

Chemical Reaction Engineering - Part 13 - intro to Plug Flow Reactors

Richard K. Herz, rherz@ucsd.edu, ReactorLab.net

Continuous flow reactors and PFRs

So far we have been studying batch reactors. Batch reactors probably produce the greatest dollar value of product, mainly because they often produce very high value products even if only in relatively small quantities. However, batch reactors are not the best choices when we want to make very large amounts of product every day during the year. Starting, stopping, cleaning and reloading batch reactors - the changeover process - takes a lot of production time out of the year and may involve a lot of operators (people). If we can, we would like a reactor that runs continuously and produces product continuously without having to shut it down more than once or twice a year for maintenance.

For example, we want to process crude oil and make gasoline and diesel fuel continuously and not in batches.

There are two main types of continuous flow reactors: plug flow reactors (PFR) and continuous stirred tank reactors (CSTR). We are going to start with PFRs and then go to CSTRs a little later.

Plug flow is obtained when the fluid velocity is constant across a plane normal to the flow direction. Plug flow is an ideal case and could only be exactly obtained in the lab with, e.g., a piston and cylinder.

Plug flow can be approached in the following cases:

- turbulent flow in a pipe
- laminar or turbulent flow in a packed bed of solid particles: inert packing or catalyst particles

We will model these situations with a PFR and usually get useful results. For more detailed models, we would need to include the process of "dispersion" of components along the flow axis, such as that caused by axial mixing due to fluid eddies in turbulent flow or between solid particles.

Usually we think about reactors in chemical process plants. However, natural systems such as reactions in groundwater flow through soil can be modeled with a PFR.

Laminar flow reactors

What about laminar flow in a pipe? Reactions in laminar flow are more complex to model than reactions in plug flow, so we will save this until later.

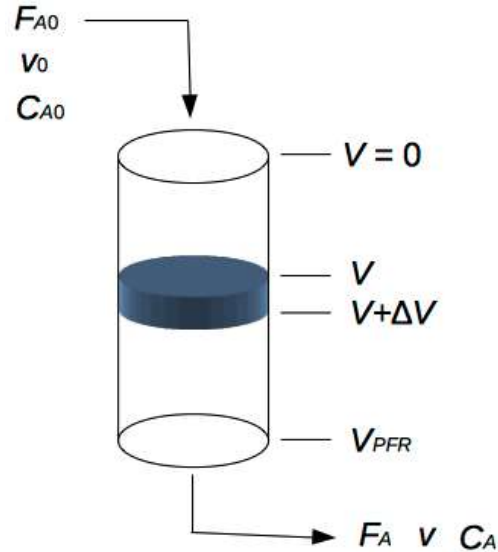
Component balance in a PFR

We need to write a component balance - for our reactant A of course - around a proper control volume. A control volume is a region in space in which conditions are uniform. For a well-mixed batch reactor, then reactor contents are at uniform conditions and the control volume is the reactor.

For a PFR, however, conditions vary along the direction of flow. For a PFR, conditions are uniform across the diameter of the reactor, ignoring here the possibility of radial temperature gradients.

The control volume for a PFR is a differential slice of the reactor.

Consider the following PFR. Most PFRs have constant cross-sectional areas but some don't, such as the spherical reactors we have seen in class.



We are going to use the volume of the reactor as measured from the entrance as our position variable, capital V . For packed beds of catalyst particles, we could also use the mass of catalyst, W . The volumetric flow rate is lower-case v .

F_A (mol/s) is the molar flow rate of component A.

These are important relationships to remember for PFRs:

$$F_A \text{ (mol/s)} = v \text{ (m}^3\text{/s)} C_A \text{ (mol/m}^3\text{)}$$

$$C_A \text{ (mol/m}^3\text{)} = F_A \text{ (mol/s)} / v \text{ (m}^3\text{/s)} \quad (\text{vs. } C_A = N_A / V \text{ for batch})$$

F_A and C_A will vary with V as A is converted.

The volumetric flow rate v might be constant or might vary. For liquids, we will assume v is constant. For gases, v will vary down the reactor if there is a change in total moles with reaction, or a change in T or significant change in P . Fluid flow down a pipe requires a drop in pressure but that drop may be negligible in some cases.

Here is the component balance for A around the control volume from any V to $V+\Delta V$ for a case where we can neglect accumulation of A over the surfaces of solid packing or catalyst, if any.

$$\frac{dN_A}{dt} = \Delta V \frac{dC_A}{dt} = [F_A]_V - [F_A]_{V+\Delta V} + r_A \Delta V$$

Divide by ΔV and take the limit as ΔV becomes very small

$$\frac{dC_A}{dt} + \frac{dF_A}{dV} = r_A$$

This is a partial differential equation (PDE) since it has two independent variables, t and V .

