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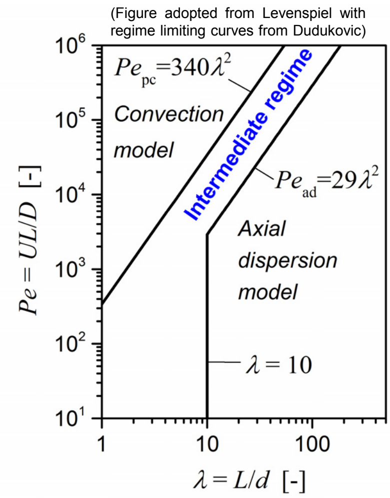
A model for the residence time distribution of convection dominated laminar flows with near-wall diffusion effects

1 - Motivation

- Liquid flows in microchannels are often laminar and the molecular diffusivity of solutes is small
- The residence time distribution (RTD) is strongly affected by convection (laminar velocity profile) while diffusion effects are especially important near walls
- In this **intermediate regime** neither the pure convection model nor the axial dispersion model are appropriate



d = pipe diameter
L = pipe length
U = mean velocity
D = molecular diffusivity
D_{ax} = axial dispersion coefficient

$$Pe = \frac{UL}{D}$$

$$Bo = \frac{UL}{D + D_{ax}}$$

$$D_{ax} = \frac{d^2U^2}{192D} = \frac{D}{192}\frac{Pe^2}{\lambda^2}$$

- Goal: Development of a general theoretical model for the RTD in the intermediate regime

2 - From concentration equation to RTD

- Normalized concentration equation

$$\frac{\partial C}{\partial \theta} + \underbrace{2(1-Y^2)}_{=V(Y)}\frac{\partial C}{\partial X} = \frac{1}{Pe}\left(4\lambda^2\frac{\partial^2 C}{\partial Y^2} + 4\lambda^2\frac{1}{Y}\frac{\partial C}{\partial Y} + \frac{\partial^2 C}{\partial X^2}\right)$$

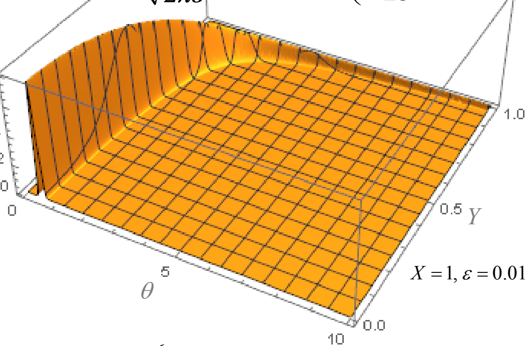
$$C = c/c_0,\ \theta = tU/L,\ X = x/L,\ Y = r/0.5d,\ V = u(r)/U$$

- Solution for flux impulse injection $C_{\uparrow}(\theta, X, Y)$
- Differential RTD $E(\theta) = \int_0^1 2Y \cdot V(Y) \cdot C_{\uparrow}(\theta, 1, Y) \cdot \mathrm{d}Y$

3 – Pure convection regime ($D = Pe^{-1} = 0$)

$$C_{\uparrow\varepsilon}(0, X, Y) = V(Y)\delta_\varepsilon(X) = \frac{V(Y)}{\sqrt{2\pi\varepsilon}}\exp\left(-\frac{X^2}{2\varepsilon}\right)$$

$$C^{pc}_{\uparrow\varepsilon}(\theta, X, Y) = \frac{1}{\sqrt{2\pi\varepsilon}}2(1-Y^2)\exp\left(-\frac{1}{2\varepsilon}\left(X - 2(1-Y^2)\theta\right)^2\right)$$



$$\lim_{\varepsilon\to 0} E^{pc}_{\varepsilon}(\theta) = \lim_{\varepsilon\to 0}\left\{\frac{1}{4\theta^3}(1+\varepsilon)\left[\operatorname{erf}\left(\frac{2\theta-1}{\sqrt{2\varepsilon}}\right) - \operatorname{erf}\left(-\frac{1}{\sqrt{2\varepsilon}}\right)\right]\right.$$
$$\left. - \frac{1}{2\theta^3}\sqrt{\frac{\varepsilon}{2\pi}}\left[(1+2\theta)\exp\left(-\frac{(1-2\theta)^2}{2\varepsilon}\right) - \exp\left(-\frac{1}{2\varepsilon}\right)\right]\right\} = \frac{1}{2\theta^3}$$

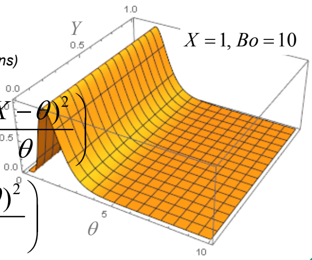
4 – Axial dispersion regime

$$\frac{\partial \bar{C}}{\partial \theta} + \frac{\partial \bar{C}}{\partial X} = \frac{1}{Bo}\frac{\partial^2 \bar{C}}{\partial X^2}$$

(with open-open boundary conditions)

$$\bar{C}^{ad}_{\uparrow}(\theta, X) = \frac{1}{2}\sqrt{\frac{Bo}{\pi\theta^3}}\exp\left(-\frac{Bo}{4}\frac{(X-\theta)^2}{\theta}\right)$$

$$E^{ad}(\theta) = \frac{1}{2}\sqrt{\frac{Bo}{\pi\theta^3}}\exp\left(-\frac{Bo}{4}\frac{(1-\theta)^2}{\theta}\right)$$

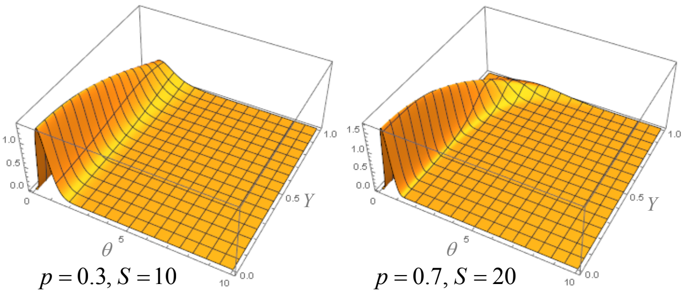


5 – Present model

- Model for concentration distribution ($0 \le p \le 1$)

$$C_{\uparrow}(\theta, 1, Y) = \sqrt{\frac{S}{\pi\theta^{3(1-p)}}}\frac{1+p(1-2Y^2)}{2^{1+p}}\exp\left(-\frac{S}{4}\frac{\left[1-\theta-p(1-2Y^2)\theta\right]^2}{\theta^{1-p}}\right)$$

- $p = 1, S = 2/\varepsilon$ → pure convection case (see ③)
- $p = 0, S = Bo$ → axial dispersion case (see ④)



- Differential RTD integral in ② can be evaluated analytically
- Relations between p, S, Bo, Pe and λ must be established
- Model RTD will be compared with measured RTDs