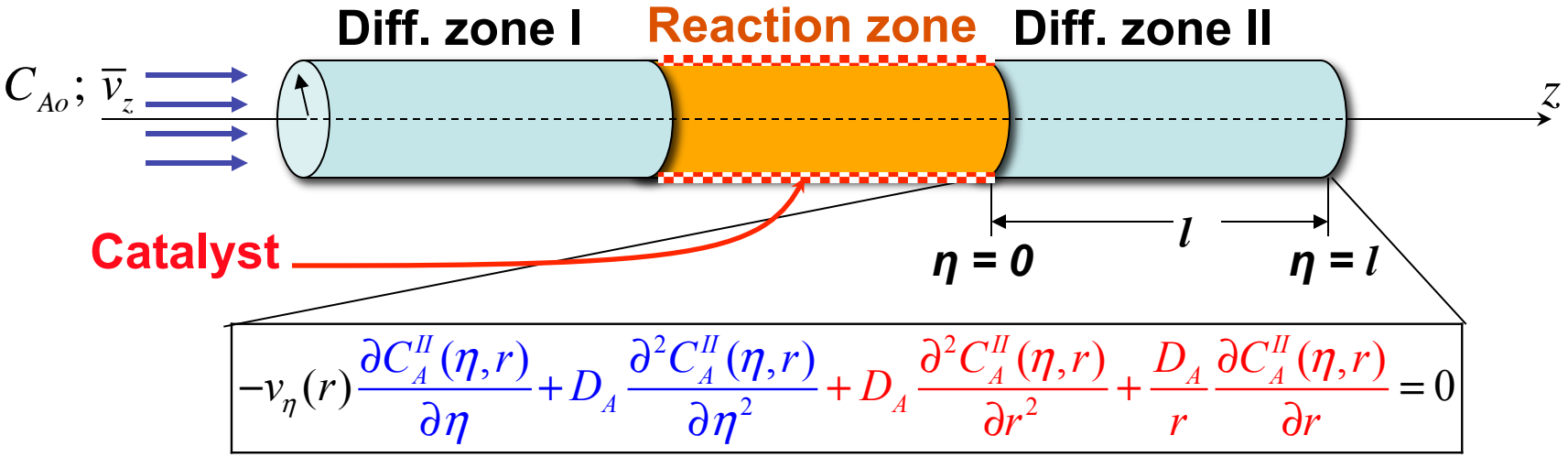
$$@r=0 \quad \frac{\partial C_A^I(\xi,0)}{\partial r}=0;$$

$$@\xi=l \quad \frac{\partial C_A^I(l,r)}{\partial \xi}=\frac{\partial C_A(0,r)}{\partial z};\ C_A^I(l,r)=C_A(0,r)$$

$$@r=R \quad \frac{\partial C_A^I(\xi,R)}{\partial r}=0$$

$$@any\,\xi \Rightarrow v_\xi(r)=\frac{R^2}{4\cdot\mu}\left(\frac{\Delta P}{L}\right)\cdot\left[1-\frac{r^2}{R^2}\right]=2\bar{v}_z\left[1-\frac{r^2}{R^2}\right]$$

# Solid Catalyzed Reactions – Open-Open BC




$$-v_\eta(r)\frac{\partial C_A^{II}(\eta,r)}{\partial \eta}+D_A\frac{\partial^2 C_A^{II}(\eta,r)}{\partial \eta^2}+D_A\frac{\partial^2 C_A^{II}(\eta,r)}{\partial r^2}+\frac{D_A}{r}\frac{\partial C_A^{II}(\eta,r)}{\partial r}=0$$

$$@\eta=0 \quad \frac{\partial C_A^{II}(0,r)}{\partial \eta}=\frac{\partial C_A(L,r)}{\partial z};\; C_A^{II}(0,r)=C_A(L,r) \qquad @r=0 \quad \frac{\partial C_A^{II}(\eta,0)}{\partial r}=0;$$

$$@\eta=l \quad \frac{\partial C_A^{II}(l,r)}{\partial \eta}=0;\; and \;\; or \;\; \bar{C}_A^{II}(l)=C_A^* \qquad @r=R \quad \frac{\partial C_A^{II}(\eta,R)}{\partial r}=0$$

$$@any\,\eta \Rightarrow v_\eta(r)=\frac{R^2}{4\cdot\mu}\left(\frac{\Delta P}{L}\right)\cdot\left[1-\frac{r^2}{R^2}\right]=2\bar{v}_z\left[1-\frac{r^2}{R^2}\right]$$