We are going to make life simple and consider only steady-state operation of a PFR.

$$\frac{dF_A}{dV} = r_A \quad \text{at steady state}$$

Given a rate equation and inlet conditions, we can integrate this equation to find how conditions vary down the reactor. For a non-isothermal reactor, we would have to integrate this equation along with the energy balance. We will get to the energy balance later.

Define the reactor "space time" τ

$$\tau(s) = \frac{V(\text{m}^3)}{v_0(\text{m}^3/\text{s})} \quad \text{or, for reactors packed with catalyst pellets,} \quad \tau(\text{kg s/m}^3) = \frac{W(\text{kg})}{v_0(\text{m}^3/\text{s})}$$

For constant density fluid flow, $v = v_0 = \text{constant}$, and the space time is the residence time of fluid in the PFR. However, this definition of space time holds even when the fluid flow rate changes down the reactor.

We can write the component balance this way after multiplying both sides by v_0

$$\frac{dF_A}{d\tau} = r_A v_0$$

For constant density fluid flow, $F_A = v_0 C_A$, and we get

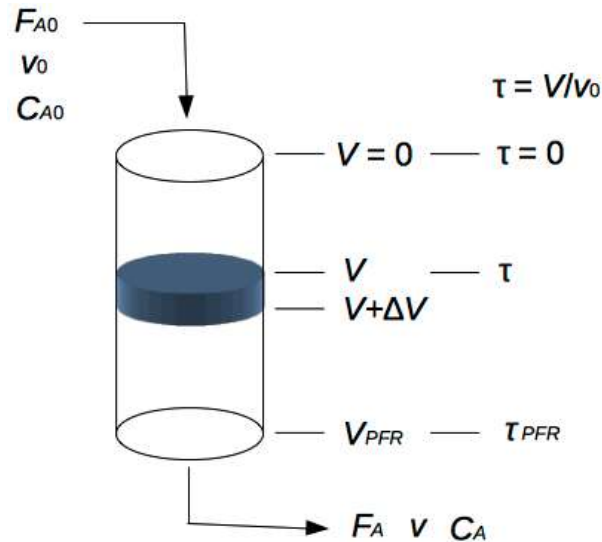
$$\frac{dC_A}{d\tau} = r_A \quad \text{steady-state PFR with constant volumetric flow rate}$$

Compare this to the component balance for A in a constant volume batch reactor

$$\frac{dC_A}{dt} = r_A \quad \text{batch reactor with constant volume}$$

Space time τ is the time a small packet of fluid has been in the PFR, where τ varies from 0 at the inlet to τ_{PFR} at the outlet. Time t is the time fluid has been reacting in the batch reactor.

Position down a PFR, as measured by τ , is equivalent to reaction time in a batch reactor.



We get the same equation for a steady-state PFR with constant v as for an unsteady-state batch reactor with constant V . How can this be? Think of a train of small batches of fluid moving down a PFR.

The result is that almost everything we learned about batch reactors applies to PFRs. Good. We don't have to start over.

We can apply what we learned about stoichiometry, integration, reversible reactions, data analysis, thermal effects and multiple reactions. We can even apply what we learned about semi-batch reactors to PFRs with side inlet streams and PFRs whose walls are selectively permeable membranes: "membrane reactors."

What is different between batch reactors and PFRs?

The difference is mainly with gases. PFRs have constant volume but may have variable volumetric flow rate with gases. Here, we assume liquids have constant density and, thus, constant flow rate. This may not be the case with some liquids but those cases are rare.

For gases, volumetric flow rate will change down a PFR when any of the following occur: change in total moles with reaction, change in temperature, change in pressure. Often we will be able to use the ideal gas law to account for changes in volumetric flow rate with changes in these variables.

Fluid flow down a pipe requires a pressure gradient, i.e., a drop in pressure (pressure drop) down the pipe. For liquids, pressure drop costs money for pumping but doesn't affect reaction rates. For gases, pressure drop results in expansion of the gas and an increase in volumetric flow rate with position down the reactor.

Remember the equation $C_A \text{ (mol/m}^3\text{)} = F_A \text{ (mol/s)} / v \text{ (m}^3\text{/s)}$. An increase in volumetric flow rate means

a decrease in concentration, which affects the reaction rate.

