Solution to Project 2

This project looks at the molar flow rates associated with a reactor/separator system. We are examining the dehydrogenation reaction of propane to propene + H2, with a side reaction using up some of this H2 and propane to make methane. In part 1 we are just looking at the reactor itself, while in part 2 we look at the complete system.

Contents

Part 1

Let's take pa to be propane, pe to be propene, h to be hydrogen and m to be methane. We have four molar balances over the reactor. The fractional conversions will be taken as c1=0.3 and c2=0.05. The total molar flow rate is tot=100. So:

```
clear

tot=100;
pa(1)=.9*tot;
pe(1)=.05*tot;
h(1)=0.03*tot;
m(1)=0.02*tot;

% The concentration on the downstream side of the reactor is just that due
% to the reaction:
c1=0.3;
c2=0.05;
pa(2)=pa(1)*(1-c1-c2);
pe(2)=pe(1)+pa(1)*c1;
h(2)=h(1)+pa(1)*(c1-2*c2);
m(2)=m(1)+pa(1)*3*c2;

%We can present this in table form:
table1=num2str([pa;pe;h;m]);
left=str2mat('propane    ','propene    ','hydrogen    ','methane    ');
table1=[left,table1];
top='component stream1    stream2';
table1=str2mat(top,table1)
```

```
table1 =

component stream1    stream2
propane      90         58.5
propene       5           32
hydrogen      3           21
methane       2         15.5
```

Part 2

Now we work on the complete problem. We have four components in 6 streams, so that gives us a total of 24 unknowns. Because streams 5 & 6 can be directly calculated from streams 2 and 3, however, we can actually solve the reduced problem for streams 1-4, and then calculate streams 5 & 6 later. This gives us a 4x4=16 element solution vector.

```
% We shall take this solution vector to be the column vector x.  The first
% four elements will be pa, the second four pe, third four h, and final
% four m.  We thus convert the 16 equations into matrix form.  Each molar
% balance will represent one row of our matrix.

a=zeros(16,16);
b=zeros(16,1); %The right hand side...

% We will replace the zeros in a and b (where appropriate) one at a time.
% Note that we could do this in an excel worksheet, and then simply upload
% the array into matlab.  Either approach works fine: you just have to get
% the matrix right!  Anyway:

% The propane balances:
% Mixer: pa(1)-pa(4)=feed
a(1,1)=1; a(1,4)=-1;b(1)=100;
% Reactor: pa(2)+(c1+c2-1)*pa(1)=0
a(2,1)=(c1+c2-1); a(2,2)=1;
% First separator: pa(3)-pa(2)=0
a(3,2)=-1; a(3,3)=1;
% Second separator: pa(4)-0.95*pa(3) = 0
a(4,3)=-0.95; a(4,4)=1;

% The propene balances:
% Mixer: pe(1)-pe(4)=0
a(5,5)=1; a(5,8)=-1;
% Reactor: pe(2)-pe(1)-c1*pa(1)=0
a(6,6)=1; a(6,5)=-1; a(6,1)=-c1;
% First separator: pe(3)-pe(2)=0
a(7,7)=1; a(7,6)=-1;
% Second separator: pe(4)-0.05*pe(3)=0
a(8,8)=1; a(8,7)=-0.05;

% The hydrogen balances:
% Mixer: h(1)-h(4)=0
a(9,9)=1; a(9,12)=-1;
% Reactor: h(2)-h(1)-(c1-2*c2)*pa(1)=0
a(10,10)=1; a(10,9)=-1; a(10,1)=-(c1-2*c2);
% First separator: h(3)-0.05*h(2)=0
a(11,11)=1; a(11,10)=-0.05;
% Second separator: h(4)-h(3)=0
a(12,12)=1; a(12,11)=-1;

% The methane balance:
% Mixer: m(1)-m(4)=0
a(13,13)=1; a(13,16)=-1;
% Reactor: m(2)-m(1)-3*c2*pa(1)=0
a(14,14)=1; a(14,13)=-1; a(14,1)=-3*c2;
% First separator: m(3)-0.05*m(2)=0
a(15,15)=1; a(15,14)=-0.05;
% Second separator: m(4)-m(3)=0
a(16,16)=1; a(16,15)=-1;
```

```
%So we get the matrix:
a

%Note that there are ones down the main diagonal, as well as a number of
%entries down the first subdiagonal (either -1 if there was no removal, or
%a smaller value if some of the material was extracted) and entries in the
%first column corresponding to the reaction.  The solution vector is just:

x=a\b

%We can decompose this into the different components, as well as adding in
%the last two streams (5 & 6):
pa=[x(1:4);0;0.05*x(3)];
pe=[x(5:8);0;0.95*x(7)];
h=[x(9:12);0.95*x(10);0];
m=[x(13:16);0.95*x(14);0];

%And we can put this together in matrix form:
table2=num2str([pa,pe,h,m]);
left=str2mat('stream 1:  ','stream 2:  ','stream 3:  ','stream 4:  ','stream 5:  ','
table2=[left,table2];
top='stream     Propane       Propene       Hydrogen      Methane';
table2=str2mat(top,table2)

% Thus, from our feed of 100 moles/s of propane we recover 78.4 moles/s of
% propene and 52.3 moles/s of hydrogen.
```

```
a =

  Columns 1 through 8

    1.0000         0         0   -1.0000         0         0         0         0
   -0.6500    1.0000         0         0         0         0         0         0
         0   -1.0000    1.0000         0         0         0         0         0
         0         0   -0.9500    1.0000         0         0         0         0
         0         0         0         0    1.0000         0         0   -1.0000
   -0.3000         0         0         0   -1.0000    1.0000         0         0
         0         0         0         0         0   -1.0000    1.0000         0
         0         0         0         0         0         0   -0.0500    1.0000
         0         0         0         0         0         0         0         0
   -0.2000         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
   -0.1500         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0

  Columns 9 through 16

         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
```

```
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
         0         0         0         0         0         0         0         0
    1.0000         0         0   -1.0000         0         0         0         0
   -1.0000    1.0000         0         0         0         0         0         0
         0   -0.0500    1.0000         0         0         0         0         0
         0         0   -1.0000    1.0000         0         0         0         0
         0         0         0         0    1.0000         0         0   -1.0000
         0         0         0         0   -1.0000    1.0000         0         0
         0         0         0         0         0   -0.0500    1.0000         0
         0         0         0         0         0         0   -1.0000    1.0000


x =

  261.4379
  169.9346
  169.9346
  161.4379
    4.1280
   82.5593
   82.5593
    4.1280
    2.7520
   55.0396
    2.7520
    2.7520
    2.0640
   41.2797
    2.0640
    2.0640


table2 =

stream      Propane        Propene        Hydrogen       Methane
stream 1:   261.4379       4.127967       2.751978       2.063983
stream 2:   169.9346       82.55934       55.03956       41.27967
stream 3:   169.9346       82.55934       2.751978       2.063983
stream 4:   161.4379       4.127967       2.751978       2.063983
stream 5:          0              0       52.28758       39.21569
stream 6:   8.496732       78.43137              0              0
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