# The Origin of Characteristic Times

Consider the governing differential equation for a microchannel reactor in which a chemical reaction take place in a catalyst layer at the walls of the microreactor.

$$-v_z(r)\frac{\partial C_A(z,r)}{\partial z}+D_A\frac{\partial^2 C_A(z,r)}{\partial z^2}+D_A\frac{\partial^2 C_A(z,r)}{\partial r^2}+\frac{D_A}{r}\frac{\partial C_A(z,r)}{\partial r}=0$$

$$where\ at\ any\ z \Rightarrow v_z(r)=2\bar{v}_z\left[1-\frac{r^2}{R^2}\right]$$

After the change of variables and all substitutions:

$$r^*=\frac{r}{R};\quad z^*=\frac{z}{L};\quad C_A^*=\frac{C_A}{C_{Ao}} \quad\Rightarrow\quad r=r^*R;\quad z=z^*L;\quad C_A=C_A^*C_{Ao};$$

one can obtain:

$$-\frac{\bar{v}_z}{L}2\left[1-\left(r^*\right)^2\right]\frac{\partial C_A^*}{\partial z^*}+\frac{D_A}{L^2}\frac{\partial^2 C_A^*}{\partial\left(z^*\right)^2}+\frac{D_A}{R^2}\frac{\partial^2 C_A^*}{\partial\left(r^*\right)^2}+\frac{D_A}{R^2}\frac{1}{r^*}\frac{\partial C_A^*}{\partial r^*}=0$$

# The origin of Characteristic Times

The coefficients in the normalized differential equation represent the characteristic times that we consider earlier:

$$-\left(\frac{\bar{v}_z}{L}\right)2\left[1-\left(r^*\right)^2\right]\frac{\partial C_A^*}{\partial z^*}+\left(\frac{D_A}{L^2}\right)\frac{\partial^2 C_A^*}{\partial\left(z^*\right)^2}+\left(\frac{D_A}{R^2}\right)\left[\frac{\partial^2 C_A^*}{\partial\left(r^*\right)^2}+\frac{1}{r^*}\frac{\partial C_A^*}{\partial r^*}\right]=0$$

or equivalently:

$$-\frac{1}{\tau_I}2\left[1-\left(r^*\right)^2\right]\frac{\partial C_A^*}{\partial z^*}+\frac{1}{\tau_{D,z}}\frac{\partial^2 C_A^*}{\partial\left(z^*\right)^2}+\frac{1}{\tau_{D,r}}\left[\frac{\partial^2 C_A^*}{\partial\left(r^*\right)^2}+\frac{1}{r^*}\frac{\partial C_A^*}{\partial r^*}\right]=0$$

**mean resident time**

**diffusion time in *z***

**diffusion time in *r***

# The origin of Characteristic Times

Similarly, from the boundary condition: $$-\left.\frac{\partial C_A(z,r)}{\partial r}\right|_R = \left.\frac{R\cdot s}{2D}k''C_A\right|_R$$

and change of variables: $$r = r^* R; \quad z = z^* L; \quad C_A = C_A^* C_{Ao}$$

one can obtain: $$-2\left(\frac{D}{R^2}\right)\left.\frac{\partial C_A^*}{\partial r^*}\right|_R = \left(s\cdot k''\right)C_A^*\Big|_R$$

or equivalently: $$-2\frac{1}{\tau_{D,r}}\left.\frac{\partial C_A^*}{\partial r^*}\right|_R = \frac{1}{\tau_A}C_A^*\Big|_R$$

diffusion time in *r*

reaction time

where: $$s = \frac{surface\ of\ catalyst\ [m^2]}{volume\ of\ reactor\ [m^3]} = \frac{S_c}{V_r}\ \left[m^{-1}\right]$$

Oregon State UNIVERSITY OSU College of Engineering

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*Thank you for your attention!*