Getting started solving problems

I recommend you start with these equations

$$\frac{dF_A}{dV} = r_A \text{ (mol/m}^3\text{/s)}$$

$$C_A \text{ (mol/m}^3\text{)} = F_A \text{ (mol/s)} / v \text{ (m}^3\text{/s)} \quad (\text{vs. } C_A = N_A / V \text{ for batch)}$$

or, for reactors packed with catalyst pellets, "packed-bed" reactors

$$\frac{dF_A}{dW} = r_A \text{ (mol/kg/s)}$$

Replace concentrations in the rate equation with F and v . Then write a stoichiometric table using F_i instead of N_i .

For gases, include inerts in the table and sum to get how F_{tot} varies with conversion X_A . For gases, use the ideal gas law in this form

$$Pv = F_{tot} RT \quad \text{for gases in flow reactors} \quad (PV = N_{tot} RT \text{ for batch})$$

First-order, essentially irreversible reaction

$A \rightarrow B$, $r_A = -kC_A$. Find the volume and space time of a PFR required to reach a conversion of 90% given the following: $k = 0.001 \text{ s}^{-1}$, $v_0 = 0.001 \text{ m}^3\text{/s}$, $C_{A0} = 1 \text{ mol/m}^3$.

Write the entry for A in the stoichiometric table

$$F_A = F_{A0}(1 - X_A)$$

Put this into the component balance for A

$$\frac{dF_A}{dV} = r_A$$

$$-F_{A0} \frac{dX_A}{dV} = -kC_A = -k \frac{F_{A0}(1 - X_A)}{v_0}$$

$$\frac{dX_A}{dV} = \frac{k}{v_0}(1 - X_A)$$

Separate variables and integrate

$$-\ln(1 - X_A) = k \frac{V}{v_0} = k \tau$$

$$V = -\ln(1 - X_A) \frac{v_0}{k} = 2.30 \text{ m}^3$$

$$\tau = \frac{V}{v_0} = 2300 \text{ s}$$

Reaction of gases with change in total moles

A + B → P, $r_A = -kC_A$. Find the volume and space time of a PFR required to reach a conversion of 90% given the following: $k = 0.001 \text{ s}^{-1}$, $v_0 = 0.001 \text{ m}^3/\text{s}$, $C_{A0} = C_{B0} = 1 \text{ mol/m}^3$. No P or inert fed to reactor.

Write the full stoichiometric table

$$F_A = F_{A0} - F_{A0} X_A$$

$$F_B = F_{B0} - F_{A0} X_A$$

$$F_P = F_{P0} + F_{A0} X_A$$

$$F_I = F_{I0}$$

$$F_{tot} = F_{tot,0} - F_{A0} X_A = 2 F_{A0} - F_{A0} X_A$$

We have gases with a change in total moles.

Use the ideal gas law? Double-check: gases? Yes, gases.

$$P v = F_{tot} R T = 2 F_{A0} - F_{A0} X_A$$

$$v = \frac{2 F_{A0} - F_{A0} X_A R T}{P}$$

$$v = \frac{2 F_{A0} R T}{P} (1 - 0.5 X_A)$$

$$v = v_0 (1 - 0.5 X_A)$$

Put this into the component balance for A

$$\frac{dF_A}{dV} = r_A$$

$$-F_{A0} \frac{dX_A}{dV} = -k C_A = -k \frac{F_{A0} (1 - X_A)}{v_0 (1 - 0.5 X_A)}$$

$$\frac{dX_A}{dV} = \frac{k(1-X_A)}{v_0(1-0.5X_A)}$$

$$\frac{(1-0.5X_A)}{(1-X_A)} dX_A = \frac{k}{v_0} dV$$

$$\int_0^x \frac{(1-0.5X_A)}{(1-X_A)} dX_A = \frac{kV}{v_0} = k\tau$$

$$0.5(X - \ln(1-X)) = k\tau$$

$$0.5(0.9 - \ln(1-0.9)) = k\tau$$

$$\frac{0.5(0.9 - \ln(1-0.9))}{k} = \frac{1.60}{0.001 \text{ s}^{-1}} = 1600 \text{ s} = \tau$$

$$V = v_0 \tau = 1.6 \text{ m}^3$$

How would V change for the same conditions and reaction kinetics except $A + B$ forms $2P$ instead of P ?

Now there is no change in total moles such that the volumetric flow rate is constant at the initial conditions. Since all the parameter values are the same as for the "First-order, essentially irreversible reaction" case above, we will find the V is larger, 2.3 m^3 , with no decrease in total moles.

