Homework No.3

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1 Problem Statement

The equation of conservation of chemical species under a chemical reaction of decomposition can be represented with the PDE given below.

$$\frac{\partial C}{\partial t} = \vec{\nabla} \cdot (D\vec{\nabla}C) - \vec{v} \cdot \vec{\nabla}C - kC^n$$

If a tubular catalytic chemical reactor initially filled with an inert solvent ($C = 0$) is fed by a stream of component "A" with a concentration of $1kmol/m^3$ ($C = 1$) and speed of $1m/s$ ($v = 1$), calculate the distribution of "A" across the reactor and as a function of time $C(x, t)$. The dispersion coefficient of the component "A" is $0.02m^2/s$ ($D = 0.01$), the kinetic decomposition coefficient $0.05s^{-1}$ ($k = 0.05$). The chemical decomposition kinetics is first order ($n = 1$).

2 Sketch

3 Assumptions and Approximations

4 Physical constants

5 Physical Transport or Thermodynamic Properties

6 Calculations

6.1 PDEPE solver

The molar balance in axial direction for a 1D flow can be written as:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - kC^n$$

The initial condition IC is:

$$C|_{t=0} = 0,\ 0 \leq x \leq 1$$

The boundary conditions BCs are:

$$C|_{x=0} = 1,\ t > 0$$

$$\left.\frac{\partial C}{\partial t}\right|_{x=L} = 0,\, t \geq 0$$

6.2 FEATool solver

7 Discussion