THE USE OF THE SOFTWARE MATLAB TO IMPROVE CHEMICAL ENGINEERING EDUCATION

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ABSTRACT - *In all the Brazilian Universities involved with the project "Prodenge – Reenge", the main objective is to improve teaching and learning procedure for engineering disciplines. The Chemical Engineering College of Campinas State University focused its effort on the use of engineering softwares. The work developed by this project has allowed all Chemical Engineering undergraduates to deal with commercial softwares which make engineering calculations and estimates easier. The following work aims Chemical Engineering Process Simulation and Control improvement through the use of the commercial software MATLAB.*

The main concern is to develop some useful case studies which are able to bring out the important characteristics for the control structure design and implementation. Beyond the process simulation and control application, the user has the main concepts related to control theory readily available in an interactive fashion.

The present work has been divided in two parts. The first one consists of Process Control fundamental theory so that an undergraduate can either review or have a first contact with the subject. The second part of the work is an ideal binary distillation column study where some important aspects of the control theory have been implemented.

Part One

The first part consists of some important   process control definitions. Some of them are presented bellow.

Types of variables

The process variables can be divided in 3 groups: manipulated variables, controlled variables and load variables.

• Manipulated variables

They are independent variables which are entering or leaving the process and can be changed to make the control.

• Controlled variables

They are the variables in which the control will be made. This control can be made either maintaining these variables as constant as possible or making them follow a desired trajectory.

Example: Temperature inside a reactor.

• Load variables

It is not possible to manipulate with these variables. Although the effects of the load variables, the control system must be prepared to work perfectly.

What is a controller ?

The construction and operation details of a controller change from manufacturer   to manufacturer, but its basic functioning is the same.

All controller aims to compare the signal which comes from the transmitter with the set-point and sends a signal to the control valve. The way that the controller compares the process signal with the set point depends on the type of action wanted. Basically there are 3 kinds of actions in a feedback controller: proportional action, integral action and derivative action.

Proportional controller (P)

The output signal is compared to the set-point and is changed proportionally to the input signal error. A

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proportional controller just acts when an error is measured. The equation of this type of controller is:

$$m(t) = \overline{m} + Kc\left(C_{sp} - C\right) \qquad (1)$$

where:

$m(t)$ = controller output signal which adjusts the control valve

$\overline{m}(t)$ = controller output signal when the error is zero

Kc = controller gain

C = process signal from transmitter

C_{sp} = set-point signal (process desired signal)

$C - C_{sp}$ = error ($e(t)$)

$$m(t) = \overline{m} + \frac{1}{\tau_I} \, e(t) \, dt$$

(2)

where:

τ_I = integral time

Proportional Integral Derivative Controller (PID)

All of the three actions (proportional, integral and derivative) are included. The derivative action is an anticipative action where the controller aims to anticipate the future system characteristic based on the derivative of the error (the time rate of change of the error). This action is quick and is always in the opposite direction of the error occurred in the system. The equation of a proportional integral controller is:

$$m = \overline{m} + Kc\left[e + \frac{1}{\tau_I} \, edt + \tau_D \frac{de}{dt} \right]$$

(3)

where:

τ_D = derivative time

Control Strategies

There are many control strategies. Some of them are presented bellow.

Feedback Control

The variable wanted to be controlled is measured and compared to a desired value (the set- point). The error between the process variable and the set-point is turned into an input so that the controller can act in the system. Therefore, the controller does not make any action until an error in the system is detected. It is an action to bring the system back to the set-point.

Feedforward Control

The variable is measured and a corrective action is taken before it upset the process. It is basically an action to maintain the system in the set-point. The

Proportional Integral Controller (PI)

An integral controller has a proportional plus an integral action. In an integral action the control valve moves based on the time integral of the error. This action aims to bring back the system to the set-point and also avoids it to go away from the set point. One important characteristic of such controller is that, due to the integral action, the response can be very slow. The equation of this type of controller is:

great advantage of this strategy is that it allows, theoretically, a perfect control. However, in many applications this is not feasible.

Feedforward / Feedback control

Feedforward control is often used in combination with feedback control. Each type of control compensates the disadvantages of the other one.

Ratio control

This is a special type of feedback control. The objective is not to control the performance of two independent variables M, L but to control the ratio R_a:

$$R_a = \frac{M}{L}$$

(4)

Some applications of ratio control are, for instance, the control of a specific reflux ratio for a distillation column or the holding of a fuel air ratio to a furnace at an optimum value.

