A PROJECT REPORT

ON

"MODELLING AND SIMULATION OF LUMPED PARAMETER SYSTEM"

BACHELOR OF TECHNOLOGY
IN
CHEMICAL ENGINEERING

SANT GADGE BABA AMRAVATI UNIVERSITY,

AMRAVATI

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2013-14

CERTIFICATE

*This is to certify that the project report entitled "**Modelling and simulation Lumped Parameter System**" Which is submitted in partial fulfillment for the award of the **Degree of Bachelor of Technology in Chemical Engineering** of Sant Gadge Baba Amravati University Amravati. This is the result of the original project work completed by **Mr. Suyog D. Dhupekar, Ms. Sadhana B. Bhosale, Mr. Tulsidas A. Madavi, Mr. Vijaykumar P. Meshram** Students of Final Year, Chemical Engineering of Anuradha Engineering College, Chikhli, Dist-Buldhana, during 2013-2014 under my supervision and guidance. The work embodied in the project report has not formed earlier for the basis of the award of any degree or compatible certificate or similar title of this for my other diploma/examining or university to the best of knowledge and belief.*

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2013-14

DECLARATION

We are Students of Chemical Engineering, Anuradha Engineering College, Chikhli, hereby declare that we have completed project work entitled **"MODELLING AND SIMULATION OF LUMPED PARAMETER SYSTEM"** under the guidance of **'Prof. V. D. Gurudasani'** and submitted in partial fulfillment for the award of the Degree of Bachelor of Technology' in Chemical Engineering of Sant Gadge Baba Amravati University, Amravati. It has not previously submitted for the basis of the award of any degree or diploma or other similar title of this for any other diploma/examining body or university.

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We are thankful to **Dr. A. N. Nanhai**, Principal of Anuradha Engineering College, Chikhli without whose backing and encouragement, the work could have been completed in the enthusiasm that now it has been distinguished and accomplished.

Last but not least we would like to thanks to all the teaching and non-teaching staff members of our department and our colleagues those who helped us directly or indirectly for completing of this project successfully.

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ABSTRACT

The terms "modelling" and "simulation" are often used interchangeably. The use of modeling and simulation (M&S) within engineering is well recognized. Simulation technology belongs to the tool set of engineers of all application domains and has been included in the body of knowledge of engineering management. M&S has already helped to reduce costs, increase the quality of products and systems, and document and archive lessons learned

Chemical process modeling is a computer modeling technique used in Chemical Engineering process design. It typically involves using purpose-built software to define a system of interconnected components, which are then solved so that the steady-state or dynamic behavior of the system can be predicted.

The time optimal control problem for water tank system, Unsteady-state steam heating of a liquid and jacket cooled continuous flow of stirred tank reactor (CSTR) with an exothermic, irreversible; second-order, homogeneous, liquid-phase reaction will be solved with the maximum principle and phase plane analysis. Computer simulation studies will be conducted. In that we will conduct the modeling and simulation of Lumped parameter systems.

CHAPTER 1

INTRODUCTION

This project focused on the modelling and simulation studies of a lumped parameters systems. Simulations have big advantages now days with the increasing computation power and speed of the computers followed by the decreasing costs. The simulation process usually starts with the modelling of the system. The result of the modelling is the mathematical model of the system which describes the most important variables and relations between them. The mathematical model of the examined lumped parameter system is described by the set of linear ordinary differential equations (ODE). The simple iteration method was used for the steady state analysis. Similarly the dynamic analysis was performed by Runge - Kutta's standard method.

Simulation is the technical; discipline which shows the behavior and reactions of any system on its model. There are many types of systems, the main categories for real system is investigation of its behavior as a result of input simulation. There simulations are done on the real model of the system. Computer simulation has a great importance today and MATLAB is big too; which can help you with computer simulation. It starts with creation of mathematical model and the obtained equations are solved by using an appropriate calculation method. The importance of computer simulation will grow in the future when computers are faster.

The most of chemical processes has nonlinear properties. Computer simulation is one way how to examine this behavior which obtained by steady-state and dynamic analysis. Model of the system is usually represented by the set of the partial or ordinary the differential equations.

Numerical simulation shows that the whole structure presents a good performance in presence of parametric variation, which is often presented in chemical processes.

1.1 WHAT IS MODELLING?

Modelling is the process of producing a model; A Model representation of construction and working of some system of interest. A model is similar to but simpler than the system it represents. One purpose of the model is to enable the analyst to predict the product of the effect of changes to the system. On the one hand, the model system should be close to approximation to the real system and incorporate to its salient features. On the other hand, It should not be so complex that it is impossible to understand and experiment with it. A good model is judicious trend off between realism and simplicity. Simulation practitioners recommend increasing the complexity of model iteratively. An important issue in modelling is model validity. Model validation techniques include

simulating model under know input conditions and comparing model output with system output. Generally, A model intended for a simulation study is mathematical model developed with help of simulation software. Mathematical model classification include deterministic (input and output variable are fixed values) or stochastic (at last one the input or output variable is probabilistic); static (time is not taken into account) or dynamic (time-varying interactions among variables are taken into account) typically, simulation models are stochastic and dynamics.

Modelling is subdivided into two groups:

- Physical modelling
- Mathematical modelling

Physical Modelling:

In physical modelling, the experiment is carried out directly on the real process. The process of interest is reproduced on different scales, and the effect of physical Feature and linear dimensions is analysed.

Mathematical Modelling

A mathematical model of a real chemical process is a mathematical description which combines experimental facts and establishes relationships among the process variables. The objective of a mathematical model is to predict the behaviour of a process and to work out ways to control its course. Mathematical modelling is an activity in which qualitative and quantitative representations or abstractions of the real process are carried out using mathematical symbols.

Mathematical modelling involves three steps:

- mathematical formulation
- development of an algorithm for the process
- Testing of the model and the solution derived from it.

1.2 WHAT IS SIMULATION?

A Simulation of a system is the operation of a model of the system. The model can be reconfigured and experienced with; usually, this is impossible, too expensive or impractical to do in the system it represents. The operation of the model can be studied, and hence properties concerning the behavior of the actual system or its subsystem can be inferred. In its broadest sense, simulation is tool to evaluate the performance of a system existing or proposed, under different configuration of interest and over long periods of real time.

