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

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:

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

The boundary conditions BCs are:

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

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

6.1 PDEPE solver

The built in function PDEPE, solves a general problem of a 1-D (parabolic or elliptic) partial differential equation, for a Cartesian, cylindrical or spherical coordinates of the from:

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t}=\frac{1}{x^m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right)+s\left(x,t,u,\frac{\partial u}{\partial x}\right)$$

Where,
$m = 0$ represents the symmetry of the problem (0 for slab, 1 for cylindrical, or 2 for spherical)
$c = 1$ is a diagonal matrix
$f = D\frac{\partial u}{\partial x}$ is the flux term
$s = -v\frac{\partial u}{\partial x} - ku^n$ is the source term
c, f, and s correspond to coefficients in the standard PDE equation form expected by pdepe. These coefficients are coded in terms of the input variables x, t, u, and $dudx$. Listing 1 implements a function that calculates the values of the coefficients c, f, and s.

```
function [c, f, s] = DiffusionPDEfun(x, t, u, dudx, P)
    % Parameters
    D  = P(1);
    k  = P(3);
    vo = P(4);

    % PDE
    c = 1;
    f = D .* dudx;
    s = - k * u - vo * dudx;
end
```

Listing 1: PDE function for equations

PDEPE requires an 'initial condition function', which is defined as a function that defines the initial condition. For $t = t_o = 0$ and all x, the solution satisfies the initial condition of the form:

$$u(x,t_o) = u_o(x)$$

PDEPE calls the initial condition function with an argument x, which evaluates the initial values for the solution at x in vector u_o. The number of elements in u_o is equal to the number of equations. Listing 2 implements the constant initial condition.

```
function u0 = DiffusionICfun(x, P)
    % u0 = u0(x)
    u0 = 0;
end
```

Listing 2: Initial condition function

The third function required by the PDEPE solver is the 'boundary condition function'. The boundary condition function spefifies the boundary conditions for all t, the solution satisfy the boundary condition of the form:

$$p(x,t,u)+q(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right)=0$$

Listing 3 implements a function that defines the terms p and q of the boundary conditions. $u1$ is the approximate solution of the left boundary, ur is the approximate solution of the right boundary, pl and ql are vectors corresponding to p and q evaluated at xl, and pr and qr are vectors corresponding to p and q evaluated at xr.

```
function [pl, ql, pr, qr] = DiffusionBCfun(xl, u1, xr, ur, t, P)
    % BCs: No flux boundary at the right boundary and constant
    % concentration on the left boundary
    c0 = P(2);
    pl = u1 - c0;
    ql = 0;
    pr = 0;
    qr = 1;
end
```

Listing 3: Boundary condition function

6.2 FEATool solver

7 Discussion