Continuous Stirred Tank with Recycle

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September 27, 2020

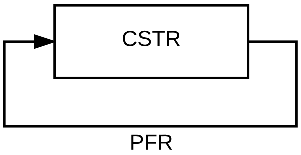

Figure 1: CSTR with PFR recycle.

Consider a CSTR of volume V with a recycle through a PFR of length L and cross-sectional area A at a superficial velocity v, see figure 1. Two models of such a system are proposed:

1. Delay differential equation model
2. Partial differential equation model

The goal is to compare the PDE model with the analytical solution of the corresponding DDE model to illustrate the effect of numerical diffusion when solving the PDE model numerically. The model experiment is a tracer experiment in which a pulse of substance $c_\delta\, V$ is introduced into the tank momentarily and then the concentration response is observed.

DDE Model

A DDE model of the system is stated in equation (1).

$$\frac{\mathrm{d}c(t)}{\mathrm{d}t} = \frac{v\,A}{V}\left[c(t - \frac{L}{v}) - c(t)\right],\ \text{for } t \geq 0,\ c(t<0) = 0 \text{ and } c(t=0) = c_\delta \tag{1}$$

$\frac{v\,A}{V}$ is observed to be the dilution rate of the CSTR, $\frac{L}{v}$ the residence time in the PFR and c_δ is the pulse concentration. Eventually the pulse will be evenly distributed in the entire volume resulting in a final concentration c_∞ according to equation (2).

$$c_\infty = \frac{c_\delta\, V}{L\,A + V} \tag{2}$$

Equation (1) may be brought to a dimensionless form as stated in equation (3) by introducing the dimensionless variables $\theta = \frac{L}{v}\,t$ and $x = \frac{c - c_\infty}{c_\delta - c_\infty}$ as well as the dimensionless constant $\phi = \dfrac{L\,A}{V}$ which is the ratio of the PFR volume to the CSTR volume.

$$\frac{\mathrm{d}x(\theta)}{\mathrm{d}\theta} = \phi\left[x(\theta-1) - x(\theta)\right], \text{ for } \theta \geq 0,\; x(\theta<0) = -\phi^{-1} \text{ and } x(\theta=0) = 1 \tag{3}$$

This delay differential equation with constant delay may be solved analytically by the method of steps.

Equation (2) may be expressed as equation (4) using the dimensionless constant ϕ.

$$c_\infty = c_\delta \frac{1}{\phi+1} \tag{4}$$

In dimensionless terms c_∞ corresponds to $x = 0$.

PDE Model

A PDE model of the system is stated in equations (5a) and (5b).

$$\frac{\mathrm{d}c}{\mathrm{d}t} = \frac{v\,A}{V}\left[c_{\mathrm{PFR}}(z=L) - c\right] \tag{5a}$$

$$\frac{\partial c_{\mathrm{PFR}}}{\partial t} = -\frac{\partial N}{\partial z}, \quad N = v\,c_{\mathrm{PFR}} \tag{5b}$$

Equations (5a) and (5b) have the associated initial conditions $c(t<0) = 0$, $c_{\mathrm{PFR}}(t<0, z) = 0$ for $z \in [0, L]$ and boundary conditions $N(t, z=0) = v\,c$, $\frac{\partial c_{\mathrm{PFR}}(t,z=L)}{\partial z} = 0$. This model may be brought to a dimensionless form using the same dimensionless variables as for the DDE model along with $\lambda = \dfrac{z}{L}$ yielding equations (6a) and (6b).

$$\frac{\mathrm{d}x}{\mathrm{d}\theta} = \phi\left[x_{\mathrm{PFR}}(\lambda=1) - x\right] \tag{6a}$$

$$\frac{\partial x_{\mathrm{PFR}}}{\partial \theta} = -\frac{\partial \Pi}{\partial \lambda}, \quad \Pi = x_{\mathrm{PFR}} \tag{6b}$$