Simulation is used before an existing system is altered or a new system built, to reduce the chances of failure to meet specification, to eliminate unforeseen bottlenecks, to prevent under or over-utilization of resources, and to optimize system performance. For instance, simulation can be used to answer questions like; what is the best design for a new telecommunication network? What are the associate d resource requirements? How will a telecommunication network perform when the traffic load by 50%? How will a new routing algorithm affect its performance? Which network protocol optimize network performance? What will be the impact of a failure? The subject of this tutorial is discrete event simulation in which the central assumption is that the system changes instantaneously in response to certain discrete events. For instance, in an M/M/1 queue – a single server queuing process in which time between arrivals and service time are exponential – an arrival cause the system continuously over time in response to control. Discrete event simulation but it is much simpler to implement, hence, is used in a wide variety of situation.

The steps involved in developing a simulation model, designing a simulation experiment, and performing simulation analysis etc:

1. Verbal Level

   In which purpose of model Are outlined verbally and objective are defined.

2. Model building

   Any design process that is ought to be effectively simulated must be first modeled properly. Model will not only provide information but also help the users to obtain a wider understanding a reality and enable them to communicate about reality in model building the abstraction of the system into mathematical logical relationship in accordance with the product.

3. Date Acquisition

   Identification, specification, collection of data, deciding constant and variables, determining complex inter dependence, etc.

4. Modes Translation

   It involves the preparation of model for computer processing.

5. Verification

   Process of verifying that computer program process as intended

6. Validation

   The process of establishing that the desire accuracy or correspondence exist between thw simulation and real systems.

7. Strategic and tactical

   The process of establishing the experiment condition of using the model

8. Experimentation

   The execution of simulated model giving all input to obtain desired output.

9. Analysis of result
   Analyzing simulated output
10. Implementation and documentation
    Preparing real and physical model

Lumped Parameter Models

Processes in which the basic process variables vary only with time are represented by lumped parameter (LP) models, which are formulated as ordinary differential equations.

1.3 Advantages

The advantages of using mathematical models can be summarized as follow

1. A process can be analyzed in depth, determining which variables or parameter critical and have a diverse effect on overall system behavior.
2. They are of great help in the search for optimum operating conditions.
3. Limit or extreme conditions, for away from the normal operating conditions, are studied safely to analyze their consequences.
4. They can be used for teaching purpose operator training etc.
5. Processes that are too large, complex, or hazardous for the laboratory are simulated on the computer.
6. Realistic time and budget constraints can be built into the simulation, giving and of " real world" engineering problem
7. Emphasis of the laboratory exercise can change experimental design and analysis rather than the practical collection of data.
8. Computer simulation is relatively inexpensive compared with the cost of maintaining expensive experimental equipment.

CHAPTER 2

LITERAURE REVIEW

Process simulation are becoming basic tools in chemical engineering program Senior-level design projects typically involves the use of either a commercial simulator or an academic simulator such as ASPEN-PLUS, ChemShare, ChemCAD, FORTRAN, HYSYS, and Prollow / PROVISION. Many design textbooks now include exercises specifically prepared for a particular simulator. For example the text by seider, seader. And Lewin has examples written for use of HYSYS, ASPEN-PLUS, GAMES, and DYNA-PLUS.

Professor Lewin has prepared a new CDROM version of this courseware giving interactive self-paced tutorials on the use HYSYS and ASPEN-PLUS throughout the curriculum.

In the past, most chemical engineering programs views process simulation as a tool to be taught and used solely in senior design courses, lately, however, the chemical engineering community has been a strong movement towards vertical integration of design throughout the curriculum. Some of these initiatives are driven by the new ABNET criteria. This integration could be highly enhanced by early introduction to process simulation.

Process simulation can also be used in lower-level courses as a pedagogical aid. The thermodynamics and separation areas have a lot to gain from simulation packages one of the advantages of process simulation software is that it enables the instructor to present information in an inductive manner. For example, in a course on equilibrium staged operation one concept which must be learnt is the optimum feed location. Standard texts such as Wankat present these concepts in deductive manner.

Some course in chemical engineering, such as process dynamics and control and process optimization, are computer intensive and can benefit from dynamic process simulators and other software packages. Henson and Zhang present an example problem in which HYSYS plant (a commercial dynamic simulator) is used in the process control course. The process features the production of e3thylene glycol in a CSTR and purification of the product through distillation. The authors use this simple process to illustrate concepts such as feedback control and open-loop dynamics. Clough present a good overview does the use of dynamic simulation in teaching plant wide control strategies.

A potential pedagogical drawback to packages such as HYSYS and ASPEN is that it is possible to construct and use models successfully without really understanding the physical phenomena within each unit operation.

CHAPTER 3

OBJECTIVE

We know that automation is keyword of today's industry. As the technology developing treatment pace keeping with latest trends must for everyone. Now a day's embedding of computer system in production area is essential part of any industry.

The knowledge of CAD and simulation software is essential for today's engineer. It is more important for chemical engineer since many reactions are time consuming costly and dangerous to carry out. The inputs for our model are only operating parameters. Thus based on this process design aspects of continuous stirred. Tank reactors in series, concentration and conversion can be calculated.

We have tried our best to remove any errors in this model. Thus suggestions for further improvement are welcomed.

CHAPTER 4

MODELLING AND SIMULATION OF LUMPED PARAMETER SYSTEM

4.1 MODELLING AND SIMUALTON OF WATER TANK SYSTEM

Modelling of water tank system;

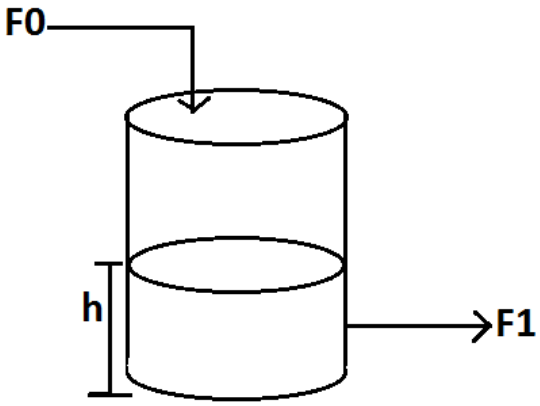


Fig 4.1 : Water tank system.

