Lesson 14

The Kolmogorov scale λ is dependent on the viscosity $\nu^{3/4}$
And the t_μ (micromixing time scale) depends on λ^2 and overall to the viscosity $\nu^{1.5}$.

Fast reaction rate

It will be reactions that are very fast and inevitably we will have $Da_\mu >> 1$ ($t_r << t_\mu$) so we are in a macromixed space. So the reaction is dominated ~~...~~ by an apparent kinetic which is dominated by the diffusional process.

$$r_{app} \simeq \frac{D}{\lambda^2} \cdot C_A$$

Arrhenius diagram

$$r(C_A, C_B) = k_0 e^{-\frac{Ea}{RT}} \cdot f(C_A, C_B)$$

slow: $r_{app} \simeq r(C_A, C_B)$

Axial dispersion model

molar flux of a compound

$$N(z) = \underbrace{\overset{\text{mean velocity}}{U} C}_{\text{convective term}} - \underbrace{D \frac{dC}{dz}}_{\text{dispersion term}}$$

diffusion → individual molecules moves because of a gradient concentration.

dispersion → fluid pockets that due to the turbulent nature of the flow (eddies) will move in different directions, and each pocket brings itself all his content.

we can analize which term ~~has~~ is more relevant.

axial dispersion time $t_D = \frac{L^2}{D}$ convective time $t_c = \frac{L}{U}$

Peclet number $Pe = \frac{t_D}{t_c} = \frac{UL}{D}$

- when $Pe \to 0$, this mean slow flow with large eddies good mixing to dispersion → CSTR
- when $Pe \to \infty$, dispersion is negligible

Lower Pe, more dispersion strength

we can obtain Pe from the RTD, for example if we put an impulsive tracer on a PFR we obtain the dirac function. So, a different response to that one is due to dispersion and we can measure it.

Lesson 15

1) Pe from RTD.

If we add H_2 and PAH, in the diffusion case we will have at the exit H_2 before PAH because it has bigger diffusivity due to its weight. On dispersion is different, we will have H_2 + PAH at the same time because the eddies moves all together.

Reactor tracing

we have a equation to solve and some boundaries conditions (adimensional).

$$\frac{\partial C^*}{\partial \theta} + \frac{\partial C^*}{\partial x} = \frac{1}{Pe} \frac{\partial^2 C^*}{\partial x^2} \qquad \theta = \frac{t}{\tau} \quad x = \frac{z}{L} \quad C^* = \frac{C}{C_0}$$

we have two processes in parallel, the theoretical model and the experimental data. $E_\theta = E_\theta(\theta, Pe)$

The two converge when thanks to non linear regression analysis we minimize the deviation.

$$\min \sum_i \left(E_{\theta_{th}}(\theta_i) - E_{\theta_{exp}}(\theta_i)\right)^2 \Longrightarrow Pe$$

we need a first guess for Pe. And anyway not always we get a result.

So, we propose other method → van der Laan

using Laplace we reduce the order of the equation.

$$sC^* + \frac{dC^*}{dx} = \frac{1}{Pe} \frac{d^2C^*}{dx}$$

Analizing:

$$-\frac{dC^*}{ds}\Big|_{s=0} = \bar{\theta} = \frac{\bar{t}}{\tau} \quad \text{first moment}$$

$$\sigma^2_\theta = \frac{\sigma^2_t}{t^2} \quad \text{second moment}$$

We can stablish the relationship between $\sigma_\theta^2 \rightarrow Pe$
we have a tool to relate the theoretical model in the Laplace domain with the σ_θ^2 of the real reactor (experiment).
Usefull because:

1. we can do it without the non lineal regression.
2. without going back from Laplace to time domain.

The adimensional moments are:

$\bar{\theta} = \int_0^{+\infty} \theta E(\theta) d\theta$ (tita bar) $\sigma_\theta^2 = \int_0^{+\infty} (\theta - \bar{\theta})^2 E(\theta) d\theta$ (sigma square)

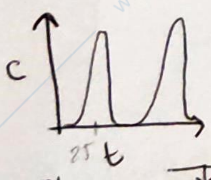
If the vessels is close $\bar{\theta}$ don't depend on Peclet number and for the other cases the dependence is not strong.
So, we will use σ_θ^2 and matching with the experimental result.

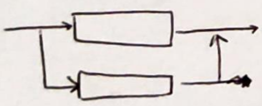
For small deviations from ideal flow ($Pe \rightarrow +\infty$, PFR) we have that: $\bar{\theta} = 1$, $\sigma_\theta^2 = \frac{2}{Pe}$ from $Pe \simeq 40-50$

Lesson 16 parte otro profesor

Ejemplo **12.2**

1.



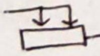


$E(t) = \frac{Q_1}{Q} \delta(t - \tau_1) + \frac{Q_2}{Q} \delta(t - \tau_2)$

$\tau_1 = \frac{V_1}{Q_1} = 0'25 min$ $\frac{Q_1}{Q} = \frac{A_1}{A_1 + A_2} = 0'4$ $V_1 = Q_1 \tau_1 = 0'1 m^3$
$V_2 = 0'9 m^3$

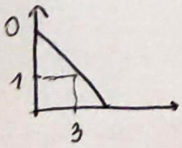
$1 m^3 V$ ✓ no dead zones.

2. Also



Twisteering reactor

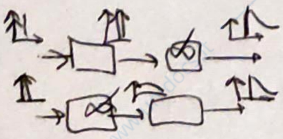
12.3

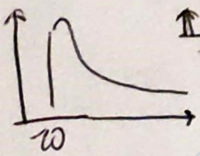


$t > t$ mean residence time > space time

$\circ \begin{cases} V \text{ or } Q \text{ not correct} \\ \text{no proper tracer} \\ \text{no closed vessel} \end{cases}$ CSTR $\begin{cases} C = A \exp\left(-\frac{t}{\tau_{CSTR}}\right) \\ \log C = \log A - \frac{t}{\tau_{CSTR}} \log e \end{cases}$

12.5





$E(t) = \frac{1}{\tau_{CSTR}} \exp\left(-\frac{t - \tau_{PFR}}{\tau_{CSTR}}\right) u(t - \tau_{PFR})$

$\bar{t} = \tau_{PFR} + \tau_{CSTR} = 50s$ $\bar{t} \not\approx \tau$ dead zones !!

$V_{dead} = V - V_{CSTR} - V_{PFR} = V - Q\tau_{PFR} - Q_{CSTR} = \square$