PERFORMANCE ANALYSIS
OF A
CONTROLLED MULTI-PURPOSE CHEMICAL PLANT

by

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ABSTRACT

An available package was used as the basis of this work and it was further developed to obtain the CHPDSC package introduced in this study to investigate the dynamic behaviour of a typical multi-purpose chemical plant at different values of processing parameters.

The package presented here, CHPDSC, permits to simulate a plant which can contain a reactor and a distillation column as major processing units. Furthermore a heat exchanger and two tanks may also be included in the flowsheet as auxiliary equipment. The CHPDSC package also permits to investigate the dynamic behaviour of and the effect of various control strategies on chemical plants which may have two, three or four components.

The continuous production of di-buthyl phtalate was simulated using the four component CHPDSC package. In these simulations the dynamic behaviour and control objectives and structures for this process were also evaluated.

Furthermore, various flow-sheets and control structures were simulated using the CHPDSC package for processes having two, three and four species to study the system dynamics and process control in an effort to complete the work done earlier on the software which was the precursor of the CHPDSC.

ÖZET

Bu çalışmada daha önce hazırlanmış bir paket program temel alınmış ve etkinlikleri geliştirilmiştir. CHPDSC program paketi tipik bir kimyasal fabrikanın değişik süreç parametreleri altında dinamik davranışını inceleme olanağı sağlamaktadır.

Sunulan paket, CHPDSC, ana süreç birimleri olarak, bir sürekli karıştırmalı tank reaktörü ve bir destilasyon kolonu ile yardımcı birimler olarak iki tank ve bir ısı değiştirici içeren bir fabrikanın dinamik davranışını ve değişik denetim stratejilerinin etkilerini incelemeye de olanak tanımaktadır.

Bu çalışmada ayrıca di-butil ftalat üretim süreci matematiksel benzetimi yapılarak program paketine uygulanmış ve prosesin dinamik davranışı değişik süreç yapıları altında değerlendirilmiştir.

Daha önce yapılan çalışmayı tamamlamak üzere , üç ve dört bileşen içeren çeşitli sistemlerin değişik akım şemaları ve denetim yapıları altında matematiksel benzetimi yapılarak sistem dinamikleri ve denetime etkileri incelenmiştir.

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A_R	Reactor heat transfer area, (m^2)
A_R	Steady-state reactor heat tranfer area, (m^2)
B	Distillation column bottom product rate, (kgmole/hr)
C_{pJ}	Heat capacity of reactor jacket fluid, (J/kg K)
D^L	Distillation column distillate product rate, (kgmole/hr)
E	Activation energy, (kJ/kgmole)
F_J	Cooling fluid flow rate in the reactor jacket, (m^3/hr)
F_{RC}	Flow rate of recycle stream, (kgmole/hr)
F_{RO}, F_R	Input and output flow rates of the reactor, (kgmole/hr)
F_{st}	Steam flow rate to the reboiler, (kg/hr)
F_{Ti}	Outflow rate of the tank i, (kgmole/hr)
F_{wc}	Cooling fluid flow rate in the reboiler, (m^3/hr)
h_{RC}	Enthalpy of recycle stream, (kJ/kgmole)
$h_{R,O}$, h_R	Enthalpies input and output streams of the reactor, (kJ/kgmole)
k	Reaction rate coefficient
k_O	Arhenius constant
L	Heat of reaction, (kJ/kgmole)
M_R	Molar holdup of the reactor, (kgmole)
Q_B	Heat transfer rate fro reboiler, (kW)
Q_C	Rate of heat removal by the condenser, (kW)
Q_R	Heat transfer rate from the reactor, (kW)
r	Rate of reaction, (kgmole/hr)
R	Reflux rate, (kgmole/hr)
R_O	Universal gas constant, (J/kgmole K)
R_i	Rate of deplation of component i in the reactor,
ro_J	Density of fluid in reactor jacket (kgmole/hr)

T_B	Bottom temperature of the column, (K)
T_D	Reflux drum temperature, (K)
T_{J0}, T_J	Temperature of the jacket fluid at the inlet and outlet, (K)
T_R	Reactor temperature, (K)
T_{Ti}	Temperature of the tank i, (K)
$T_{w,0}$	Condenser cooling water inlet temperature, (K)
U_R	Reactor overall heat transfer coefficient, (J/m^2 s K)
V_R	Reactor volume, (m^3)
V_R	Steady-state reactor volume, (m^3)
x_A	Mole fraction of component A
x_B	Mole fraction of component B
$x_{B,i}$	Mole fraction of component i in the bottom stream of the column
$x_{D,i}$	Mole fraction of component i in the distillate stream of the column
x_{Ri}	Mole fraction of component i in the reactor
$x_{i,RC}$	Mole fraction of component i in the recycle stream
x_{Ri}	Mole fraction of component i in the reactor
$x_{i,0}$	Mole fraction of component i in the input stream of the reactor
$x_{Tj,i}$	Mole fraction of component i in the output stream of tank j
FC	Flow controller
LC	Level controller
TC	Temperature controller

CHAPTER I

INTRODUCTION

During the last two decades, numerous works have dealt with the design and investigation of dynamic behaviour of control systems to regulate specific unit operations (eg. distillation) and to bring a system (eg. reactor) back to the desired operating point to guarantee optimal profiles.

Hovewer, the design of control systems for complete chemical processes have been recognized for a long time as an important and difficult problem. The problem is difficult because :

1 . Chemical processes are non-linear, and multiple couplings exist among variables,

2 . The measurements and manipulation of process variables are limited to a relatively small number of variables,

3 . The control objectives may not be clearly stated (or even known) at the beginning of the control system design,

4 . Evaluation of the control system is based on a number of different objectives including ; (a) safety, (b) reliabilty, (c) goodness of control (including stability), (d) range of control, (e) ease of start-up and shut-down, (f) cost of operation, and (g) ease of operation of the system (including training)

5 . The process structure may effect the controllability of the process.

6 . There may be considerable uncertainty in the prediction of process behaviour.

In this work, considering the factors described above, the dynamic behaviour of some hypothetical plants are investigated. For this purpose, an existing package [1], precursor to CHPDSC is used. The package permits to simulate a general chemical plant which contains a continuous stirred tank reactor and a distillation column as the mojor equipment and two tanks and a heat exchanger as auxiliary equipment with two or three components in the process streams. The precursor package is enlarged so that the package CHPDSC now permits to handle four component systems. CHPDSC also permits sinusoidal upsets, in addition to step change upsets already incorporated in the original version.

In Chapter III, the developements to the precursor package and the scope of the CHPDSC are given.

The simulation results (Chapter IV) of this study is divided into three parts. In Examples (1,5) a four component system is investigated using the enlarged version of CHPDSC.

In the second part of this chapter, a realistic case from industrial application is introduced (Examples

6-9). The production of di-buthyl pthalate under different process structures and different controller gains are investigated. From this realistic example, it is determined that different types of process structure change the operability and controllability of the production. It is also concluded that economic variables such as cost of operation, rate of return must be considered, before the decision made about process structure (flowsheet).

Examples (10-12) in the third part of Chapter IV study new cases of some examples introduced by Akman [1]. These new cases investigate Akman's examples under different control structures and also for different process flow sheets which are alternate cases to Akman's.

CHAPTER II

PROCESS CONTROL OF COMPLETE CHEMICAL PLANTS : A SUMMARY SURVEY

Until the mid of 1950's, it was believed that controling perfectly every unit in an overall process, will result in the perfect control of the overall process. In 1956, it was indicated by Buckley [2] that the application of servomechanism theory to each individual loop in a chemical plant led to severe difficulties. Each loop which is designed for the fastest response and return to a specified operation condition may lead the process to instability and oscillations. Even with the controls damped or detuned sufficiently to eliminate this oscillation, the plant was often found to be very touchy and hard to operate.

Up to mid of 50's, researchers both in academia and in industry tried to hold constant all flows, temperatures, pressures, in order to control an overall chemical process. They argued that the product qualifications would be constant. However the problems are, whether it is possible to hold these variables constant, or whether it is neccesary to hold them constant, or whether there are same inconsistencies in holding them constant. Buckley [3], named this approach as "set point enviromental control". He introduced a new approach termed "dynamic process control" to contrast it.

Dynamic process control implies a considerably different way of designing and operating plants from that usually used previously. Buckley's approach is summarized below. From the plant manager's standpoint the plant must fulfill two primary requirements. First, it must produce a product whose quality (compositions, viscosities, color, etc.) meets sales specifications. Secondly, it must maintain a "material balance". Second statement is termed "material balance control" by Buckley. Material balance control implies three things ; i) inventories must be maintained between the minimum and maximum limits, ii) production rate must be adjusted to exactly equal, on a long term basis, the sales rate. iii) The resulting adjustment in process flows must be sufficiently smooth and gradual to avoid upsetting process equipment. Buckley indicated that, product quality controller acts as high-pass filters for disturbances; that is, the gain of the transfer function was very small at both low and high frequencies. On the other hand, the level controller systems commonly used for material balance control are low-pass filters ; the gain is large at low frequencies and very small at high frequencies. Buckley realized that this difference in the behaviour could be used to develop a new control strategy for chemical plants. Thus by selecting the break frequencies of the material balance controllers to be an order of magnitude lower than the resonant frequency of the product quality controllers, the two kinds of control systems will not interact. This means that, by interspering storage units and level control systems in the appropriate way between units where the product quality controllers are located, it can be effectively eliminated all dynamic interactions between units and provide essentially complete compensation for disturbances. This also implies that the overall controllability and operability of a plant is strongly dependent upon the intermediate material balance controllers.

In 1960, Williams and Otto [13] proposed a hypotetical chemical plant for the investigation of computer control. The plant contains a reaction, a heat exchanger, a multiple separation step and recycle streams.

In 1961, Gould and Kipinak [6] using the reactor in the Williams plant studied dynamic optimization (and control) of a continuous stirred tank reactor.

Foss [1973] , Kestanbaum et al. [1976], and Lee and Weekman [1976] have reviewed the existing theories and concluded that they are not directly adressing the overall process control system design problem.

In his review paper, Foss [4] criticizes the gap between the theory of process control and its application, and emphasis that the problem of chemical process control appears to involve the regulation of complex, often poorly understood physicochemical processes in the face of many unknown and uncharacterized disturbances.

Kestanbaum et al. [8], also emphasise the lack of application of the modern control system techniques in the industry due to the normal time lag between the conception of modern control system design tecniques in the academic community and their industrial application. Their review paper concentrate especially on the design of analog controllers for single-input single-output (SISO) systems and overdamped systems.

Lee and Weekman [9], emphasise the difficulties encountered in chemical process control . Firstly, understanding the process which is complex due to the physicochemical complexities, nonlinearity, high interaction and continuously disturbances by many uncharacterized noises. Second difficulty is to apply the theory to commercial plants. They present a commentary on the status of application of modern control theories to industrial chemical processes.

Synthesis of control structure based on aspects of structural controllability and observability to yield a controllable and observable system has been presented by

Morari and Stephanopoulos [11] in 1980 . They proposed "decomposition criteria" for the synthesis of control structures for a chemical plant. In their paper, they indicate that decomposing the overall process into independently controlled groups in terms of regulation or optimization, is useful when determining the alternative process control structures.

Govind and Powers [5], approach to the control system synthesis problem as a non-numerical problem solving procedure. Their paper describes a systematic procedure to generate control structures based on the cause-and-effect represantation of process. In the language of non-numerical problem solving, control system synthesis problem becomes one of using specific rules to generate a search tree of alternate control structures. The final product is a set of control schemes from which the final system may be selected or evolved. The authors emphasise that to test these ideas, computer programs are being developed which, interacting with the control engineer, will generate and evaluate alternate control systems.

Stephanopoulos [12] reviews the history of the systhesis of the process control systems in chemical engineering. In his review paper, he presents the scope of process synthesis problem and then proceeds to discuss the various facets of process control system synthesis. In the paper, earlier problem formulations, solutions and methodologies, outlining their assumptions, extent of applicability, advantages and short comings are evaluated. Then the need for a change in the process control curricula is examined and some new provocative questions for future researh are raised. Stephanopoulos implies that this subject is to a large extent still an "art" of engineering.

Akman developed a dynamic simulation and control package for a multi-purpose hypothetical chemical plant in 1987 [1]. He introduced a complete chemical plant which may have a chemical reactor, a separation unit, two mixing tanks to reduce in fluctuations in some terminal variables, and a heat exchanger unit before the separation unit to help stabilize any temperature fluctuations in the column feed in addition to help atttain the desired thermal condition of the feed. He developed the control structure for the proposed chemical plant, using a systematic integration procedure of the modal control structures for complete plant. In doing this he considered the interactions between different pieces of equipment in the flow sheet and eliminated the overspecifications and concluded on two different noninteracting control configurations for the distillation column.

Akman especially emphasizes that for multivariable systems with multiple inputs and multiple outputs (MIMO) of alternative control structures may not lead to one unique solution but several solutions the validities of which should be tested by simulation tecniques. It is only after simulations that a decision for the final control structure can be made.

In the view of survey on overall chemical plant control, it is surprisingly concluded that, although the term "overall process control" was used in 1950 for the first time, the published material on this subject is very limited. Most authors claim that this subject is still an art. Considering the rapid development in modern control science in the last three decades and the requirements of chemical industries, the lack of detailed studies in this subject does not seem very realistic. In the view of these facts ,it may be concluded that there must be a lot of unpublished studies on this subject.

CHAPTER III

SCOPE OF THE CHPDSC PACKAGE

In this chapter, the scope of precursor package will be given. Then the details of the developments made to the package are introduced. General scope of developed software CHPDSC is given in the last part of the chapter.

3.1 SCOPE OF THE PRECURSOR SOFTWARE

The proposed chemical plant by Akman [1] simulates a typical process which is shown in Figure 3.1 The major equipments are the continuous stirred tank reactor and a distillation column. Two mixing tanks and a heat exchanger unit are the proposed auxiliary equipments. Recycle streams may also be considered.

The simulation package (CHPDSC) was developed in the FORTRAN programing language on the CDC mainframe computer. For the calculation of the initial conditions of each equipment and for the dynamic behaviour of each unit evaluated in different SUBROUTINES which introduces the model equations. The properties of the interconnecting streams is transfered by the COMMON blocks between the subroutines. Package uses six different data files. Data files, INTANK1, INCSTR, INTANK2, INHEX, and INDIST give the initial conditions, spesification of the equipment, and controller gains for

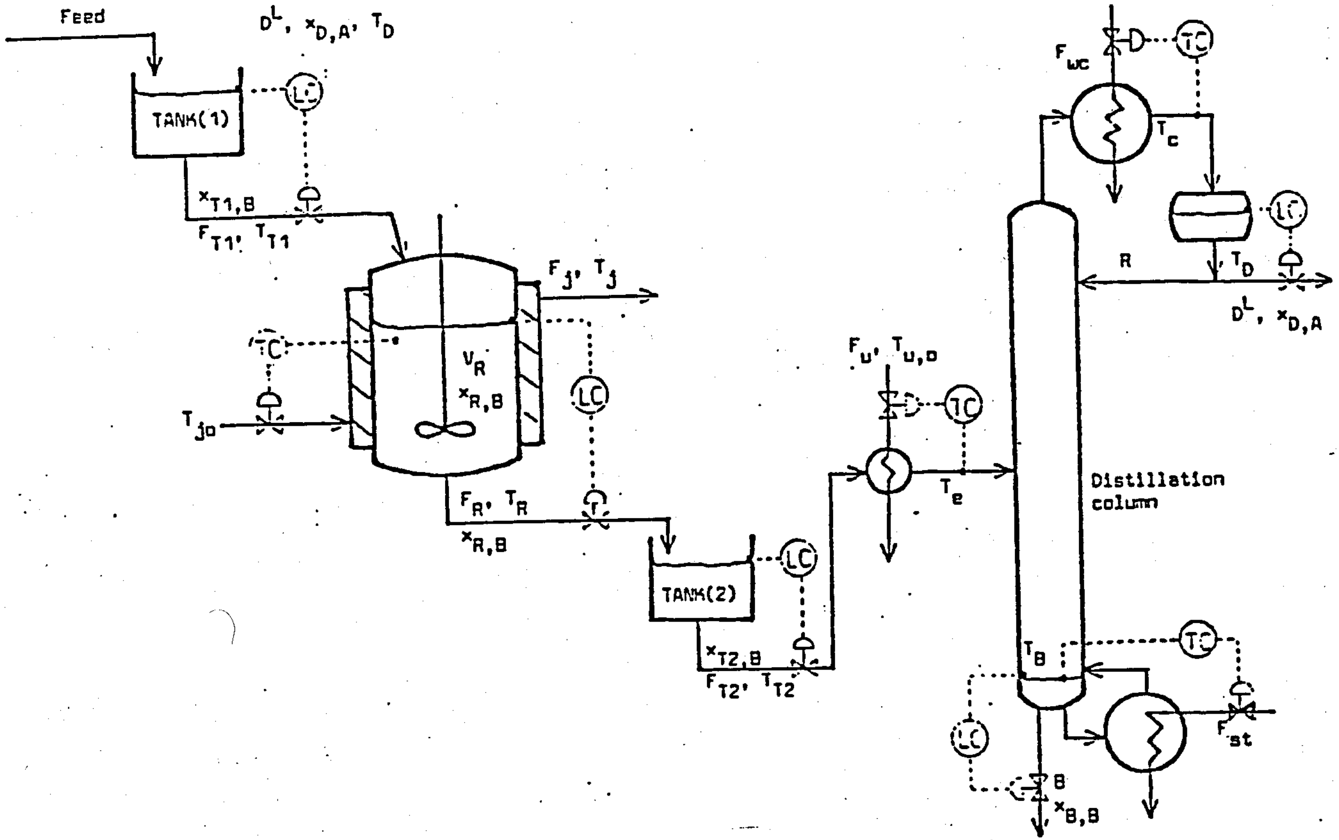


Figure 3.1 The complete plant.

each individualy unit. Data file INSYST describes the flowsheet of the desired plant, pysical properties of the components and the integration parameters.

Although Akman's multi-purpose plant is much a realistic model observable in chemical industries, the component number which is limited at three in the package limits the use of package for the adaptation to real-life-process situations.

3 .2. Further Developments of the Precursor Package

In this section, model equations of continuous stirred tank reactor used in the developed version of CHPDSC, is introduced.

Model equations for the continuous stirred tank reactor is expressed as follows for a irreversible, second order, exothermic reaction. The assumtions is that the reactor is perfectly mixed and nonisothermal.

Heat transfer between the process at temperature T_{FR} and the avarage jacket temperature T_J is described by an overall heat transfered coefficent :

$$Q_{FR}=U_{FR}*A_{FR}*(T_{FR}-T_J) \qquad (3.1)$$

where Q_{FR} : heat transfer rate

U_{FR} : overall heat transfer coefficient

A_{FR} : heat transfer area

If the heat trnsfer area varies with the reactor hold up it would be included as another variable. This will require another equation.

$$A_{FR}=(A_{FR}/V_{FR})*V_{FR} \qquad (3.2)$$

where A_{FR} : steady-state heat transfer area

V_{FR} : steady-state reactor volume

V_{FR} : reactor volume

The rate of reaction can be expressed in molar basis for the following cases;

1. The reaction is overall second order

$$r=k*x_A*x_B*(M_{FR}^2/V_{FR}) \qquad (3.3)$$

2. Reaction is second order with respect to component A

$$r=k*x_A^2*(M_{FR}^2/V_{FR}) \qquad (3.4)$$

3. Reaction is second order with respect to component B

$$r=k*x_A^2*(M_{FR}^2/V_{FR}) \qquad (3.5)$$

in these expressions ;

M_R = molar hold-up of the reactor

x_A, x_B = mole fractions

$$k = k_0 * \exp(-E/R_g * T_g) \qquad (3.6)$$

where E : activation energy

k_0: Arhenius constant

R_g: gas constant

Total and component continuity equations in the cases;

1. Reaction is; A + B ——> C + D

$$\frac{d(M_R)}{dt} = F_{R,0} - F_R + F_{RC} \qquad (3.7)$$

where $F_{R,0}$: fresh feed flow rate

F_R : output flow rate

F_{RC} : recycle flow rate

$$\frac{d(M_R)}{dt} = F_{R,0} * x_{i,0} - F_R * x_i + F_{RC} * x_{i,RC} - R_i \qquad (3.8)$$

i = A,B,C,D

where R_i = rate of depletion of component i and $R_A = r$

$R_B = r$

$R_C = -r$

$R_D = -r$

2. Reaction is; $2A + B \longrightarrow C + D$

$$\frac{d(M_R)}{dt} = F_{R,o} - F_R + F_{RC} - R \qquad (3.9)$$

$$\frac{d(M_R)}{dt} = F_{R,o}*x_{i,o} - F_R*x_i + F_{RC}*x_{i,RC} - R_i \qquad (3.10)$$

where $R_A = 2r$

$R_B = r$

$R_C = -r$

$R_D = -r$

3. Reaction is; $A + B \longrightarrow 2C + D$

$$\frac{d(M_R)}{dt} = F_{R,o} - F_R + F_{RC} + R \qquad (3.11)$$

$$\frac{d(M_R)}{dt} = F_{R,o}*x_{i,o} - F_R*x_i + F_{RC}*x_{i,RC} - R_i \qquad (3.12)$$

where $R_A = r$

$R_B = r$

$R_C = -2r$

$R_D = -r$

Energy balance equation;

$$\frac{d(M_R.h_R)}{dt} = F_{R,0}*h_{R,0} - F_R*h_R + F_{RC}*h_{RC} - L*r - Q_R \qquad (3.13)$$

where $h_{R,0}, h_R, h_{RC}$ = liquid enthalpies of fresh feed, output, and recycle streams respectively

L = heat of reaction

Jacket energy balance equation ;

$$ro_J*c_{pJ}*V_J*\frac{d(T_J)}{dt} = ro_J*c_{pJ}*F_J*(T_{J0}-T_J)+Q_R \qquad (3.14)$$

where ro_J = density of jacket fluid

c_p = heat capacity of jacket fluid

For reactor volume controller;

$$F_R = f_c(V_R)$$

and for reactor temperature controller;

$$F_J = f_c(T_R)$$

two required equations must be introduced in the program according to the type of controller.

The difference in the equations of reactor model from the previous work is in total continuity, component continuity, and kinetic equations. In this work, the number of component is expanded to four. Furthermore, reaction types $A + B \longrightarrow C + D$, $2A + B \longrightarrow C + D$, $A + B \longrightarrow 2C + D$ are evaluated. Also the kinetic model for the second order reaction (if the reaction is second order overall, or second order with respect to A, or second order with respect to B) is evaluated in the program. The program reads the reaction type and reaction kinetic parameters from data file INCSTR.

The details of the mathematical models of process units in the flowsheets are given in Akman's study [1]. In this work, the main difference in the unit models with respect to those given by Akman is that Akman's units were modelled to handle binary and tertiary mixtures, whereas here these models were extended to also handle four component mixtures.

3.3 GENERAL SCOPE OF CHPDSC

The CHPDSC package is prepared on the CDC main frame using FORTRAN as the programming language. The package is a combination of a number of subroutines. The MAIN program is a divider program which reads the number of components, physical properties, flow-sheeting parameters, integration step size, printing and plotting time intervals by calling the data file INSYST. The MAIN program also calls the integration subroutine RUNGE. The integration routine is Runge-Kutte by Gills method. Subroutine BUFFER is called by subroutine RUNGE and calls the unit subprograms in the sequence as they appear in flow-sheeting parameters. Subroutines T1MAIN, T2MAIN, RMAIN, DMAIN and HMAIN read the input parameters calling the data files for the related equipment and calculate the initial conditions. Data files are prepared for each individual unit. These are INTANK1 for the first tank, INTANK2 for the second tank, INCSTR for continuous stirred tank reactor, INDIST for the distillation column and INHEX for the heat exchanger. Subroutines TANK1, TANK2, CSTR, DIST and HEX perform the calculations in connection with mathematical models for each unit and solution procedure for simulation. Subroutine FEEDD matches the output stream properties of CSTR, TANK2 and HEX to the feed stream properties of DIST. Subroutine HYDRAU calculates the liquid flow rates from each tray, from each holdups, by use of Francis' weir formula. Subroutine ENTCOEF calculates the coefficients in the liquid and vapor molar enthalpy expressions from molecular weights, liquid and vapor heat capacities, boiling points, and from the heat of vaporization of components. Subroutine ENTH calculates the molar enthalpies of liquid and vapor streams as a function of temperature and composition. Subroutine TEMPENT evaluates temperatures from liquid and molar enthalpies. Subroutine MWDENS calculates the avarage weights and densities based on molar fractions. Subroutine EQUIL performs the vapor-liquid equilibrium calculations by Raoult's Law employing the Newton-Raphson covergence method. Subroutine CONDENS performs the calculations pertinent to the condenser of the distillation column. Subroutine CONVERG is called by CONDENS and performs the convergence calculations by Wengstein convergence method. Subroutine STEAM contains the data taken from staem tables and calculates the heat of vaporization and the temperature of saturated stream from steam density in the reboiler of the distillation column. Subroutines PRINTT, PRINTR and PRINTD prints the variables pertinent to the related equipments. The output files are OUTTANK for tanks, OUTCSTR for the reactor and OUTDIST for the distillation column.

CHAPTER IV

RESULTS OF SIMULATIONS AND THE RELATED DISCUSSIONS OF SYSTEM DYNAMICS

In this chapter, various example plants simulated by CHPDSC is introduced.

4.1. Result of Simulations for Four Component Systems

In this section two example flowsheet was simulated using the enlarged version of CHPDSC, will be introduced and discussed. The type of reaction is in the form $A + B \longrightarrow C + D$, and the reaction is second order with respect to component B.

The controller gains in the following examples were determined via the "Online Trail and Error " procedure as outlined by Luyben [10] which seems to be a modified Ziegler-Nichols analysis. The controller gains determined in this manner are given in the Appendices for each case.

EXAMPLE 1

In this example, the continuous stirred tank reactor and the distillation column are the processing units. The flowsheet is as shown in Figure 4.1 .