Let,

A=Area of tank,

H=Height of liquid in the tank

Input of A, moles/time = ρF_0

Output of A, moles/time =ρF_1

Material balance around the tank

Input - output = accumulation

$$\rho F_0 - \rho F_1 = \frac{d(\rho V)}{dt}$$

As density is constant,

$$F_0 - F_1 = \frac{dV}{dt}$$

$$F_0 - F_1 = \frac{d(Ah)}{dt}$$

$$\frac{Ad(h)}{dt} = F_0 - F_1$$

Above equation also written as,

$$\frac{dh}{dt} = \frac{F_0 - F_1}{A}$$

Above equation is mathematical model of water tank system.

SIMULATION OF WATER TANK SYSTEM IN TURBO C++

```
#include<stdio.h>
#include<math.h>
#include<conio.h>
#include<stdlib.h>
#include<iostream.h>
#include<graphics.h>
#include<dos.h>
void main()
{
int gdriver=DETECT,gmode;
initgraph(&gdriver,&gmode,"C:\\TURBOC3\\BGI");
float func(float,float,float,float);
float t,t1,tn,H1=0,h2,k1,k2,k3,k4,q0,q1,A,h,H2,d,ih,c;
int j,ht,n,i;
clrscr();
cout<<"       SIMULATION OF WATER TANK SYSTEM\n\n";
cout<<"Ratio for tank height with respect to level of water in the tank is, 26:1\n\n";
cout<<"Enter the height for tank in foot(ft):";
cin>>ht;
ht=100+ht;
j=ht-1;
n=100;
clrscr();
cout<<"      MODELLING AND SIMULATION OF WATER TANK SYSTEM\n\n";
cout<<"Enter the initial value of time in second;";
cin>>t1;
cout<<"Enter the initial level of water in foot(ft):";
cin>>H1;
cout<<"Enter the time interval in second(s):";
cin>>h;
h2=h/2;
cout<<"Enter the value of inlet flow rate of water in (ft3/s) q0:";
cin>>q0;
cout<<"Enter the value of outlet flow rate of waterin (ft3/s) q1:";
cin>>q1;
cout<<"Enter the c/s area of the tank in (ft2):";
cin>>A;
clrscr();
line(230,80,300,80);
line(300,80,300,95);
line(230,85,295,85);
line(295,85,295,95);

line(250,100,250,ht);
line(250,ht,400,ht);
line(400,ht,400,100);

line(400,ht-10,470,ht-10);
line(470,ht-10,470,ht);
line(400,ht-5,465,ht-5);
```

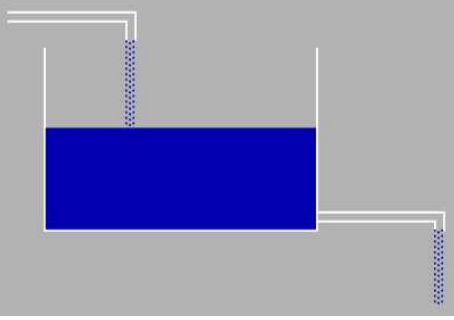
```
line(465,ht-5,465,ht);

H2=H1;
ih=H1;
cout<<"      SIMULATION OF WATER TANK SYSTEM\n\n";
cout<<"change in height with respect to time is as follows:\n";
 for(int s=96;s<ht;s=s+3)
 {
 putpixel(295,s,1);
 putpixel(297,s+1,1);
 putpixel(299,s,1);
 delay(25);
 }
 for(t=t1;;t+=h)
 {
 i=0;
 if(j>=n)
 {
 k1=h*func(q0,q1,H1,A);
 k2=h*func(q0,q1,H1+(k1/2),A);
 k3=h*func(q0,q1,H1+(k2/2),A);
 k4=h*func(q0,q1,H1+k3,A);
 H1=H1+(k1+k2*2+k3*2+k4)/6;
 d=(26*(H1-H2));
 if(H2==ih&&H2!=0)
 {
 c=0;
 while(c<=d)
 {
 setcolor(1);
 line(251,j,399,j);
 c++;
 j--;
 delay(50);
 if(j<n)
 {
 cout<<"Overflow";
 n=1;
 break;
 }
 }
 for(int p=ht;p<ht+40;p=p+3)
 {
 putpixel(465,p,1);
 putpixel(467,p+1,1);
 putpixel(469,p,1);
 delay(100);
 }
 getch();
 if(n==1)
 {
 break;
```

```
}
}
cout<<"t="<<t+h<<"\t"<<"H="<<H1<<"\n";
c=0;
while(c<=d)
{
setcolor(1);
line(251,j,399,j);
j--;
c++;
delay(50);
if(j<n)
{
cout<<"Overflow";
n=1;
break;
}
}
for(int p=ht;p<ht+40;p=p+3)
{
putpixel(465,p,1);
putpixel(467,p+1,1);
putpixel(469,p,1);
delay(100);
}
H2=H1;
getch();
if(n==1)
break;
}
else
{
cout<<"overflow";
getch();
}
}
}
float func(float q0,float q1,float H,float A)
{
float ftH;
ftH=(q0-q1)/A;
return (ftH);
getch();
}
```

OUTPUT:

```
      SIMULATION OF WATER TANK SYSTEM

Ratio for tank height with respect to level of water in the tank is, 26:1

Enter the height for tank in foot(ft):100
Enter the initial value of time in second;0
Enter the initial level of water in foot(ft):0
ENter the time interval in second(s):2
Enter the value of inlet flow rate of water in (ft3/s) q0:10
Enter the value of outlet flow rate of waterin (ft3/s) q1:7
Enter the c/s area of the tank in (ft2):12
```

```
      SIMULATION OF WATER TANK SYSTEM

change in height with respect to time is as follows:
t=2     H=0.5
t=4     H=1
t=6     H=1.5
t=8     H=2
```



CHAPTER 4.2

MODELLING AND SIMULATION UNSTEADY-STATE STEAM HEATING OF A LIQUID

(Dynamic Lumped Parameter Rigid Analytical Model)

Consider a closed kettle Fig. 4.2 of total surface area **A** m^2 is heated through this surface by condensing steam at temperature *T,* K. The kettle is charged with M kg of liquid of heat capacity **C,** J/kg at a temperature of *To* K. If the process is controlled by a heat-transfer coefficient *h* W/m^2K, Here we formed mathematical model for system that how does the temperature of the liquid vary with time?

