Lecture 15: Reactors in Series and Parallel

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begun: September 25, 2009
last updated: September 26, 2011

I. Parallel

Identical reactors in parallel behave just like a single reactor. Only the through-put is multiplied by the number of reactors. This is true for BRs, CSTRs and PFRs.

II. Series

II.A. CSTRs in series

Example.

Consider a set of identical CSTRs in series.

II.A.1. If we have one reactor with a volume of 10 liters, with the parameters given by the following input file

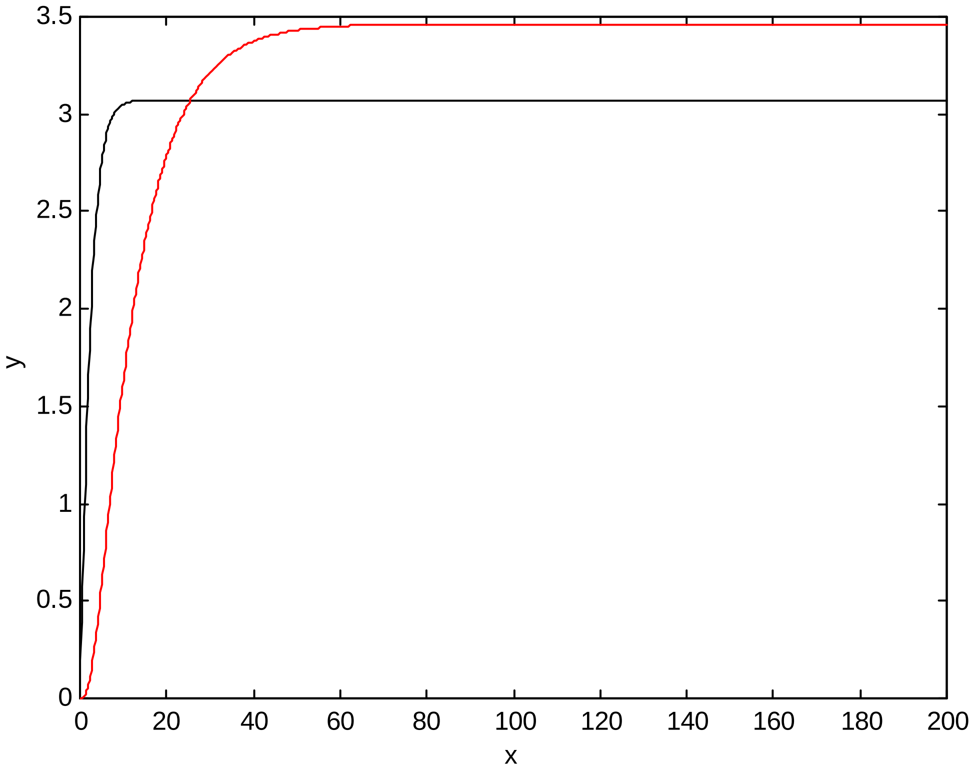
```
function dydt = sysodeinput(x,y,nvec);
%
%  one reaction
%  2A --> B
%
%  example usage:
%  [y,x] = sysode(2,1000,0,100,[0,0]);
%
CA = y(1);
CB = y(2);
nuA = -2.0;
nuB = 1.0;
% constant volume;
F = 1; % liter/sec
Fin = F;
Fout = F;
CAin = 10.0; % mol/liter
CBin = 0.0; % mol/liter
V = 10; % liter
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-1; % liter/mol/sec
Ea = 2500; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CA;
```

```
%
%  molar balances
%
dydt(1) = Fin/V*CAin - Fout/V*CA + nuA*rate;
dydt(2) = Fin/V*CBin - Fout/V*CB + nuB*rate;
```

We can type at the command line prompt

```
[y,x] = sysode(2,1000,0,200,[0,0]);
```

and obtain the following output:



The final concentration of A is 3.072 moles/liter.

II.A.2. If we have two reactors in series each with a volume of 5 liters, with all other parameters remaining unchanged and given by the input file