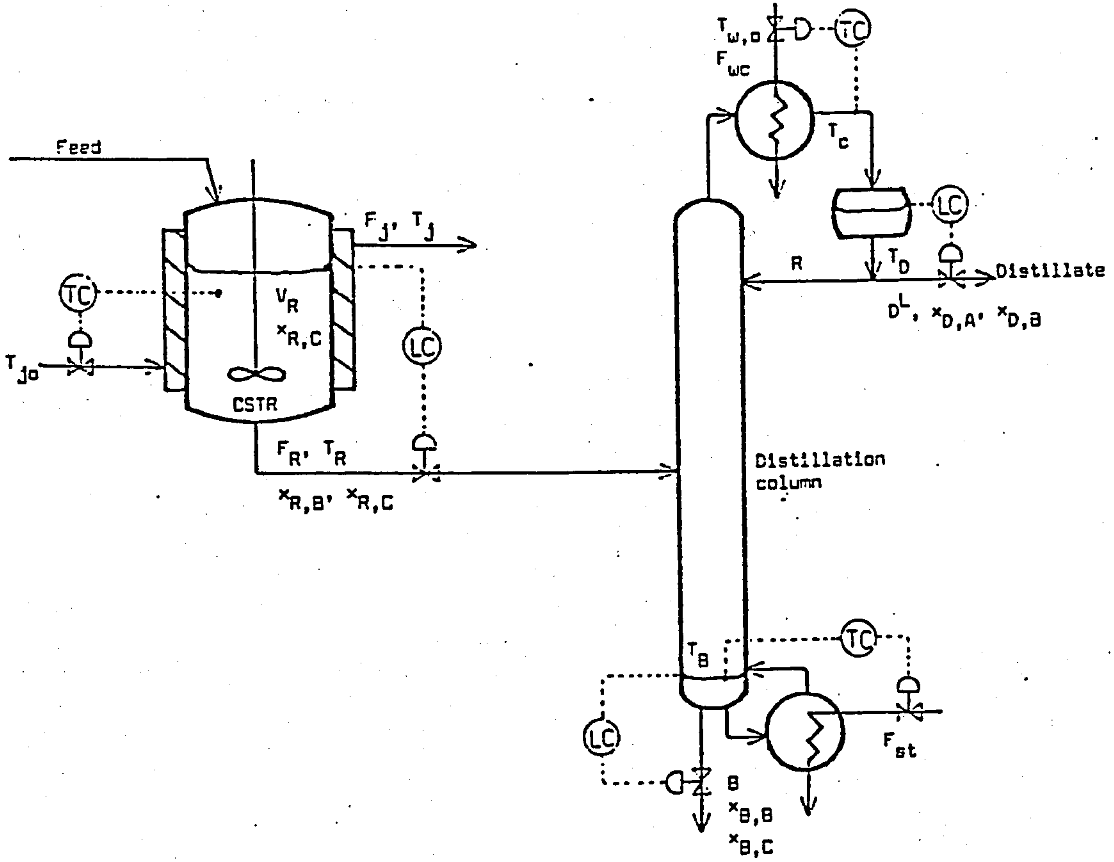


Figure 4.1 Flowsheet of the plants in Examples 1, 3 to 8.

The reaction occuring in the reactor is in the form ; A + B ——> C + D , is second order with respect to component B. The reaction is sligthly exothermic. Since the energy which is produced by the reaction is inadequate to supply the reaction temperature in the continuous reactor, the reactor must be heated. This is provided by the jacket of the reactor in which a heating liquid is passed. Temperature of the reactor is controlled by a PI controller which manipulates the heating liquid flow rate. The set point for the temperature controller is 373.2 K.

The reactor effluent is pumped to the distillation column. The bottom temperature of the column is controlled at 606.2 K which is close to the boiling point of heaviest component C, by a PID cotroller which manipulates the flow rate of heating liquid in the reboiler. The condenser subcools the vapor leaving the top tray of the column and the set point for the temperature of subcooled liquid leaving the condenser is 375.6 K. A PI controller is used to manipulate the flow rate of condenser water.

A mixture of components A and B with the molar ratio is 10.02 : 1 is fed to the process to produce component C as the main product. The product is taken from the bottom stream of the column which contains 90.72 % component C.

The physical properties of the components , the initial steady-state conditions and the technical specifications of the process equipment are given in Tables A.1, A.2, A.3.

The upset given is a 5 % step decrease in the feed flow to the reactor from 45.36 kgmole/hr .

The various terminal variables are plotted as functions of time and shown from Figure 4.2 to Fig. 4.4 .

When the feed flow rate to the reactor decreases, the outflow rate of the reactor decreases as shown in Figure 4.2 .

When the feed flow rate decreases, the reactor temperature initially increases and then return to its set value with oscillation. The initial increase in the reactor temperature is due to the increase in residence time in the reactor. Since the reactor temperature is controlled by manipulating the heating liquid flow rate to the reactor jacket, increasing reactor temperature will result in the decrease of flow rate of heating liquid. The changes in jacket liquid flow rate and the jacket temperature is shown in Figure 4.2. The changes in the reactor temperature and the jacket temperature give an indication of the heat transfer between the reactor and its jacket.

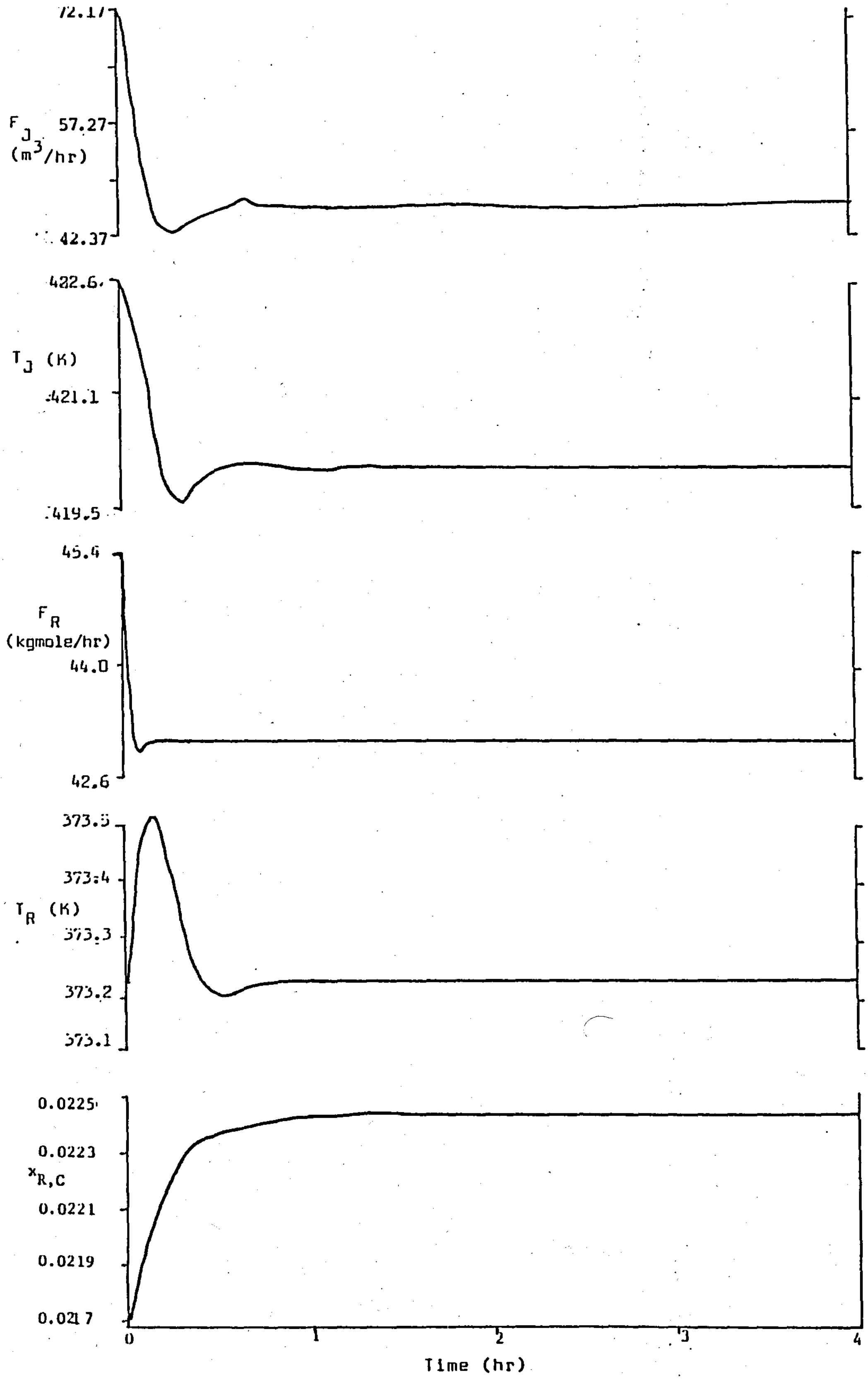


Figure 4.2. Response of the reactor in Example 1

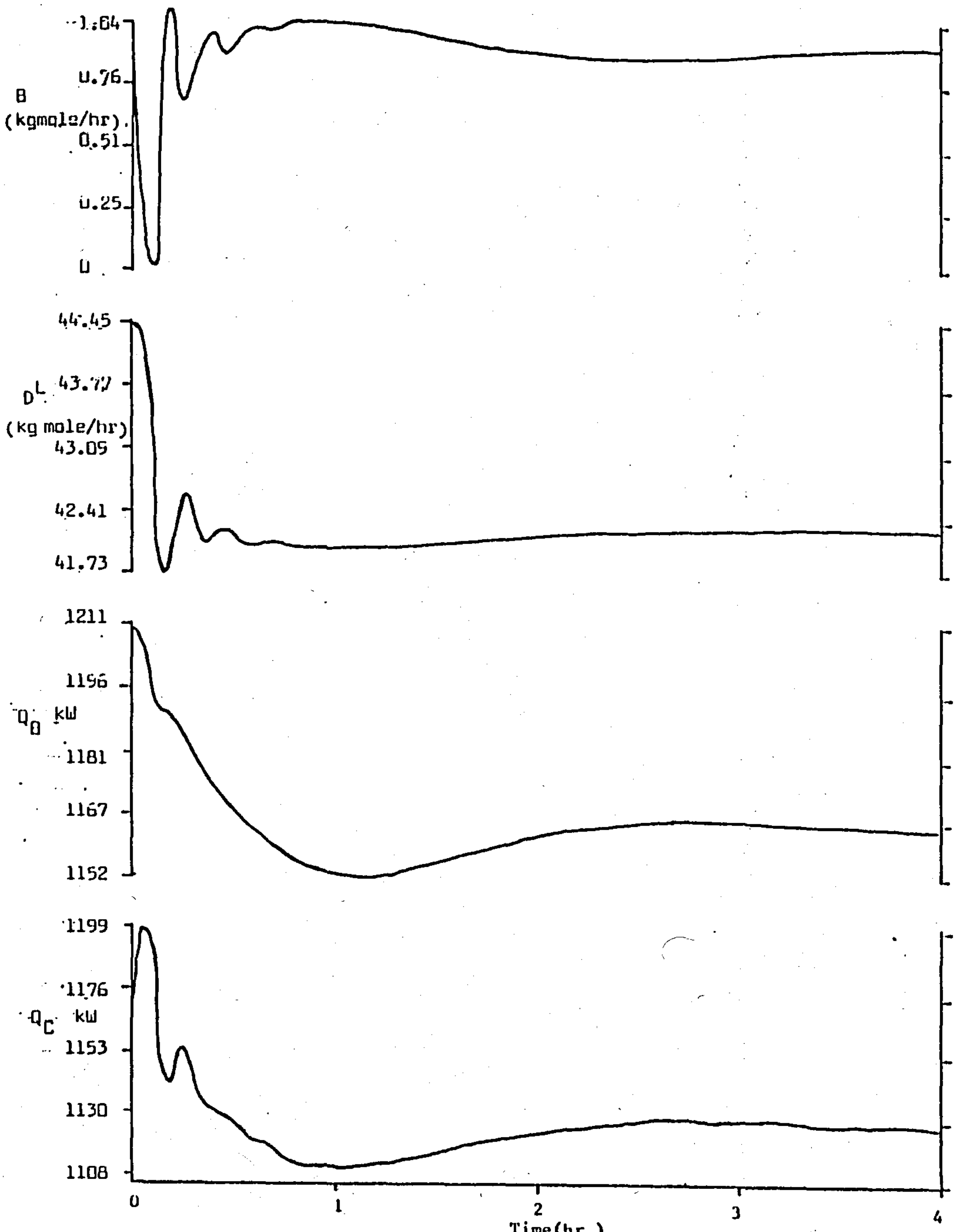


Figure 4.3 Response of the column (flows and heats)in Example 1

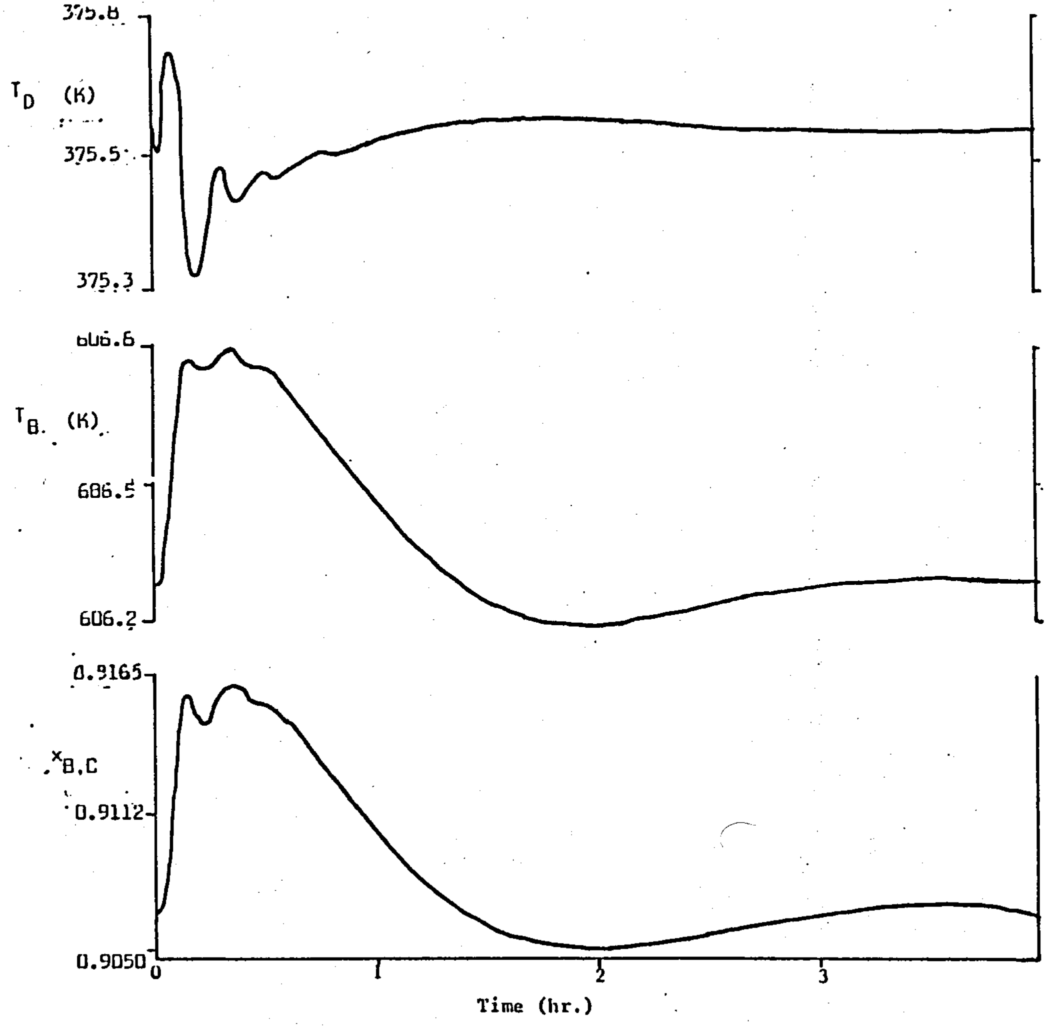


Figure 4.4 Response of the column (temperatures and main product fraction at the bottom) Example 1 .

Due to the increase in residence time in the reactor, the conversion in the reactor increases. The response in the mole fraction of main product, $x_{R,C}$, is shown in Figure 4.2. The mole fraction increases continuously without oscillation until the new steady-state reached.

When the feed flow decreases, the distillate, D^L, and the bottom stream of the column, B, also decreases as shown in Figures 4.3 . It can be noted in Figure 4.3, that the increase in bottoms flow rate is much little than the increase in distillate stream.

When the flow rate decreases, the inventories of the column start to decrease. Since the liquid rate from the first tray to the column base will decresae, the steam flow will be more than the required amount at steady-state. Since the flow of steam is manipulated by bottoms temperature controller, it will take some time for the steam flow to decrease. Meanwhile, the excess heat input will cause excessive vaporization and the loss of liquid at the bottom. The bottoms flow rate and the heat given to the bottom is shown in Figure 4.3 .

The bottom temperature and the mole fraction of the heaviest component is shown in Figure 4.4. The bottoms temperature initially increases due to the excess heat input to the bottom, and then decreases to its set value with oscillations.

The response in distillate temperature controlled by a PI controller manipulating the condenser cooling liquid flowrate is a typical controlled response and oscillatory as shown in Figure 4.4 .

As can be shown from graphs, mole fraction of component C in the bottom stream follows the bottom temperature response. This means that temperature can be used as a secondary control variable at the bottom of the column to control the composition.

EXAMPLE 2

The only difference in Example 2 and Example 1, is an intermediate tank between the reactor and the column added to the process. Flowsheet which is simulated is shown in Figure 4.5 . The physical properties of the components , the initial steady-state conditions and the technical spesifications of the equipments are as given in Tables A.2, A.3, A.4, A5.

The volume of the tank is 0.78 m^3 and the volume is controlled by a P type level controller.

The responses in the variables in the tank and in the column are shown in Figures 4.6, 4.7, 4.8 for this example.

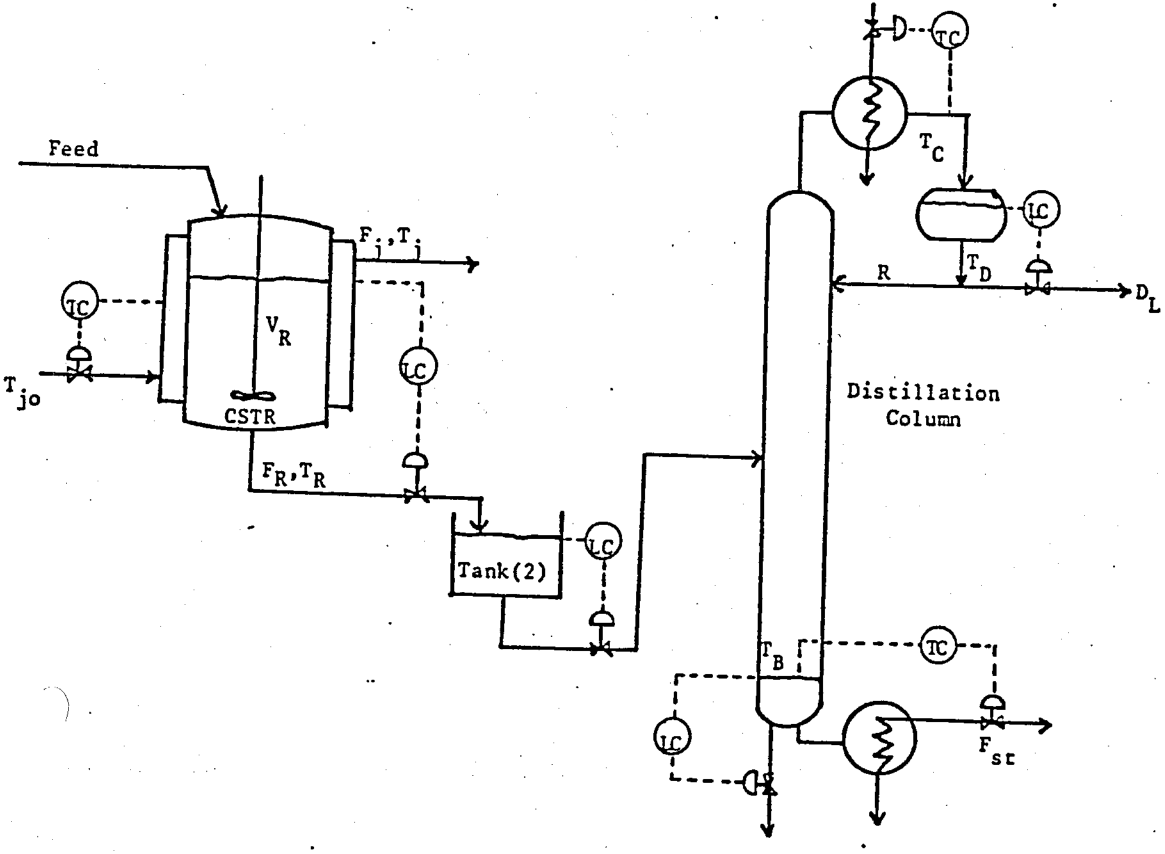


Figure 4.5 Flowsheet of the plants in Examples 2, 10.

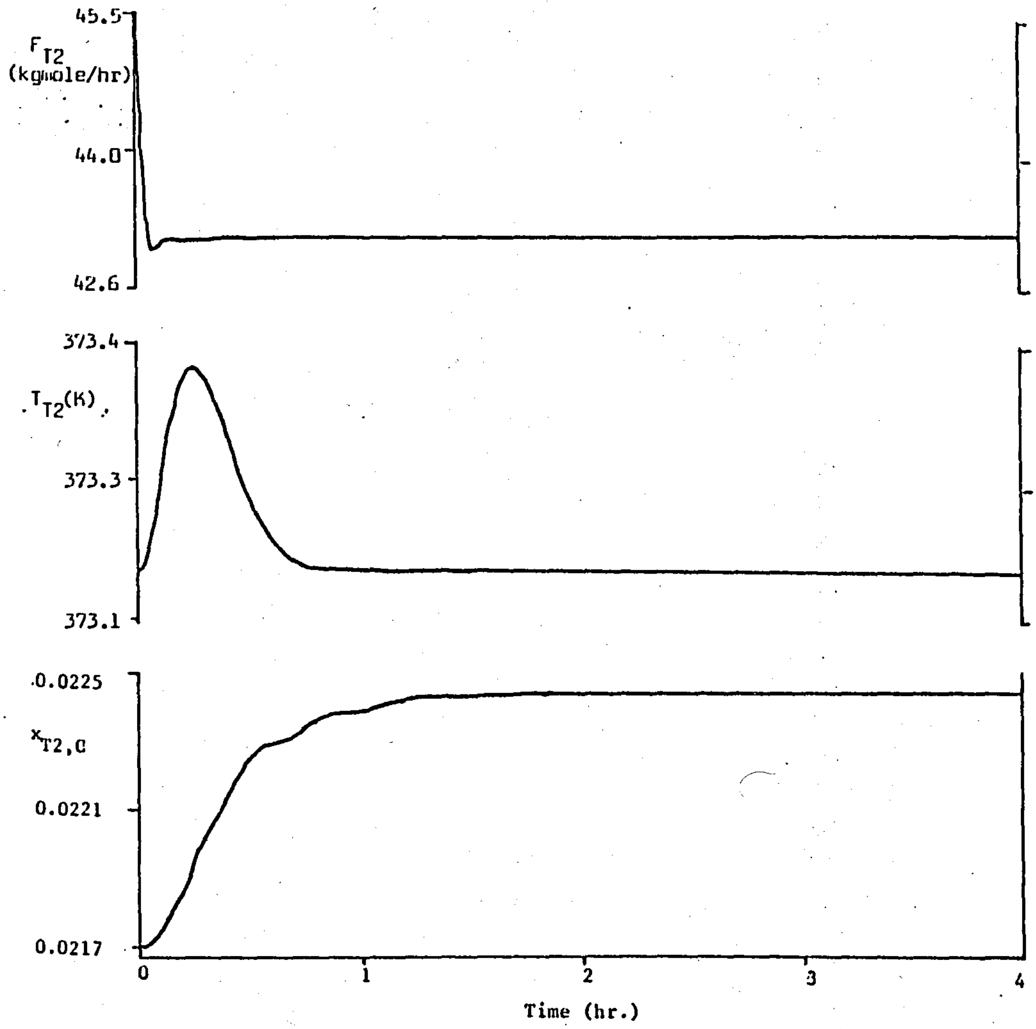


Figure 4.6 Response of the tank in Example 2

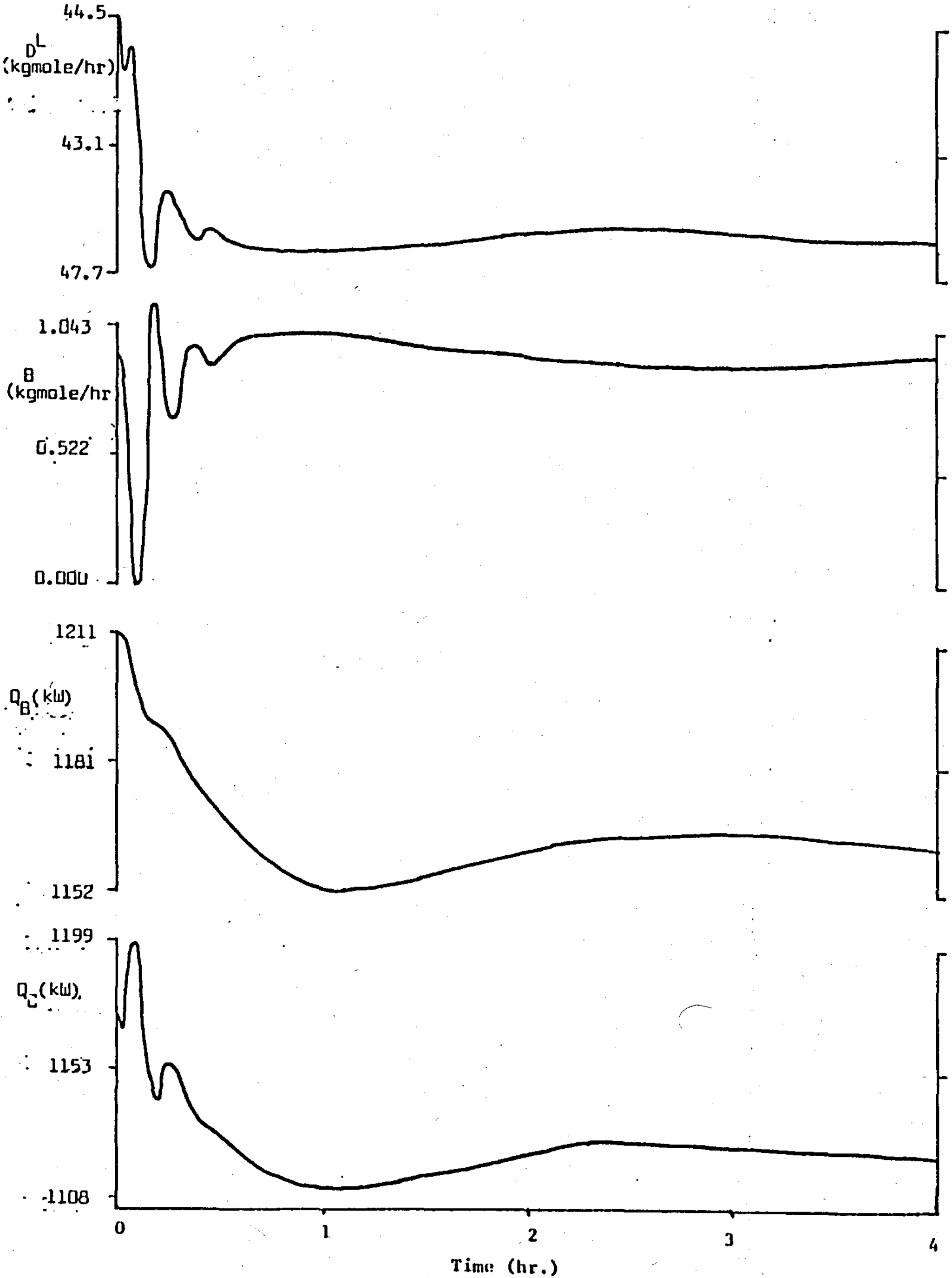


Figure 4.7: Response of the column (flows and heats) in Example 2

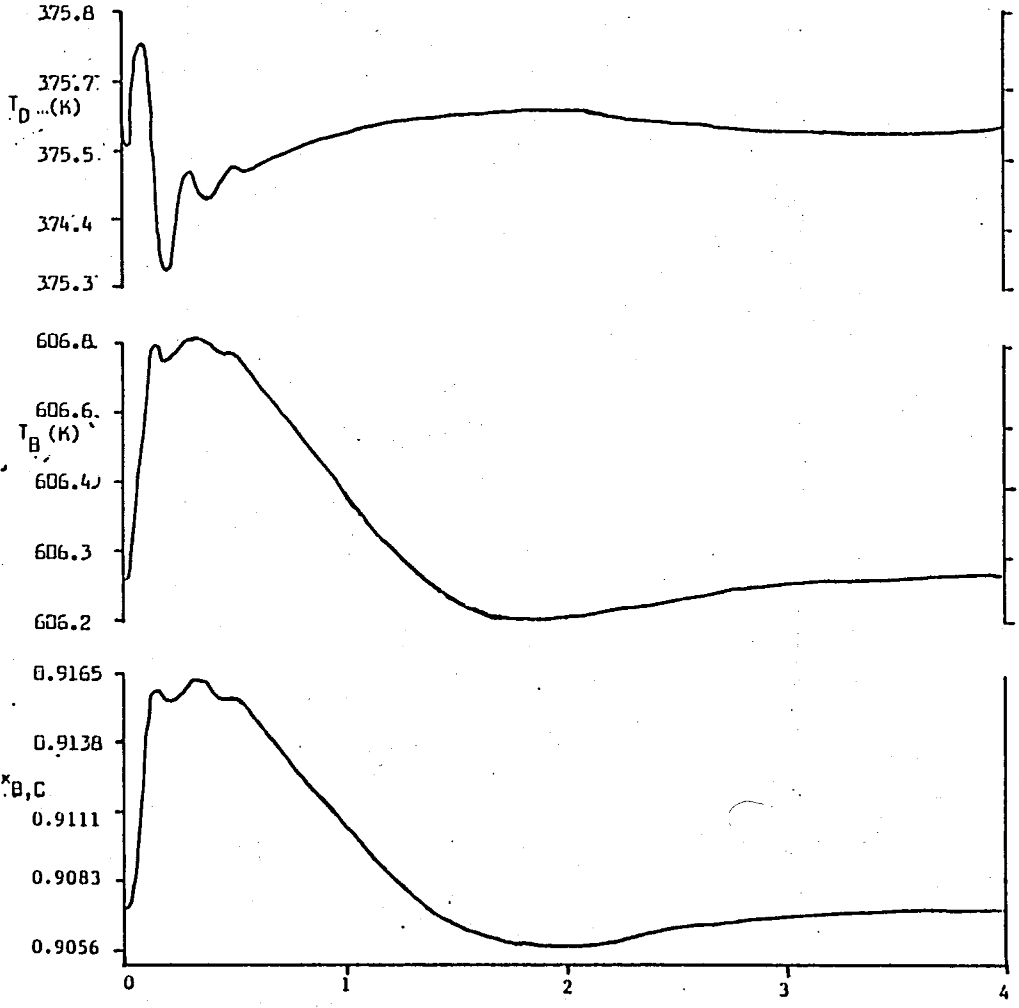


Figure 4.8 Response of the column (temperatures and main product fraction at the bottom) in Example 2

It can be noted that the amplitude of the fluctuation in tank temperature is lower than the amplitude in the reactor. Hence the intermediate tank reduces the fluctuations in the temperature of the stream which comes from reactor.