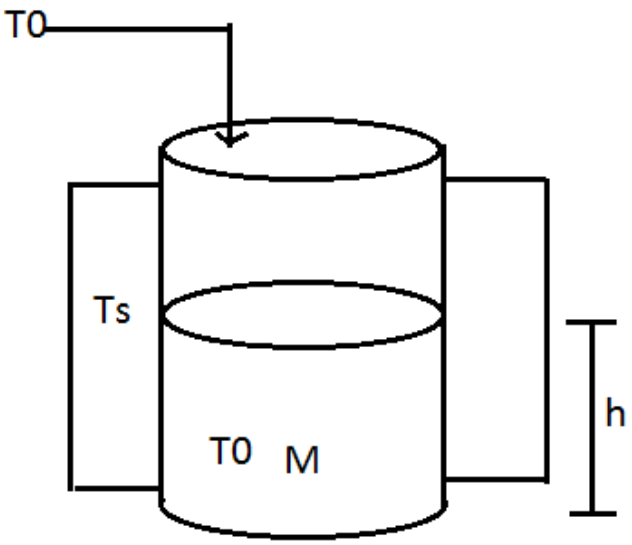


Fig 4.2 : Unsteady-state Steam Heating of a Liquid

Let,

A =total surface area, m2

T =steam at temperature, K.

M =Mass of liquid, kg

C_p=heat capacity, J/kg

To =liquid at entering temperature, K.

h =heat-transfer coefficient, W/m2K

Heat input (J) =$hA(T_s - T)dt$

Heat output (J) = 0

Heat accumulation (J) $= MC_p \frac{dT}{dt} dt$

Material balance around the steam heating tank

Input - output = accumulation

$$hA(T_s - T)dt = MC_p \frac{dT}{dt} dt$$

On separating the variables, we get

$$\frac{hA}{MC_p} = \frac{dT}{(T_s - T)}$$

On integrating and rearranging, we get

$$-ln(T_s - T) = \frac{hA}{MC_p} + B$$

B can be evaluated by using the boundary conditions, i.e., when t = *0*, T = To.

Therefore,

$$-ln(T_s - T_0) = B$$

Substituting ***B*** from Eq. (5.31) into Eq. (5.30), we get

$$-ln(T_s - T) = \frac{hA}{MC_p} t - ln(T_s - T_0)$$

$$ln \frac{(T_s - T)}{(T_s - T_0)} = \left(-\frac{hA}{MC_p} t \right)$$

Or

$$\frac{(T_s - T)}{(T_s - T_0)} = exp\left(-\frac{hA}{MC_p} t \right)$$

This is the expression for variation of *T* with ***t*** (time).

Above equation is mathematical model of Unsteady-state Steam Heating of a Liquid.

SIMULATION OF HEATING WATER TANK SYSTEM IN TURBO C++

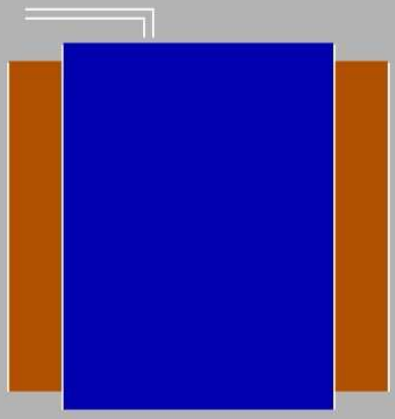
```
#include<stdio.h>
#include<math.h>
#include<conio.h>
#include<stdlib.h>
#include<iostream.h>
#include<graphics.h>
#include<dos.h>
void main()
{
int gdriver=DETECT,gmode;
initgraph(&gdriver,&gmode,"C:\\TURBOC3\\BGI");
float func(float,float,float);
float t1,p,q,t,tn,T1=25,k1,h2,k2,k3,k4,U,Cp,Ts,M,c,d,ih,T2,A,h,pow,x;
int j,ht,n,i;
clrscr();
h=0.2;
cout<<"Enter the height for tank in meter(m):";
cin>>ht;
ht=100+ht;
j=ht-1;
printf("\nEnter the value of temp Ts in kelvin: ");
scanf("%f",&Ts);
printf("\nEnter the value of area A m2:");
scanf("%f",&A);
printf("\nEnter the value of mass flow M:");
scanf("%f",&M);
printf("\nEnter the initial time t1 and and inital temp T1 in  kelvin:");
scanf("%f%f",&t1,&T1);
printf("\nEnter the value of last term of tn:");
scanf("%f",&tn);
printf("\nEnter the value of Cp inJ/kg/k:");
scanf("%f",&Cp);
printf("\nEnter the value of U in wattm2/k:");
scanf("%f",&U);
clrscr();

line(230,80,300,80);
line(300,80,300,95);
line(230,85,295,85);
line(295,85,295,95);

line(250,100,250,ht);
line(250,ht,400,ht);
line(400,ht,400,100);

line(220,110,220,ht-10);
line(220,ht-10,250,ht-10);
line(220,110,250,110);

line(400,ht-10,430,ht-10);
```

```
line(430,ht-10,430,110);
line(430,110,400,110);

cout<<"      SIMULATION OF WATER HEATING TANK SYSTEM\n\n";
cout<<"change in TEMPERATURE with respect to time is as follows:\n";
for(p=109;p<=ht-10;p++)
{
setcolor(6);
line(221,p,249,p);
line(401,p,429,p);
}

for(q=99;q<=ht;q++)
{
setcolor(1);
line(251,q,399,q);
}
 for(t=t1;t<tn;t+=h)
 {
k1=func(x,Ts,T1);
k2=func(x,Ts,T1+(k1/2));
k3=func(x,Ts,T1+(k2/2));
k4=func(x,Ts,T1+k3);

T1=T1+(k1+2*k2+k3*2+k4)/6;
x=(-(U*A)/(Cp*M));

  while(T1>=Ts)
  {
  setcolor(1);
  line(251,j,399,j);
  T1++;
  j--;
  delay(25);
}
printf("\nt=%5.1f,T=%6.2f",t,T1);
}
getch();
}
float func(float x,float Ts,float T1)
{
float ftT;
ftT=(pow(2.7128,x)*(Ts-T1));
return(ftT);
}
```