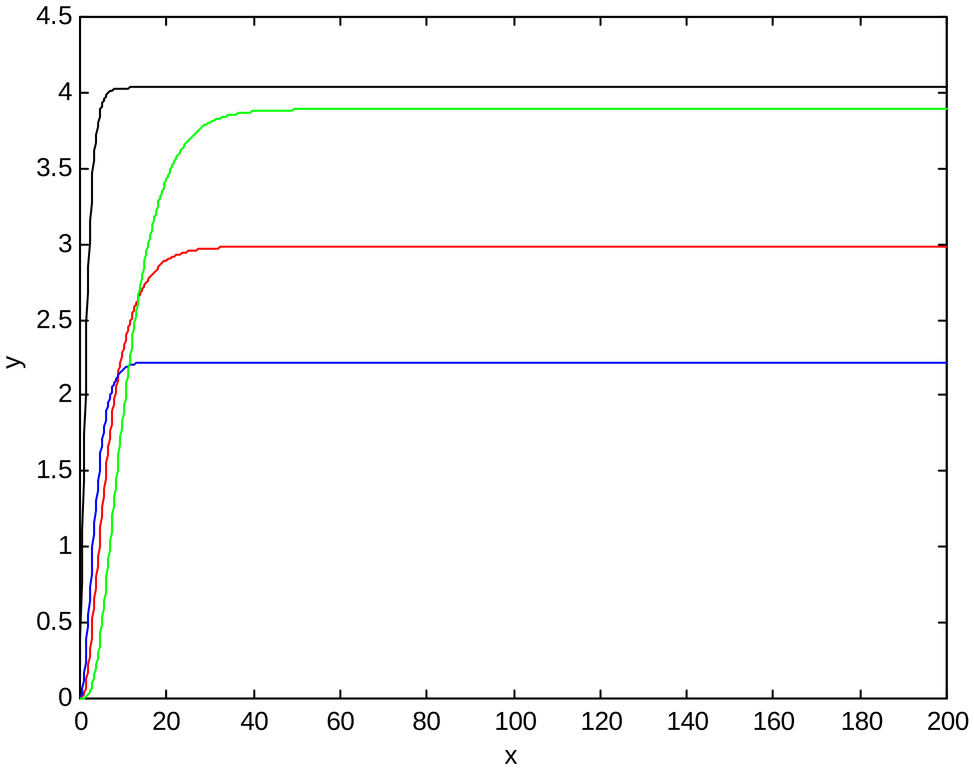
```
function dydt = sysodeinput(x,y,nvec);
%
%  CSTR in series
%  one reaction
%  2A --> B
%
%  example usage:
```

```
%  [y,x] = sysode(2,1000,0,100,[0,0,0,0]);
%
CA1 = y(1);
CB1 = y(2);
CA2 = y(3);
CB2 = y(4);
nuA = -2.0;
nuB = 1.0;
% constant volume;
F = 1; % liter/sec
Fin1 = F;
Fout1 = F;
Fin2 = F;
Fout2 = F;
CAin1 = 10.0; % mol/liter
CBin1 = 0.0; % mol/liter
CAin2 = CA1; % mol/liter
CBin2 = CB1; % mol/liter
V1 = 5; % liter
V2 = 5; % liter
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-1; % liter/mol/sec
Ea = 2500; % J/mol
k = ko*exp(-Ea/(R*T));
rate1 = k*CA1*CA1;
rate2 = k*CA2*CA2;
%
%  molar balance on reactor 1
%
dydt(1) = Fin1/V1*CAin1 - Fout1/V1*CA1 + nuA*rate1;
dydt(2) = Fin1/V1*CBin1 - Fout1/V1*CB1 + nuB*rate1;
%  molar balance on reactor 2
dydt(3) = Fin2/V2*CAin2 - Fout2/V2*CA2 + nuA*rate2;
dydt(4) = Fin2/V2*CBin2 - Fout2/V2*CB2 + nuB*rate2;
```

We can type at the command line prompt

```
[y,x] = sysode(2,1000,0,200,[0,0,0,0]);
```

and obtain the following output:



The final concentration of A is 2.221 moles/liter.

II.A.3. If we have five reactors in series each with a volume of 2 liters, with all other parameters remaining unchanged and given by the input file (Here we have generalized the input file to work for an arbitrary number of reactors, by simply changing the variable nr.)