It can be seen that in Figures 4.7 and 4.8, the response of the column in this example is very similar with the previous example and the differences in the amplitute of the fluctuations is very little and have no significant importance. This is due to the column is primarly affected by the decrease in feed flow rate and the changes in concentration in feed flow.

EXAMPLE 3

In this example, the flowsheet which is simulated is shown in Figure 4.1. The processing units are the continuous stirred tank reactor and the distillation column. The process is the same as in Example 1. The physical properties of the components , the initial steady-state conditions and the technical spesifications of the equipments are as given in Tables A.1, A.2, A.3. The difference in this example is the upset which is given to process.

In this example, the upsets are;

a) The feed flow rate to the reactor is decreased 5 % from 45.36 kgmole/hr. by a step change,

b) The fresh feed temperature is increased to 299.8 K from 297.0 K by a step change.

It can be noted that the only difference in this example from Example 1, is an additional upset. (i.e. increase in feed temperature)

The various terminal variables are plotted as functions of time from Figure 4.9 to Figure 4.11.

When the upsets are given, the output flow of the reactor decreases as shown in Figure 4.9 .

When the upsets are given, the reactor temperature initially increases and then returns to its set value with oscillation. The initial increase in reactor temperature occurs by two reasons. Firstly, increase in residence time in the reactor causes higher conversion and hence higher heat generation due to the exothermic reaction. Secondly, the upset in feed temperature causes an initial increase in the reactor temperature. The temperature controller of the reactor manipulates the flow of heating liquid to the reactor jacket. When the reactor temperature increases, the flow of jacket liquid decresaes. The changes in the flow rate of jacket liquid, F_J and the jacket temperature, T_J, are shown in Figure 4.9 . The changes in the reactor temperature and

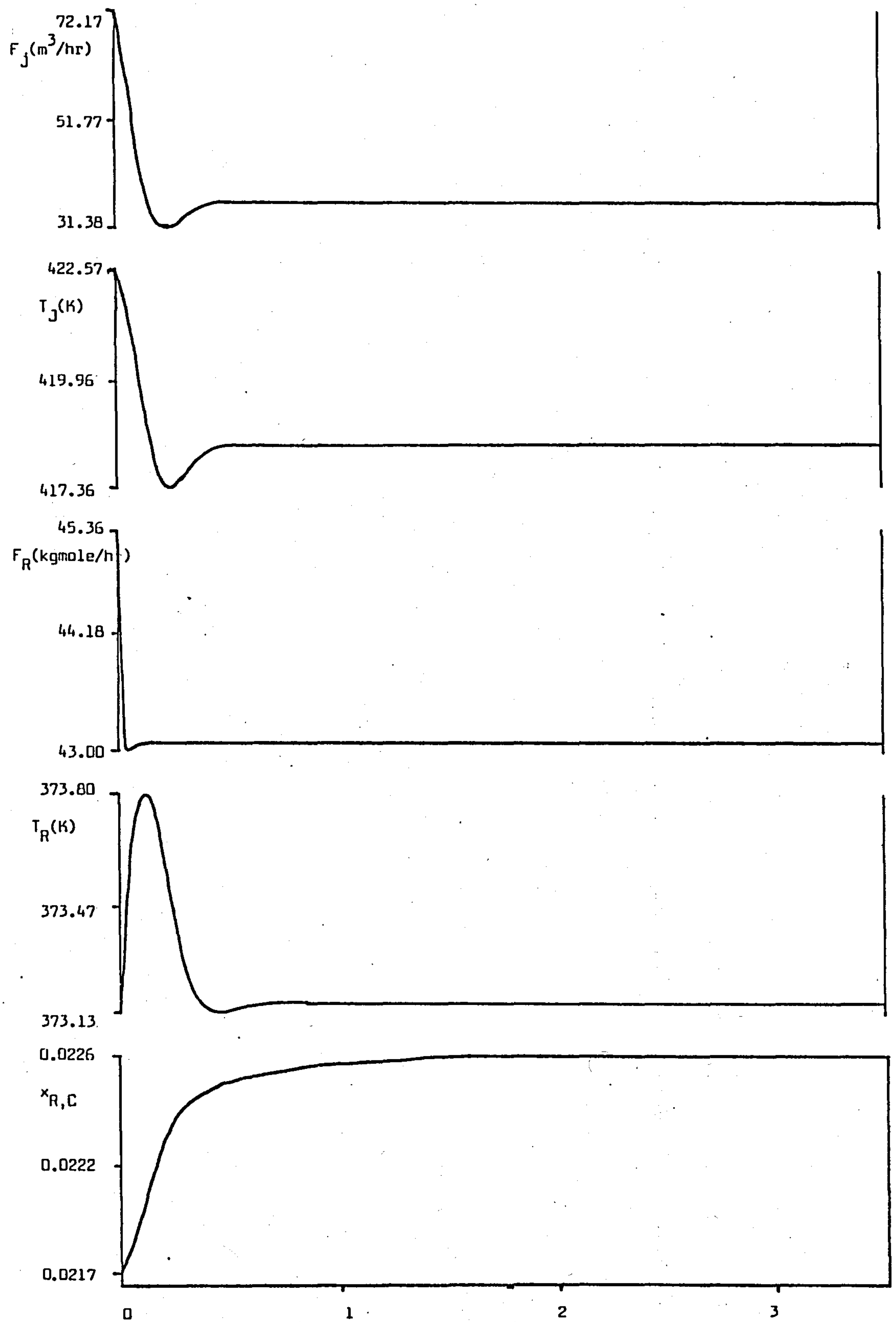


Figure 4.9 Response of the reactor in Example 3

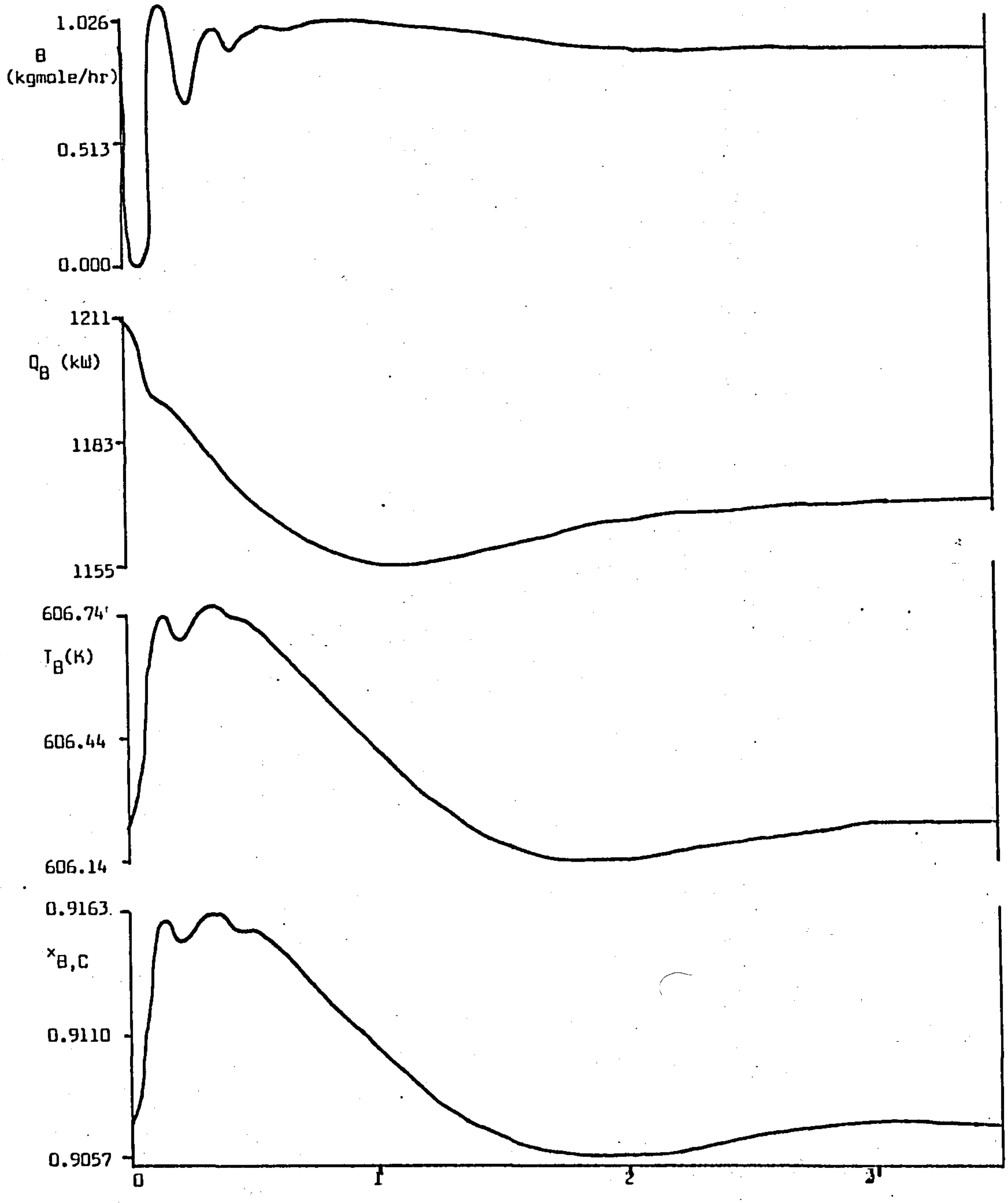


Figure 4.10 Response of the column (bottoms) in Exaple 3

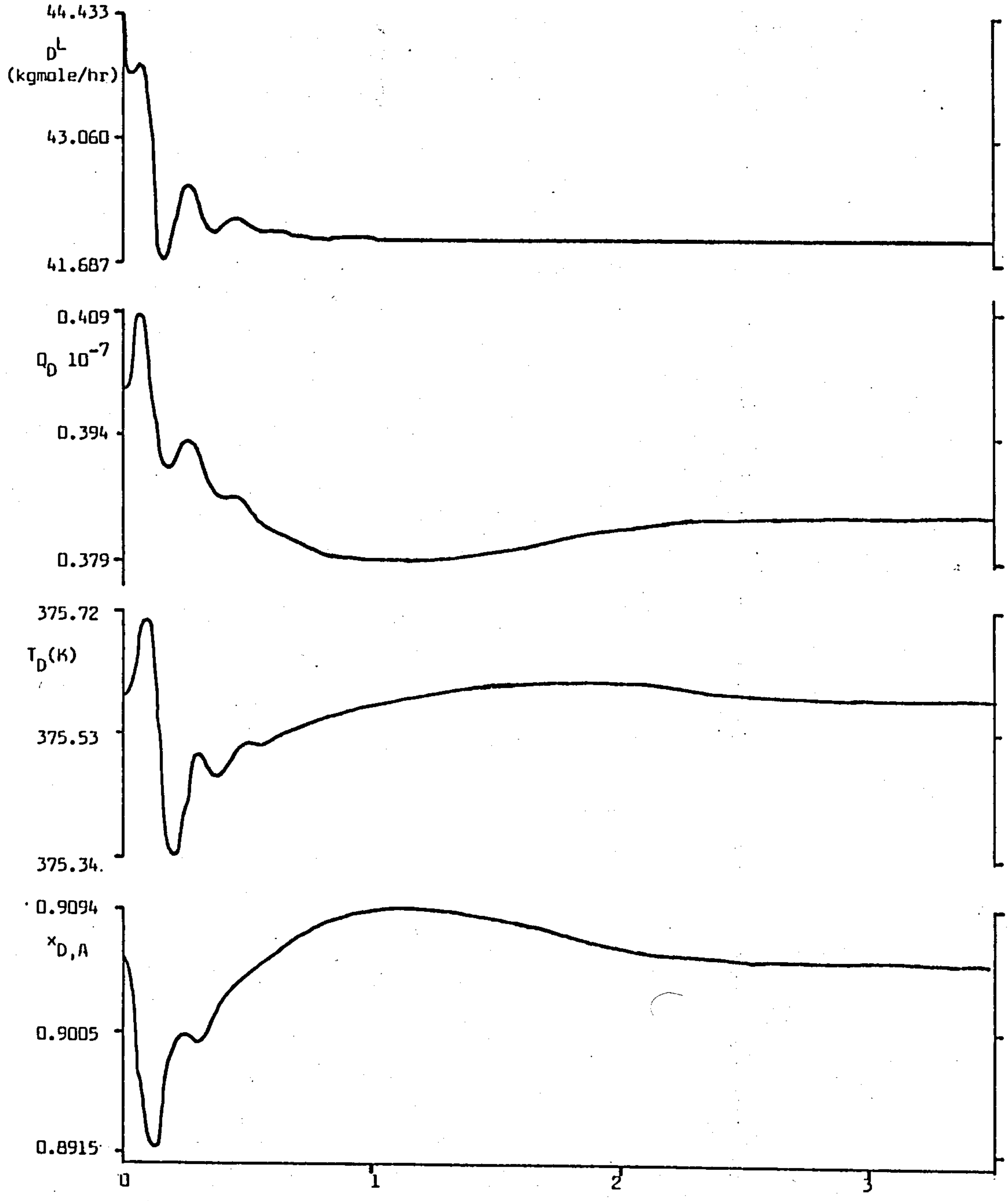


Figure 4.11 Response of the column (distillate) in Example 3

the jacket temperature give an indication of heat transfer between the reactor and the jacket.

The changes in the variables of the distillation column are primarily due to the changes in feed flow rate and in feed composition. As it was discussed in the previous examples, when the flow rate decreases, the flow rate of bottom and the distillate streams decrease with oscillations. When the feed flow decreases, the inventories of the column start to decrease. Since the liquid rate from the first tray to the column base will decrease, the steam flow will be more than the required amount at steady-state. Since the flow of steam is manipulated by the bottom temperature controller, it will take some time for the steam flow decrease. Meanwhile the excess heat input will cause excessive vaporization and loss of liquid at the at the column base. The response in the bottoms flow rate and the heat given to the bottoms as shown in Figure 4.10.

The bottom temperature initially increases and then decreases with oscillation. The response in the bottom temperature and the mole fraction of the heaviest component at the bottom (main product) are shown in Figure 4.10 . Again in this example, the mole fraction of heaviest component follows the bottoms temperature.

The response in the distillate temperature, T_D, and the mole fraction of the component C, $x_{D,C}$ (greatest amount in the feed stream) are shown in Figure 4.11 . The response in the distillate temperature has strong relation with the condenser temperature which is controlled by the manipulations of the cooling water flow in the condenser. Since the condenser temperature is controlled by a PI controller, the response in the reflux drum temperature is a typical controlled response and oscillatory as shown in Figure 4.11 .

EXAMPLE 4

Again in this example, the processing units are the continuous stirred tank reactor and the distillation column and the flowsheet is as shown in Figure 4.1.

The process is the same in Example 1 and initial conditions are also the same . The physical properties of the components , the initial steady-state conditions and the technical specifications of the equipments are as given in Tables A.1, A.2, A.3. The difference in this example is the upset which is given to process.

In this example, the upset given to process is 5 % step increase in the feed flow.

The various terminal variables are plotted as functions of time from Figure 4.12 to 4.14 .

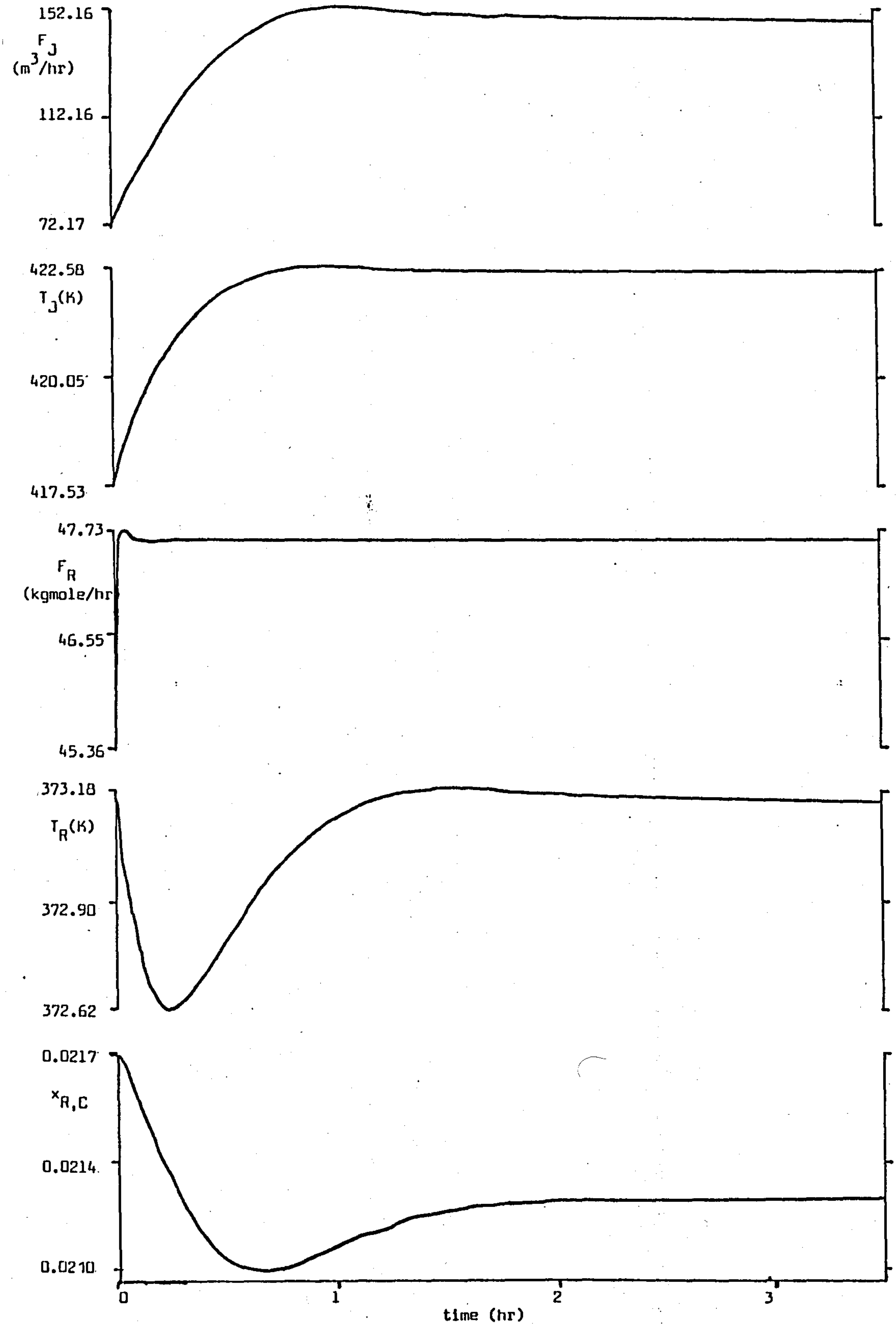


Figure 4.12 Response of the reactor in Example 4

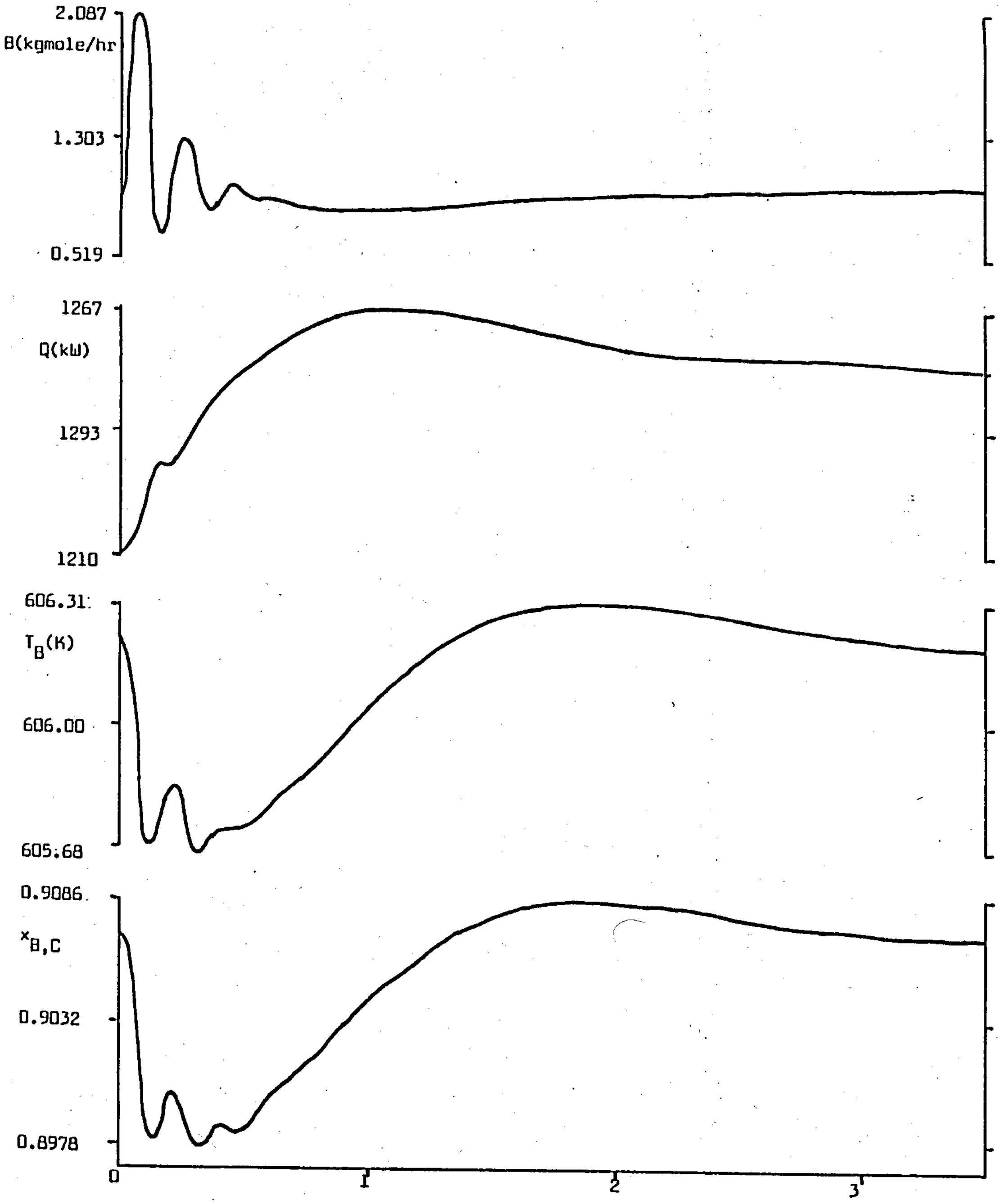


Figure 4.13 Response of the column (bottoms) in Example 4

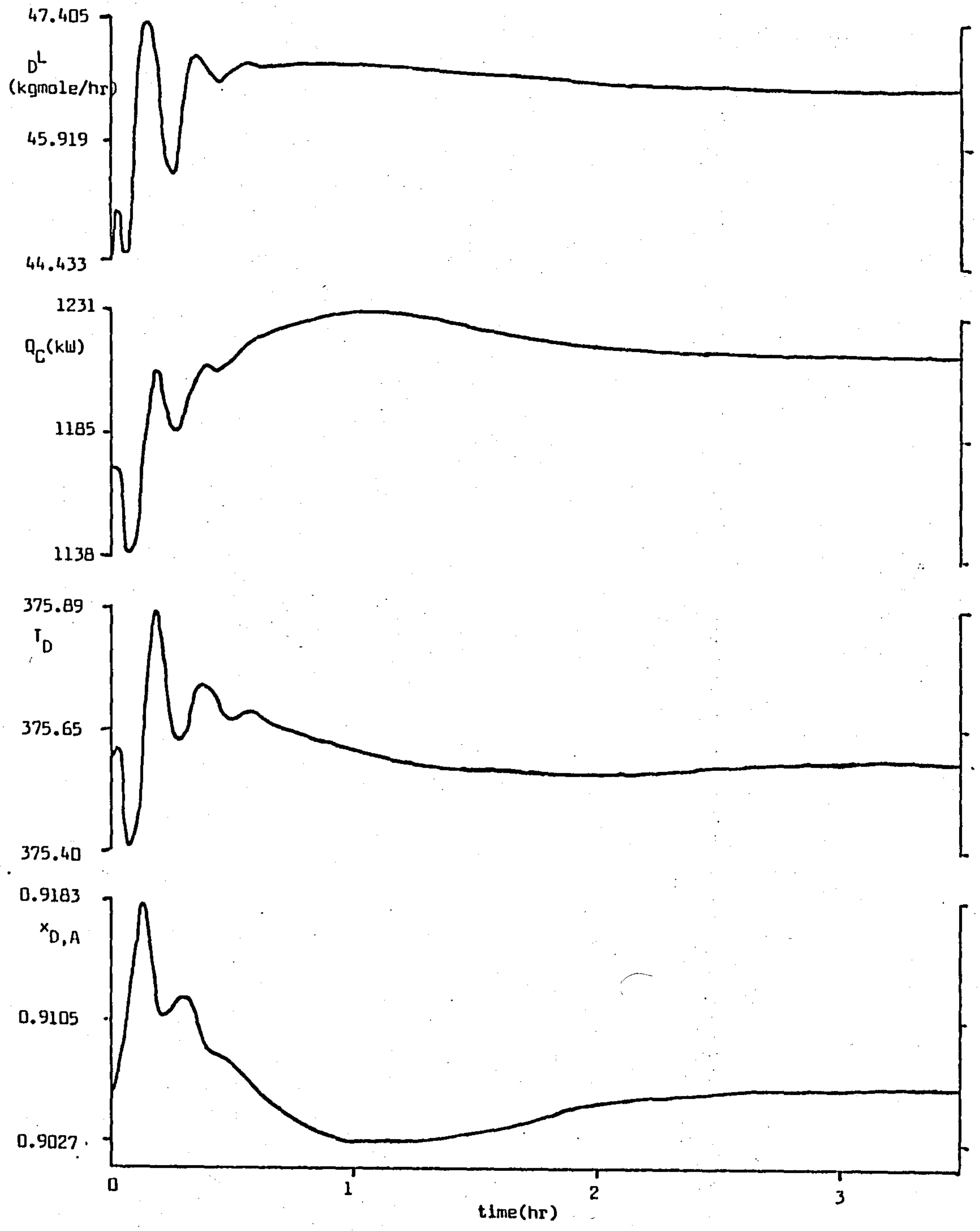


Figure 4.14 Response of the column (flows) in Example 4

When the feed flow rate to the reactor increases, the outflow rate of the reactor increases as shown in Figure 4.12 .