The corresponding dimensionless initial conditions are $x(\theta<0) = -\phi^{-1}$, $x_{\mathrm{PFR}}(\theta<0, \lambda) = -\phi^{-1}$ for $\lambda \in [0,1]$ and boundary conditions $\Pi(\theta, \lambda=0) = x$, $\frac{\partial x_{\mathrm{PFR}}(\theta,\lambda=1)}{\partial \lambda} = 0$. The dimensionless model may be discretized according to the method of lines using a central difference scheme yielding equations (7a) and (7b).

$$\frac{\mathrm{d}x}{\mathrm{d}\theta} = \phi\left[x_{\mathrm{PFR},\,n} - x\right] \tag{7a}$$

$$\frac{\partial x_{\mathrm{PFR},\,i}}{\partial \theta} = -\frac{\Pi_{i+\frac{1}{2}} - \Pi_{i-\frac{1}{2}}}{\Delta\lambda}, \quad \Pi_{\frac{1}{2}} = x, \quad \Pi_{i+\frac{1}{2}} = x_{\mathrm{PFR},\,i}, \quad i \in 1, \ldots, n \tag{7b}$$

where $\Delta\lambda = n^{-1}$. The discretized PFR model is equivalent to a finite series of CSTRs. This analogy explains the numerical diffusion which is observed for numerical simulation of the distributed PFR model.

Simulation

Both models are implemented in MATLAB® R2017a, see appendix A.

A simulation of a tracer experiment is presented in figure 2 for different combinations of ϕ and n. The numerical simulation approaches the analytical solution for increasing n

as the degree of numerical diffusion diminishes. Increasing ϕ, corresponding to a large PFR volume relative to CSTR volume, increases the amount of oscillations before the final steady state concentration of tracer is reached because the relatively large PFR volume hinders mixing in the CSTR. Increasing n appears to improve the agreement between the analytical and the numerical solution.