OUTPUT:

```
      MODELING AND SIMULATION OF WATER HEATING TANK SYSTEM

Enter the height for tank in meter(m):200

Enter the value of temp Ts in kelvin: 100

Enter the value of area A m2:10

Enter the value of mass flow M:60

Enter the initial time t1 and and inital temp T1 in  kelvin: 0 25

Enter the value of  last term of tn:2

Enter the value of Cp inJ/kg/k:2145

Enter the value of U in wattm2/k:245
```

```
      SIMULATION OF WATER HEATING TANK SYSTEM

change in TEMPERATURE with respect to time is as follows:

t=  0.0,T= 71.88
t=  0.2,T= 89.27
t=  0.4,T= 95.91
t=  0.6,T= 98.44
t=  0.8,T= 99.40
t=  1.0,T= 99.77
t=  1.2,T= 99.91
t=  1.4,T= 99.97
t=  1.6,T= 99.99
t=  1.8,T=100.00
```



CHAPTER 4.3

MODELLING AND SIMULATION OF SINGLE CONTIUOUS STIRRED TANK

Consider a Single continuous stirred tank reactor with constant holdup as shown in fig 4.3. The reaction is carried in reactor, A→Product. To form the mathematical model of given system we made assumption.

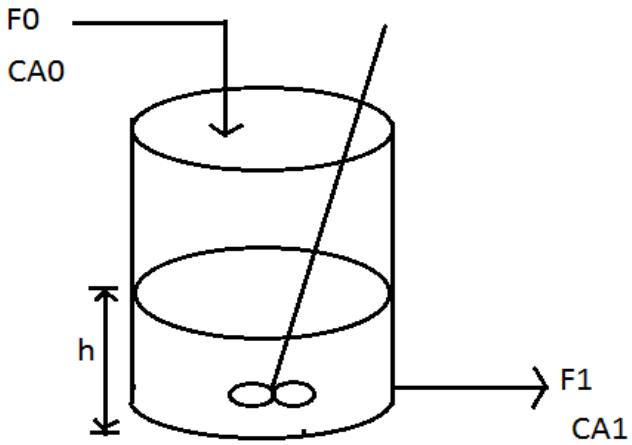


Fig : Single continuous stirred tank system

Assumption:

- Perfect mixing in the tank
- Density is constant through the system
- First order kinetics
- Isothermal operation
- Constant holdup

Let,

V = Volume of liquid in the tank,

F_0 = Mass flow at inlet

F_1 = Mass flow at outlet

C_A = Concentration at inlet

C_{A1} = Concentration at outlet

ρ = Density of fluid

k = Rate constant

Material balance around the tank

$$\begin{pmatrix} Mass\ flow \\ into\ the\ tank \end{pmatrix} - \begin{pmatrix} Mass\ flow \\ out\ of\ the\ tank \end{pmatrix} = \begin{pmatrix} Time\ rate\ of\ change \\ of\ mass\ inside\ the\ tank \end{pmatrix}$$

$$\rho F_0 - \rho F_1 = \frac{d(\rho V)}{dt}$$

But, Volume is constant

$$\frac{d(\rho V)}{dt} = 0$$

$$F_0 - F_1 = F$$

$$\begin{pmatrix} Flow\ of \\ moles\ of\ A \\ into\ the\ tank \end{pmatrix} = \begin{pmatrix} Flow\ of\ moles \\ of\ A\ out \\ of\ the\ tank \end{pmatrix} + \begin{pmatrix} Rate\ of\ moles \\ of\ A\ from \\ chemical\ reaction \end{pmatrix} = \begin{pmatrix} Time\ rate\ of \\ change\ of\ moles \\ of\ A\ inside\ the\ trank \end{pmatrix}$$

$$F_0 C_{A0} - F_1 C_{A1} + (-r_A)V = \frac{d(VC_{A1})}{dt}$$

$$\frac{Vd(C_{A1})}{dt} = F(C_{A0} - C_{A1}) - kC_{A1}V$$

$$\frac{Vd(C_{A1})}{dt} = F(C_{A0} - C_{A1}) - kC_{A1}V$$

$$\frac{d(C_{A1})}{dt} = \frac{F}{V}(C_{A0} - C_{A1}) - kC_{A1} \dots\dots\dots\dots (1)$$

But, $\frac{F}{V} = \tau$

$$\frac{d(C_{A1})}{dt} = \tau(C_{A0} - C_{A1}) - kC_{A1} \dots\dots\dots . (2)$$

Equation (1) and (2) represent mathematical model of the system

Data:

$$C_{A0} = 1.8kg\ moles\ \frac{of\ A}{m}$$

$$\tau = 5\ m^2$$

$$k = 0.5m^{-1}$$

Replacing in equation (2), we obtain

$$\frac{d(C_{A1})}{dt} = 0.9 - C_{A1}$$

SIMULATION OF SINGLE CONTIUOUS STIRRED TANK IN TURBO C++

```
#include<stdio.h>
#include<math.h>
#include<conio.h>
#include<stdlib.h>
#include<iostream.h>
#include<graphics.h>
#include<dos.h>
void main()
{
int gdriver=DETECT,gmode;
initgraph(&gdriver,&gmode,"C:\\TURBOC3\\BGI");
float t0,CA0,h,t,tn,CA,k1,k2,k3,k4,ht,q,ih,CA1,h2,t1;
float func(float, float);
int j,n,i;
cout<<"Enter the height for tank in foot(ft):";
cin>>ht;
ht=100+ht;
j=ht-30;
n=100;
cout<<"ENter the time interval in second(s):";
cin>>h;
h2=h/2;
printf("\nEnter the initial value of t(minimium) and CA(kgmole/m3):");
scanf("%f%f",&t0,&CA0);
printf("\nEnter the value of last term of tn:");
scanf("%f",&tn);
CA=CA0;
printf("\n  t(min)  CA(kgmole/m3)   \n");
clrscr();

line(230,80,300,80);
line(300,80,300,95);
line(230,85,295,85);
line(295,85,295,95);

line(250,100,250,ht);
line(250,ht,400,ht);
line(400,ht,400,100);

CA1=CA;
ih=CA1;
cout<<"      SIMULATION OF CSTR SYSTEM\n\n";
cout<<"change in concentration with respect to time is as follows:\n";
  for(q=99;q<=ht;q++)
{
setcolor(1);
line(251,q,399,q);
}
  for(t=t0;t<tn;t+=h)
```

```
  {

 k1=func(t,CA);
k2=func(t,CA+(k1/2));
k3=func(t,CA+(k2/2));
k4=func(t,CA+k3);
CA=CA+(k1+2*k2+k3*2+k4)/6;
  while(CA0<=CA)
  {
  setcolor(1);
  line(251,j,399,j);
  CA++;
  j--;
  delay(50);
  }
  printf("\nt=%5.1f,CA=%6.2f",t,CA);
}
getch();
}
float func (float t,float CA)
{
float ftCA;
ftCA=(0.9-CA);
return (ftCA);
 }
```