When the feed flow increases, the reactor temperature initially decreases and then return to its set value. The initial increase in the reactor temperature is due to the decrease in residence time in the reactor. This will cause lower conversion and hence lower heat generation by the exothermic reaction. Since the reactor temperature is controlled by manipulating the heating liquid flow rate to the reactor jacket, decreasing the reactor temperature will result to an increase in the flow rate of the heating liquid to the reactor jacket as shown in Figure 4.12 . The changes in the flow rate of the jacket liquid, F_J, and the jacket temperature, T_J are shown in Figure 4.12 . The changes in the reactor temperature and the jacket temperature give an indication of heat transfer between the reactor and the jacket.

The response in the molar fraction of main product, $x_{R,C}$, is shown in Figure 4.12 . Due to the decrease in residence time as explained above, the molar fraction of product decraeses after upset.

The changes in the variables of the distillation column are primarily affected by the changes in the feed flow and the changes in composition.When the feed flow rate increases, the flowrates of the distillate and the bottom streams increases as shown in Figures 4.13, 4.14. It can be noted that the increase in the flow rate of bottom is lower. Contrary to the previous examples where the feed flow rate was decreased, in this example bottoms temperature initially increases. Since, when the feed flow is increased, the liquid flow rate from first tray to the column base also increases, the steam flow will be lower than the required amount at steady-state. Since the steam is manipulated by the bottom temperature controller, it will take some time for the steam flow to decrease. Meanwhile, the lower heat input will cause lower vaporization and accumulation of the liquid at the column base. On the other hand, the liquid level controller of the bottom will affect and the flow rate of the bottom will increase as shown in Figure 13. The heat given to the bottom is shown in Figure 13.

Again, in this example where increasing flow rate upset is applied , we can say that the temperature controller at the bottom of the column may be considered as a secondary controlled variable for the heaviest component. The response in the heaviest component which is also the main product and the temperature of the bottom are shown in Figure 4.13.

The response in the distillate temperature, T_D, and the mole fraction of the component C, $x_{D,C}$ (greatest amount in the feed stream) are shown in Figure 4.14 . As the previous examples, the response in the distilate temperature has strong relation with the condenser temperature which is controlled by the manipulations of the cooling water flow in the condenser. Since the condenser temperature is controlled by a PI controller, the response in the reflux drum temperature is a typical controlled response and oscillatory as shown in Figure 4.14.

EXAMPLE 5

In this example, the process, the flowsheet, technical spesifications of the equipments and the initial conditions are the same with the previous example. The physical properties of the components , the initial steady-state conditions and the technical spesifications of the equipments are as given in Tables A.1, A.2, A.3. The difference in this example is the upset which is given to process. The difference from Example 4, two additional upset are given. The upsets in this example are the followings .

a) The feed flow is increased 5 % by a step change from 45.36 kgmole/hr.

b) The temperature of fresh feed is decreased to 294.3 K from 297.0 K by a step change.

c) The heating liquid temperature which is utilized to heat the reactor is increased to 433.2 K from 427.6 K by a step change.

The various terminal variables are plotted as functions of time in Figures 4.15 to 4.17 .

When the feed flow rate to the reactor increases, the outflow rate of the reactor increases as shown in Figure 4.15 .

Contrary to previous examples, the temperature of reactor in this example initially increases and then returns to its set point as shown in Figure 4.15. This initial increase is due to the upset given to the heating liquid temperature. At the same time, due to the increase in heating liquid temperature, the flow rate of jacket fluid decreases as shown in Figure 4.15. Like in the previous example, the response in the molar fraction of the product, $x_{FR,C}$ decreases due to the decrease in residence time as shown in Figure 4.15. Compared to the previous example, the decrease rate of the concentration of the product is more slow. This is due to the different responses in reactor temperature which will affect the conversion. Cosidering the two examples together, it can be say that, the changes in residence time much more affected the conversion than the temperature changes.

Various terminal variables of the distillation column is shown in Figures 4.16 and 4.17. It can be noted that the response in the variables for the bottom is very

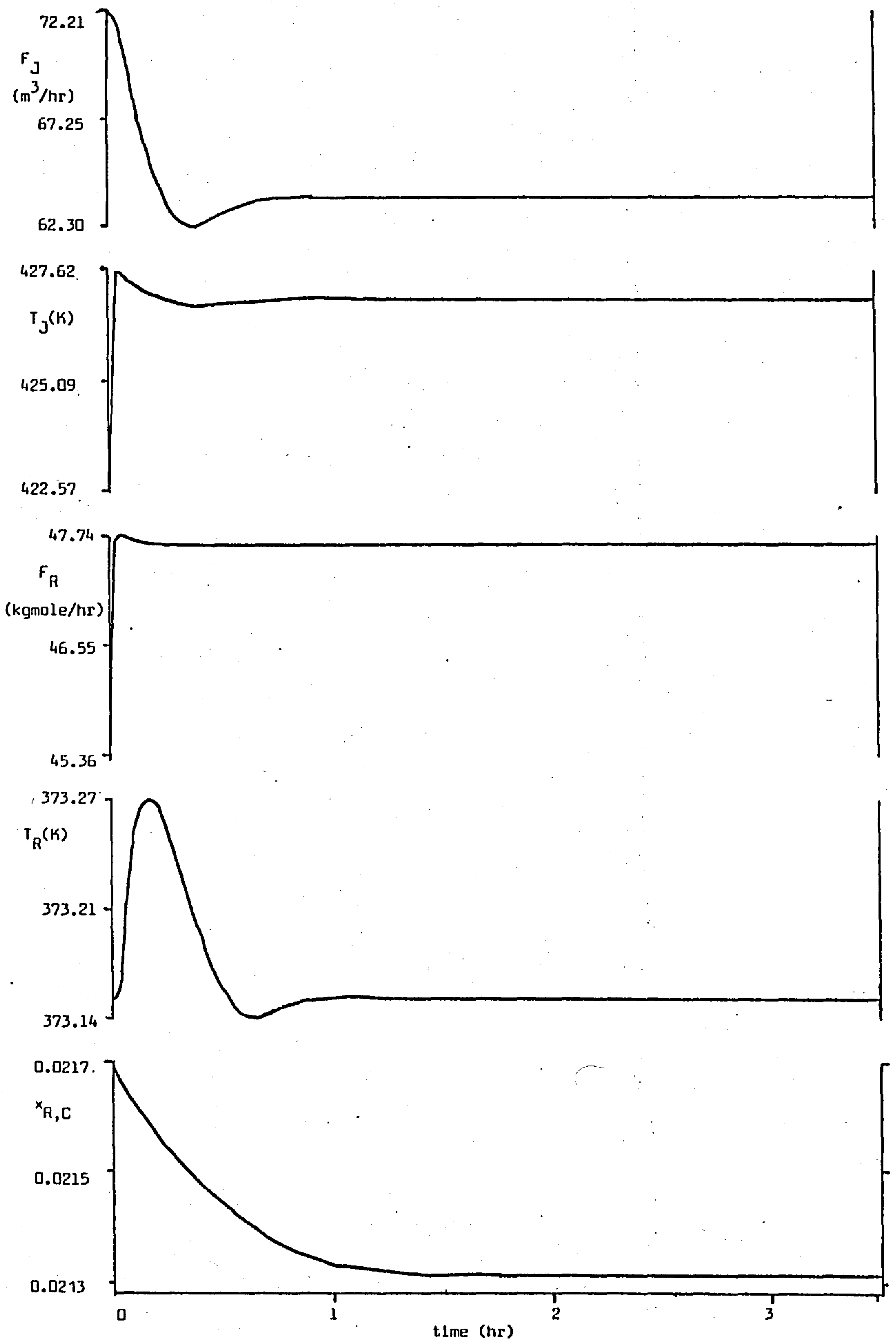


Figure 4.15 Response of the reactor in Example 5

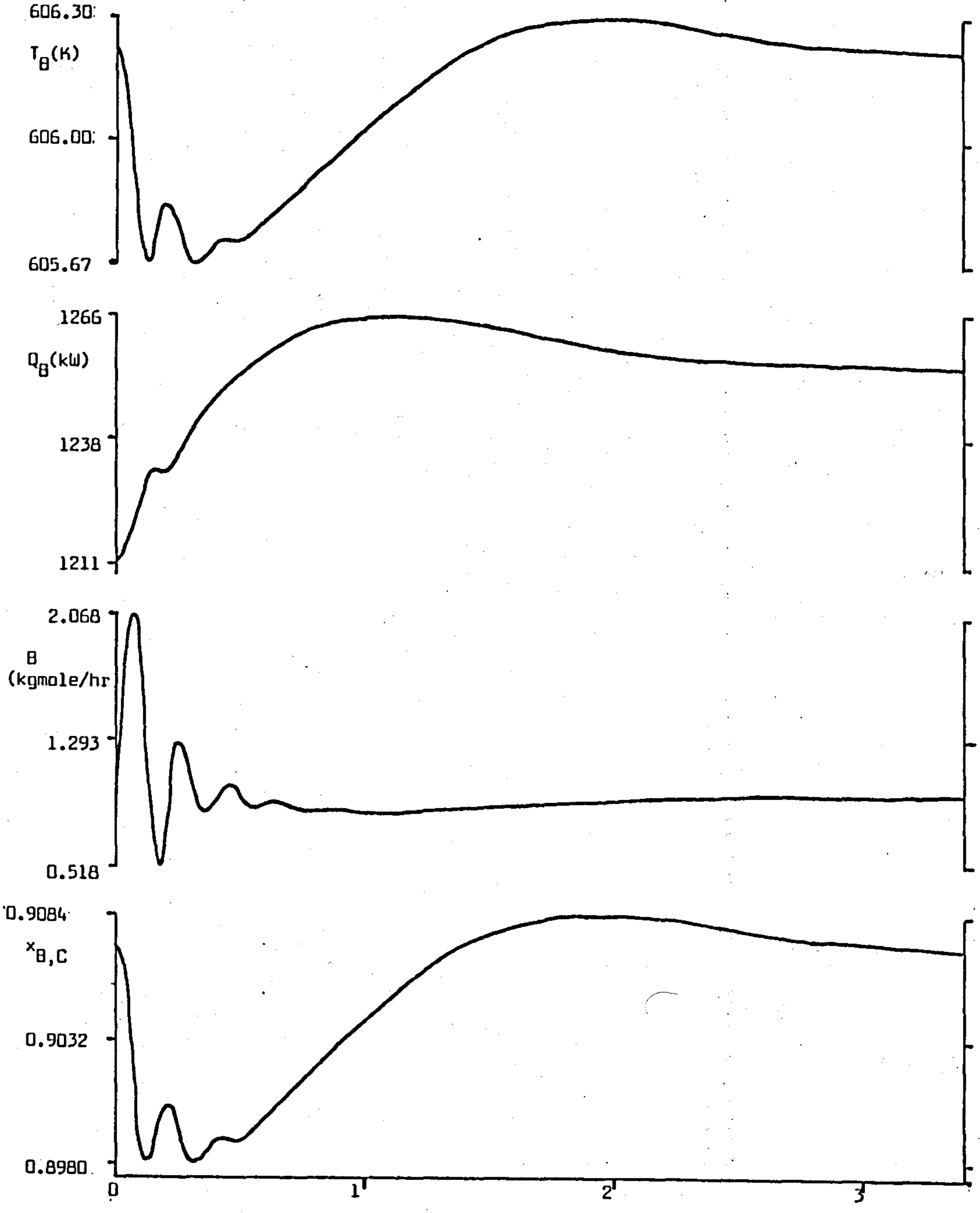


Figure 4.16 Response of the column (bottoms) in Example 5

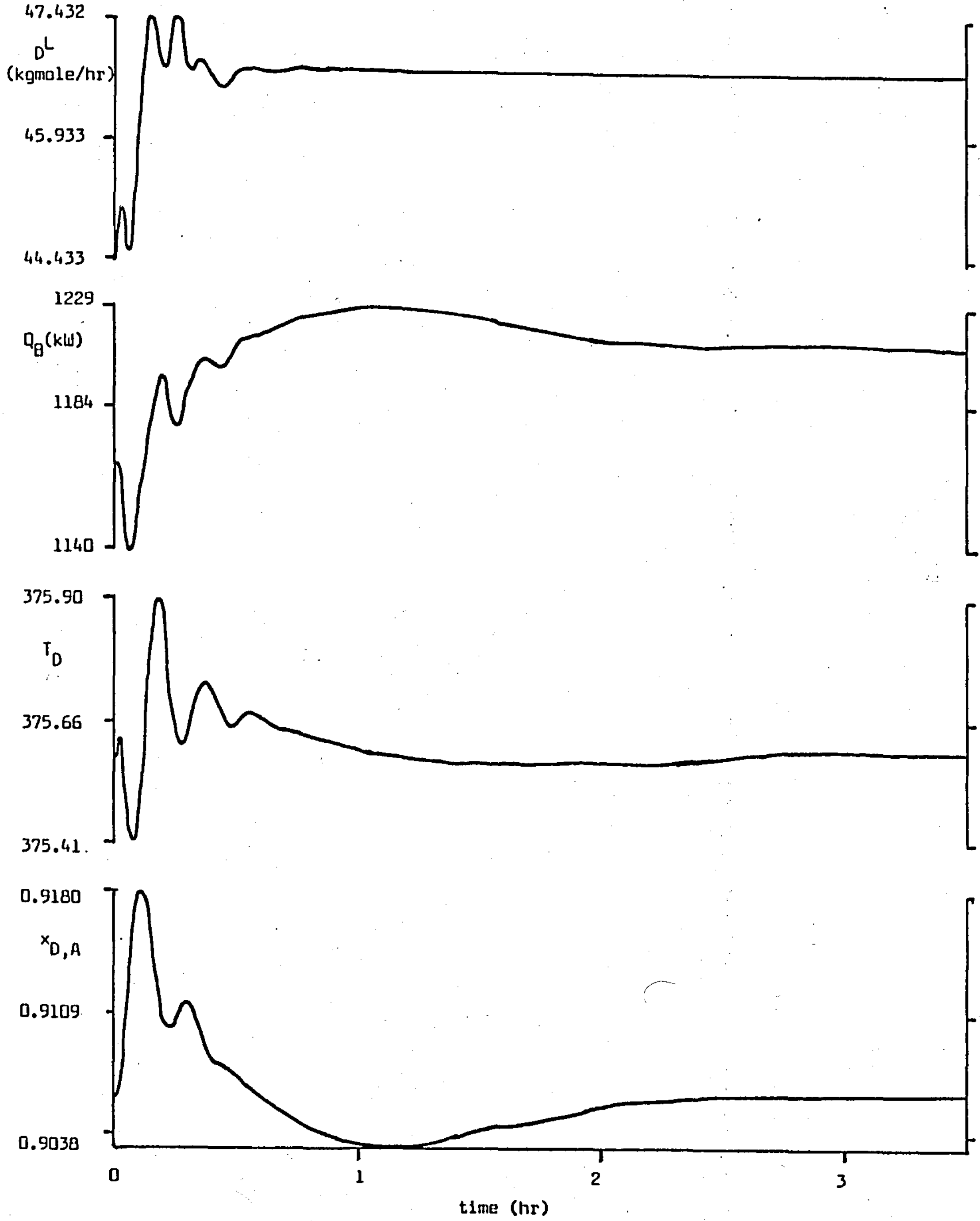


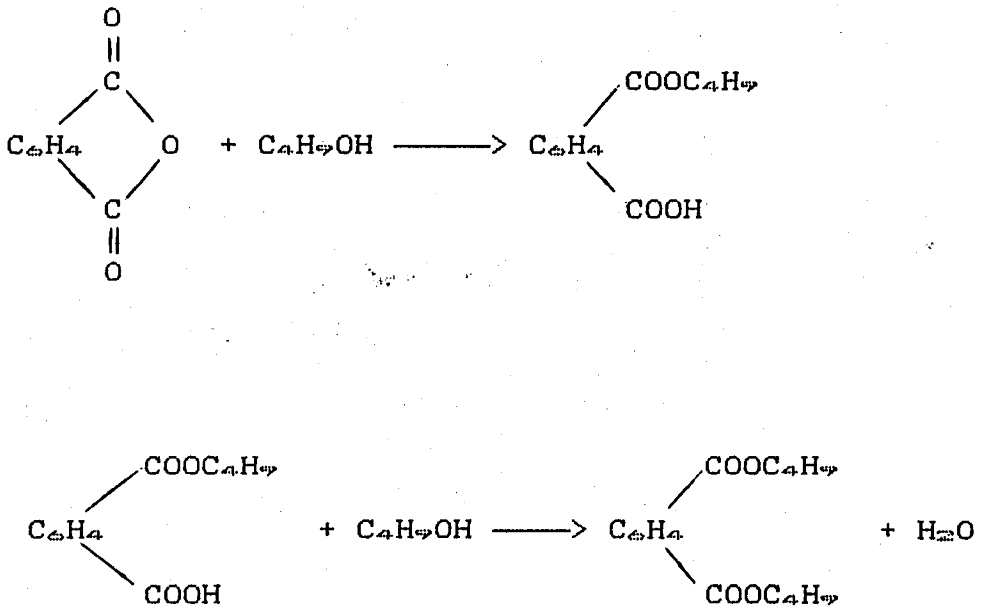
Figure 4.17 Response of the column (distillate) in Example 5

similar to the previous example. On the other hand, the changes at the top of the column is not similar. This is due to the different changes rate in the feed composition which affects the top of the column due to the reflux stream.

4. 2. Simulations of Dibuthyl Phtalate Production : An Industrial Example to a Four Component Systems

In this part, a production process is introduced. The production of di-butyl phthalate under two different process structure and different controller gains are investigated.

The reaction of production of di-butyl phthalate proceeds in two steps. It is reported that [2], the



first step proceeds to completion with ease by heating a mixture of the two components. The esterification of second carboxyl group is much slower, requiring either high temperature or a catalyst [7]. The mechanism and the rate of the esterification reaction is controlled principally by the temperature, the catalyst concentration, and the molar ratio of reactants. It is reported that [2], the reaction of mono- to dibutyl phthalate with excess butanol as solvent had been found to be second order with respect to monoester up to 85 % conversion at temperature range 80° to 150 °C.

EXAMPLE 6

In this example, the flowsheet which is simulated is shown in Figure 4.1. The continuous stirred tank reactor and the distillation column are the processing units.

General description of the process is as follows.

A mixture stream which contains buthyl alcohol and phtalic anhydride with the molar ratio of 10.02:1 at initial steady state is pumped to the continuous stirred tank reactor to produce dibuthyl pthalate. The set point for the volume of the reactor is 2.83 m^3. The volume is controlled by a PI controller. The reaction taking place in the reactor;

2 Buthyl alcohol + Phthalic anhydride ——> Di-buthyl pthalate + Water

is second order with respect to pthalic anhydride. Reaction is sligthly exothermic. Since the energy which is produced by the recaction is inadequate to supply the reaction temperature in the continuous reactor, the reactor must be heated. This is provided by the jacket heater. Temperature in the reactor is controlled by a PI controller which manipulate the flow rate of heating liquid (Downtherm A). The set point for the reaction temperature is 374.8 K. The reactor effluent is pumped into the distillation column. The column has ten trays (with Murphree vapor phase efficiencies of 68 % for the stripping section, and of 76 % for the rectifiying section). The diameter of the column is 1.83 m. and the weir of each tray is 1.22 m. The weir heights in the stripping and rectifiying sections are 3.18 cm. and 4.45 cm. respectively. The liquid feed enters the column from the fifth stage. The bottoms temperature of the column is controlled at 605.4 K which is close to boiling point of the dibuthyl phthalate (heaviest component), by a PID conroller which manipulates the flow rate of heating liquid. The set point for the bottoms level controller is 0.5 m^3. and the reflux drum level controller is 0.28 m^3. These conrollers has only proportional action. The condenser subcools the vapor leaving the top tray of the column and the set point for the temperature of subcooled liquid leaving the condenser is 374.8 K. A PI controller is used to manipulate the flow rate of condenser water.

The product of the process is the bottom stream of the distillation column which contains 95.19 % di-buthyl pthalate and 4.81 % pthalic anhydride at initial steady state. The distillate stream which is rich in butanol, contains 90.55 % butanol, 6.71 % pthalic anhydride and 2.74 % water.

The physical properties of the components , the initial steady-state conditions and the technical spesifications of the equipments are given in Tables A.6, A.7, A.8.

In this example, the upset given to process is 5 % step deacrese in feed flow rate to the reactor from 45.36 kgmole/hr.

When the feed flow rate to the reactor decreases, the output flow of the reactor decreases as shown in Figure 4.18 . It can be noted that, although the feed flow rates are 45.36 and 43.09 kgmole/hr. at two steady-state the outflow rates are lower than these values. This is due to the reaction type which is un-equimolar.