Why would V be smaller for a decrease in total gas moles? When there is a decrease in total gas moles, the decrease in volumetric flow rate has the effect of increasing $C_A = (F_A/v)$ such that the reaction rate increases and we need a smaller reactor with less reaction time.

How would V change for the same conditions and reaction kinetics except $A + B$ forms $4P$ instead of $2P$? That's for you to answer.

Volumetric flow rate for ideal gases

These are really the only things you need to remember: writing the stoichiometric table and the ideal gas law.

$$F_{tot} = F_{tot,0} + (\sum v_i) F_{A0} X_A \quad \text{compare to} \quad N_{tot} = N_{tot,0} + (\sum v_i) N_{A0} X_A \quad \text{for a batch reactor}$$

$$Pv = F_{tot} RT \quad \text{compare to} \quad PV = N_{tot} RT \quad \text{for a batch reactor}$$

The rest of the equations below show what can happen with flow rate. You don't have to remember them. The values you need will appear from writing the stoichiometric table and the ideal gas law while

working a problem.

Continuing with this development

$$v = F_{tot} RT/P$$

$$\frac{v}{v_0} = \frac{F_{tot} RT/P}{F_{tot,0} RT_0/P_0}$$

$$v = v_0 \left(\frac{F_{tot}}{F_{tot,0}} \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right) \quad \text{compare to} \quad V = V_0 \left(\frac{N_{tot}}{N_{tot,0}} \right) \left(\frac{T}{T_0} \right) \quad \text{for a constant } P \text{ batch reactor}$$

$$F_{tot} = F_{tot,0} + \left(\sum v_i \right) F_{A0} X_A \quad \text{compare to} \quad N_{tot} = N_{tot,0} + \left(\sum v_i \right) N_{A0} X_A \quad \text{for a batch reactor}$$

$$v = v_0 \left(1 + \epsilon X_A \right) \left(\frac{T}{T_0} \right) \left(\frac{P_0}{P} \right)$$

$$\epsilon \stackrel{\text{def}}{=} y_{A0} \sum v_i$$

$$y_{A0} \stackrel{\text{def}}{=} \frac{F_{A0}}{F_{tot,0}}$$

Pressure drop

Fluid flow down a pipe requires a pressure gradient, i.e., a drop in pressure (pressure drop) down the pipe. For liquids, pressure drop costs money for pumping but doesn't affect reaction rates. For gases, pressure drop results in expansion of the gas and an increase in volumetric flow rate with position down the reactor.

We already know how a change in pressure affects volumetric flow rate for gases. See the last few equations above. What we need now is an equation that says how the pressure can change down the PFR. Your fluids textbook has equations for pressure drop.

We need to add to our differential equations a differential equation for dP/dz , where z (m) is linear position down the reactor.

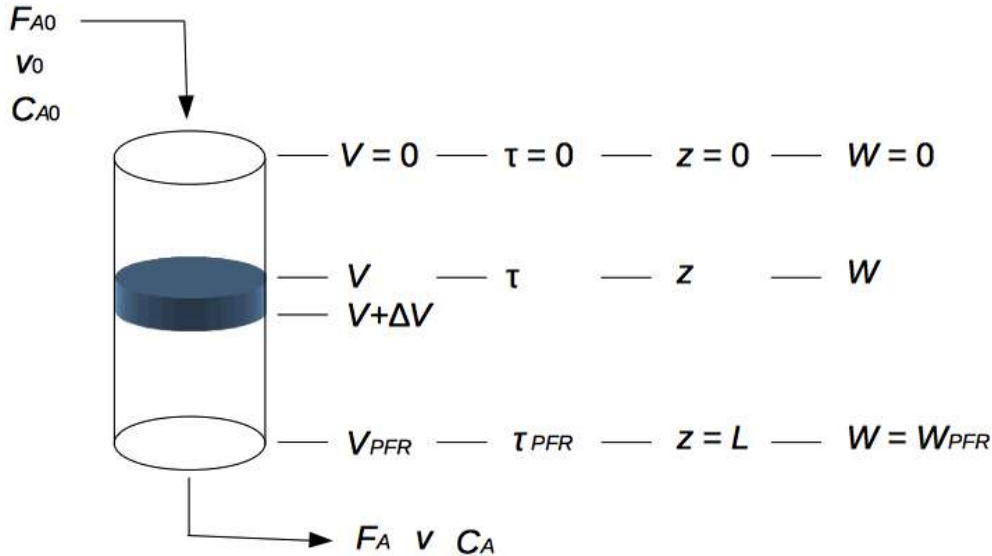
V (m^3), τ (s) and z (m) are directly proportional to each other for a tube of constant cross-sectional area A_x (m^2), so you should have no problem switching between them as independent variables.