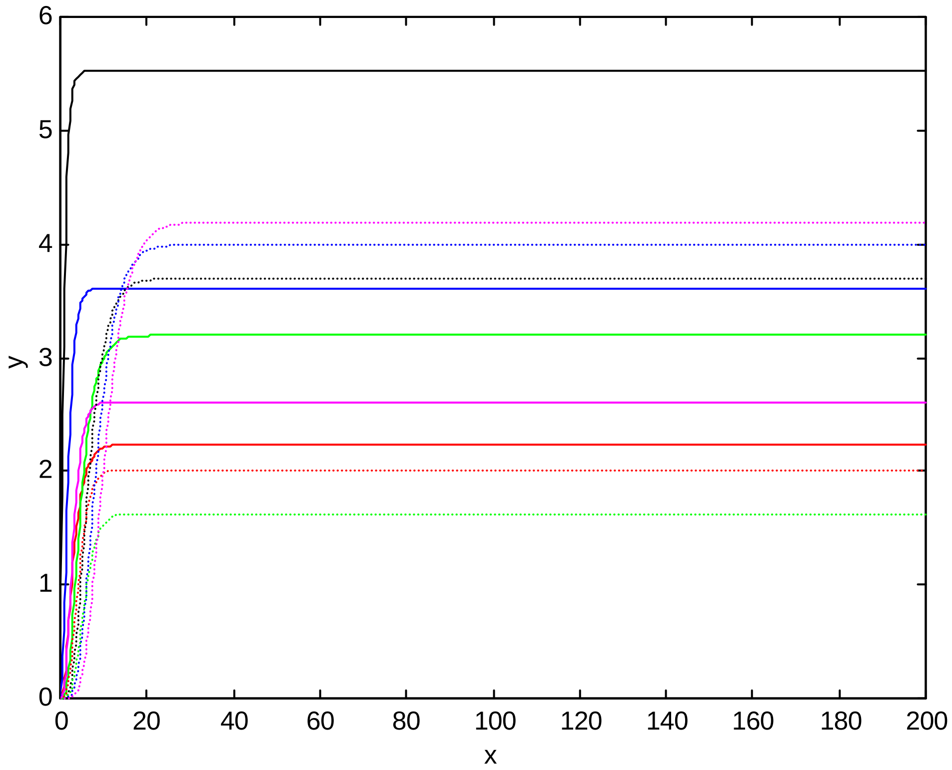
```
function dydt = sysodeinput(x,y,nvec);
%
%  CSTR in series
%  one reaction
%  2A --> B
%
%  example usage:
%  [y,x] = sysode(2,1000,0,100,[0,0,0,0,0,0,0,0,0,0]);
%
% number of reactors = nr
nr = 5;
for i = 1:1:nr
   CA(i) = y(2*i-1);
   CB(i) = y(2*i);
end
%
nuA = -2.0;
nuB = 1.0;
% constant volume;
F = 1; % liter/sec
for i = 1:1:nr
```

```
   Fin(i) = F;
   Fout(i) = F;
end
CAin(1) = 10.0; % mol/liter
CBin(1) = 0.0; % mol/liter
for i = 2:1:nr
   CAin(i) = CA(i-1);
   CBin(i) = CB(i-1);
end
Vtot = 10; % liter
for i = 1:1:nr
   V(i) = Vtot/nr;
end
%
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-1; % liter/mol/sec
Ea = 2500; % J/mol
k = ko*exp(-Ea/(R*T));
for i = 1:1:nr
   rate(i) = k*CA(i)*CA(i);
end
%
%  molar balance on reactor 1
%
for i = 1:1:nr
              dydt(2*i-1) = Fin(i)/V(i)*CAin(i) - Fout(i)/V(i)*CA(i) + nuA*rate(i);
              dydt(2*i)   = Fin(i)/V(i)*CBin(i) - Fout(i)/V(i)*CB(i) + nuB*rate(i);
end
```

We can type at the command line prompt

```
yo = zeros(1,10);
[y,x] = sysode(2,1000,0,200,yo) ;
```

and obtain the following output:

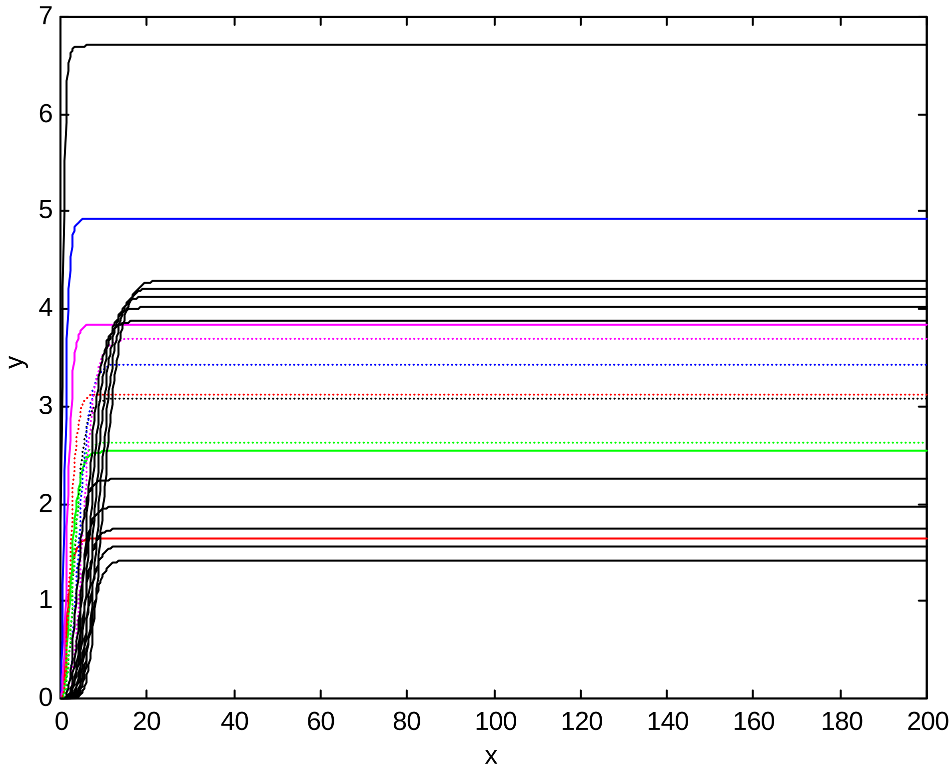


The final concentration of A is 1.626 moles/liter.

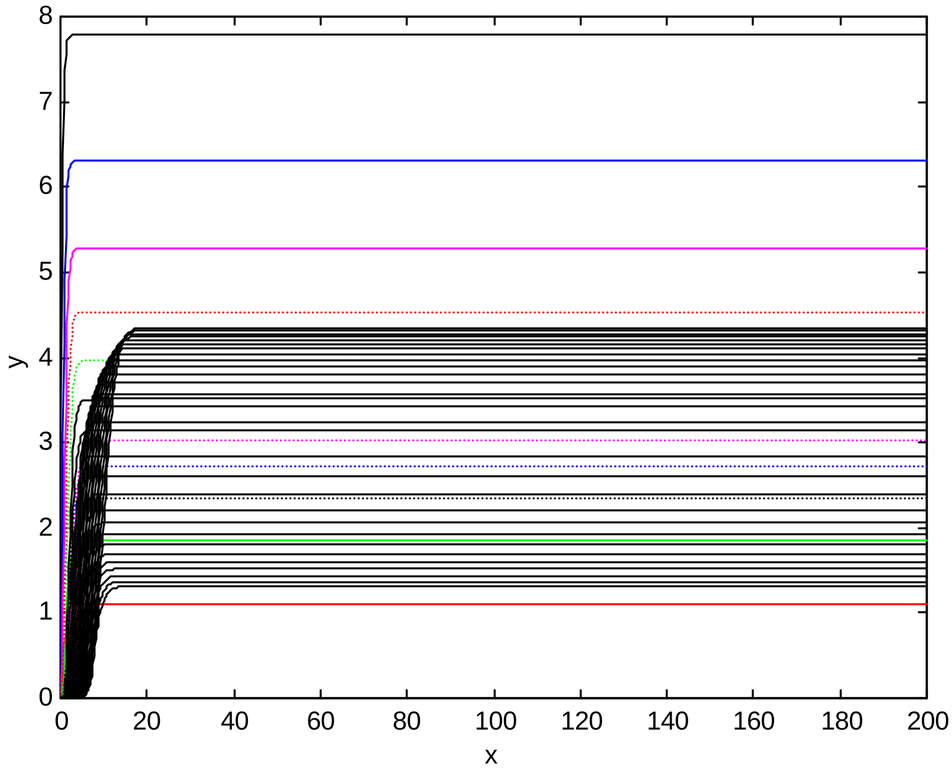
II.A.4. If we have 10, 20, or 100 reactors in series each with a volume of respectively 1, 0.5 or 0.1 liters, with all other parameters remaining unchanged and given by the same input file used in the 5 reactor example above with the single change that nr now is set equal to 10, 20, or 100, then we can type at the command line prompt, respectively

```
yo = zeros(1,20);
[y,x] = sysode(2,1000,0,200,yo) ;

yo = zeros(1,40);
[y,x] = sysode(2,1000,0,200,yo) ;

yo = zeros(1,200);
[y,x] = sysode(2,1000,0,100,yo) ;
```