When the feed flow rate decreases, the reactor temperature, T_{RC}, initially increases and the return to its set value is as shown in Figure 4.19 . The initial increase in the reactor temperature is due to the increase in residence time in the reactor which will cause higher conversion and hence higher heat generation due to the exothermic reaction. The temperature controller of the reactor manipulates the flow of heating liquid in the reactor jacket. When the reactor temperature increases, the flow of heating liquid decreases. The changes in the jacket flow, F_J, and the jacket temperature, T_J, are shown in Figure 4.18 . The

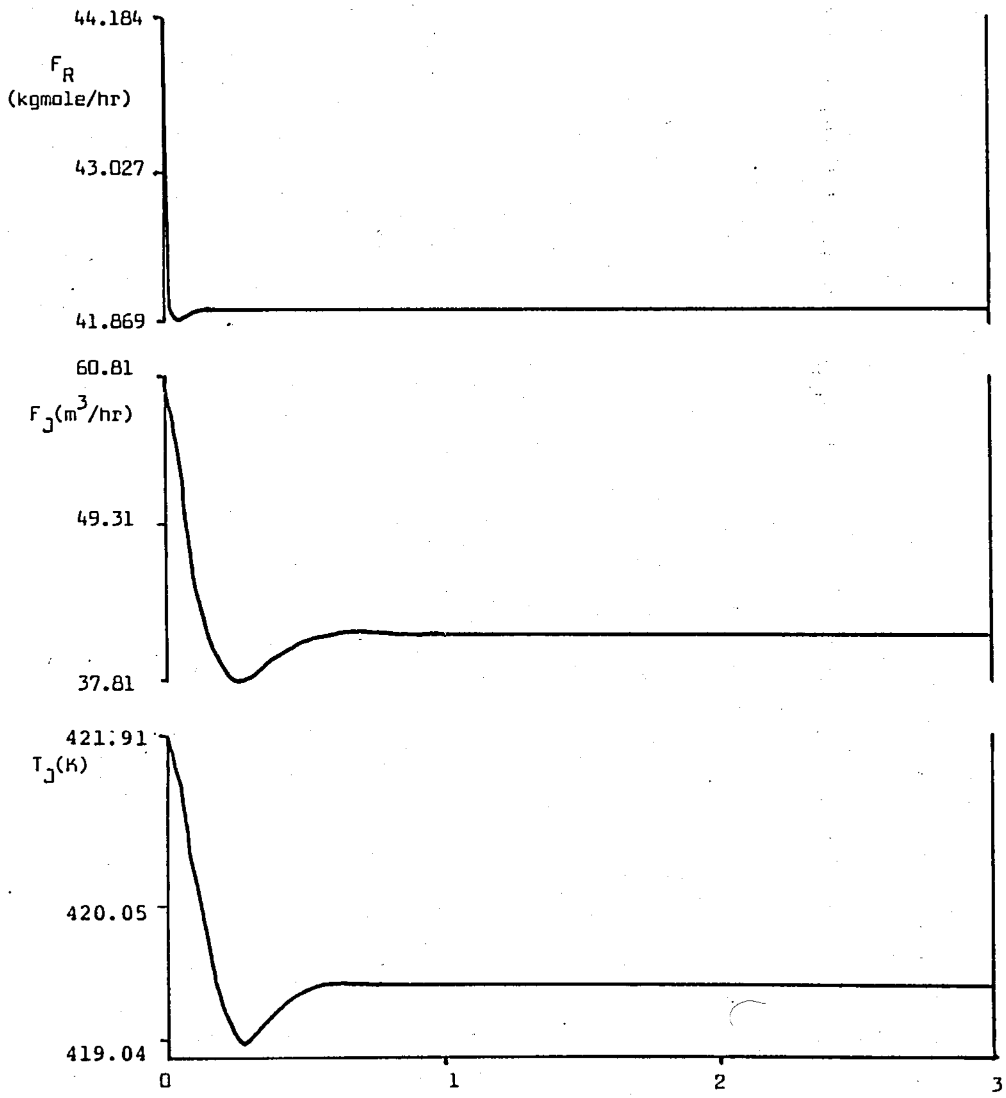


Figure 4.18 Response of the reactor (flows and jacket temperature) in Example 6

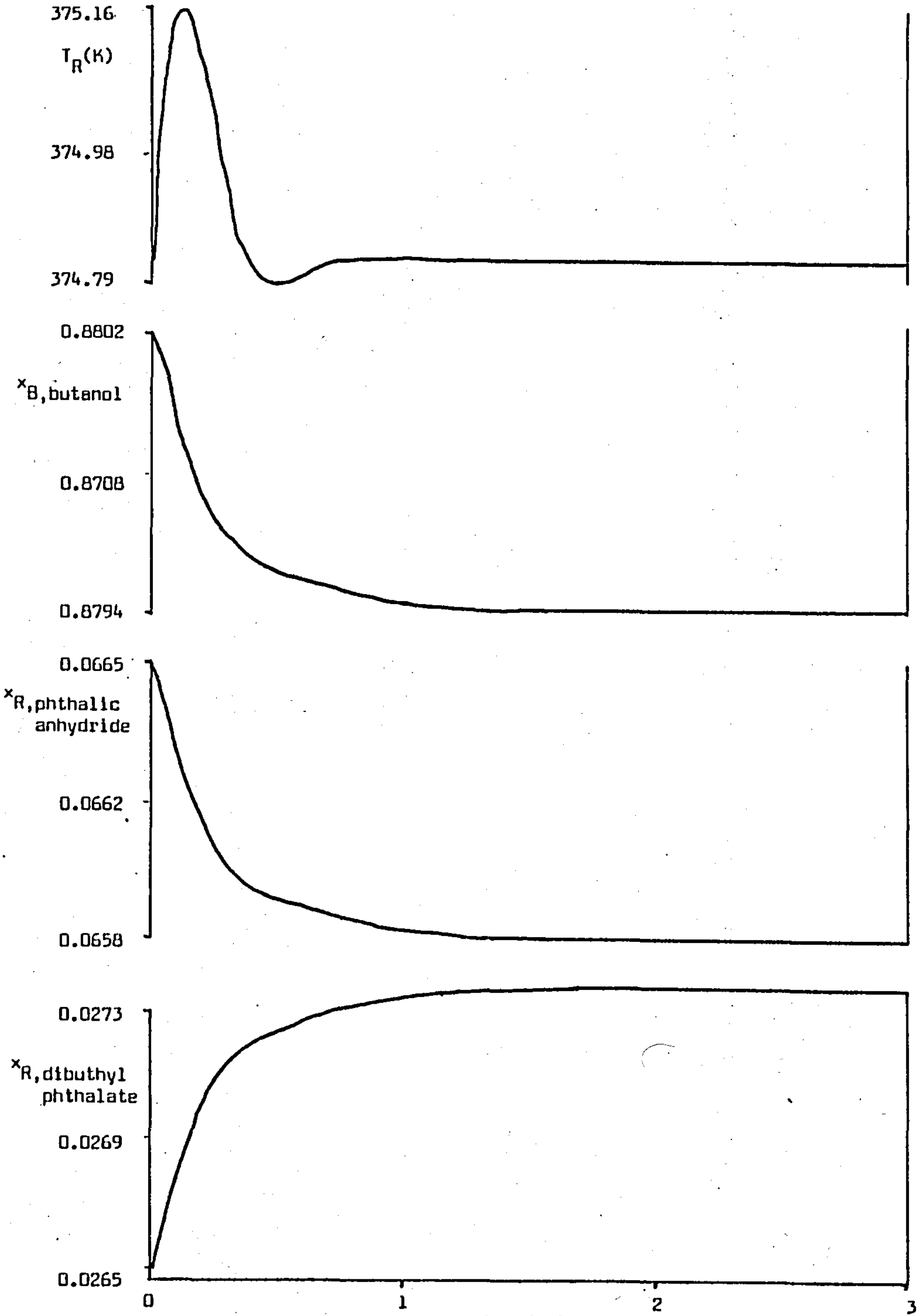


Figure 4.19 Response of the reactor (temperature and compositions) in Example 6

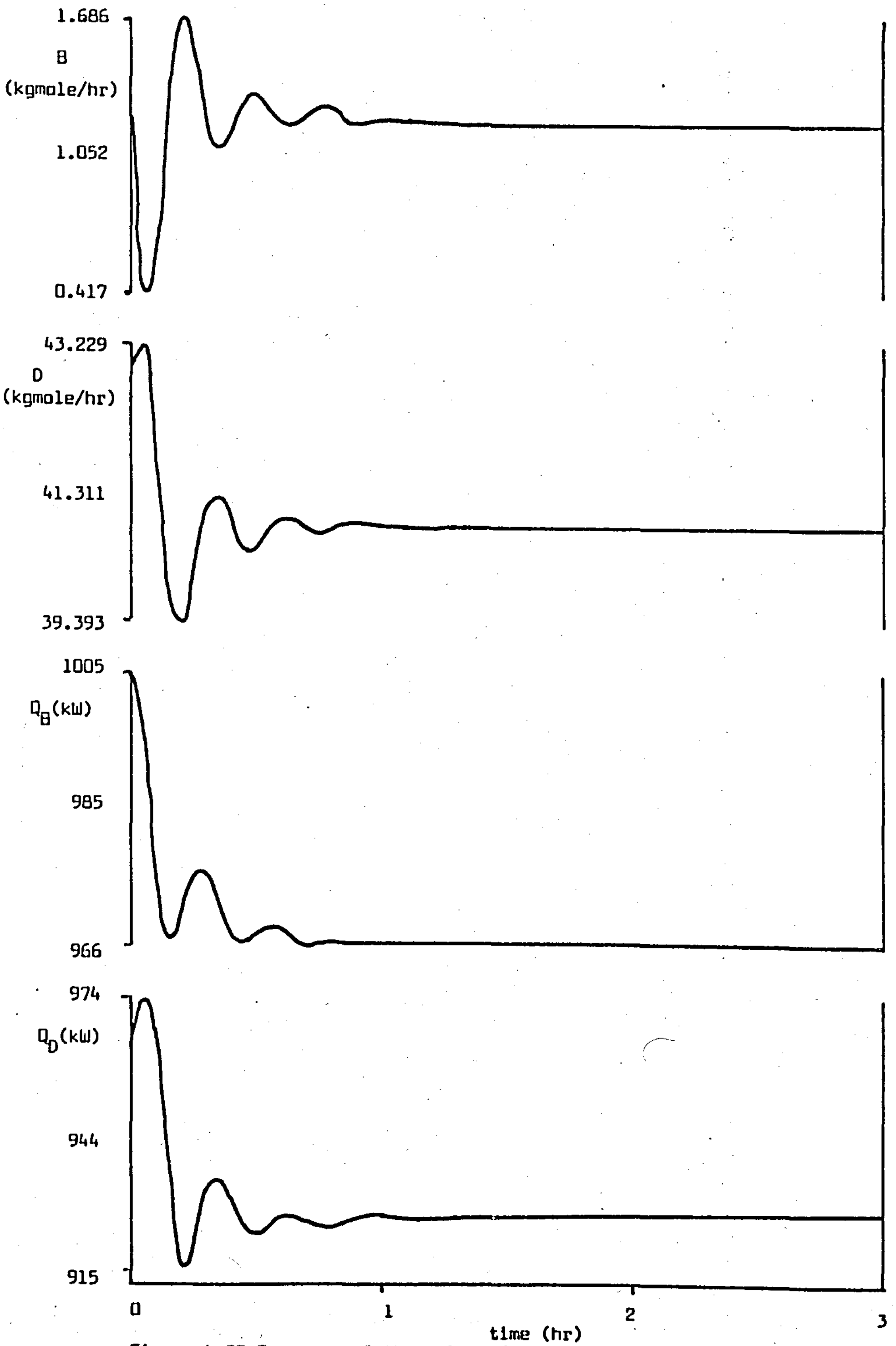


Figure 4.20 Response of the column (flows) in Example 6

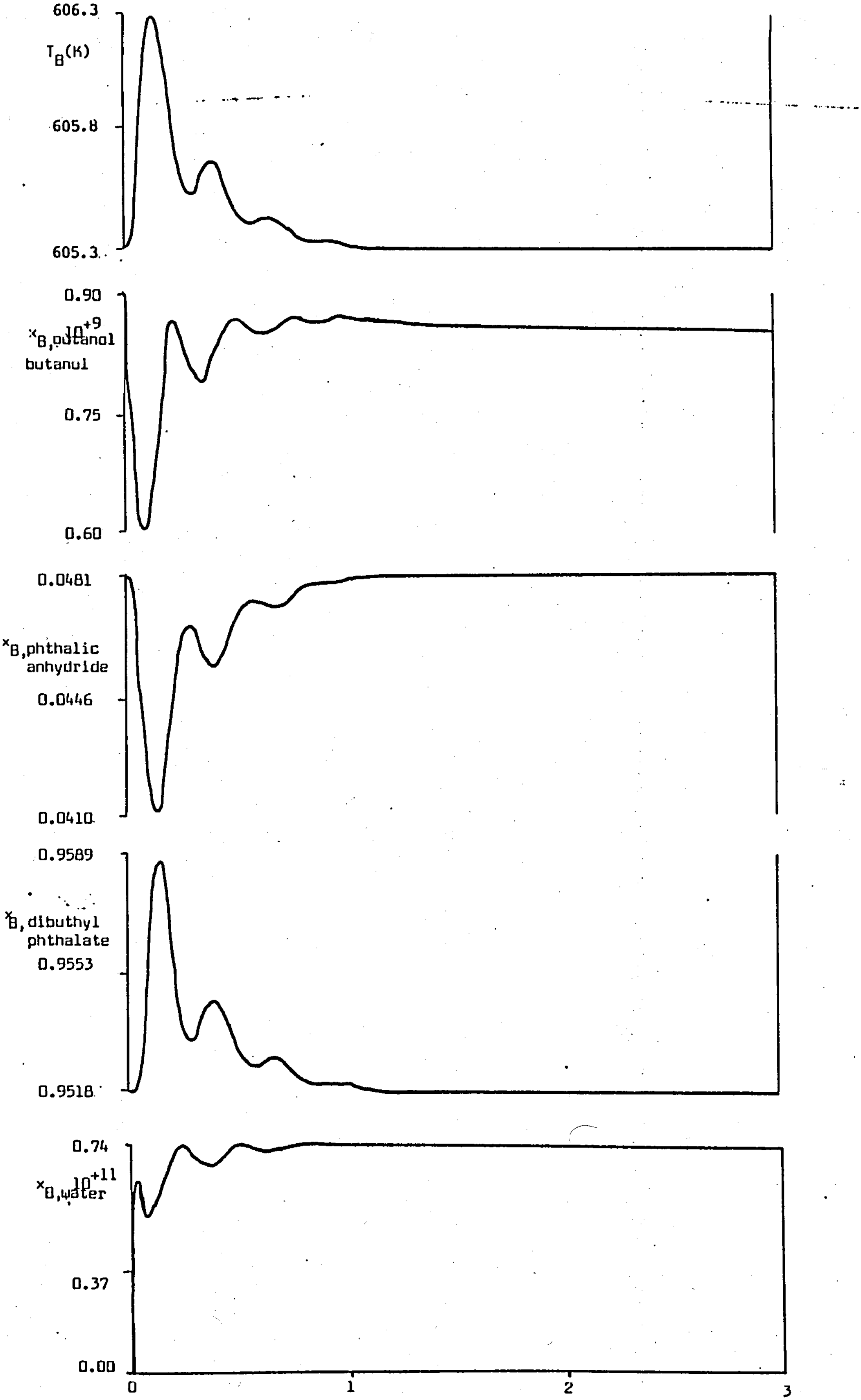


Figure 4.21 Response of the column (bottoms temperature and compositions) in Example 6

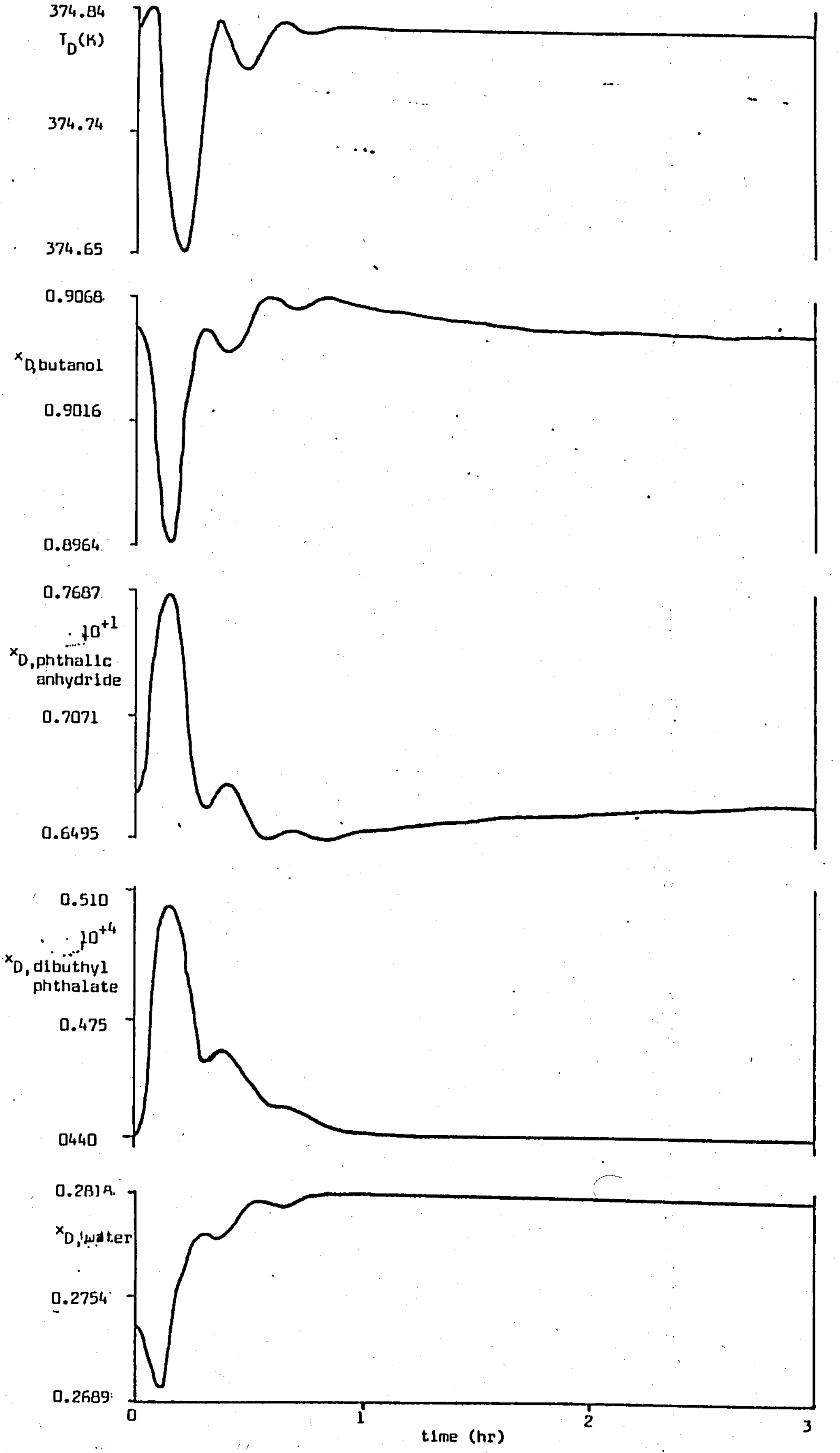


Figure 4.22 Response of the column (distillate temperature and composition) in Example 6

changes in the reactor temperature and the jacket tempearture give an indication of heat transfer between the reactor and the jacket.

When the feed flow rate decreases, due to the increase in residence time, the molar fraction of reactants will decrease and molar fraction of products will decrease as shown in Figure 4.19 .

The changes in the variables of the distillation column are primarily due to the changes in feed flow rate and the composition. When the feed flow rate decreases, the flow rate of distillate decraeses with oscillation as shown in Figure 4.22 . When the flow rate decreases, the inventories of the column start to decrease. Since the liquid rate from the first tray to the column base will decrease, the steam flow will be more than the required amount at steady-state. Since the flow of steam is manipulated by the bottoms temperature controller, it will take some time for the steam flow to decrease. Meanwhile, the excess heat input will cause excessive vaporization and loss of liquid at the base. The bottom flow rate and the heat given to the bottom is as shown in Figure 4.20. The excess heat input will cause an initial increase in the bottoms temperature. The bottom temperature then decreases with oscillation as shown in Figure 4.21.

The mole fractions of the components at bottom are shown in Figure 4.21. It can be noted that the response of the mole fraction of the heaviest component (di-buthyl phtalate) follows the bottoms temperature. Again, this conclusion justify that temperature can be used as secondary control variable at the bottom of the column when the main product is heaviest component.

The response in the distillate temperature, T_D, and the mole fractions of components in the distillate stream are shown in Figure 4.22. The response in the distillate temperature has strong relation with the condenser temperature which is controlled by the manipulations of the cooling water flow in the condenser. Since the condenser temperature is controlled by a PI controller the response in the reflux drum temperature is a typical controlled response and oscillatory.

From the plots it can be seen that all variables reach their new steady-state conditions in almost 2 hours of operation after the upset.

EXAMPLE 7

In this example, the continuous stirred tank and the distillation column are the processing units. The flowsheet is the same in Figure 4.1 and the process is the same in Example 6.

The physical properties of the components , the initial steady-state conditions and the technical spesifications of the equipments are as given in Tables A.6, A.7, A.8.

In this example, the upset given is in the feed composition to the reactor. The molar ratio of butanol to pthalic anhydride, (B/P), is decreased from 10.02 to 9.00. (molar fraction of phthalic anhydride is increased from 0.09074 to 0.1).

The various terminal variables are plotted as functions of time and shown from Figure 4.23 to Figure 4.27 .

After the step change is given, the reaction rate constant which is related to the (B/P) ratio, is affected and the reaction rate decreased at first. Since the reaction is exothermic, decrease in reaction rate will cause decrease in reactor temperature at this step. The temperature controller actuates the reactor by manipulating the heating liquid flow rate in order to keep reaction temperature constant. The changes in the flow rate of the heating liquid in the reactor jacket, F_J, and in the jacket temperature, T_J, are shown in Figures 4.24.

Since the molecular model of the reaction is in the form; $2\ A + B \longrightarrow C + D$, the molar feed rate to the