For packed beds of catalysts of constant cross-sectional area, the catalyst mass W (kg), V (m^3), τ (s), and z (m) are directly proportional to each other.

$$W \text{ (kg)} = \rho_{bed} \text{ (kg/m}^3\text{)} V \text{ (m}^3\text{)} = \rho_{bed} A_x \text{ (m}^2\text{)} z \text{ (m)} = \rho_{solid} (1 - \epsilon) A_x z$$

where ϵ is the fraction of the bed volume that is filled with fluid between the solid particles, the "bed

void fraction."



The volumetric flow rate of gases will change and as P , T and X_A (for reactions with change in total moles) change with flow down the reactor. This change in the volumetric flow rate of gases will change the rate of pressure drop, component concentrations, and reaction rate. So component balances, the energy balance, and the pressure drop equation for gases are coupled to each other and must be integrated together.

For turbulent flow in an open tube,

$$\frac{dP}{dz} = -v \left[f_F \left(\frac{32m}{\pi^2 d_{tube}^5} \right) \right] \quad \text{turbulent flow in open tube [Pa/m = kg/m}^2\text{/s}^2]$$

where f_F is the Fanning friction factor and m is the constant mass flow rate. The rate of pressure drop is directly proportional to the volumetric flow rate v , which is a function of P , T and F_{tot} for gases. The Fanning friction factor varies with Reynolds number and roughness of the inner tube wall for turbulent flow, and can be found from plots in references.

For fluid flow through a packed bed, laminar or turbulent, use the Ergun equation, where d_{pellet} is the diameter of the packing particles or "pellets."

$$\frac{dP}{dz} = -v \left[600 \left(\frac{\mu(1-\epsilon)^2}{\pi d_{tube}^2 d_{pellet}^2 \epsilon^3} \right) + 28 \left(\frac{m(1-\epsilon)}{\pi^2 d_{tube}^4 d_{pellet} \epsilon^3} \right) \right] \quad \text{fluid flow in packed bed [Pa/m = kg/m}^2\text{/s}^2]$$

In both cases, for constant viscosity and Fanning friction factor,

$$\frac{dP}{dz} = -v [\text{constant}]$$

P always decreases with increasing z . The rate of decrease is proportional to the volumetric flow rate.

There are a few cases that can simplify calculations.

When the pressure drop is small, say less than 10%, we may be able to get a reasonable answer by assuming the pressure is constant at the average value, as long as we know the inlet and outlet pressures. In this case, we don't need a separate equation for change in pressure down the reactor.

When the pressure drop is somewhat larger - there are no fixed percentages - then we may be able to get a reasonable answer by assuming that the pressure changes linearly with position down the reactor, as long as we know the inlet and outlet pressures. In this case, we don't need a separate equation for change in pressure down the reactor since we can express pressure as a function of V or τ .

Adiabatic PFRs

For adiabatic reactors, you can use the "adiabatic temperature rise equation" to get T vs. X .

$$T = T_0 + \frac{C_{A0}(-\Delta H_{rxn})}{\rho C_{pm}} X_A$$

This is the same equation that we derived for the batch reactor. Then you can replace T in the component balance (in the rate coefficient Arrhenius equations) with this equation so that the component balance becomes a function of X only.

Adiabatic conditions can be approached in large diameter PFRs where the surface (for heat transfer) to volume (where reaction occurs) ratio is small.

Non-isothermal, non-adiabatic PFRs

In many cases, we will want to remove the heat of reaction for exothermic reactions, or supply the heat of reaction for endothermic reactions. Then we will get a non-isothermal, non-adiabatic reactor.

In most batch reactors, we have a mixer that circulates reactant fluid past heat exchange surfaces. In PFRs, we have to rely on fluid flow past tube walls for heat transfer, although this can be enhanced in some cases with "static mixers." Since we have to rely on the usual fluid flow in a PFR, we need to use relatively small diameter tubes in order to increase the surface to volume ratio.

This means that PFR's where we need heat transfer are often constructed in a manner similar to shell-and-tube heat exchangers. Heat transfer fluid is on one side and the reaction mixture (and possibly solid catalysts) is on the other side.

Consider the case of a PFR that is composed of many parallel tubes in a shell, with reactants on the tube side and heat transfer fluid on the shell side. We will assume that conditions in all of the parallel tubes are identical. That means we only have to write equations for one tube. The tube diameter is d_{tube} .