OUTPUT;

```
      MODELING AND SIMULATION OF CSTR SYSTEM

Enter the height for tank in foot(ft):100
ENter the time interval in second(s):2
Enter the initial value of t(minimium) and CA(kgmole/m3):0 5
Enter the value of  last term of tn:20
```

```
      SIMULATION OF CSTR SYSTEM

change in concentration with respect to time is as follows:

t=  0.0,CA=  2.44
t=  2.0,CA=  1.48
t=  4.0,CA=  1.12
t=  6.0,CA=  0.98
t=  8.0,CA=  0.93
t= 10.0,CA=  0.91
t= 12.0,CA=  0.90
t= 14.0,CA=  0.90
t= 16.0,CA=  0.90
t= 18.0,CA=  0.90
```

CHAPTER 4.4

MODELLING AND SIMULATION OF THREE CONTIUOUS STIRRED TANK

REACTORS IN SERIES WITH VARIABLE HOLDUP

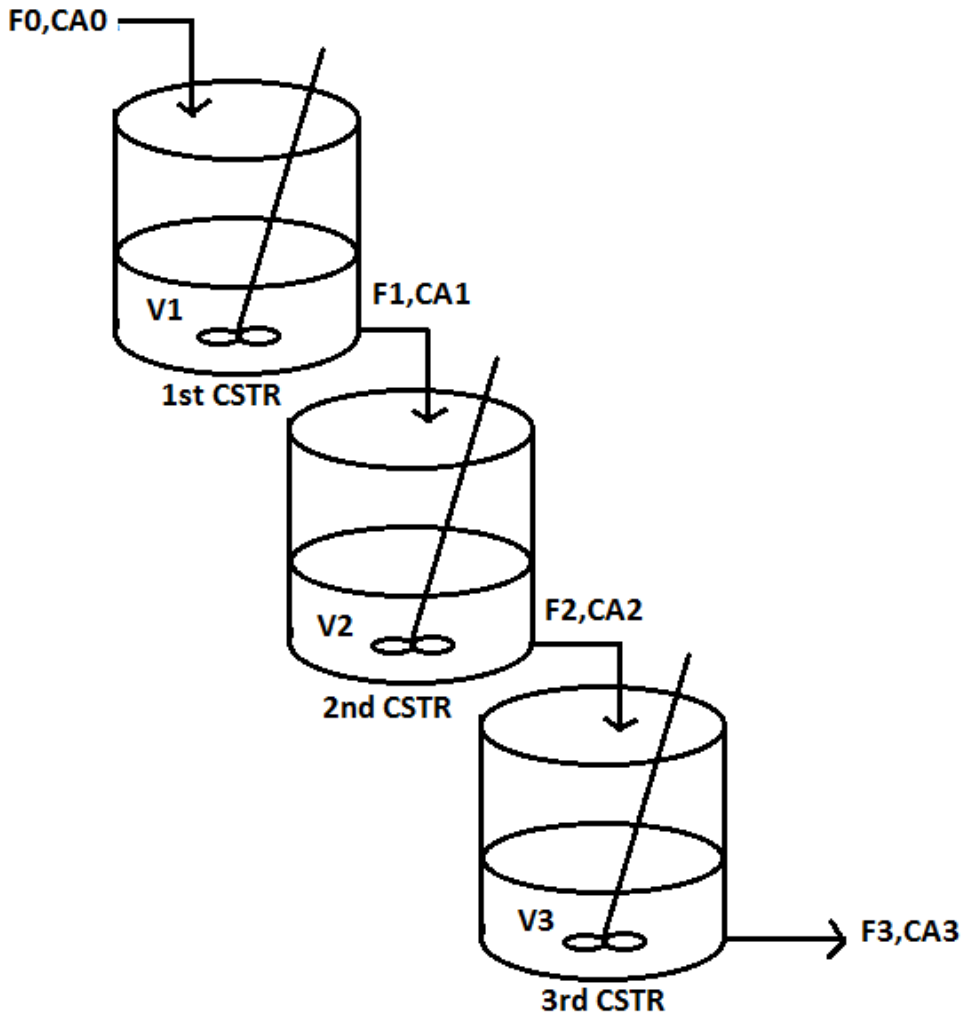


Fig : Three continuous stirred tank system in series

Assumption:

- Perfect mixing in the tank
- Density is constant through the system
- First order kinetics
- Isothermal operation
- Constant holdup

Let,

F_0=Input flowrate,m3/m

$F_1F_2F_3$= Flowrate of first, second and third CSTR respectively,m3/m

$V_1V_2V_3$= Volumes of first, second and third CSTR respectively, m3

C_{A0}=Concentration at inlet kgmoles/m3

$C_{A1}C_{A2}C_{A3}$= Concentration of first, second and third CSTR respectively, kg.moles/m3

$k_1k_2k_3$=Rate constant of first, second and third CSTR respectively,m-1

Material balance around the first continuous stirred tank reactor

$$\begin{pmatrix} mass\ flow\ into \\ first\ CSTR \end{pmatrix} - \begin{pmatrix} mass\ flow\ out \\ of\ first\ CSTR \end{pmatrix} = \begin{pmatrix} time\ rate\ of\ change\ of \\ mass\ inside\ first\ CSTR \end{pmatrix}$$

$$\rho F_0 - \rho F_1 = \frac{d(\rho V_1)}{dt}$$

$$F_0 - F_1 = \frac{d(V_1)}{dt}$$

Similarly , for second continuous stirred tank reactor

$$F_1 - F_2 = \frac{d(V_2)}{dt}$$

And for third continuous stirred tank reactor

$$F_2 - F_3 = \frac{d(V_3)}{dt}$$

Component Material balance on A around the first continuous stirred tank reactor

$$\begin{pmatrix} Flow\ of \\ moles\ of\ A \\ into\ first\ CSTR \end{pmatrix} = \begin{pmatrix} Flow\ \ of\ moles \\ of\ A\ out \\ of\ first\ CSTR \end{pmatrix} + \begin{pmatrix} Rate\ of\ formation \\ ofmoles\ \ of \\ A\ from \\ chemical\ reaction \end{pmatrix} = \begin{pmatrix} Time\ rate\ of \\ change\ of\ moles \\ of\ A\ inside \\ first\ CSTR \end{pmatrix}$$

$$F_0C_{A0} - F_1C_{A1} + (-r_A)_1V_1 = \frac{d(V_1C_{A1})}{dt}$$

$$\frac{V_1dC_{A1}}{dt} + C_{A1}\frac{dV_1}{dt} = F_0C_{A0} - F_1C_{A1} + k_1V_1C_{A1}$$