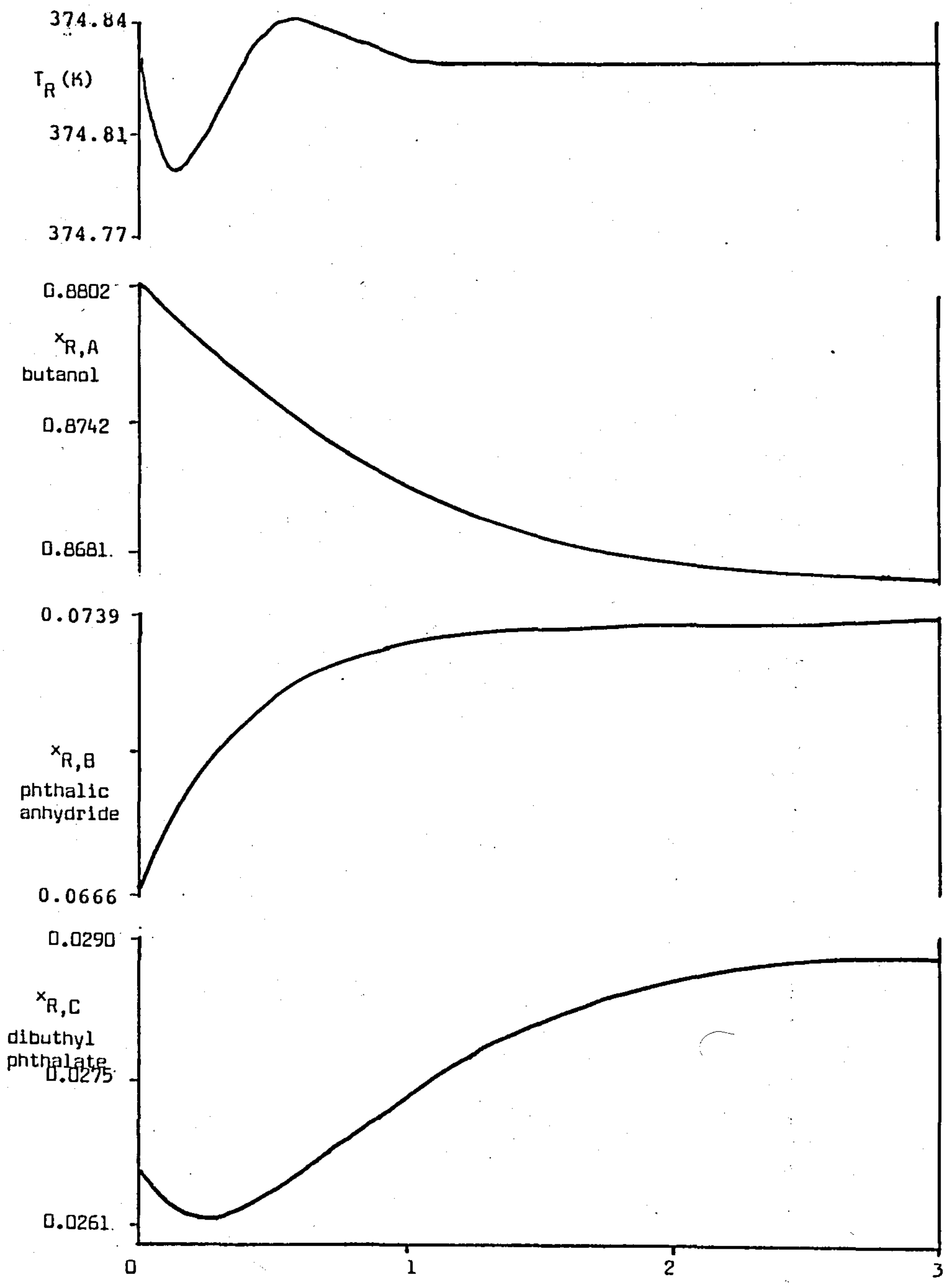


Figure 4.23Response of the reactor (temperature and composition)in Example 7

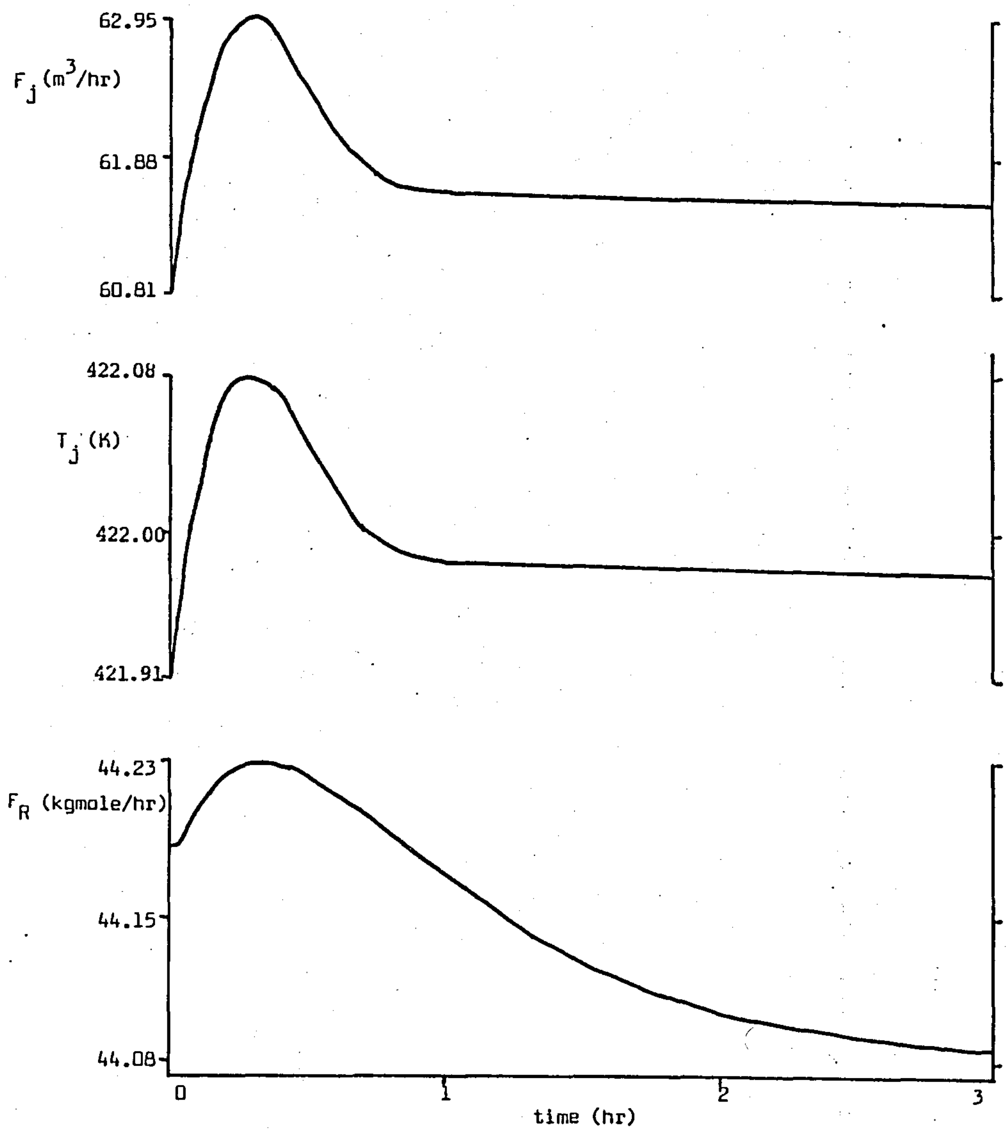


Figure 4.24 Response of the reactor (flows and jacket temperature)in Example 7

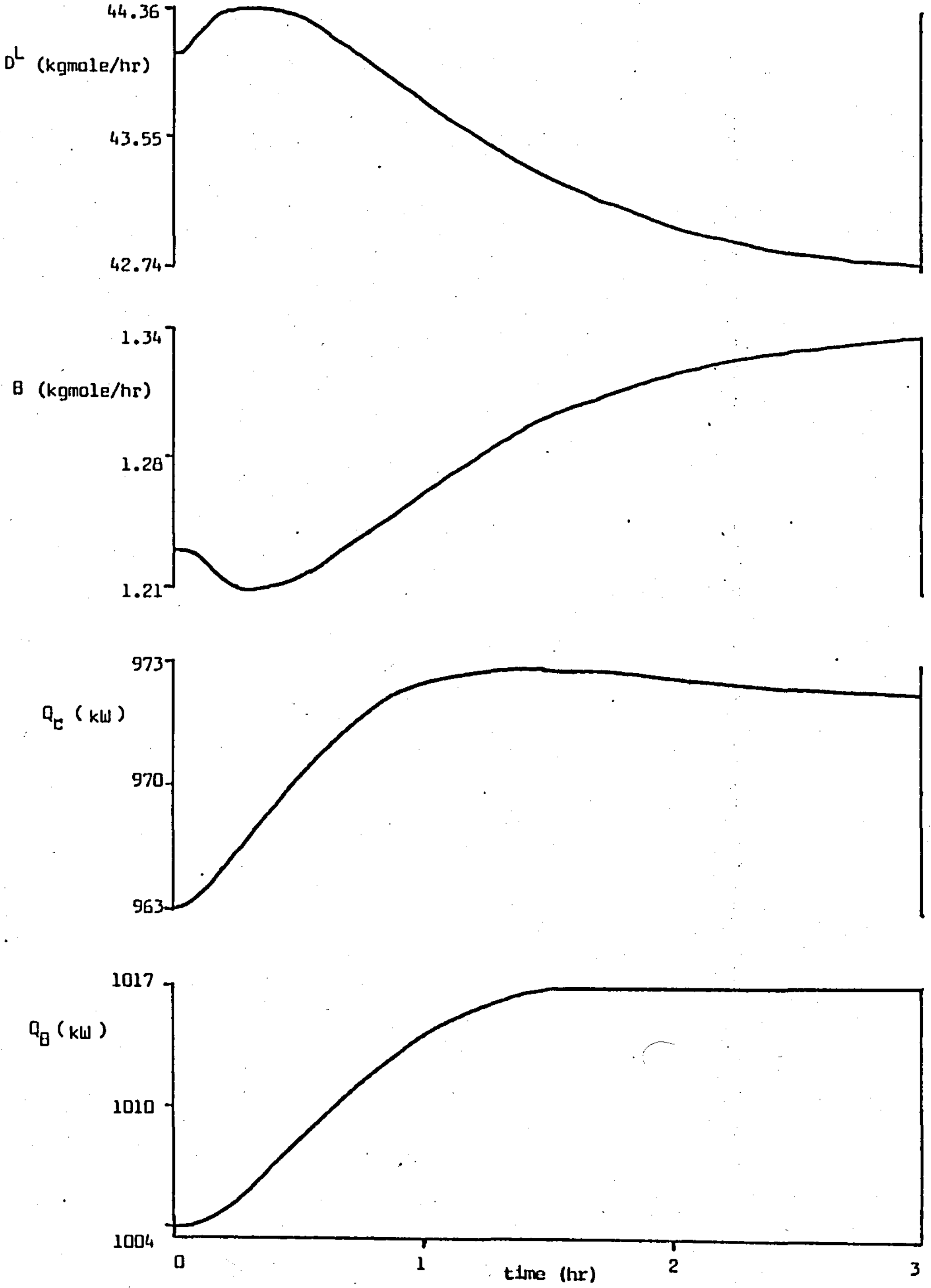


Figure 4.25 Response of the column (flows and heats) in Example 7

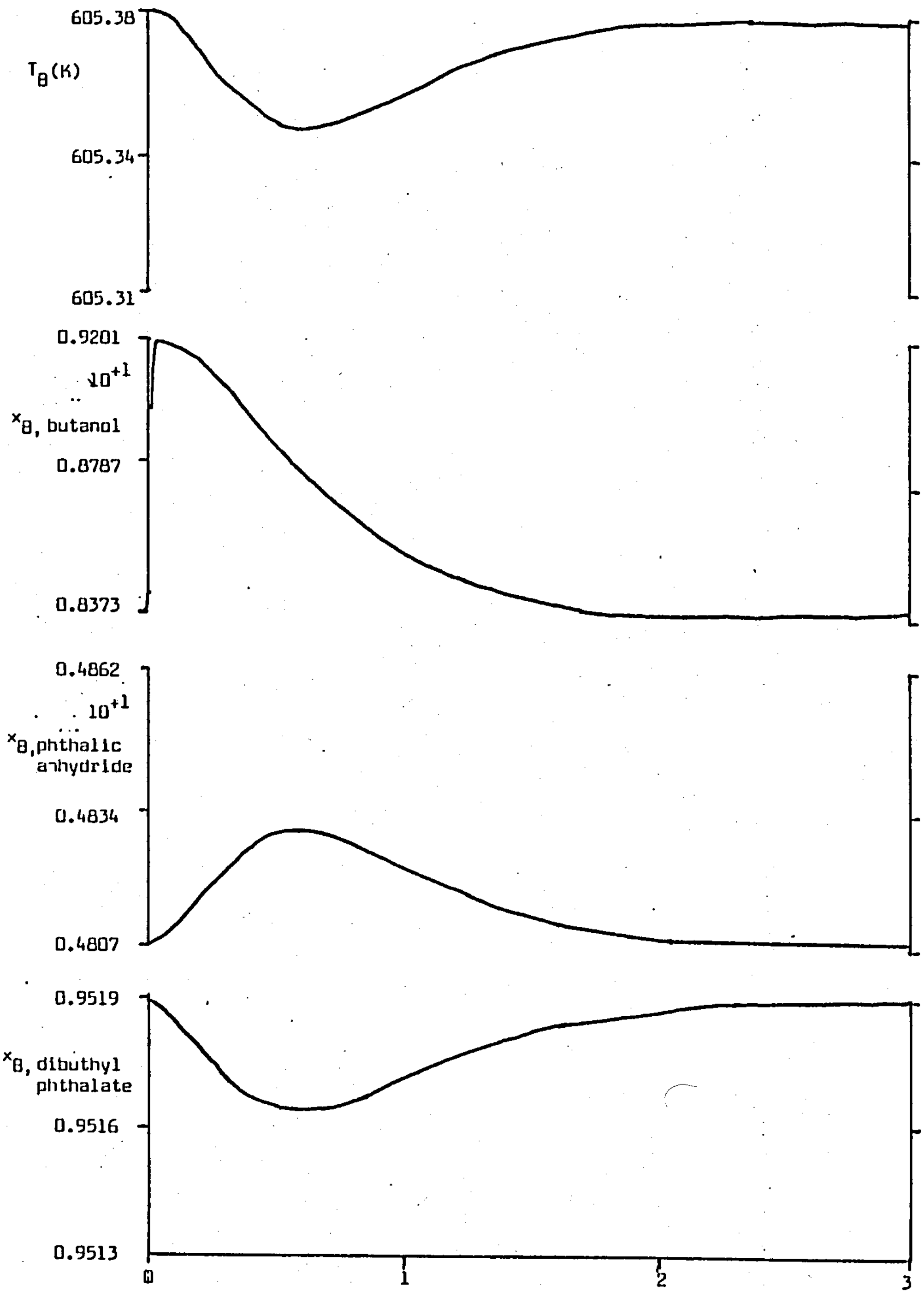


Figure 4.26 Response of the column (bottoms temperature and compositions) in Example 7

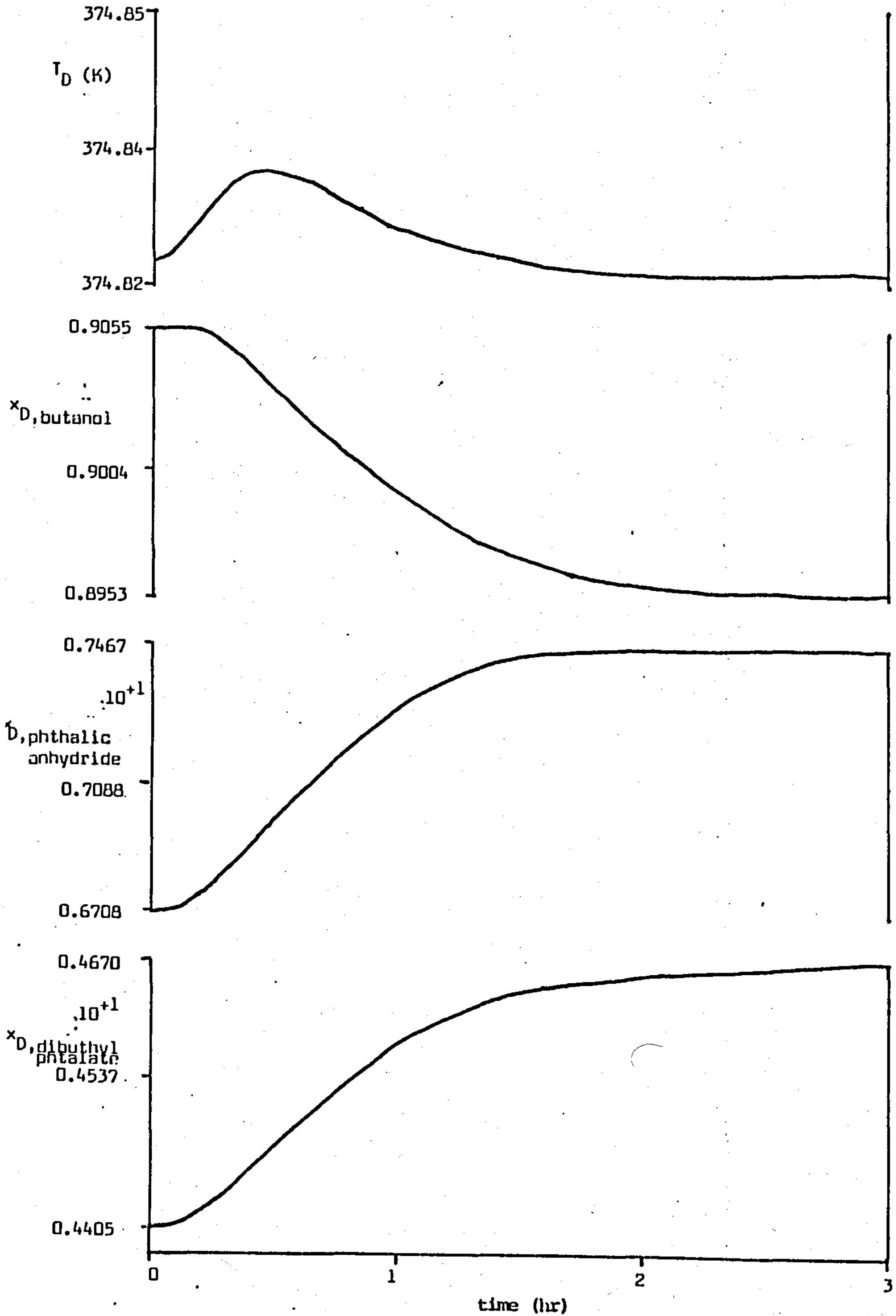


Figure 4.27 Response of the column (distillate temperature and compositional) in Example 7.

reactor is greater than the molar outflow rate which is proportional to the reaction rate. The reaction rate decrease causes the lower conversion and the outflow rate increases as can be seen in Figure 4.23.

It was discussed earlier that the initial decrease in the reaction rate constant due to the step change in the composition of the feed flow was affected the reactor at first. On the other hand, increase in the mole fraction of pthalic anhydride in the reactor will affect the system and the reaction rate will start to increase finally. At this step, outflow rate will decrease due to the increasing conversion until the new steady-state condition is reached.

The terminal variables of the reactor are ; reactor temperature, T_R, flow rate of heating liquid in the jacket, F_J, jacket temperature, T_J, molar fraction of components and the outflow rate of the reactor can be seen from Figure 4.23 to Figure 4.24 . As can be seen in Figure 4.23 , the behavoir of reactor temperature, T_R, is a typical controlled response and oscillatory.

The operation of the column is primarily affected by the composition and the flow rate distribution. At first step, when the feed flow rate increases, distillate stream, D^L, increases as shown in Figure 4.25. The change in flow rate of distillate stream are similar to the change in the flow rate. However, the response in the flow rate of the bottom stream is different due to the excessive boil-up rate. After upset, the feed flow rate increases at first and the column inventories begin to increse. At the same time, mole fraction of phthalic anhyride will increase in the trays troughout the equilibrium relationships. This will cause excessive vaporization at the column base and the bottom product will decresae. The mole fraction of phthalic anhydride is much more from the initial steady-state and to the heat of vaporization of this new mixture in the bottom, temperature will decrease. Meanwhile, since the heating liquid is manipulated by the bottom temperature controller, it will take some time for the heating liquid flow to increase. When the outflow rate from the reactor to the column begin to decrease, and the fraction of dibuthyl pthalate begins to increase, the bottom product begin to increase and the distillate stream decreases. Figure 4.25. As can be seen, dibuthyl phtalate (heaviest component) follows the bottoms temperature. This justifies that the use of bottoms temperature to be selected as the secondary controlled variable to infer for the controlled composition. (Figure 4.26).

The response in the distillate temperature and the mole fractions of light components are shown in Figure 4.27.

In this example, after a given upset, all the variables reach their new steady-state conditions nearly in 3.0 hours.

EXAMPLE 8

In this example, the equipments and the flowsheet is the same as in Example 7. Flowsheet is shown in Figure 4.1. Technical spesifications of the process, reaction in the reactor, and the initial conditions for the simulation are the same in Example 7. Step change which is given to the reactor is also the same. The only difference in this example from previous example is in the gains of the controllers of the reactor and of the distillation column.

In the reactor, the temperature and level controller gains are decreased. Also in the distillation column, for the distillate and bottoms, the temperature and level controllers are set for low gains.

The physical properties of the components, the initial conditions and the technical spesifications of the process are as given in Tables A.6, A.9, A.10.

The various terminal variables as functions of time are plotted in Figures 4.28 and 4.32.

In this example, PI type controller is used to manipulate the flow of heating liquid in the reactor jacket, contrary to the previous example where a PID type controller was used. Additionaly, controller gain for

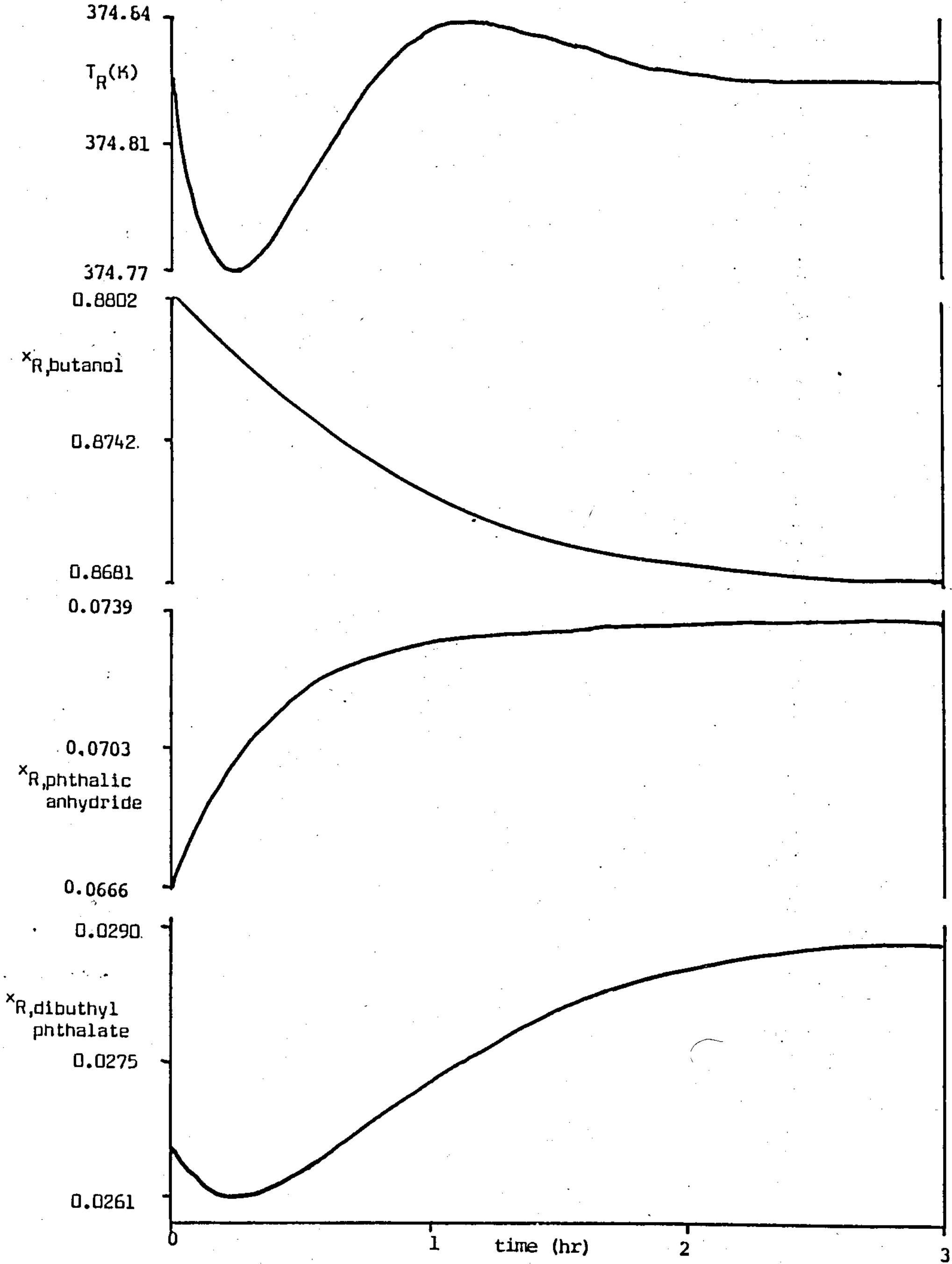


Figure 4.28 Response of the reactor in Example 8

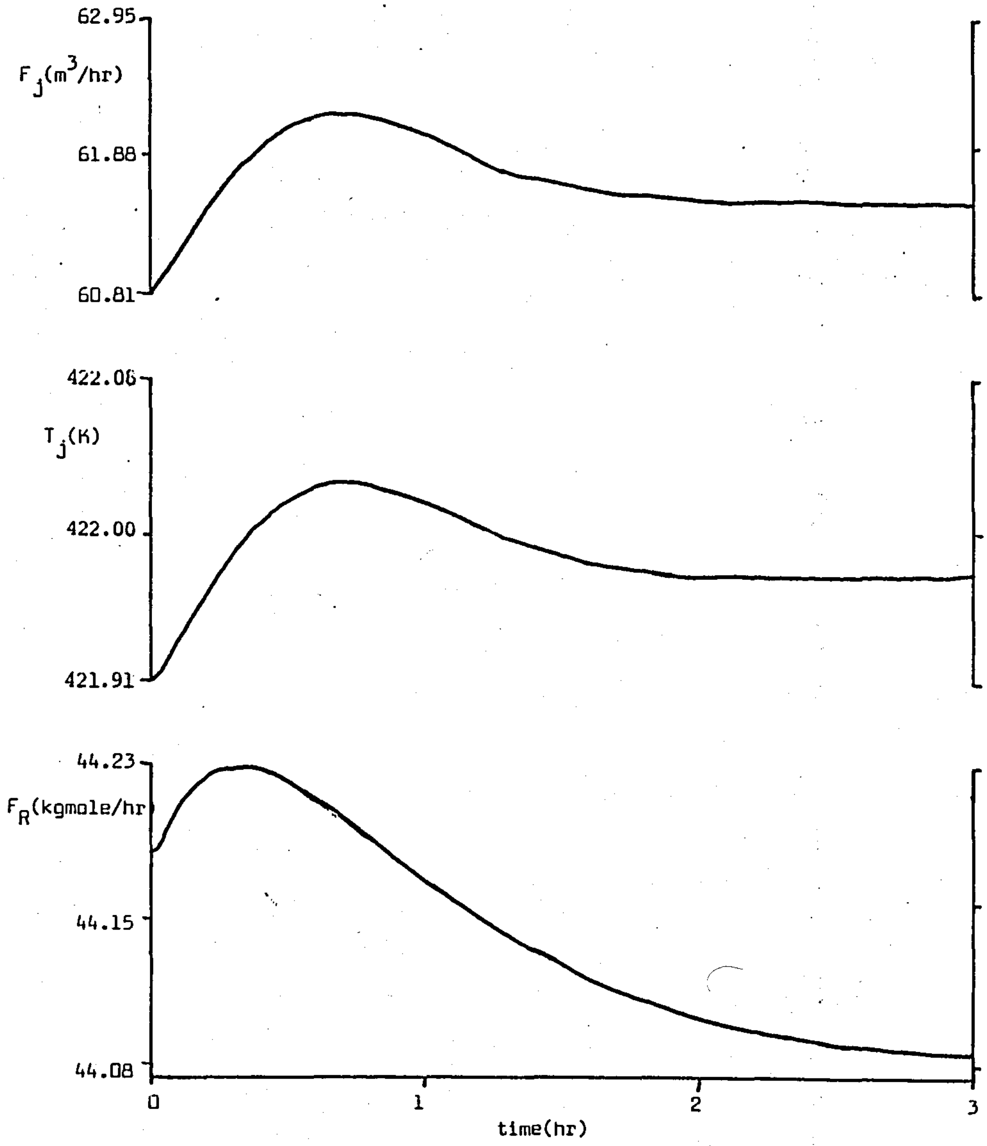


Figure 4.29 Response of the reactor (flows and jacket temperature) in Example 8

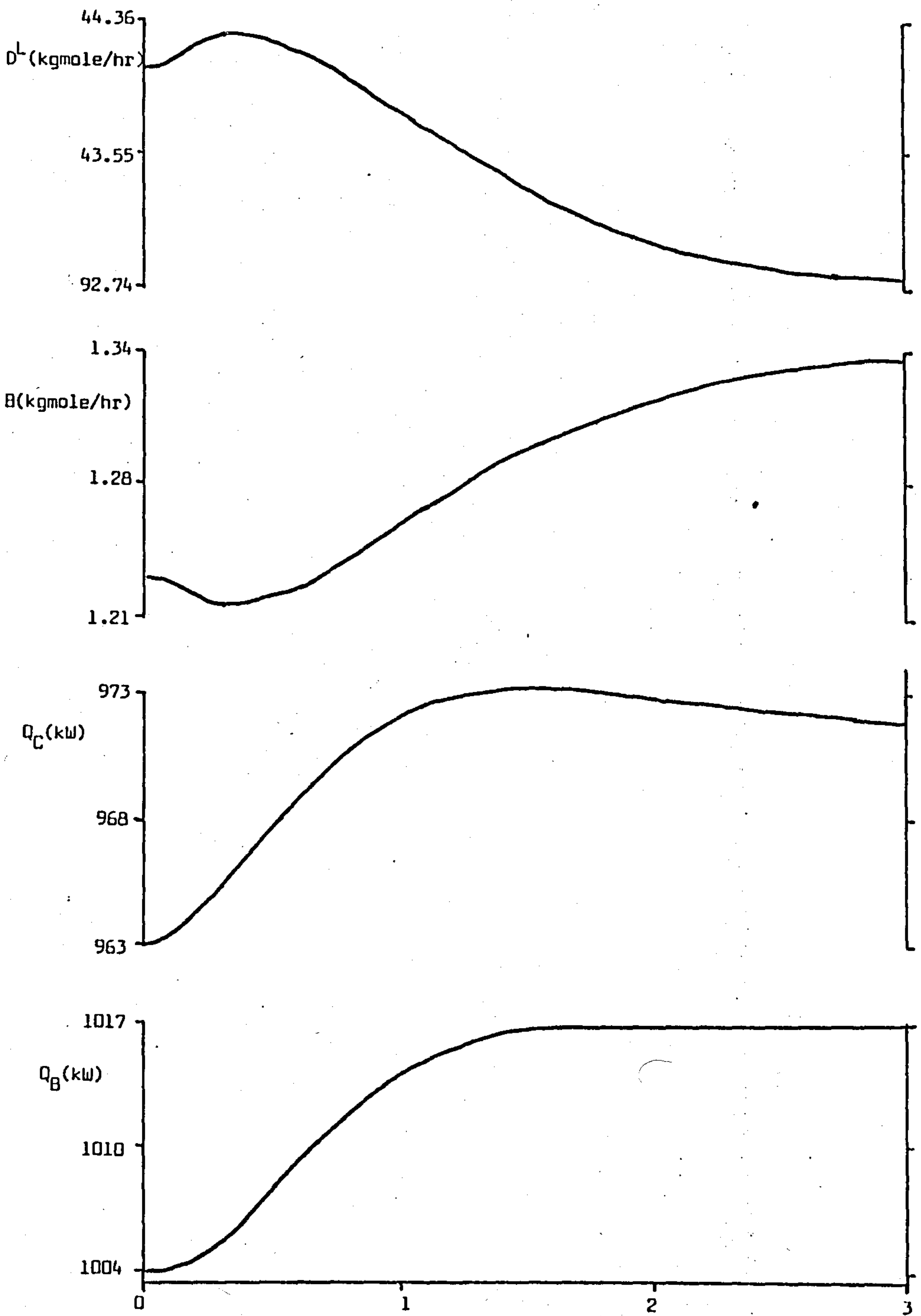


Figure 4.30 Response of the column (flows, and heat) in Example 8

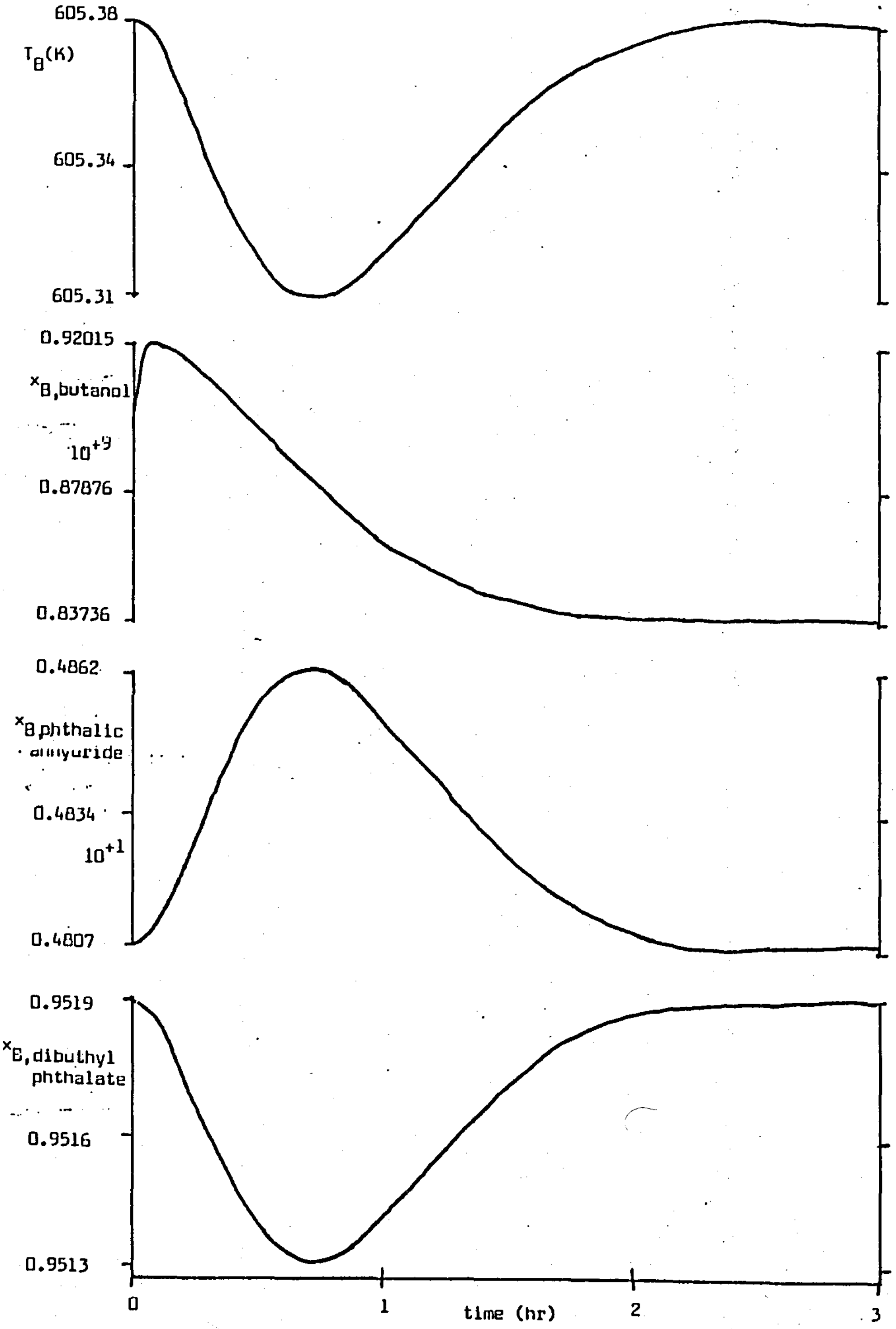


Figure 4.31 Response of the column (bottoms temperature and compositions) in Example 8