Specify that the temperature of the heat transfer fluid T_j is constant along the length of the tubes. This

may not be the case in a real reactors but it keeps things simple here so we can learn the basics.

We also specify plug flow in the tubes and, as well, that the temperature is constant across the tube diameter at any position down the length of the tube. Of course, the temperature can vary down the length of the tube.

The steady-state energy balance for the reaction mixture is

$$\frac{d}{dV}(\rho v C_{pm} T) = Ua(T_j - T) + \Delta H_{rxn} r_A$$

where a (m^2/m^3) is the wall area of the tube per unit volume of tube, and $a = 4/d_{tube}$.

The product (ρv) is the mass flow rate and is constant so we can pull this product out of the derivative along with the mass-average heat capacity, which we also assume is constant.

$$\rho_0 v_0 C_{pm} \frac{dT}{dV} = Ua(T_j - T) + \Delta H_{rxn} r_A$$

$$\rho_0 C_{pm} \frac{dT}{d\tau} = Ua(T_j - T) + \Delta H_{rxn} r_A$$

For gases with a change in volumetric flow rate, we have to account for that in the rate equation r_A . If U changes significantly, we will have to account for the variation of U down the tube.

$$\frac{dT}{d\tau} = \left(\frac{Ua}{\rho_0 C_{pm}} \right) (T_j - T) + \left(\frac{-\Delta H_{rxn}}{\rho_0 C_{pm}} \right) (-r_A) \quad \text{PFR}$$

where a (m^2/m^3) is the tube wall area per unit volume of tube, and $a = 4/d_{tube}$. Compare this to the equation for a constant volume batch reactor

$$\frac{dT}{dt} = \left(\frac{U A/V}{\rho_0 C_{pm}} \right) (T_j - T) + \left(\frac{-\Delta H_{rxn}}{\rho_0 C_{pm}} \right) (-r_A) \quad \text{Batch reactor}$$

Notice how sensitive is the rate of pressure drop in a PFR to reactor tube diameter, d_{tube} . When you want to have good heat transfer with energetic reactions and large a (m^2/m^3), you would want small diameter tubes. But these will have high pressure drop. One solution is to have many relatively short, small diameter tubes arranged in parallel in a shell-and-tube reactor. But constructing the reactor with many tubes requires many welds and is more expensive. Maybe we should just use some cheap adiabatic reactors in series with heat exchangers between them instead? So this is another interesting design optimization problem.

Putting it all together - PFR with gases, change in total moles, change in T, pressure drop

Consider the gas-phase reaction $A \rightarrow 2B$ in a PFR. The feed gas contains A but not B. The reaction is first-order in A. The reaction is exothermic and the PFR has a heat transfer jacket with a heat transfer

fluid at constant T_j .

The component balance on A, the energy balance, and the pressure drop equation can be written