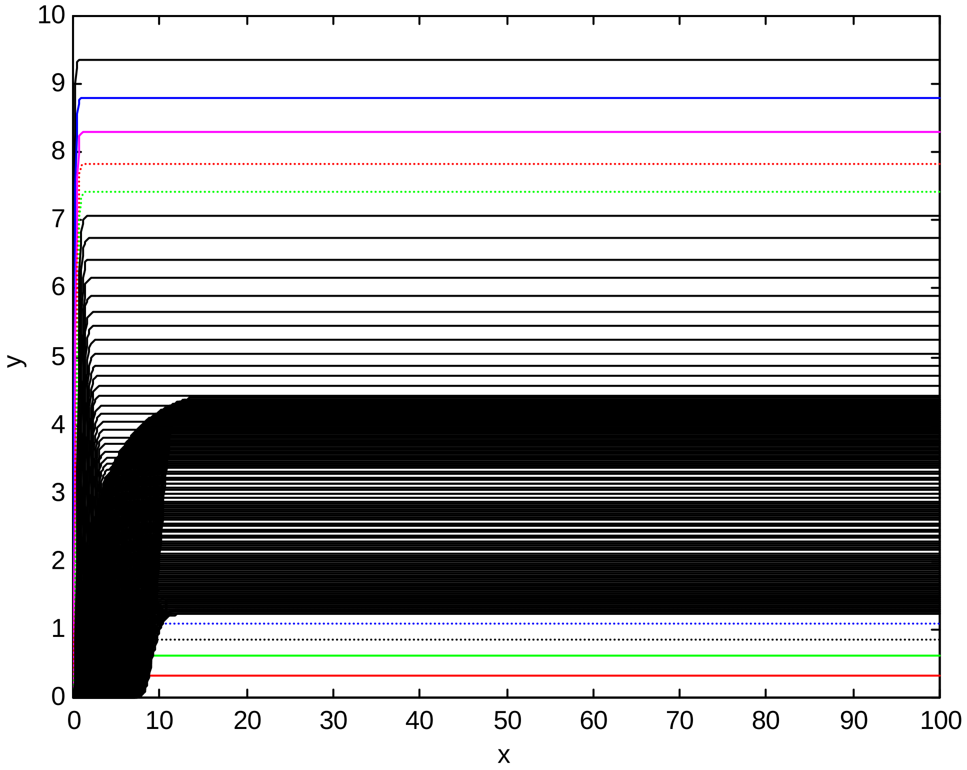
and obtain the following outputs:



output for 10 reactors



Output for 20 reactors



output for 100 reactors

The final concentration of A in 5 reactors is 1.416 moles/liter.
The final concentration of A in 10 reactors is 1.309 moles/liter.
The final concentration of A in 20 reactors is 1.221 moles/liter.

II.A.5. If we have a PFR with the same total volume as the CSTRs above (for example a diameter of 0.1 m and a length of 1.273 m) above all other parameters equal, as in the following input file,

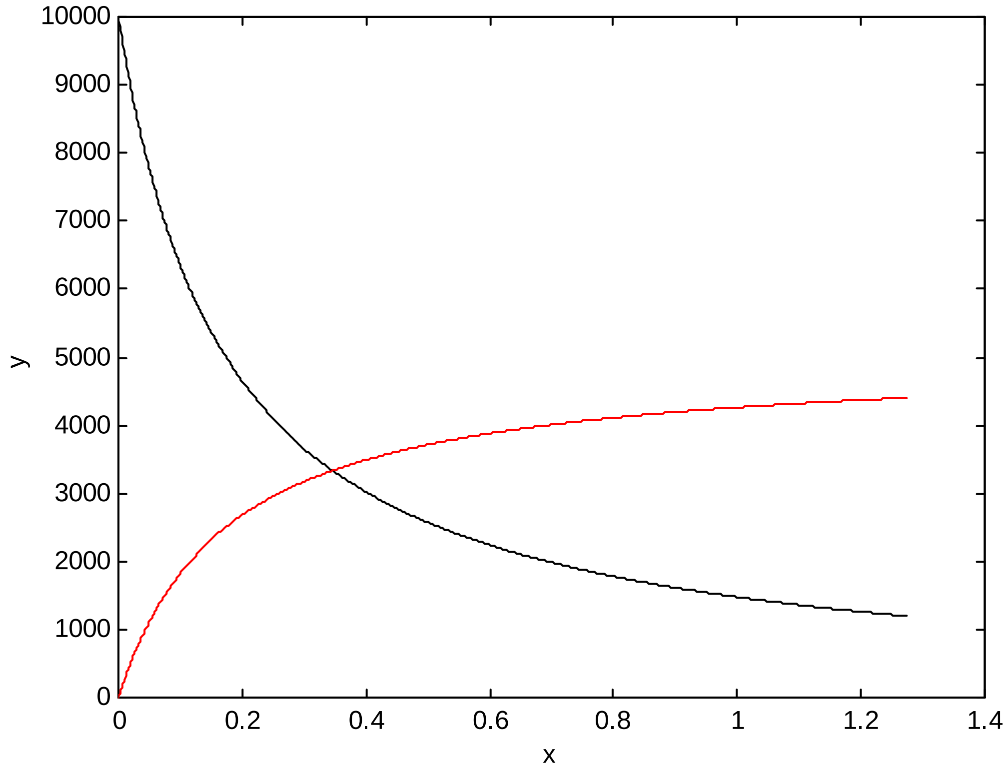
```
function dydt = sysodeinput(x,y,nvec);
%
% one reaction
% 2A --> B
%
% sample command
% [y,x] = sysode(2,1000,0,1.273,[10000,0]);
%
CA = y(1);
CB = y(2);
%
% define the stoichiometry
%
nuA = -2.0;
nuB = 1.0;
```

```
%
%  define the rate law
%
R = 8.314; % J/mol/K
T = 300; % K
ko = 1.0e-1; % liter/mol/sec
ko = ko/1000; % m^3/mol/sec
Ea = 2500; % J/mol
k = ko*exp(-Ea/(R*T));
rate = k*CA*CA;
%
%  define mole balance
%
% volumetric flowrate
F = 1; % liter/sec
F = F/1000; % cubic meters/sec
%
%  circular pipe
%
Vtot = 10.0; % liters
Vtot = Vtot/1000; % cubic meters
Dp = 0.10; % m
Across = 0.25*pi*Dp*Dp; % m^2
l = Vtot/Across; % m
%
% velocity
%
v = F/Across; % m/s
%
% residence time
%
tr = l/v; % sec
%
%  molar balances
%
% dCAdz = nuA*r/v
dydt(1) = (nuA*rate)/v;
dydt(2) = (nuB*rate)/v;
```