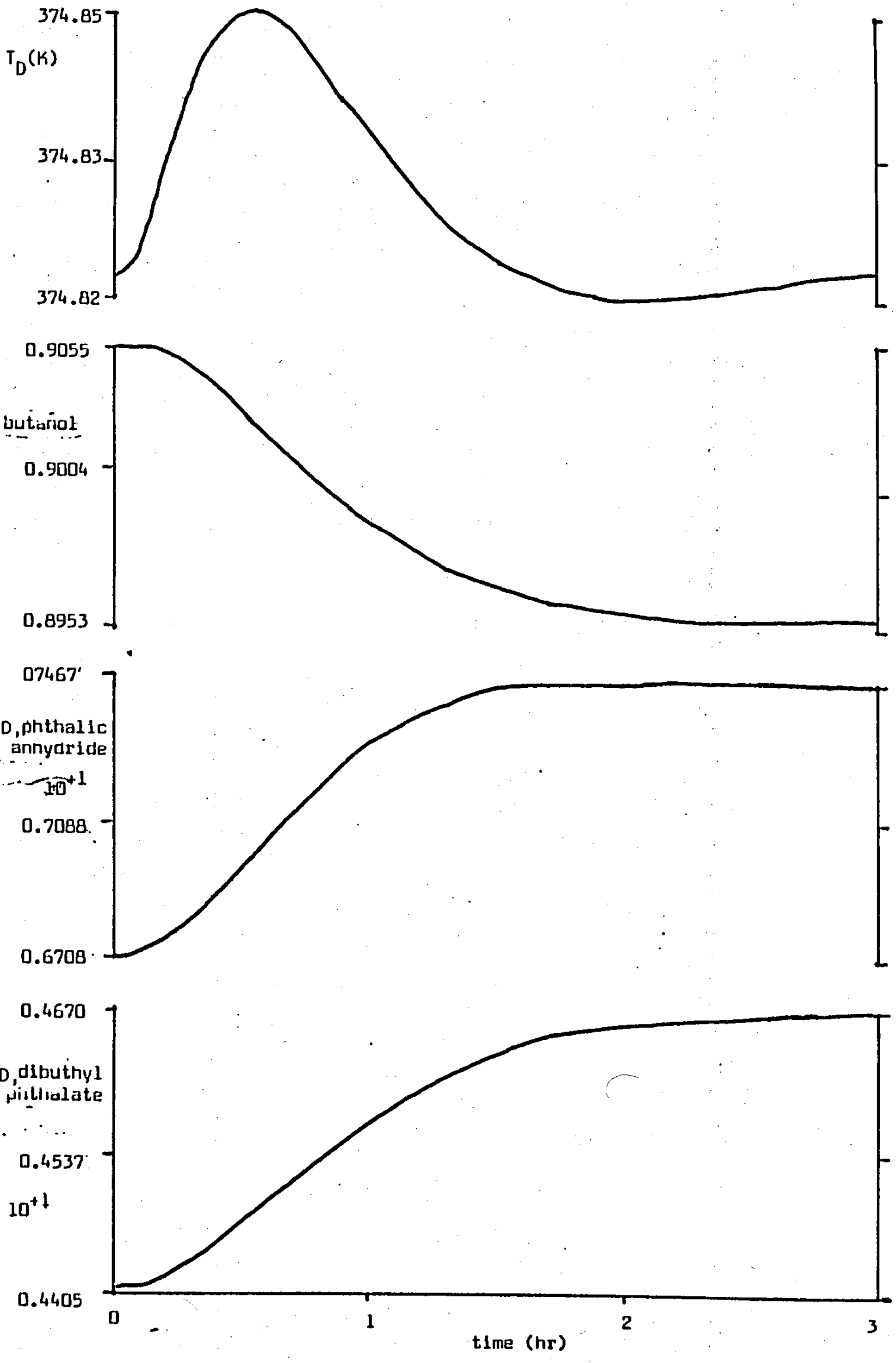


Figure 4.32 Response of the column (distillate temperature and compositions) in Example 8

jacket is decreased. As can be seen in the response of heating liquid flowrate, Figure 4.28 , rise time increases and overshoot decreases according to the previous example as expected. The controlled variable, temperature remains constant nearly 2 hours after from upset. In the previous example, this time was 1 hour. On the other hand, the responses of the outflow rate of the reactor and the effluent concentrations of the components are nearly the same as in the previous example. From this point of the view, it can be stated that reactor is primarily affected by the concentration changes, and it is not affected by temperature fluctuations which are very small due to low heat generation of the reaction.

For the column, the flow rate of bottoms and distillate are shown in Figure 4.30. Temperatures and concentrations in bottoms and distilate are shown in Figures 4.31 and 4.32. As can be seen from the graphs, the response of the concentration of phthalic anhydride follows the bottoms temperature and the low temperature controller gain affected the product quality.

EXAMPLE 9

In this example, the flowsheet which is simulated is shown in Figure 4.33. The continuous stirred tank reactor and the distillation column are major processing

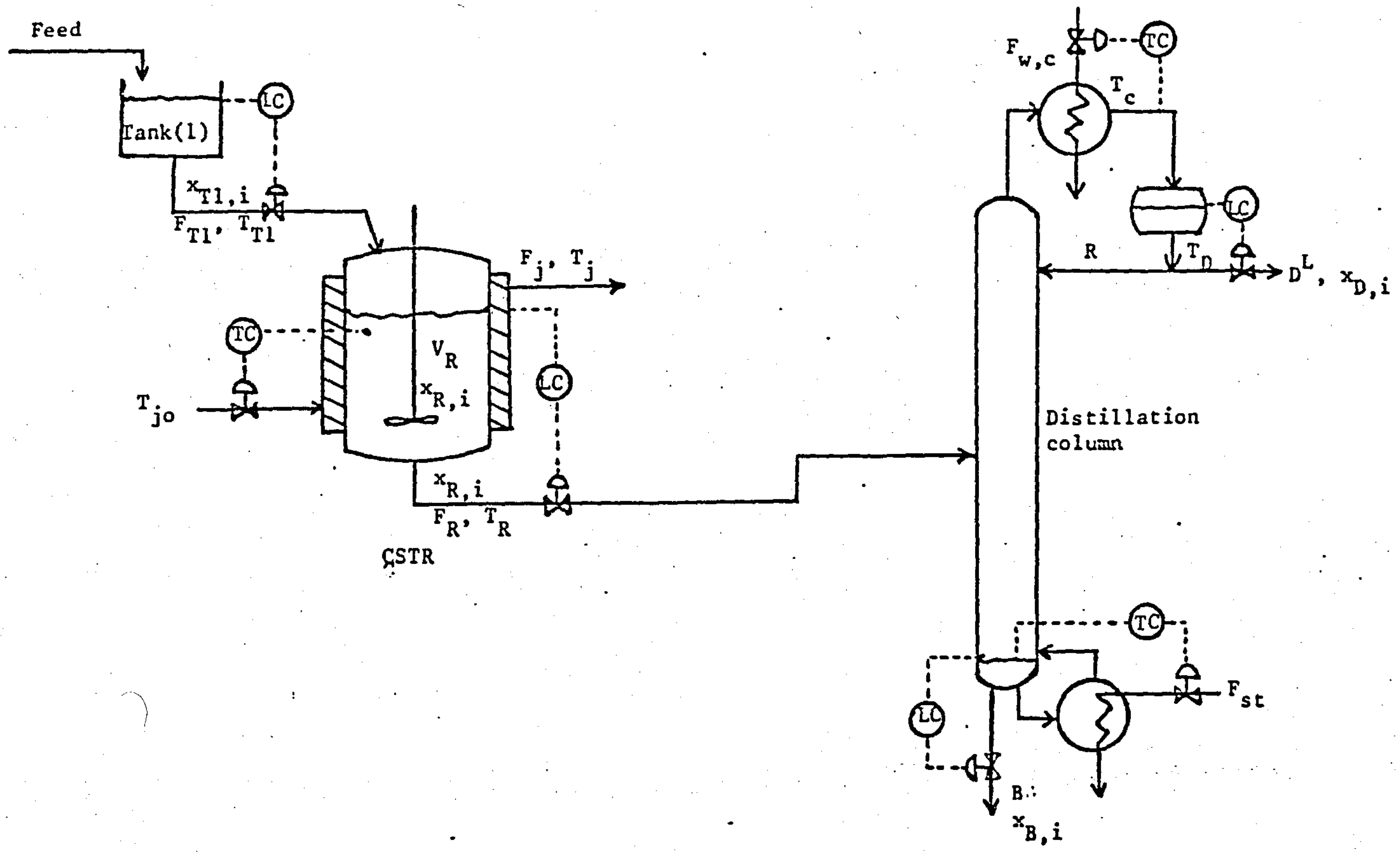


Figure 4.33 Flowsheet of the plant in Example 9.

units, and the tank is the auxillary unit.

The physical properties of the components, the initial conditions and the technical spesifications of the process are as given in Tables A.8, A.9, A.11, A.12.

A mixture of butanol and pthalic anhydride with the ratio of 10.02 respectively at the initial steady-state is pumped to the tank. The main function of this tank is to damp out the fluctuations in composition. The damping effect of the mixing tank is to improve the operation of the reactor. The volume of the tank is 2.12 m^3.

The effluent of tank is pumped into the reactor and the outflow of reactor is pumped into the distillation column. Technical spesifications of the reactor and the distillation column are the same as in Examples 7 & 8. Initial steady-state conditions for the reactor and the distillation column are the same as in Examples 7 & 8 . The controller settings for both reactor and the column are the same in Example 8. It can be noted that the only difference of this example from 8 is the tank whose effluent is pumped to reactor.

Various terminal variables are plotted from Figure 4.34 to 4.38.

Contrary to the previous Examples 7 & 8, in this example upset in concentration does not affect directly

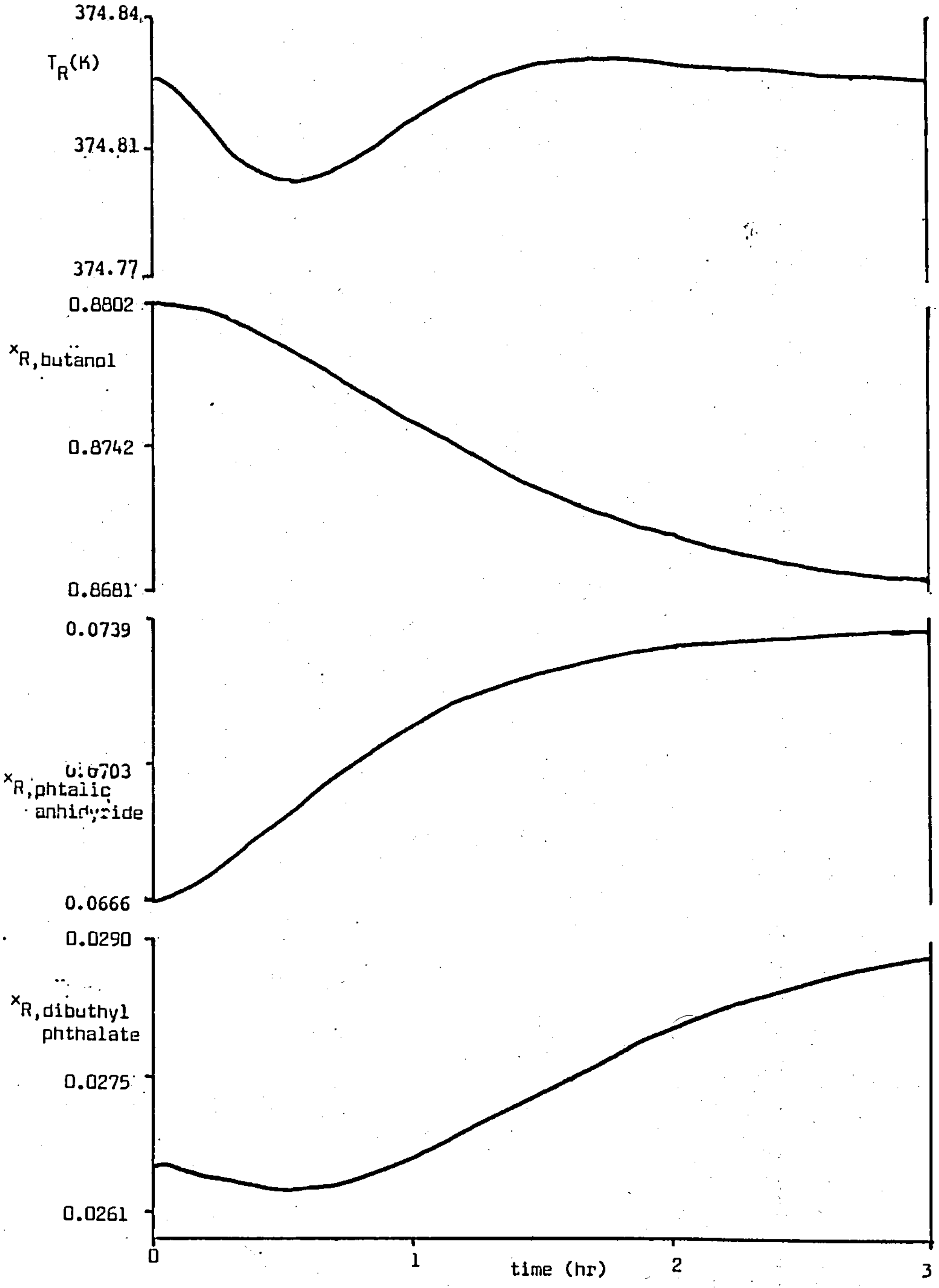


Figure 4.34 Response of the reactor in Example 9.

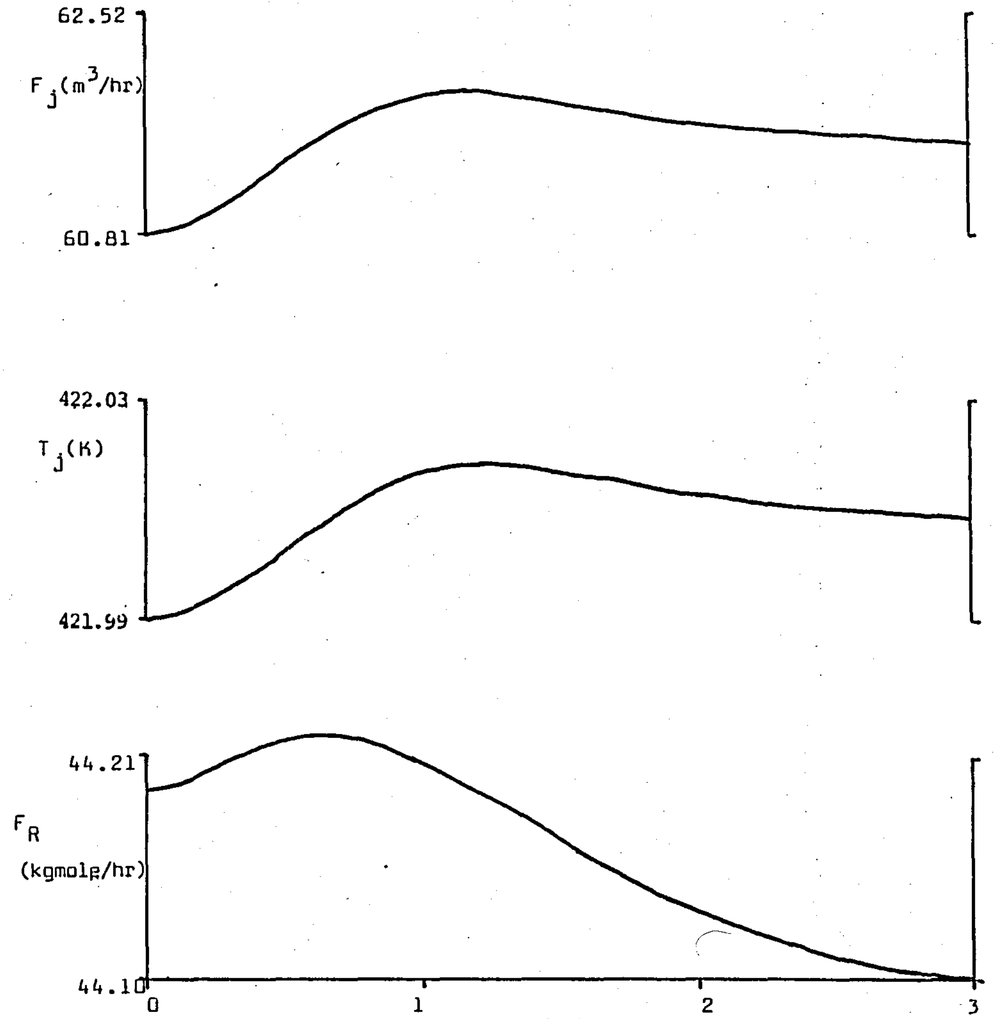


Figure 4.35 Response of the reactor (flows and jacket temperature) in Example 9

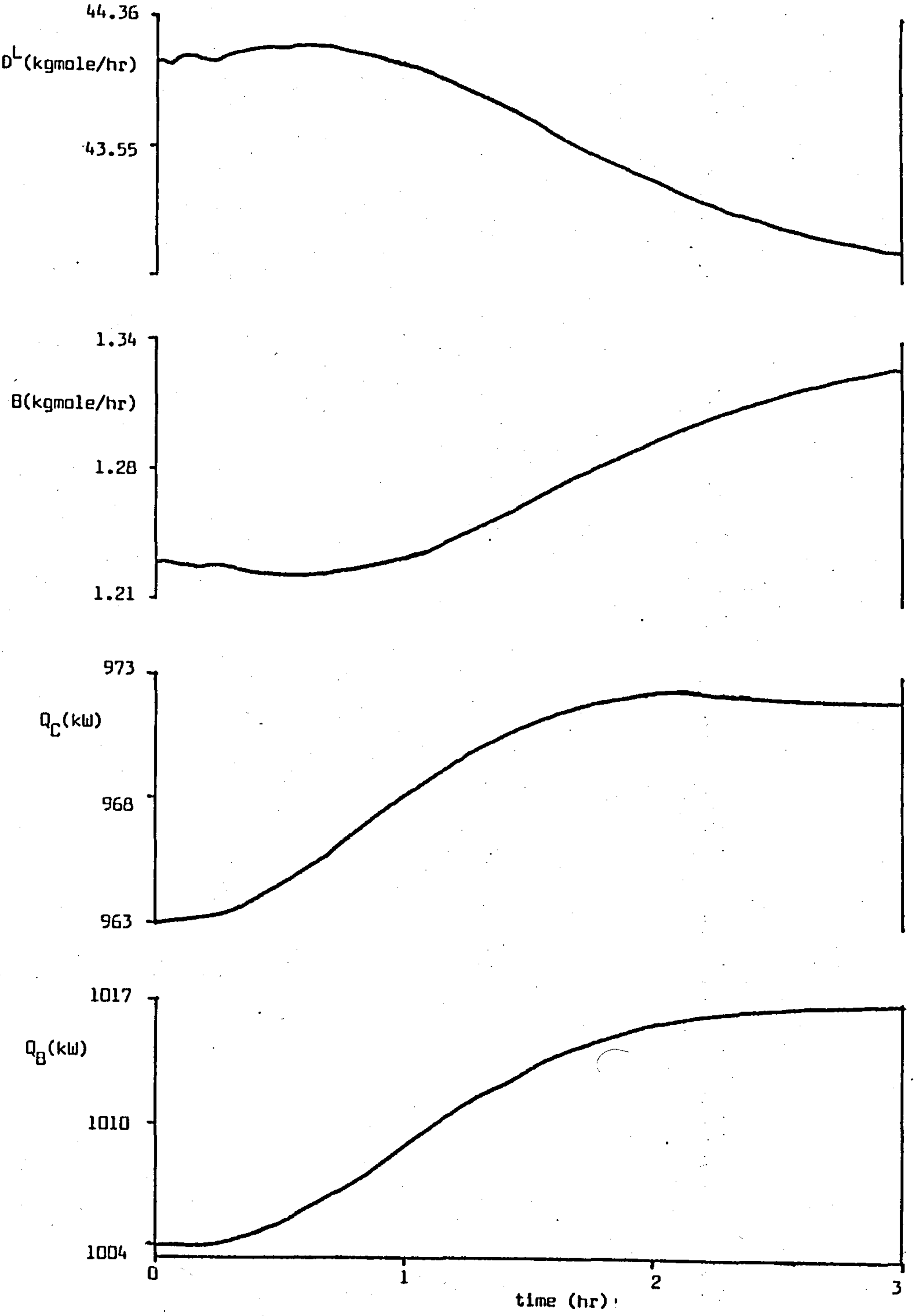


Figure 4.36 Response of the column (flows and heats) in Example 9

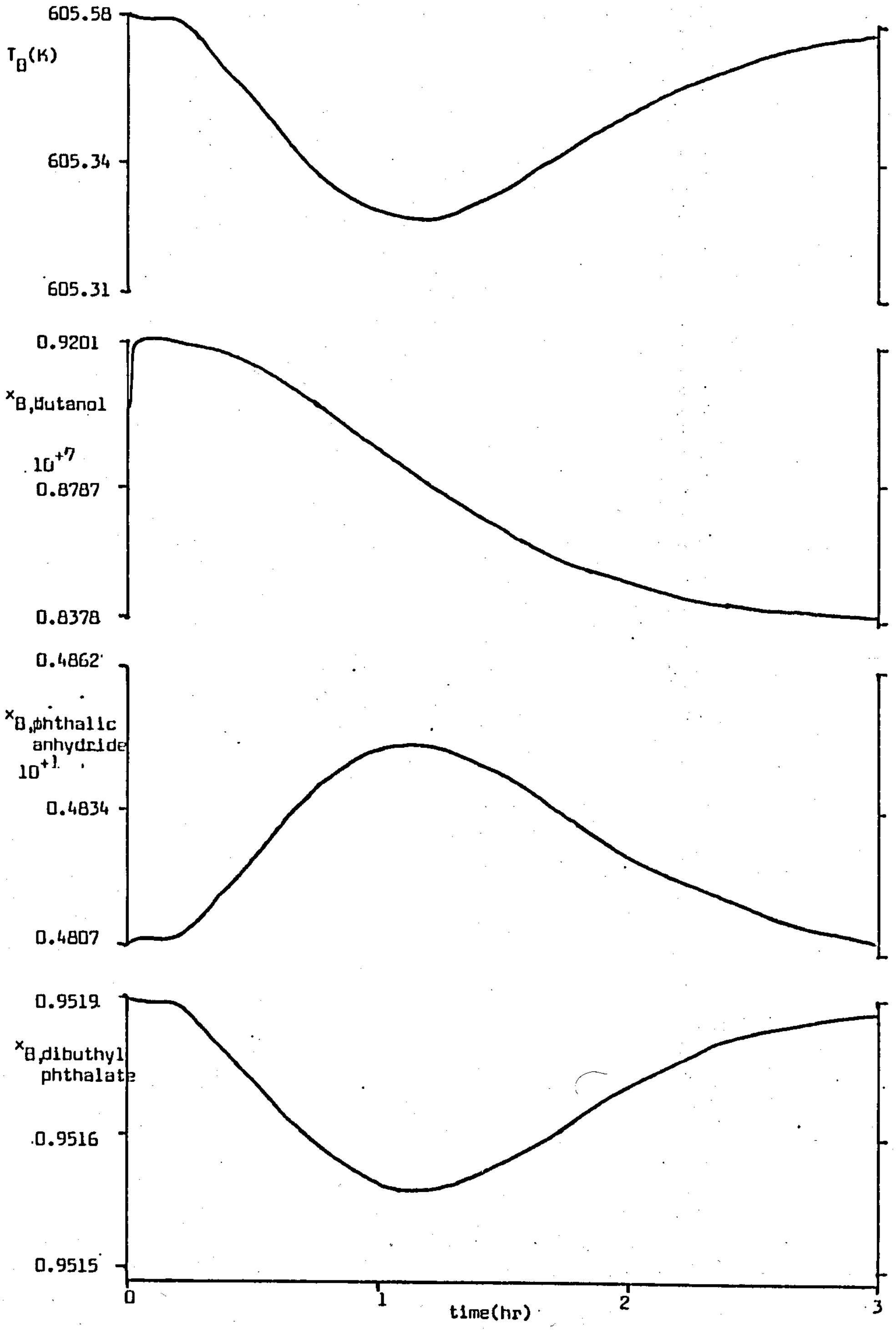


Figure 4.37 Response of the colmun (bottoms temperature and compositions) in Example 9

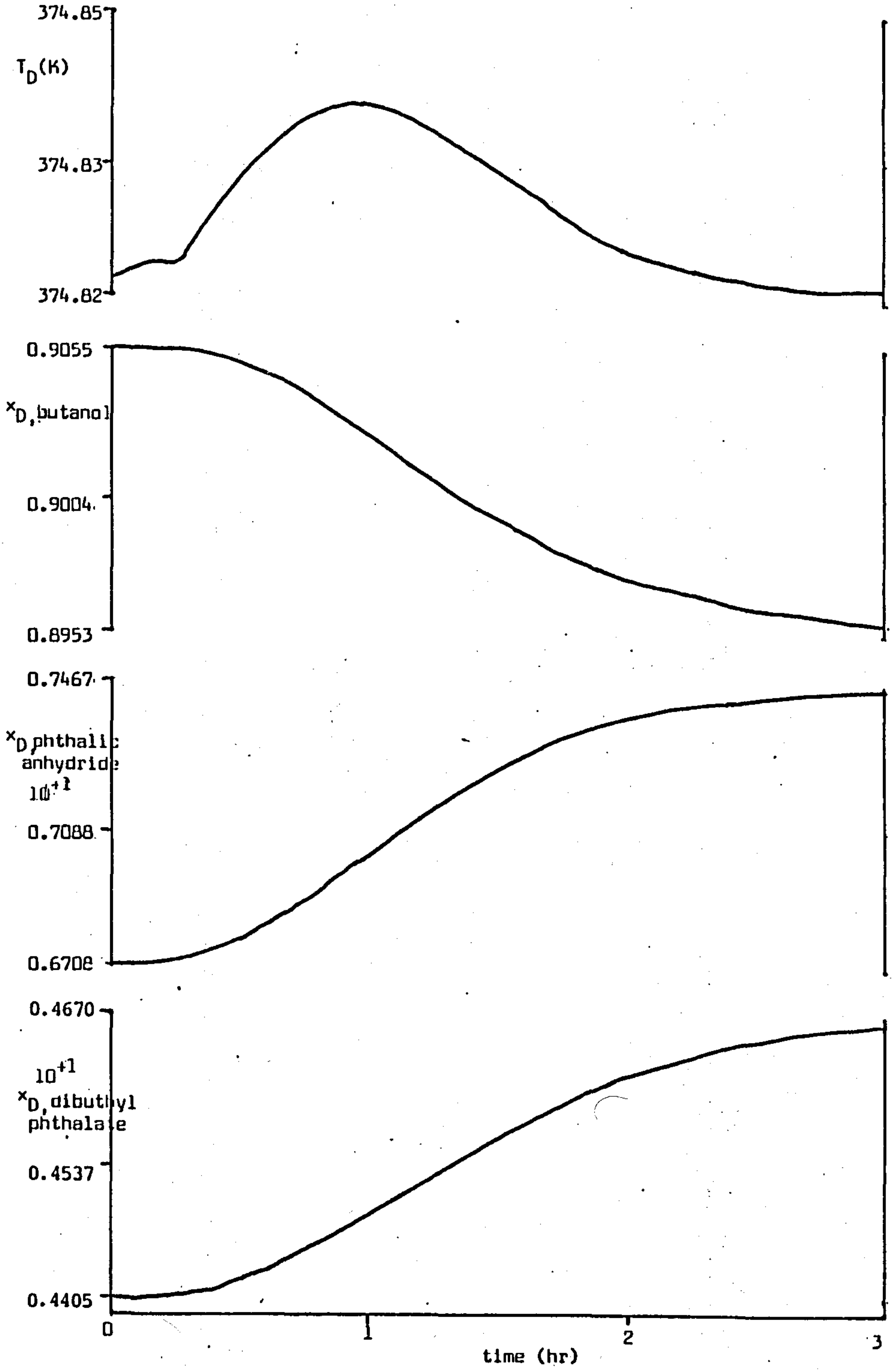


Figure 4.38 Response of the column (distillate temperature and compositional in Example 9

the reactor, but the tank makes smoother the concentration change in the feed stream. It can be noted that overshoot in the reactor temperature is smaller due to the smaller changes in the feed concentration and will cause small changes in the conversion and hence heat generated from the reaction will increase slowly. This will cause a small but late overshoot and make the reactor more operable. On the other hand, low controller gains also affect the rise time to the new steady state condition.

