Exercise: Chemical Reaction in a Reactor (PFR)

We consider the chemical reaction in a reactor, as described in Section 1.2.1 of the book [KX].

a) Solve the dimensionless ODE:

$$\frac{d}{d\tau}\tilde{C}(\tau) = 1 - \tilde{C}(\tau) - \beta\tilde{C}(\tau), \quad \tilde{C}(\tau = 0) = 0$$

dimensional ODE for concentration in a reactor

$$\frac{dC(t)}{dt} = \lambda C_{env} - \lambda C(t) - kC(t), \quad C(t = 0) = C_0$$

This models a chemical reaction in a plug flow reactor (*PFR*)

Non-dimensionalization:

$$\tilde{C} = \frac{C}{C_{env}}, \qquad \tau = \frac{t}{T}$$

But $T = \frac{1}{\lambda}$, so:

$$\tau = \mu t \;\Rightarrow \tau = \lambda t$$

Dimensionless parameter: $\beta = \frac{k}{\lambda}$

So:

$$\frac{d}{d\tau}\tilde{C}(\tau) = 1 - \tilde{C}(\tau) - \beta\tilde{C}(\tau)$$

$$\frac{d\tilde{C}(\tau)}{d\tau} = 1 - (1 + \beta)\tilde{C}(\tau) \quad (1)$$

Let $\alpha = 1 + \beta$, then:

$$\frac{d\tilde{C}(\tau)}{d\tau} = 1 - \alpha\tilde{C}(\tau) \;\Leftrightarrow\; \frac{d\tilde{C}(\tau)}{1 - \alpha\tilde{C}(\tau)} = d\tau$$

Integrate both sides:

$$-\frac{1}{\alpha}\ln\left(1-\alpha\tilde{C}(\tau)\right)=\tau+c' \Rightarrow -\ln\left(1-\alpha\tilde{C}(\tau)\right)=\alpha\tau+\alpha c' \Rightarrow$$

$$1-\alpha\tilde{C}(\tau)=e^{-\alpha\tau}e^{-\alpha c\prime} \;\; \Rightarrow \;\; \alpha\tilde{C}(\tau)=1-e^{-\alpha\tau}e^{-\alpha c\prime} \;\Rightarrow$$

$$\tilde{C}(\tau)=\frac{1}{\alpha}-\frac{e^{-\alpha c\prime}}{\alpha}e^{-\alpha\tau}$$

For $\tau=0$:

$$\tilde{C}(0)=0 \Rightarrow \frac{1}{\alpha}-\frac{e^{-\alpha c\prime}}{\alpha}=0 \Rightarrow 1-e^{-\alpha c\prime}=0 \Rightarrow e^{-\alpha c\prime}=1 \Rightarrow e^{-\alpha c\prime}=e^{0} \Rightarrow \alpha c'=0 \Rightarrow c'=0$$

So:

$$\tilde{C}(\tau)=\frac{1}{1+\beta}-\frac{1}{1+\beta}e^{-(1+\beta)\tau} \;\Rightarrow$$

$$\tilde{C}(\tau)=\frac{1}{1+\beta}\left[1-e^{-(1+\beta)\tau}\right] \tag{1}$$

(b) Provide the solution using the initial variables.

The dimensional form of the equation arises from the change of variables

$$\tilde{C}=\frac{C}{C_{env}}, \qquad \tau=\frac{t}{T}$$

and the definition $\beta=\frac{k}{\lambda}$

Thus, the solution is:

$$\frac{C(t)}{C_{\text{env}}}=\frac{1}{1+\dfrac{k}{\lambda}}\left[1+e^{-\left(1+\frac{k}{\lambda}\right)\lambda t}\right] \Rightarrow$$

$$C(t)=C_{\text{env}}\cdot\frac{\lambda}{k+\lambda}\left[1+e^{-(k+\lambda)t}\right]$$

(c) Compare the numerical and analytical solution of the problem (provide a graphical representation).

The graph shows the evolution of concentration during a chemical reaction. The solid blue line shows the solution for β = 0.0, and the blue circles show the result of the numerical solution from code.

(d) Graphically compare the solution for a small β (e.g., β = 0.2) with the solution we found for the case of negligible β.

The solution for negligible β is:

$$\tilde{C}(\tau) = 1 - e^{-\tau}$$

and the solution for any β is given by equation (1).

We observe that for large times:

- For β = 0: $\tilde{C}(\tau \to \infty) = 1$

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- For β = 0.2: $\tilde{C}(\tau \to \infty) = \frac{1}{1.2} = 0.83$

The red solid line shows the solution for $\beta = 0.2$, and the red circles show the result of the numerical solution.