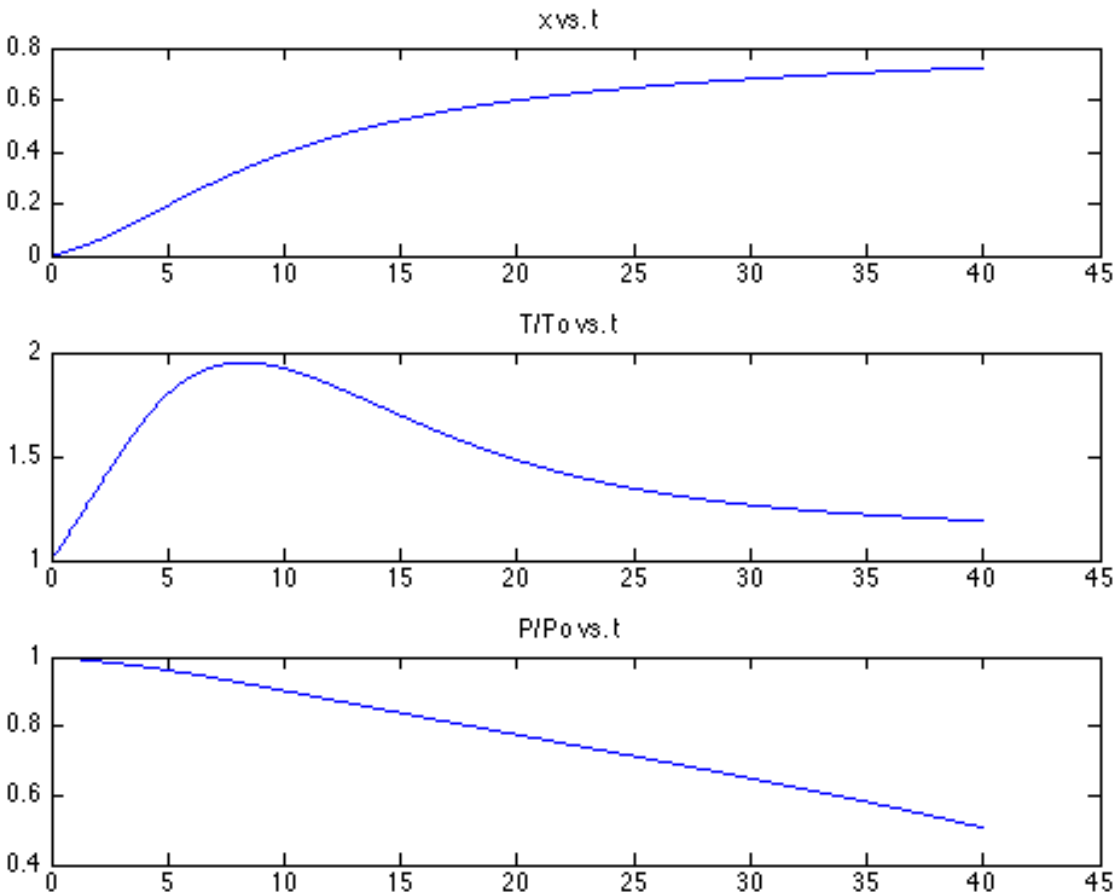
$$\begin{aligned}\frac{dX_A}{d\tau} &= \frac{r_A v_0}{-F_{A0}} \\ \frac{dT}{d\tau} &= \left(\frac{Ua}{\rho C_{pm}} \right) (T_j - T) + \left(\frac{\Delta H_{rxn} r_A}{\rho C_{pm}} \right) \\ \frac{dP}{d\tau} &= -v K_{dp}\end{aligned}$$

where K_{dp} is a constant determined from the appropriate pressure drop equation, and where τ is the space time: τ (s) = V (m^3) / v (m^3/s), or τ ($kg\ s/m^3$) = W (kg) / v (m^3/s).

The right-hand side of each of these equations is a function of all three of the dependent variables. Therefore, the three ODEs must be integrated together.

The plots below show example results. The Matlab script used to generate the plots is shown below.

Make sure you understand what is happening for each curve. How would the plots change qualitatively if the reaction were endothermic?



Listing of Matlab script using Euler's method

Euler's method of integration is useful here because it is easy to read and understand. However, you may have to do some trial and error with the step size dt when you change conditions. Take smaller steps until the solution doesn't change.

Below this script is a script that uses Matlab's standard function `ode45`. That function uses more sophisticated integration algorithms.

```
% A > 2B, gas with change in moles, T, P, rA = -kCA,
clear
% arbitrary input values here for hypothetical reaction
vo = 1; % m3/s, inlet gas volumetric flow rate at reaction conditions
V = 40; % m3, total reactor volume
rho = 10; % kg/m3, inlet gas density
Cpm = 20; % J/kg/K, mass-average heat capacity
Ua = 60; % J/K/s/m3, heat xfer coeff U * tube area/vol a
Po = 200e3; % Pa, inlet gas pressure
To = 300; % K, inlet T
Tj = 330; % K, jacket T
k300 = 2e-2; % (1/s), rate coefficient at 300 K
E = 10e3; % J/mol, activation energy
R = 8.3145; % J/mol/K, gas constant
delH = -10e3; % J/mol, heat of reaction
Kdp = 1e3; % Pa/m3, pressure drop constant
yAo = 0.5;
FAo = yAo*Po*vo/R/To;
x = 0; % conversion of A
T = To; % K, temperature
P = Po; % Pa, pressure
t = 0; % sec, space time
i = 1;
tfinal = V/vo;
dt = 1e-6*tfinal; % Euler's method shown

while t(i) <= tfinal
    % compute current values
    v = vo*(1+yAo*x(i))*(T(i)/To)*(Po/P(i));
    k = k300*exp(-(E/R)*(1/T(i) - 1/300));
    r = -k*FAo*(1-x(i))/v;

    % compute derivatives
    dxdt = r*vo/(-FAo);
    dTdt = (Ua/(rho*Cpm))*(Tj-T(i)) + (delH*r)/(rho*Cpm);
    dPdt = -v*Kdp;

    % update array values
    x(i+1) = x(i) + dxdt * dt;
    T(i+1) = T(i) + dTdt * dt;
    P(i+1) = P(i) + dPdt * dt;
    t(i+1) = t(i) +dt;
    i = i+1;
end
subplot(3,1,1),plot(t,x), title('x vs. t')
subplot(3,1,2),plot(t,T/To), title('T/To vs. t')
subplot(3,1,3),plot(t,P/Po), title('P/Po vs. t')
```

The script below is for the same case but uses the standard Matlab function ode45 for integration. The main script also calls a user-written function, which is also listed below.