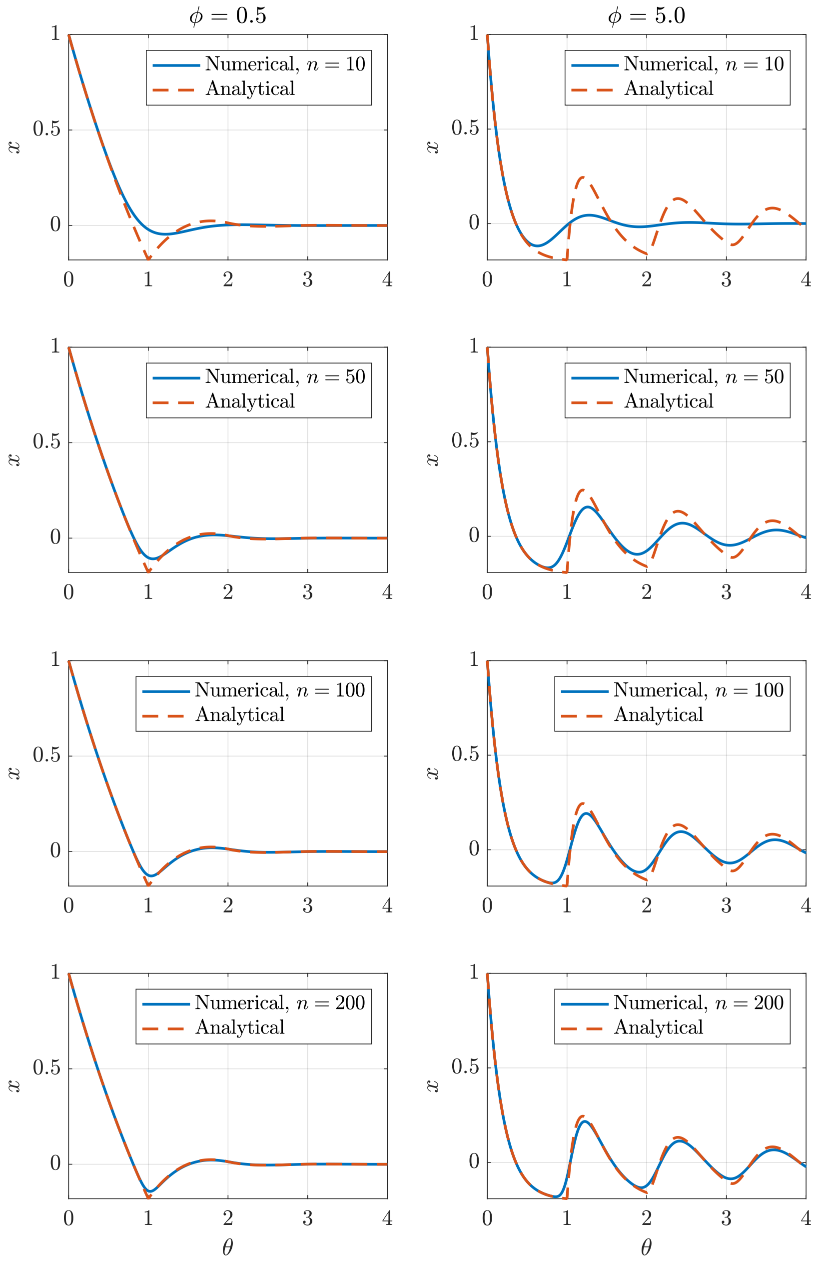

Figure 2: Tracer experiment simulated for $n = \{10, 50, 100, 200\}$ and $\phi = \{0.5, 5.0\}$.

A tracer.m

```matlab
set(0,'defaultlinelinewidth',1.7,'DefaultAxesFontSize',14,'DefaultAxesXGrid','on','DefaultAxesYGrid','
    on','defaultTextInterpreter','latex', 'DefaultFigurePosition', [0 0 600 900])
set(groot,'defaultAxesTickLabelInterpreter','latex','defaultLegendInterpreter','latex');

n_tau = 4;
t = linspace(0,n_tau,1000);
n_discrete = [10 50 100 200];
phi = [0.5 5];

%% Plot
figure(1);
for j = 1:2
    % Parameters
    P.phi = phi(j);
    P.x_delta = 1;
    x_infty = P.x_delta * 1/(P.phi+1);
    % Compute
    state_analytical = tracer_analytical(t,P,n_tau);
    for i = 1:4
        subplot(4,2,1+2*(i-1)+j-1);
        P.n = n_discrete(i);
        state = ones(1,P.n+1)*(-1/P.phi);
        state(P.n+1) = P.x_delta;
        [~,state_ode] = ode15s(@dispersion_model,t,state(:),[],P);

        plot(t,state_ode(:,end)) % Finite difference
        hold on
        plot(t,state_analytical,'--') % Analytical
        ylim([(exp(-P.phi)*(P.phi*P.x_delta+1)-1)/P.phi P.x_delta]); xlim([0 n_tau])
        legend({sprintf('Numerical, $n=%d$', P.n),'Analytical'})
        ylabel('$x$')
        if i == 1
            title(sprintf('$\\phi=%0.1f$',P.phi))
        end
    end
xlabel('$\theta$')
end
%% Analytical solution
function y = tracer_analytical(t,P,n_tau)
    % Method of steps to solve DDE analytically
    % See http://www.orcca.on.ca/TechReports/TechReports/2005/TR-05-02.pdf
    % for a brief introduction to the subject.
    syms x(l) u(l) phi_ x0_
    x0 = x0_;
    u(l) = -1/phi_;

    y = nan(size(t));
    for i = 1:n_tau
        % Solve
        u(l) = dsolve(diff(x,l)==phi_*(u(l)-x(l)),x(0)==x0);
        fun = matlabFunction(u(l));
        x0 = u(1); % Initial condition for next step
        % Compute
        indices = t>=(i-1)&t<=i;
        v = t(indices)-(i-1);
        y(indices) = fun(v,P.phi,P.x_delta);
    end
end
%% System of ODEs
function dx = dispersion_model(~,x,P)
    x_pfr = x(1:end-1); % Unpack
    dx_cstr = P.phi*(x_pfr(end)-x(end)); % CSTR
    dx_pfr = -diff([x(end); x_pfr])*P.n; % PFR
    dx = [dx_pfr; dx_cstr]; % Pack
end
```