From equation

$$\frac{V_1 dC_{A1}}{dt} + C_{A1}(F_0 - F_1) = F_0 C_{A0} - F_1 C_{A1} + k_1 V_1 C_{A1}$$

$$\frac{V_1 dC_{A1}}{dt} = F_0(C_{A0} - C_{A1}) - k_1 V_1 C_{A1}$$

$$\frac{dC_{A1}}{dt} = \frac{F_0}{V_1}(C_{A0} - C_{A1}) - k_1 V_1 C_{A1} \ldots\ldots\ldots\ldots (1)$$

Similarly , for second continuous stirred tank reactor

$$\frac{dC_{A2}}{dt} = \frac{F_1}{V_2}(C_{A1} - C_{A2}) - k_2 V_2 C_{A2} \ldots\ldots\ldots\ldots (2)$$

And for third continuous stirred tank reactor

$$\frac{dC_{A3}}{dt} = \frac{F_2}{V_3}(C_{A2} - C_{A3}) - k_3 V_3 C_{A3} \ldots\ldots\ldots\ldots (3)$$

Equation (1),(2) and (3) are the mathematical model of three continuous stirred tank reactor.

SIMULATION OF THREE CONTIUOUS STIRRED TANK REACTORS IN SERIES WITH VARIABLE HOLDUP IN TURBO C++

```
#include<stdio.h>
#include<math.h>
#include<conio.h>
#include<stdlib.h>
#include<iostream.h>
#include<graphics.h>
#include<dos.h>
void main()
{
int gdriver=DETECT,gmode;
initgraph(&gdriver,&gmode,"C:\\TURBOC3\\BGI");
float func(float,float,float,float,float,float);
float funcc(float,float,float,float);
void drawTank(int);
float
t,t1,tn,h2,k1,k2,k3,k4,CA0,CA1,CA,v,TCA0,k0,e=2.72,R=1.99,E,k11,k22,k33,k44,h,H2,f,L1,k,L,A
;
int N,j,n,i,c,temp[10],volm[10],area[10],level[10],l[10];
int stx,sty,w,ht;
stx=310;sty=46;w=80,ht=100;
clrscr();
cout<<"          SIMULATION OF CSTR CONNECTED IN SERIES\n:";
cout<<"Enter the number of reactor;";
cin>>N;
if(N<=0)
{
cout<<"Plese enter correct number of reactor!";
getch();
exit(0);
}
cout<<"Enter the area in feet2(ft2), volm in feet3(ft3) and initial level of mixture in feet(ft) and
temp of mixture in degree farade (F) for each reactor\n";
for(i=0;i<N;i=i+1)
{
cout<<"A"<<i+1<<":";
cin>>area[i];
cout<<"v"<<i+1<<":";
cin>>volm[i];
cout<<"L"<<i+1<<":";
cin>>level[i];l[i]=level[i];
cout<<"T"<<i+1<<":";
cin>>temp[i];
}
cout<<"Enter the value of frequency factor in hour-1(hr-1);";
cin>>k0;
cout<<"Enter the activation energy in {Btu/lb.mol}:";
cin>>E;
cout<<"Enter the flow rate in (ft3/hr):";
```

```
cin>>f;
cout<<"Enter the concentration of mixture before entering into reactor(lb.mol/ft3):";
cin>>CA0;TCA0=CA0;
cout<<"Enter the initial concentration of component into reactor(lb.mol/ft3):";
cin>>CA;
cout<<"Enter the initial value of time in hour;";
cin>>t1;
cout<<"Enter the time interval in second(s):";
cin>>h;
cout<<"Enter the order of reaction:";
cin>>n;
cout<<"Enter the value of last term of tn:";
cin>>tn;
clrscr();

cout<<"          SIMULATION OF CSTR CONNECTED IN SERIES\N:";
cout<<"Change in concentration and level of mixture in each reactor with respect to time is as follow:";
for(t1=0;t1<tn;t1+=h)
{
stx=310;sty=46;w=80,ht=100;
CA0=TCA0;
for(j=0;j<N;j++)
{
A=area[j];
L=l[j];
v=volm[j];
k=k0*pow(e,(-E/(R*temp[j])));

k1=h*func(f,CA0,k,n,v,CA);
k2=h*func(f,CA0,k,n,v,CA+(k1/2));
k3=h*func(f,CA0,k,n,v,CA+(k2/2));
k4=h*func(f,CA0,k,n,v,CA+k3);
CA1=CA+(k1+2*k2+2*k3+k4)/6;

k11=h*funcc(f,k,L,A);
k22=h*funcc(f,k,L+(k11/2),A);
k33=h*funcc(f,k,L+(k22/2),A);
k44=h*funcc(f,k,L+k33,A);
L1=L+(k11+2*k22+2*k33+k44)/6;

l[j]=L1;
cout<<"\nt="<<t1+h<<"\tCA"<<(j+1)<<"="<<CA1;
cout<<"\t"<<"L"<<(j+1)<<"="<<L1;
CA0=CA1;
}
CA=CA1;
drawTank(N);
for(i=0;i<N;i++)
{
j=sty+(ht-1);
c=0;
```