Part Two

The second part of this work is an ideal binary distillation column study. Several additional assumptions and idealizations were made. These hypothesis are sometimes valid but they are frequently only crude approximations. However, the purpose of studying this simplified model case is to reduce the problem to its most elementary form so that the basic structure of the equations can be clearly seen.

First of all, the column was modeled considering equimolal overflow (whenever a mole of vapor condenses, it vaporizes a mole of liquid), which eliminates an energy equation for each tray. The holdup of vapor is assumed negligible and a simple linear relationship between the liquid holdup, (M_N) and the liquid flow rate leaving the tray, L_N is also considered. A further assumption made is a pure binary system with constant molar relative volatility through the column and perfect 100 percent efficient trays. The variables used to model the column are presented bellow:

N_s = feed tray of the column
F = feed rate (moles/s)
x_F = composition of liquid in the feed tray
M_D = holdup of liquid in the reflux drum (moles)
x_D = composition of the liquid in the drum
N_T = top tray of the column
y_{NT} = composition of vapor in the top of the column
R = rate of reflux (moles/s)
D = rate of overhead distillate product removed (moles/s)
B = rate of liquid bottoms product removed (moles/s)
x_B = liquid composition in the base of the column
V = rate of vapor generated in the reboiler of the column (moles/s)
M_B = holdup in the reboiler (moles)
M_N = holdup on each tray (moles)
x_N = composition of liquid in each tray
y_N = composition of vapor in each tray
  = hydraulic constant of the trays
R_0 = initial reflux rate
$\overline{M}_N$ = constant

There are 4 equations per tray: a total and a component continuity, a liquid hydraulic equation and a vapor-liquid equilibrium equation. These equations are presented bellow.
Vapor-liquid equilibrium equation:

$$y_n = \frac{?x_n}{1 + (\quad -1)?x_n}$$

(5)

Liquid hydraulic equation:

$$L_N = \overline{L}_N + \frac{M_N - \overline{M}_N}{}$$

(6)

Total continuity:

$$\frac{d(M_N)}{dt} = L_{N+1} - L_N$$

(7)

Component continuity:

$$\frac{d(M_N ?x_N)}{dt} = L_{N+1} ?x_{N+1} - L_N ?x_N + V ?y_{N-1} - V$$

(8)

A feedback control was made through 2 controllers PI which change the reflux R and the vapor V to control overhead distillate composition x_D and bottom composition x_B. The equations for each controller are:

$$V = V_0 - Kc_B ? err_B + \frac{1}{IB} \quad err_B ?dt$$

(9)

where:

$err_B = x_{B\ set-point} - x_B$

$$R = R_0 + Kc_D ? err_D + \frac{1}{ID} \quad err_D ?dt$$

(10)

where:

$err_D = x_{D\ set-point} - x_D$

The initial conditions given for the column are:

$N_T = 20$
$x_{D\ set-point} = 0.98$
$x_{B\ set-point} = 0.02$
$x_{F\ set-point} = 0.5$
$N_F = 10$
$M_{D0} = 100$ moles
$M_{B0} = 100$ moles
$M_0 = 10$ moles
$R_0 = 128.01$ moles/s
$V_0 = 178.01$ moles/s
$F = 100$ moles/s
  $= 0.1$
  $= 2$

The constants of the 2 controller are:

$K_{CD} = 1000$
$K_{CB} = 1000$
  $_D = 5$
  $_B = 1.25$

To make the control of the given column, a program was made in the software MATLAB. The program asks the student a perturbation in the   in the composition of the feed stream. The program is listed bellow:

```
% initial variables
NT=20;NF=10;MDO=100;MBO=100;MO=10;
RO=128.01;VO=178.01;F=100;BETA=0.1;
ALFA=2;
% CONTROLLER CONSTANTS
KCD=1000;KCB=1000;
TAUD=5;TAUB=1.25;
ERINTB=0;ERINTD=0;
% Perturbation
Z=input('Enter with a perturbation between 0 and 1
Z=');
% INITIAL VALUES OF X
XB=0.02;
X=[0.035 0.05719 0.08885 0.1318 0.18622 0.24951
0.31618 0.37948 0.43391 0.47688 ...
0.51526 0.56295 0.61896 0.68052 0.74345 0.80319
0.85603 0.89995 0.93458 0.96079];
XD=0.98;
% initial conditions
for N=1:NT
M(N)=MO;
MX(N)=M(N)*X(1,N);
LO(N)=RO+F;
if N>NF
LO(N)=RO;
end;
end;
Time=0;DELTA=0.005;ERINTD=0;ERINTB=0;i=1
;
while Time<12
% LIQUID HYDRAULIC EQUATION  AND VLE
for N=1:20
Y(N)=ALFA*X(1,N)/(1+(ALFA-1)*X(1,N));
L(N)=LO(N)+(M(N)-MO)/BETA;
end;
YB=ALFA*XB/(1+(ALFA-1)*XB);
```

```
% 2 CONTROLLERS FEEDBACK PI
ERRB=0.02-XB;
ERRD=0.98-XD;
V=VO-KCB*(ERRB+ERINTB/TAUB);
R=RO+KCD*(ERRD+ERINTD/TAUD);
D=V-R;
B=L(1)-V;
if R<0 disp('level too low or unreal composition ')
end;
if V<0 disp("level too low or unreal composition ')
end;
if D<0 disp('level too low or unreal composition ')
end;
if B<0 disp('level too low or unreal composition')
end;
% CÁLCULATION OF DERIVATIVES
XBDOT=(L(1)*X(1,1)-V*YB-B*XB)/MBO;
MDOT(1)=L(2)-L(1);
MXDOT(1)=V*(YB-Y(1))+L(2)*X(1,2)-L(1)*X(1,1);
for N=2:NF-1
MDOT(N)=L(N+1)-L(N);
MXDOT(N)=V*(Y(N-1)-Y(N))+L(N+1)*X(1,N+1)-
L(N)*X(1,N);
end;
% FEED TRAY
MDOT(NF)=L(NF+1)-L(NF)+F;
MXDOT(NF)=V*(Y(NF-1)-
Y(NF))+L(NF+1)*X(1,NF+1)-L(NF)*X(1,NF)+F*Z;
for N=(NF+1):(NT-1)
MDOT(N)=L(N+1)-L(N);
MXDOT(N)=V*(Y(N-1)-Y(N))+L(N+1)*X(1,N+1)-
L(N)*X(1,N);
end;
MDOT(NT)=R-L(NT);
MXDOT(NT)=V*(Y(NT-1)-Y(NT))+R*XD-
L(NT)*X(1,NT);
XDDOT=V*(Y(NT)-XD)/MDO;
% Euler Integration
Time=Time+DELTA;
XB=XB+DELTA*XBDOT;
for N=1:NT
M(N)=M(N)+MDOT(N)*DELTA;
MX(N)=MX(N)+MXDOT(N)*DELTA;
X(1,N)=MX(N)/M(N);
end;
XD=XD+XDDOT*DELTA;
ERINTD=ERINTD+ERRD*DELTA;
ERINTB=ERINTB+ERRB*DELTA;
A(i,:)=[ Time XB X(1,10) XD R V];
i=i+1;
end;
figure(1);plot(A(:,1),A(:,2),'c-'),xlabel('Time
[hr]'),ylabel('XB');grid;
figure(2);plot(A(:,1),A(:,3),'r-'),xlabel('Time
[hr]'),ylabel('XF');grid;
figure(3);plot(A(:,1),A(:,4),'g-'),xlabel('Time
[hr]'),ylabel('XD');grid;
figure(4);plot(A(:,1),A(:,5),'b-'),xlabel('Time
[hr]'),ylabel('R (moles/hr)');grid;
figure(5);plot(A(:,1),A(:,6),'m-'),xlabel('Time
[hr]'),ylabel('rate of vapor (moles/hr)');grid;
```