We use the following command

```
[y,x] = sysode(2,1000,0,1.273,[10000,0]);
```

to obtain the following output



The final concentration of A in the PFR is 1.199 mol/liter.

We summarize the results in the following table:

reactor type	number of reactors	final concentration of A (moles/liter)
CSTR	1	3.072
CSTR	2	2.221
CSTR	5	1.626
CSTR	10	1.416
CSTR	20	1.309
CSTR	100	1.221
PFR	1	1.199

The conclusion from this set of examples is that, if the total volume is kept the same, as the number of CSTRs approaches infinity, the conversion approaches that of the PFR.

II.B. PFRs in series

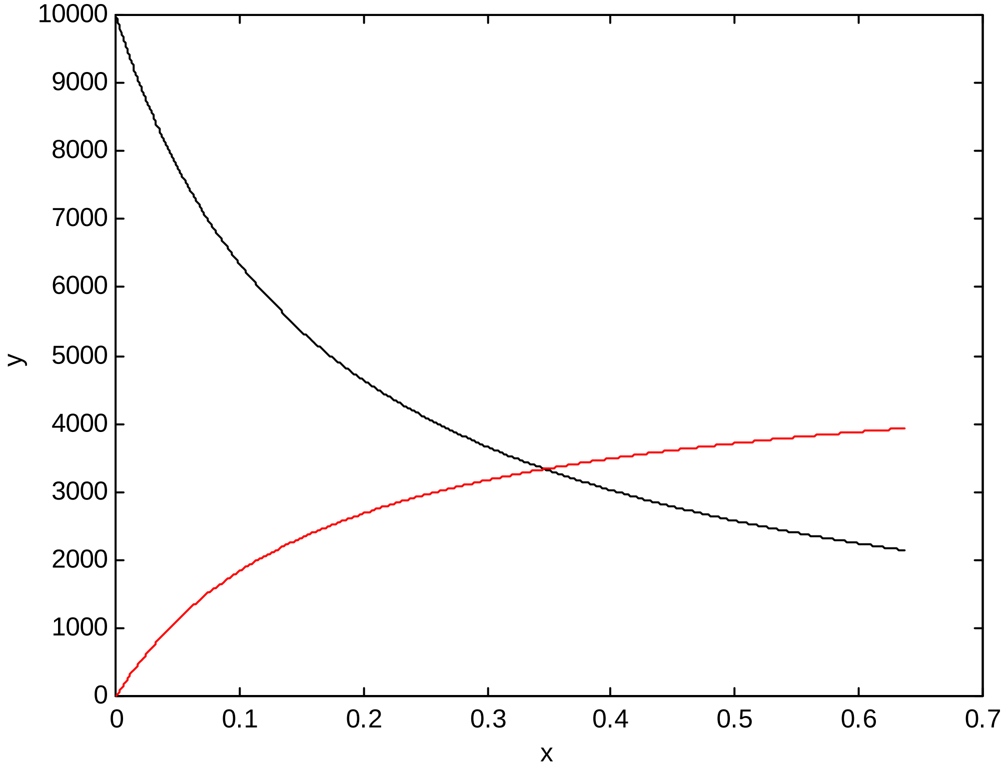
PFRs in series behave as if 1 PFR of equal volume. In the example above, we have one PFR of diameter 0.1 m and length 1.273 m. In this example, we will have two PFRs of diameter 0.1 and each half as long.