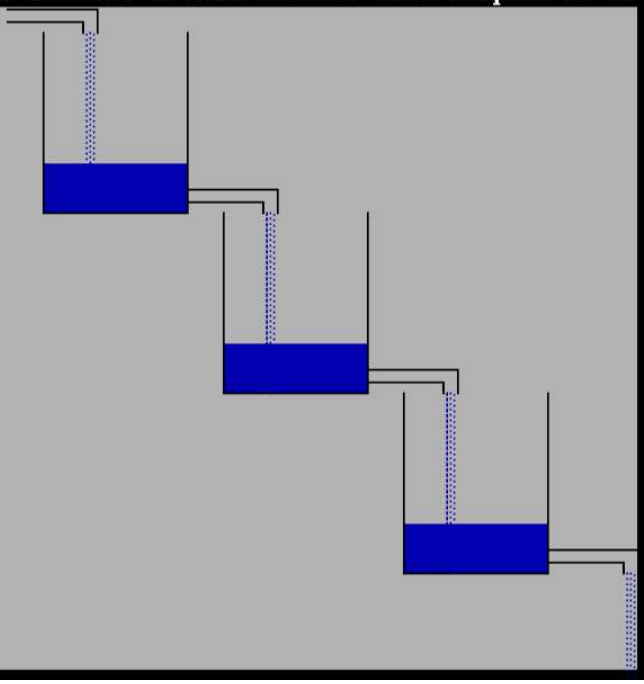
```
for(int p=sty;p<ht+sty-1;p=p+3)
{
setcolor(1);
putpixel(stx+26,p,1);
putpixel(stx+28,p+1,1);
putpixel(stx+24,p+1,1);
delay(15);
}
while(c<=(4*(L1-level[i])))
{
setcolor(1);
line(stx+1,j,stx+79,j);
j--;
c++;
delay(5);
}
stx=stx+w+20;
sty=sty+ht;
for(int s=sty;s<ht+sty;s=s+3)
{
putpixel(stx+26,s,1);
putpixel(stx+28,s+1,1);
putpixel(stx+24,s,1);
delay(10);
}
}
getch();
}
}
float func(float f,float CA0,float k,float n,float v,float CA)
{
float fCT;
fCT=(f*(CA0-CA)-k*pow(CA,n))/v;
return(fCT);
}
float funcc(float f,float k,float L,float A)
{
float ftL;
ftL=(f-(k*pow(L,0.5)))/A;
return(ftL);
}
void drawTank(int N)
{
int stx,sty,i,j,w,ht;
stx=310;sty=46;w=80,ht=100;
for(i=0;i<N;i++)
{
setcolor(0);
line(stx-20,sty-13,stx+30,sty-13);
line(stx-20,sty-6,stx+22,sty-6);
line(stx+30,sty-13,stx+30,sty);
line(stx+22,sty-6,stx+22,sty);
```

```
line(stx,sty,stx,sty+ht);
line(stx,sty+ht,stx+w,sty+ht);
line(stx+w,sty+ht,stx+w,sty);

stx=stx+w+20;
sty=sty+ht;
}
setcolor(0);
line(stx-20,sty-13,stx+30,sty-13);
line(stx-20,sty-6,stx+22,sty-6);
line(stx+30,sty-13,stx+30,sty);
line(stx+22,sty-6,stx+22,sty);
}
```

OUTPUT:

```
            SIMULATION OF CSTR CONNECTED IN SERIES
 :Enter the number of reactor;3
 Enter the area in feet2(ft2), volm in feet3(ft3) and initial level of mixture in
  feet(ft) and temp of mixture in degree farade(F) for each reactor
 A1:12
 v1:44
 L1:0
 T1:80
 A2:14
 v2:49
 L2:0
 T2:88
 A3:15
 v3:55
 L3:0
 T3:90
 Enter the value of frequency factor in hour-1(hr-1);729
 Enter the activation energy in {Btu/lb.mol}:15000
 ENter the flow rate in (ft3/hr):40
 Enter the concentration of mixtur before entering into reactor(lb.mol/ft3):1
 Enter the inital concentration of component into reactor(lb.mol/ft3):3
 Enter the initial value of time in hour;0
 ENter the time interval in second(s):1
 Enter the order of reaction:1
 Enter the value of last term of tn:3
```

```
            SIMULATION OF CSTR CONNECTED IN SERIES
 :Change in concentration and level of mixture in each reactor with respect to ti
 me is as follow:
 t=1     CA1=1.814744    L1=3.333333
 t=1     CA2=2.333332    L2=2.857143
 t=1     CA3=2.656489    L3=2.5
 t=2     CA1=1.674807    L1=6.333333
 t=2     CA2=2.104325    L2=4.857143
 t=2     CA3=2.371978    L3=4.5
 t=3     CA1=1.558905    L1=9.333333
 t=3     CA2=1.914651    L2=6.857143
 t=3     CA3=2.136333    L3=6.5
```



CHAPTER 5

APPLICATIONT TO CHEMICAL ENGINEERING

Design has been taught to chemical engineering undergraduate from many years using a traditional case studies approach which involves bisecting the design process into its various elements, imparting relevant knowledge by formal lectures, and demonstrating how experienced engineers have designed successful system. It was hoped that this approach would imbue sufficient knowledge and skills to become confident designers.

These efforts to teach design led to the realization that competence in design seemed to be caught by only a handful of who rose to the challenge and were able to apply skills, knowledge and other personal attributives often with outstanding results. The recipe for success seemed to combine such ingredients as organization, lateral thinking computation, practical experience in workshop skills, and an ability to think in abstract terms.

A problem solving foundation to engineering design provided with the necessary skills and confidence to be able to tackle any problem, design or otherwise, without felling hindered by lack of direct experience in the particular topic.

CHAPTER 6

CONCLUSION AND RESULT

Computer aided design has become increasingly important for simplifying the calculation effort. As more as more programs of greater sophistication are available. Our model is major step towards the mathematical modelling and simulation of lumped parameter systems

The program given is in turbo C++ language. In the literature many more programs are available for the models deal with in this report and further work can be undertaken to run these programmers in computers demonstrate the usefulness optimum performance of plant and machinery, insure energy conservation, reduce cost and improve productivity. However the importance of engineering knowledge and judgment in use of models, program and computer is reinforced with the demonstration occurs. The advantage of the computer is in doing fast and respective number to yield insight to performance through numerical experimentation of thermodynamics properties. Database is another pre-requisite for software development in simulation.

Simulation is the future of Chemical engineers as well as all industries. The package comes out as an aid to all working engineers and students. Problem solving can be done at very fats rate without losing the accuracy. The package simple to use also self explanatory. This model is basically simulated using TURBO C++ software; also programs can be developed to system any type industry. This package will be roadmap and a guide for the future developments.

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