Function ode45 is more robust to changes in parameter values than is Euler's method. Function ode45 uses one of the Runge-Kutta algorithms and uses an "adaptive" step size: when rates of change are small, large steps are taken, when rates are large, small steps are taken.

See http://en.wikipedia.org/wiki/Runge%E2%80%93Kutta_methods

```
% A > 2B, gas with change in moles, T, P, rA = -kCA
% uses user-written function file myODEs.m
clear
% arbitrary input values here for hypothetical reaction
vo = 1; % m3/s, inlet gas volumetric flow rate at reaction conditions
V = 40; % m3, total reactor volume
rho = 10; % kg/m3, inlet gas density
Cpm = 20; % J/kg/K, mass-average heat capacity
Ua = 60; % J/K/s/m3, heat xfer coeff U * tube area/vol a
Po = 200e3; % Pa, inlet gas pressure
To = 300; % K, inlet T
Tj = 330; % K, jacket T
k300 = 2e-2; % (1/s), rate coefficient at 300 K
E = 10e3; % J/mol, activation energy
R = 8.3145; % J/mol/K, gas constant
delH = -10e3; % J/mol, heat of reaction
Kdp = 1e3; % Pa/m3, pressure drop constant
yAo = 0.5;
FAo = yAo*Po*vo/R/To;
x = 0; % conversion of A
T = To; % K, temperature
P = Po; % Pa, pressure
t = 0; % sec, space time
i = 1;
tfinal = V/vo;
tspan = [0 tfinal];
yo = [x T P]; % initial conditions
params = [vo yAo To Po k300 E FAo Ua rho Cpm Tj delH Kdp];

% integrate using standard Matlab function ode45
[t y] = ode45('myODEs',tspan,yo,[],params);

x = y(:,1);
T = y(:,2);
P = y(:,3);
subplot(3,1,1),plot(t,x), title('x vs. t')
subplot(3,1,2),plot(t,T/To), title('T/To vs. t')
subplot(3,1,3),plot(t,P/Po), title('P/Po vs. t')
```

User-written function file myODEs.m which is called by ode45 to get current values of the derivatives

```
function dydt = myODEs(t,y,flags,params)

% extract params = [vo yAo To Po k300 E FAo Ua rho Cpm Tj delH Kdp];
vo = params(1); yAo = params(2); To = params(3); Po = params(4);
k300 = params(5); E = params(6); FAo = params(7); Ua = params(8);
rho = params(9); Cpm = params(10); Tj = params(11);
delH = params(12); Kdp = params(13);

% extract values of the dependent variables
```

```

x = y(1); T = y(2); P = y(3);

% compute current values
v = vo*(1+yAo*x)*(T/To)*(Po/P);
R = 8.3145; % J/mol/K, gas constant
k = k300*exp(-(E/R)*(1/T - 1/300));
r = -k*FAo*(1-x)/v;

% compute derivatives
dxdt = r*vo/(-FAo);
dTdt = (Ua/(rho*Cpm))*(Tj-T) + (delH*r)/(rho*Cpm);
dPdt = -v*Kdp;

% set up return values, column vector required by ode45
dydt = [dxdt; dTdt; dPdt];

```

Simulations in ReactorLab

Get ReactorLab at <http://www.ReactorLab.net>

Division 1 Isothermal Reactors

- Lab 1 Nth Order Reactions - PFR
- Lab 4 Variable Flow Rate PFR
- Lab 5 Reversible Reactions - PFR
- Lab 8 Dynamic Pipe Reactor (not exactly plug flow but close)

Division 2 Catalytic Reactors

- Lab 2 First Order Reactions (gas) - PFR
- Lab 3 First Order Reactions (liquid) - PFR (liquid so constant v)

Division 3 Thermal Effects

- Lab 2 PFR With Heat Exchange

Division 4 Flow Patterns

- Lab 1 PFR CSTR Comparison
- Lab 2 Packed Bed RTD (residence time distribution)

Division 5 Multiple Reactions

- Lab 2 Ethylene Oxidation

Division 7 Biological Reactions

- Lab 1 Enzyme Reactions - PFR