The input file is unchanged.

The length is halved in the command prompt is

```
[y,x] = sysode(2,1000,0,0.6365,[10000,0]);
```

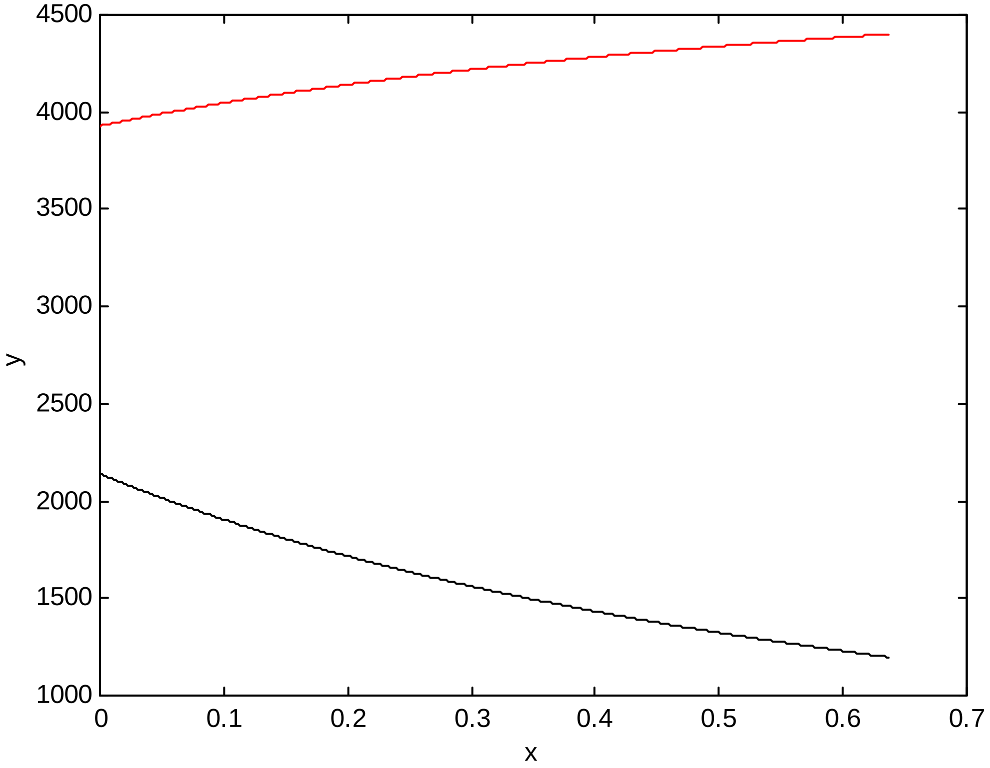
The output looks like



The output concentrations from A and B from the first PFR is 2.1415298e+003 3.9292351e+003 moles/m^3.

We use this output in the second reactor with the same input file and initial conditions that correspond to the output of the first reactor

```
[y,x] = sysode(2,1000,0,0.6365,[2141.5298,3929.2351]);
```



The final concentrations of A and B are 1199 and 4400 moles/m^3., which is the same concentration as obtained for the single PFR in the example above.

II.C. BRs in series

BRs of equal volume in series behave as a single BR of the same volume in which the reaction is allowed to take place for the sum of the residence times of the reactors in series. In essence, this is a pointless task. You are moving the contents from one pot to another pot and allowing the same reaction to continue in a new location. Of course, if there is some other physics going on, like fouling of a catalyst, moving the material to a new pot with fresh catalyst is of course not pointless.

Lecture 16: Combinations of Reactors

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Graphical Analysis of Reactors in Series

Look at graphs
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Example of Reactors in Series

Consider an elementary, irreversible isomerization reaction of A to B in a PFR followed by a CSTR, both operated at steady state. Also consider placing the CSTR first. Compare the two results.

This is an isomerization reaction of A to B.

$$A \rightarrow B$$

The stoichiometric coefficients are $\nu_A = -1$ and $\nu_B = 1$

This is an elementary reaction. Therefore the rate is of the form

$$r = kC_A$$

The mole balance for the PFR is

$$-F\frac{dC_A}{dV} = -\nu_A r$$

Substitute rate law and stoichiometry into the mole balance.

$$\frac{dC_A}{dV} = -\frac{k}{F}C_A$$

This ODE can be solved by hand.

$$\int_{C_{A,o}}^{C_A} \frac{dC_A}{C_A} = -\frac{k}{F}\int_0^{V_{PFR}} dV$$

$$\ln\left(\frac{C_A}{C_{A,o}}\right) = -\frac{k}{F}V_{PFR}$$

$$C_A = C_{A,o}\exp\left(-\frac{k}{F}V_{PFR}\right)$$

This is the outlet concentration of the PFR. This is also the inlet concentration to the CSTR.

