CHE352: SIMULATION LAB 10

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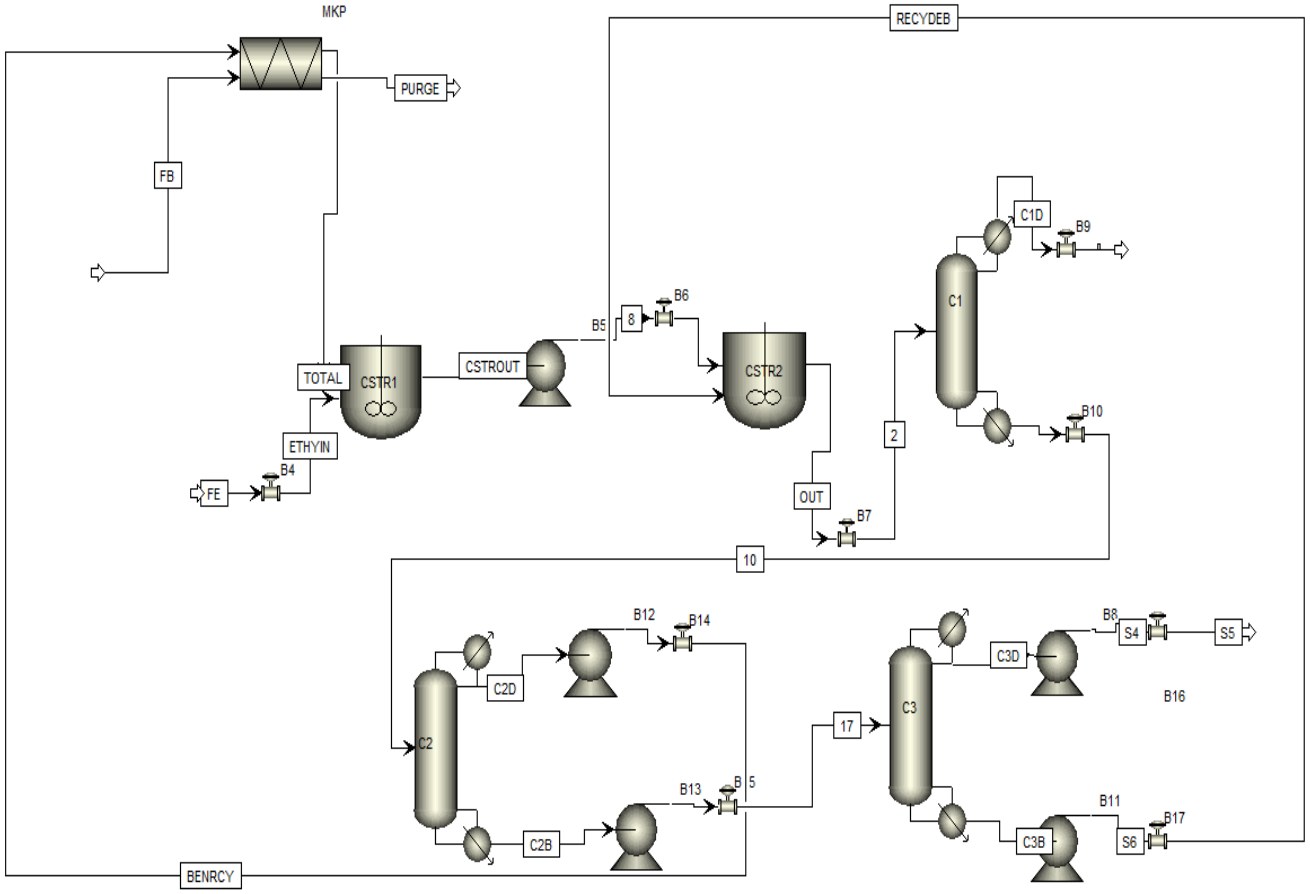
Roll No- 220007



fmincon was implemented on the code present in the appendix.