For a step perturbation in the composition of the feed stream from 0.5 to 0.55, the program gives the following graphics:
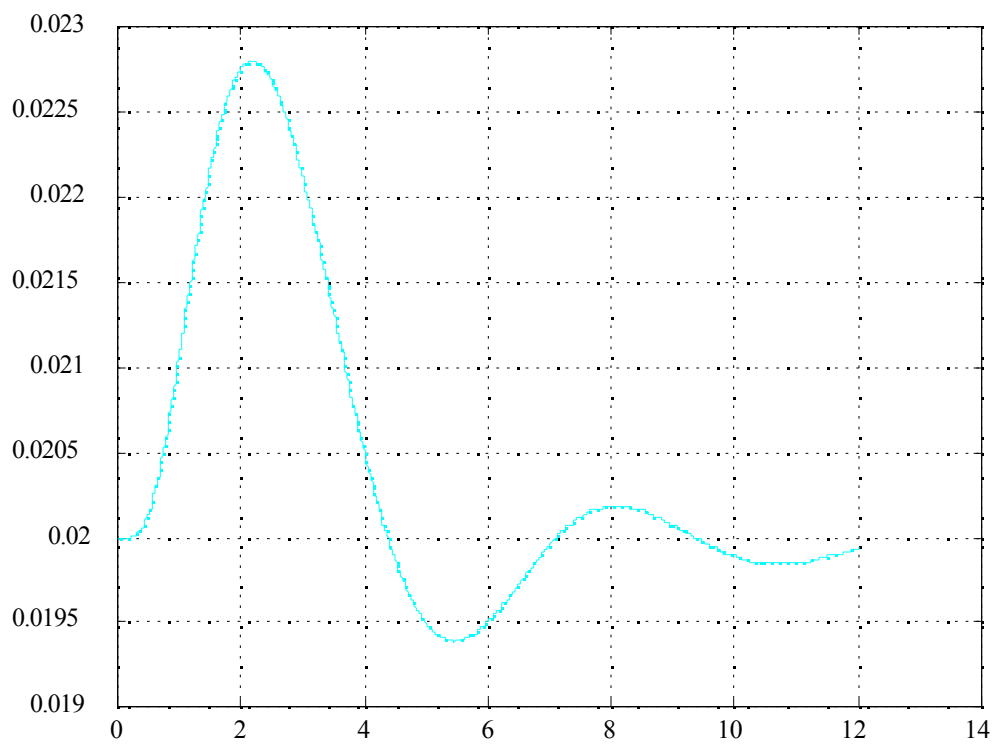
Figure 1. Graphic of composition x_B X time (hours)
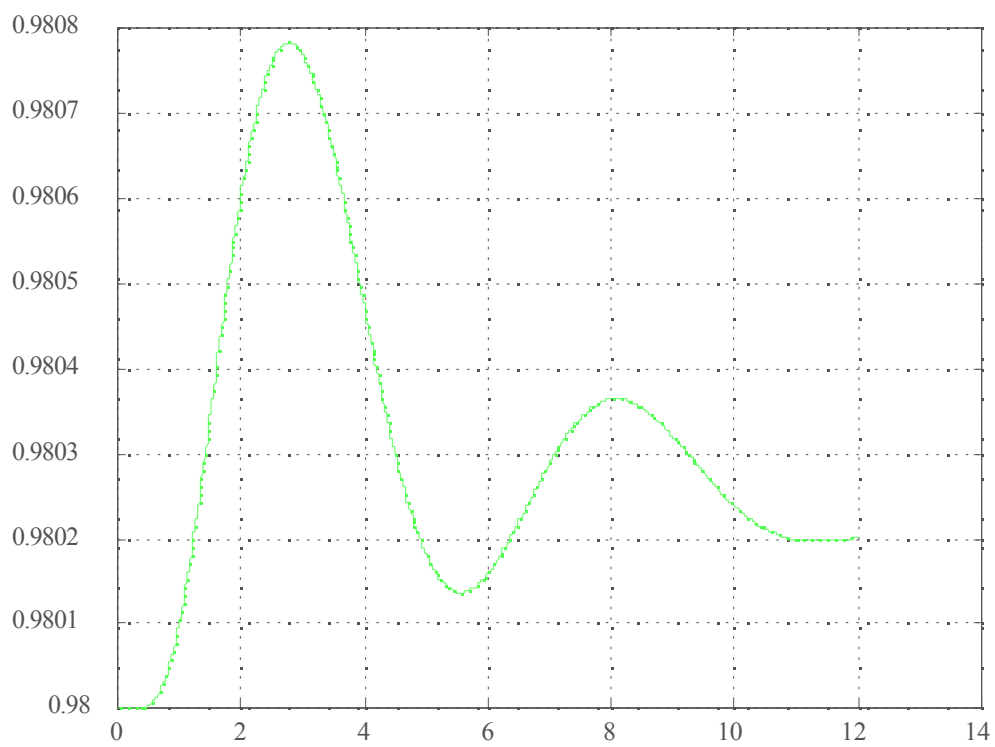

Figure 2. Graphic of composition x_D X time (hours)

Observing the graphics it can be seen that, after the perturbation, the control acts in the system and the compositions stabilize.

Other activities

All of the present work will be accessible to all Chemical Engineering undergraduates of UNICAMP through home-pages to create a deep interaction between the students and the studied subjects.
Moreover, 2 performances regarding this work were made to all professors of Chemical Engineering College of UNICAMP. In both lectures the participation of all professors in the project "Prodenge-output

Reenge" was encouraged as well as the undergraduates' contribution.

References

1) Luyben, W.L; "Process Modeling, Simulation and Contro for Chemical Engineers"*;* 2nd Edition; Mc Graw-Hill, 1974.
2) Seborg, Dale E., Thomas F. Edgar and Duncan A. Mellichamp; "Process Dynamics and Control"*;* 1st Edition; John Wiley and Sons, 1989.