The steady-state CSTR mole balance is

$$0 = \frac{F}{V_{CSTR}}C_{A.in} - \frac{F}{V_{CSTR}}C_A + \nu_A r$$

Substitute rate law and stoichiometry into the mole balance.

$$0 = \frac{F}{V_{CSTR}}C_{A.in} - \frac{F}{V_{CSTR}}C_A - kC_A$$

Solve for outlet concentration.

$$C_A = \frac{1}{\frac{F}{V_{CSTR}}+k}\frac{F}{V_{CSTR}}C_{A.in} = \frac{F}{F+kV_{CSTR}}C_{A.in} = \frac{1}{1+k\frac{V_{CSTR}}{F}}C_{A.in} = \frac{1}{1+kt_R}C_{A.in} = \frac{1}{1+Da}C_{A.in}$$

Replace the CSTR inlet concentration with the PFR outlet

$$C_A = \frac{1}{\frac{F}{V_{CSTR}}+k}\frac{F}{V_{CSTR}}C_{A.in} = \frac{F}{F+kV_{CSTR}}C_{A.in} = \frac{1}{1+k\frac{V_{CSTR}}{F}}C_{A.in} = \frac{1}{1+kt_R}C_{A.in} = \frac{1}{1+Da}C_{A.in}$$

$$C_A = \frac{1}{1+k\frac{V_{CSTR}}{F}}C_{A,o}\exp\left(-\frac{k}{F}V_{PFR}\right)$$

This is the outlet concentration of A as a function of the initial concentration, k, F, and the two volumes.

Now, let’s work the problem with the order of the reactors reversed, namely the CSTR first.

The CSTR mole balance yields

$$C_A = \frac{1}{1+k\frac{V_{CSTR}}{F}} C_{A.o}$$

The PFR mole balance yields

$$C_A = C_{A,o} \exp\left(-\frac{k}{F} V_{PFR}\right)$$

Replace the PFR inlet with the CSTR outlet

$$C_A = \frac{1}{1+k\frac{V_{CSTR}}{F}} C_{A.o} \exp\left(-\frac{k}{F} V_{PFR}\right)$$

This is the same result that we obtained above. The order of the reactors doesn't matter for this reaction. But the concentration at the intermediate point between reactors is different.

What about a second order reaction?

CSTR solution:

$$0 = \frac{F}{V_{CSTR}} C_{A,in} - \frac{F}{V_{CSTR}} C_A - 2k_{\dim er} C_A^2$$

This is a quadratic equation.

$$ax^2 + bx + c = 0$$

with solution

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$C_A = \frac{\frac{F}{V_{CSTR}} \pm \sqrt{\left(\frac{F}{V_{CSTR}}\right)^2 + 8k_{\dim er} \frac{F}{V_{CSTR}} C_{A,in}}}{-4k_{\dim er}}$$

For the PFR,

$$-F\frac{dC_A}{dV} = -\nu_A r$$

Substitute rate law and stoichiometry into the mole balance.

$$\frac{dC_A}{dV} = -2\frac{k}{F}C_A{}^2$$

This ODE can be solved by hand.

$$\int_{C_{A,o}}^{C_A}\frac{dC_A}{C_A{}^2} = -2\frac{k}{F}\int_0^{V_{PFR}} dV$$

$$-\frac{1}{C_A}+\frac{1}{C_{A,o}} = -2\frac{k}{F}V_{PFR}$$

$$C_A = \frac{1}{\frac{1}{C_{A,o}}+2\frac{k}{F}V_{PFR}}$$

These are the two results:

CSTR
$$C_A = \frac{\frac{F}{V_{CSTR}} \pm \sqrt{\left(\frac{F}{V_{CSTR}}\right)^2 + 8k_{\dim er}\frac{F}{V_{CSTR}}C_{A,in}}}{-4k_{\dim er}}$$

PFR
$$C_A = \frac{1}{\frac{1}{C_{A,o}}+2\frac{k}{F}V_{PFR}}$$

This will not give the same result, when the order is switched. For example,

Consider these parameters:

Cain	2
F	3
k	4
VPFR	5
VCSTR	6

If you put the CSTR first, your exit concentrations of A are

CSTR	0.323682
PFR	0.060891

If you put the PFR first, your exit concentrations of A are

PFR	0.072289
CSTR	0.042876

In this case, putting the PFR first resulted in the highest conversion.