The variables altered to optimise the total cost were: -

- br_p: benzene mole purity in the recycle stream from C2 distillate stream.
- deb_p: ethylbenzene impurity in C3 bottom recycle stream
- br_fr: benzene flow rate in the recycle stream

fmincon failed to optimise all the three variables for a large data set, so data set had to be estimated using multiple repetitive iterations of fmincon, varying different values.

Sl No	Initial Guess*	Lower Bound*	Upper Bound*	Optimised Values*	J=TAC final value ($)
1	[0.96 0.02 190]	[0.96 0.02 180]	0.96 0.025 200]	[0.96 0.0222 189.9902]	1747200
2	[0.96 0.0222 189.9902]	[0.95 0.0222 189.9902]	[0.97 0.0222 189.9902	[0.97 0.0222 189.9902]	1739200
3	[0.97 0.0222 189.9902]	[0.97 0.0222 189.9902]	[0.98 0.0222 189.9902]	[0.98 0.0222 189.9902]	1732100
4	[0.98 0.0222 189.9902]	[0.98 0.0222 189.9902]	[0.999 0.0222 189.9902]	[0.991 0.0222 189.9902]	1727700
5	[0.991 0.0222 189]	[0.985 0.02 185]	[0.995 0.023 195]	[0.9903 0.0219 194.9998]	1724500
6	[0.991 0.0222 189]	[0.985 0.02 185]	[0.995 0.023 210]	[0.9883 0.0216 209.9439]	1723900

*Initial Guess, Lower Bound and Upper Bound, Optimised Values in the form of [br_pr, deb_p, br_fr].

Final Optimised Values: -

- br_p: 0.9883
- deb_p: 0.0216
- br_fr: 209.9439
- J = $ 1723900

Appendix:

Code Used for optimising TAC using fmincon(MATLAB): -

```
global br_p br_fr deb_p
optim=optimset('fmincon')

optim.Display = 'iter'

[x,J] = fmincon (@(x)TAC(x),[0.91 0.02 190],[],[],[],[],[0.9 0.015 180],[0.999 0.999
210],[],optim)


function J =TAC(x)
global br_p bz_fr deb_p

br_p = x(1);
deb_p = x(2);
bz_fr=x(3);
Aspen=actxserver('Apwn.Document.40.0');
[stat,mess]=fileattrib;
Aspen.invoke('InitFromArchive2',[mess.Name '\Lab 10.bkp']);
Aspen.Visible = 0;
```

```
Aspen.SuppressDialogs = 1;

%Supplying values to the simulation

Aspen.Application.Tree.FindNode('\Data\Blocks\C2\Subobjects\Design
Specs\1\Input\VALUE\1').value=br_p;
Aspen.Application.Tree.FindNode('\Data\Blocks\C3\Subobjects\Design
Specs\1\Input\VALUE\1').value=deb_p;
Aspen.Application.Tree.FindNode('\Data\Blocks\MKP\Input\OUTMLFL').value=bz_fr;

Run2(Aspen.Engine)

Run2(Aspen.Engine)

status=Aspen.Application.Tree.FindNode('\Data\Results Summary\Run-
Status\Output\PER_ERROR').value;

if status==0
    C1Q = Aspen.Application.Tree.FindNode("\Data\Blocks\C1\Output\REB_DUTY").value;
    C2Q = Aspen.Application.Tree.FindNode("\Data\Blocks\C2\Output\REB_DUTY").value;
    C3Q = Aspen.Application.Tree.FindNode("\Data\Blocks\C3\Output\REB_DUTY").value;
    hot = (C2Q)*0.0036*24*300*8.22+(C1Q)*0.0036*24*300*9.8+(C3Q)*0.0036*24*300*9.8;

    C1_CQ =
Aspen.Application.Tree.FindNode("\Data\Blocks\C1\Output\COND_DUTY").value;
    C2_CQ =
Aspen.Application.Tree.FindNode("\Data\Blocks\C2\Output\COND_DUTY").value;
    C3_CQ =
Aspen.Application.Tree.FindNode("\Data\Blocks\C3\Output\COND_DUTY").value;
    cold=(C1_CQ+C2_CQ+C3_CQ)*0.0036*24*300*0.354;

    opx = hot - cold;

    C1_N = Aspen.Application.Tree.FindNode("\Data\Blocks\C1\Input\NSTAGE").value;
    C1_N = double(C1_N);
    C1_D = Aspen.Application.Tree.FindNode("\Data\Blocks\C1\Subobjects\Column
Internals\INT-1\Output\CA_DIAM6\INT-1\CS-1").value;

    C1_TOPT =
Aspen.Application.Tree.FindNode("\Data\Streams\C1D\Output\TEMP_OUT\MIXED").value;
    C1_BOTT =
Aspen.Application.Tree.FindNode("\Data\Streams\C1B\Output\TEMP_OUT\MIXED").value;

    C2_N = Aspen.Application.Tree.FindNode("\Data\Blocks\C2\Input\NSTAGE").value;
    C2_N = double(C2_N);
    C2_D = Aspen.Application.Tree.FindNode("\Data\Blocks\C2\Subobjects\Column
Internals\INT-1\Output\CA_DIAM6\INT-1\CS-1").value;
    C2_TOPT =
Aspen.Application.Tree.FindNode("\Data\Streams\C2D\Output\TEMP_OUT\MIXED").value;
    C2_BOTT =
Aspen.Application.Tree.FindNode("\Data\Streams\C2B\Output\TEMP_OUT\MIXED").value;

    C3_N = Aspen.Application.Tree.FindNode("\Data\Blocks\C3\Input\NSTAGE").value;
    C3_N = double(C3_N);
```

```
    C3_D = Aspen.Application.Tree.FindNode("\Data\Blocks\C3\Subobjects\Column
Internals\INT-1\Output\CA_DIAM6\INT-1\CS-1").value;
    C3_TOPT =
Aspen.Application.Tree.FindNode("\Data\Streams\C3D\Output\TEMP_OUT\MIXED").value;
    C3_BOTT =
Aspen.Application.Tree.FindNode("\Data\Streams\C3B\Output\TEMP_OUT\MIXED").value;

    Fq1=10^(0.477+0.085*log(C1_N)-0.347*log(C1_N)^2);
    A1=pi*(C1_D^2)/4;
    CP1=10^(2.994+0.446*log(A1)+0.396*log(A1)^2);

   TC_1 = CP1*C1_N*1.8*Fq1;

   Fq2=1;
   A2=pi*(C2_D^2)/4;
    CP2=10^(2.994+0.446*log(A2)+0.396*log(A2)^2);

    TC_2 = CP2*C2_N*1.8*Fq2;

    Fq3=1;
   A3=pi*(C3_D^3)/4;
    CP3=10^(2.994+0.446*log(A3)+0.396*log(A3)^2);

    TC_3 = CP3*C3_N*1.8*Fq3;

    C1_CC = TC_1+17640*C1_D^1.066*((C1_N-2)*2*0.3048*1.2)^0.802+7296*(-
C1_CQ/(0.568*(C1_TOPT-298)))^0.65+7296*(C1Q/(0.852*(527-C1_BOTT)))^0.65;
    C2_CC = TC_2+17640*C2_D^1.066*((C2_N-2)*2*0.3048*1.2)^0.802+7296*(-
C2_CQ/(0.568*(C2_TOPT-298)))^0.65+7296*(C2Q/(0.852*(457-C2_BOTT)))^0.65;
    C3_CC = TC_3+17640*C3_D^1.066*((C3_N-2)*2*0.3048*1.2)^0.802+7296*(-
C3_CQ/(0.568*(C3_TOPT-298)))^0.65+7296*(C3Q/(0.852*(527-C3_BOTT)))^0.65;

    vol_CSTR = 200;
    D_CSTR = (2*vol_CSTR/pi)^0.333;
    L_CSTR = 2*D_CSTR;
    CSTR_C = 17460*(D_CSTR^1.066)*(L_CSTR^0.802);
    cpx = C1_CC+C2_CC+C3_CC+2*CSTR_C;

    J = cpx/3+opx;

else

    J=10e10;
end
end
```