The distillation column is affected by the concentration changes which is explained above.

Abstractly, in Examples 7, 8 and 9, the responses of the dibutyl phthale production process is simulated under same upset in fresh feed concentration. In Example 7, the process units were the reactor and the column. In Example 8 also, the process units were the reactor and the column, but in this example the gains of the controllers of the process were relatively decreased.In Example 9, same controller gains which was used in Example 8 was used, and the process structure was changed so that a premixing tank is added to the process. The responses in the various terminal variables for these three examples are plotted in same graphs from Figure 4.39 to 4.43.

It can be seen in the responses of variables of reactor that, outlet composition of the reactor is not

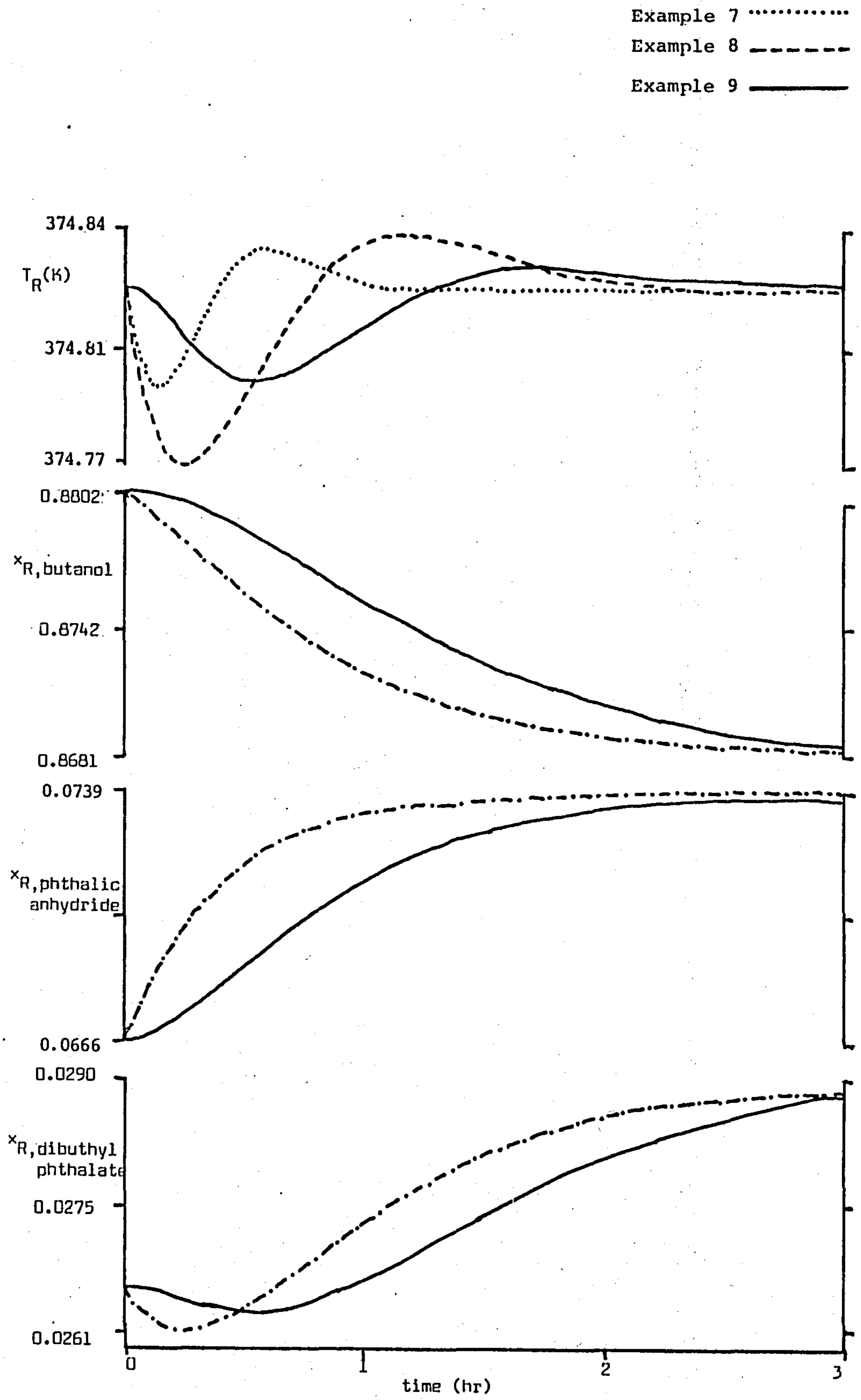


Figure 4.39 Response of reactors (temperatures and compositions) in Examples 7, 8 and 9

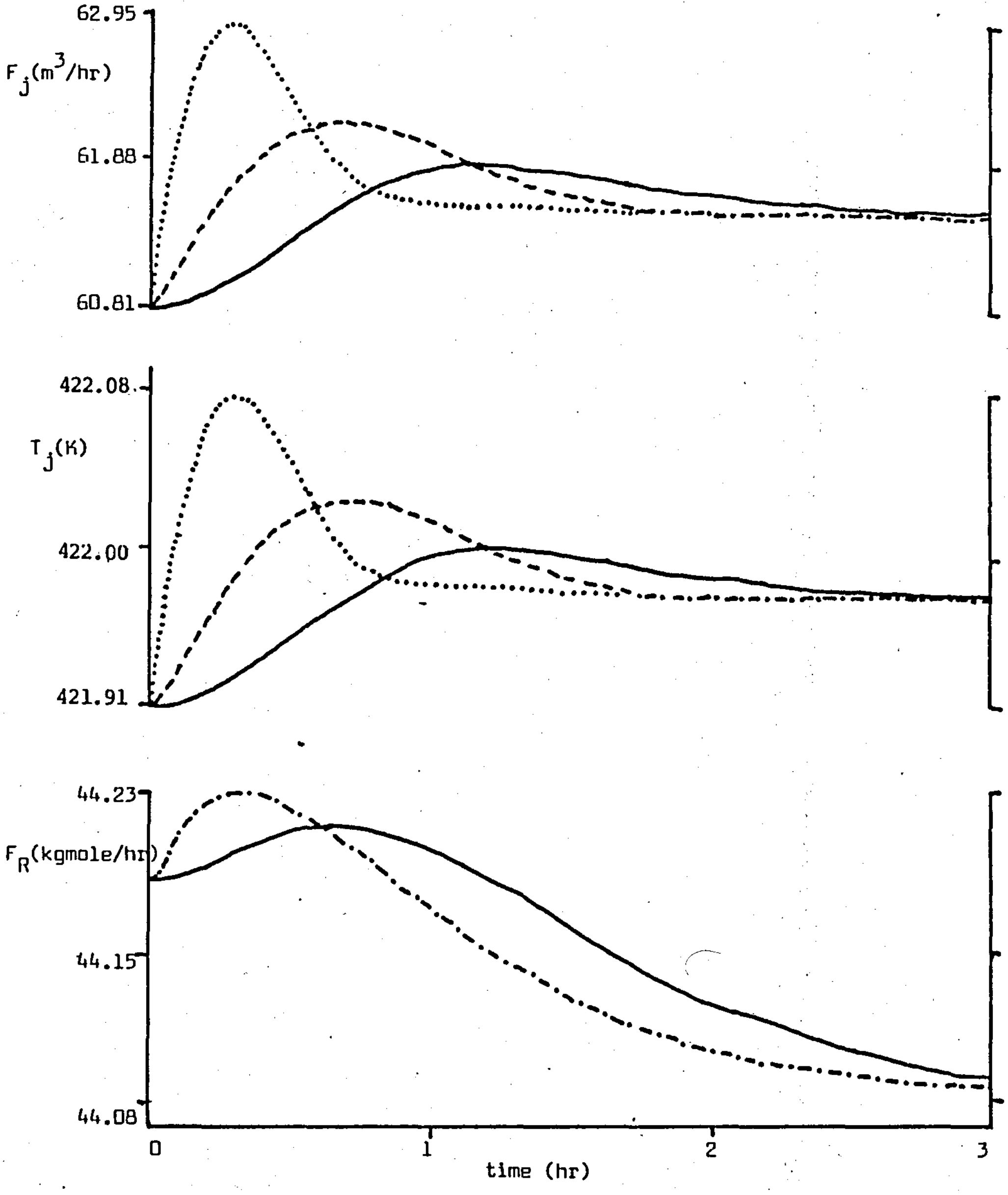


Figure 4.40 Response of the reactors (flows and jacket temperature) in Examples 7,8 and 9

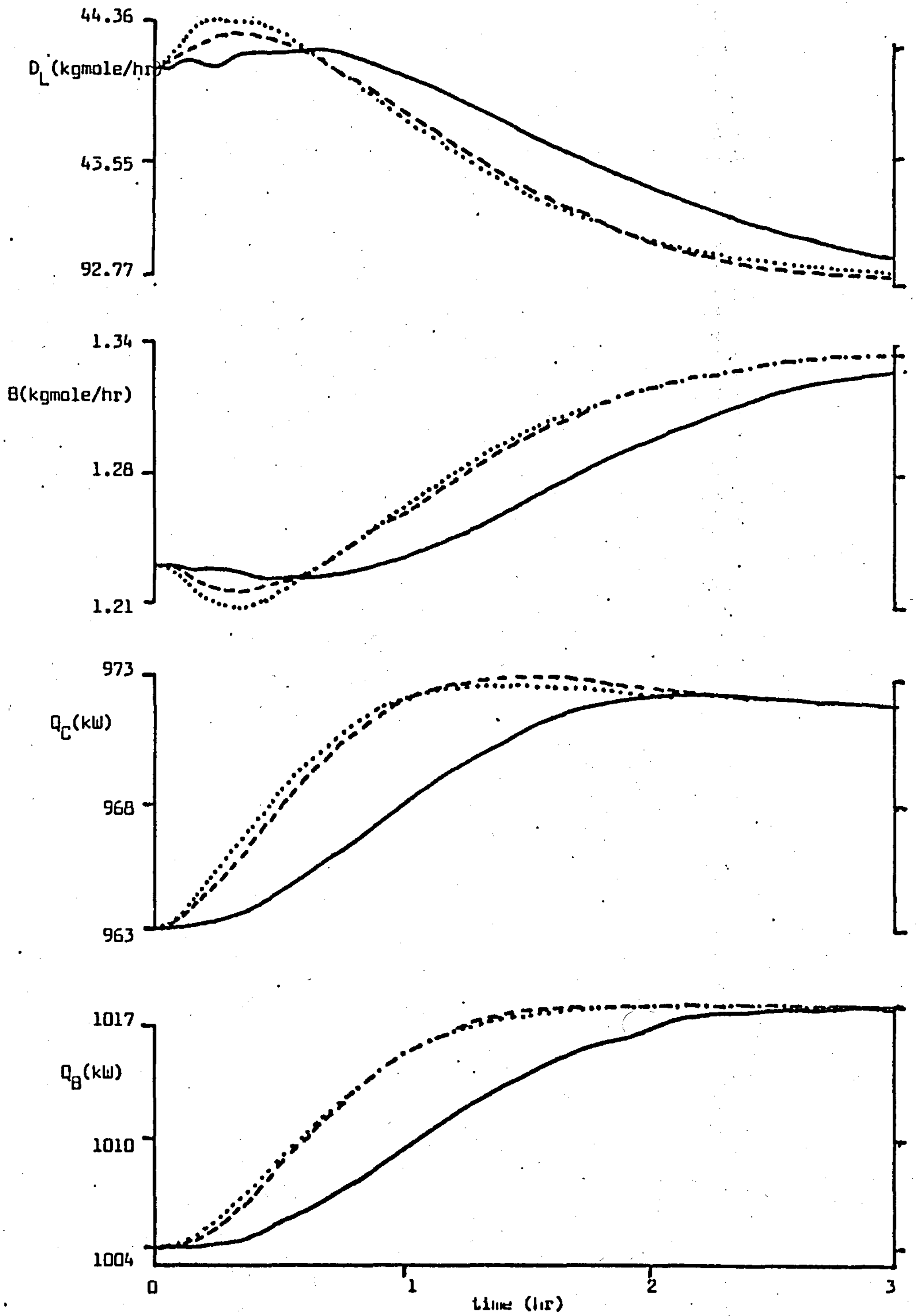


Figure 4.41 Response of the columns (flows and heats) in Examples 7,8 and 9

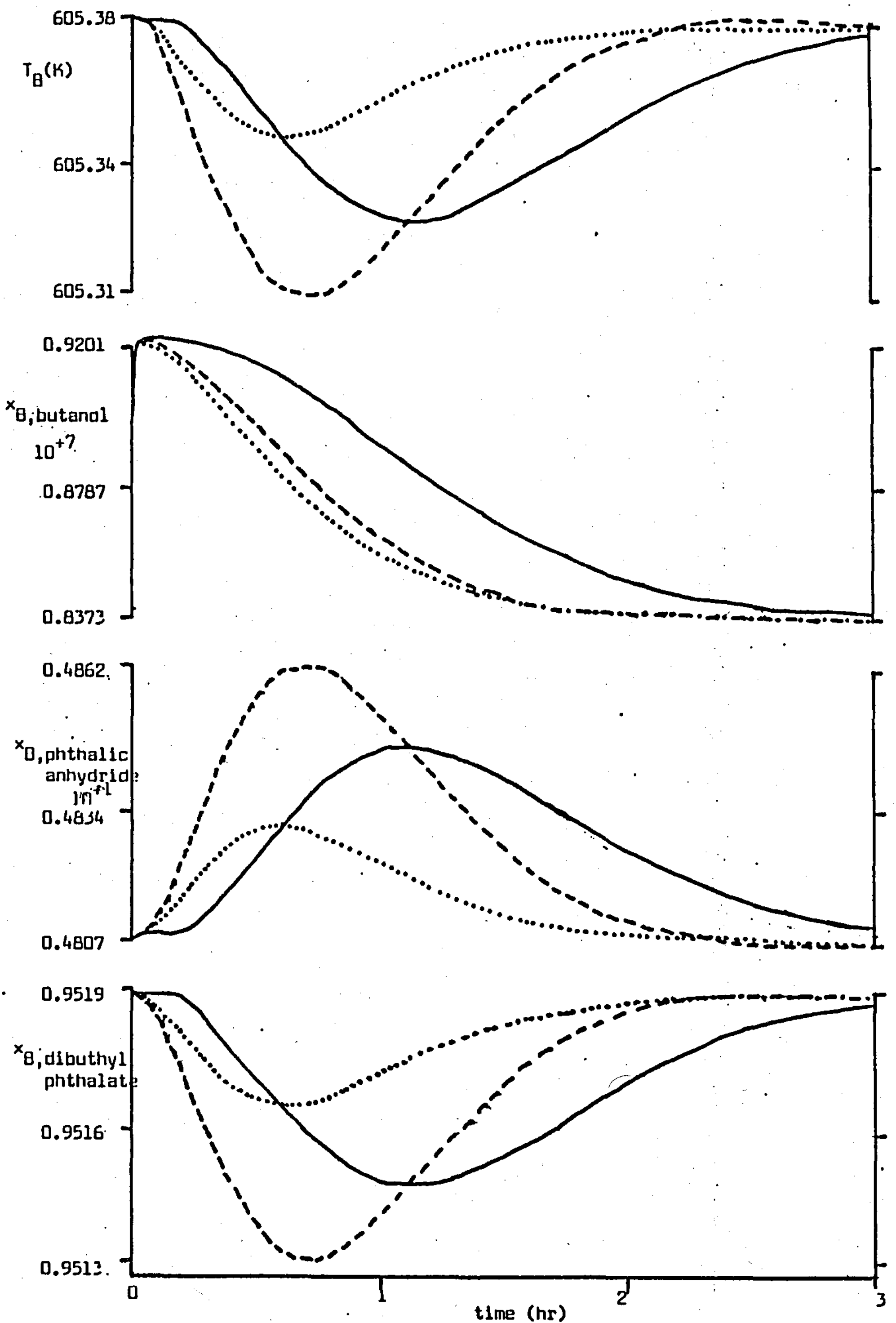


Figure 4.42 Response of the column (bottoms temperature and compositions) in Examples 7, 8 and 9

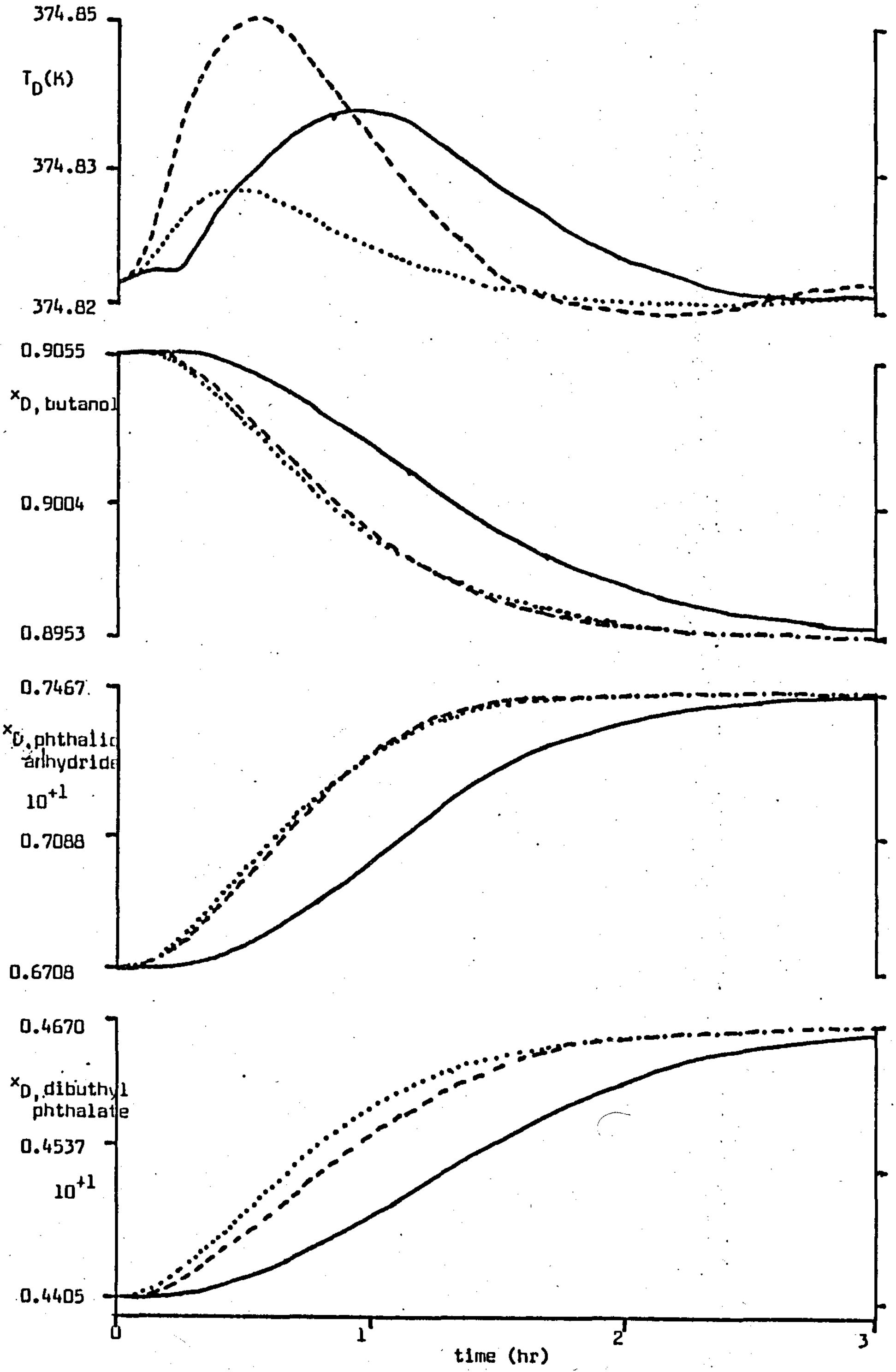


Figure 4.43 Response of the column (distillate temperature and compositions) in Examples 7, 8 and 9

affected by the changes in reactor temperature. This is due to the reaction is low exothermic and hence small fluctuations in the temperature did not affected the composition of the reactor. Outlet composition of the reactor is primarly affected by the change in feed composition. It can be noted that, although the gains of the controllers are different in Example 7 and 8, the responses in the outlet mole fractions are the same. Also, it can be noted that, responses in the mole fractions in the outflow rate of the reactor in Example 9, is different when compared with Example 7 & 8. This is due to the effect of premixing tank. It is also observed that, premixing tank affects the reactor temperature. It can be seen that, fluctuations in temperature in Example 9 are smaller. Also, the response of heating liquid flow rate is smoother. It is also possible to see the effects of premixing tank in the distillation column. The responses in distillate and bottoms temperature are smoother. An interesting point in the column is that, the heat removed from the distillate condenser and the heat given to the column at the bottom from initial steady-state to final steady-state are smaller compared with other examples.

As a conclusion, it can be said that, a premixing tank makes this production process more operable. This conclusion justifies Buckley's approach to control of chemical processes. On the other hand, here, it should be pointed out that, an extra tank will increase the investment.

4 . 3. Examples for Comparison with Previous Study

In this chapter same example flowsheets which is introduced in Akman's work will be simulated by the computer program under different control structures.Furthermore, for two different control structures the effect of intermediate tank between the reactor and the column will be investigated.

The main difference in the examples of this section from the Akman's examples is in control the structure of the distillation column. One structure which is selected by considering the overspesifications of the overall control structure of the plant is in order to control the reflux drum level constant to manipulate the distillate flow rate. The other structure is to control the reflux drum level by manipulating the reflux drum flow rate. These two different structures will affect the column individualy and will also affect the overall process in the case of recycle streams (when the distillate product of the column is used as recycle). Akman evaluates some examples in his study (Examples 1 and 4) in the first control structure which is explained above. In this section, second structure will be evaluated. The effect of an intermediate tank between the main processing units (reactor and the column) will also be evaluated.

The physical properties of the components, and the data files for processing unit showing the initial conditions are given in Appendix A.

EXAMPLE 10

This example is different than the Example 4 in the previous work [1]. The difference is in the flowsheet. An intermediate tank is added between the reactor and the column. The flowsheet which is simulated shown in Figure 4.5.

General description of the process is as follows: A feed stream containing components A and B is pumped to the continuouos stirred tank reactor to produce the component C. The reactor volume is controlled by a PI controller and the set point for the reactor volume 2.83 m^3 . The reaction taking place in the reactor $A + B \longrightarrow C$ is second order and irreversible. Since the reaction is highly exothermic, heat is removed by a jacket cooler. To control the reaction temperature a PID controller which manipulates the flow rate of cooling water, is used. The set point for temperature is 347.1 K.

The reactor effluent is pumped to the mixing tank and the effluent of tank is pumped to the distillation column. The technical spesifications of the column are the same of Example 1. The feed enters the column from the fifth stage. The bottoms temperature of the column is controlled at 398.4 K which is close to the boiling point of component C, by a PI controller which manipulates the rate of steam flow. The set points bottom level controller and the reflux drum level controller is 0.5 m^3 and 0.28 m^3 respectively. These controllers are only proportional action. The condenser temperature is 349.8 K , and a PI controller is used which manipulates the flow of cooling water in the condenser.

The product stream of the process is the bottom stream of the distillation column which is rich in component C.

The flowsheeting parameters, integration step size and the physical properties of the components are given in Table A.13 . The initial conditions and the technical spesifications of the equipment are given in Tables A.14, A.15, A.16.

The upset given is a -15 % step change from 45.36 kgmole/hr in the flowrate of fresh feed to the reactor.

The various terminal variables are plotted as functions of time in Figures 4.44 through 4.48 to follow the responses of time.

When the feed flow rate decreases, the outflow rate of reactor, F_R, also decreases as shown in Figure 4.45 .

When the feed flow rate decreases, the reactor

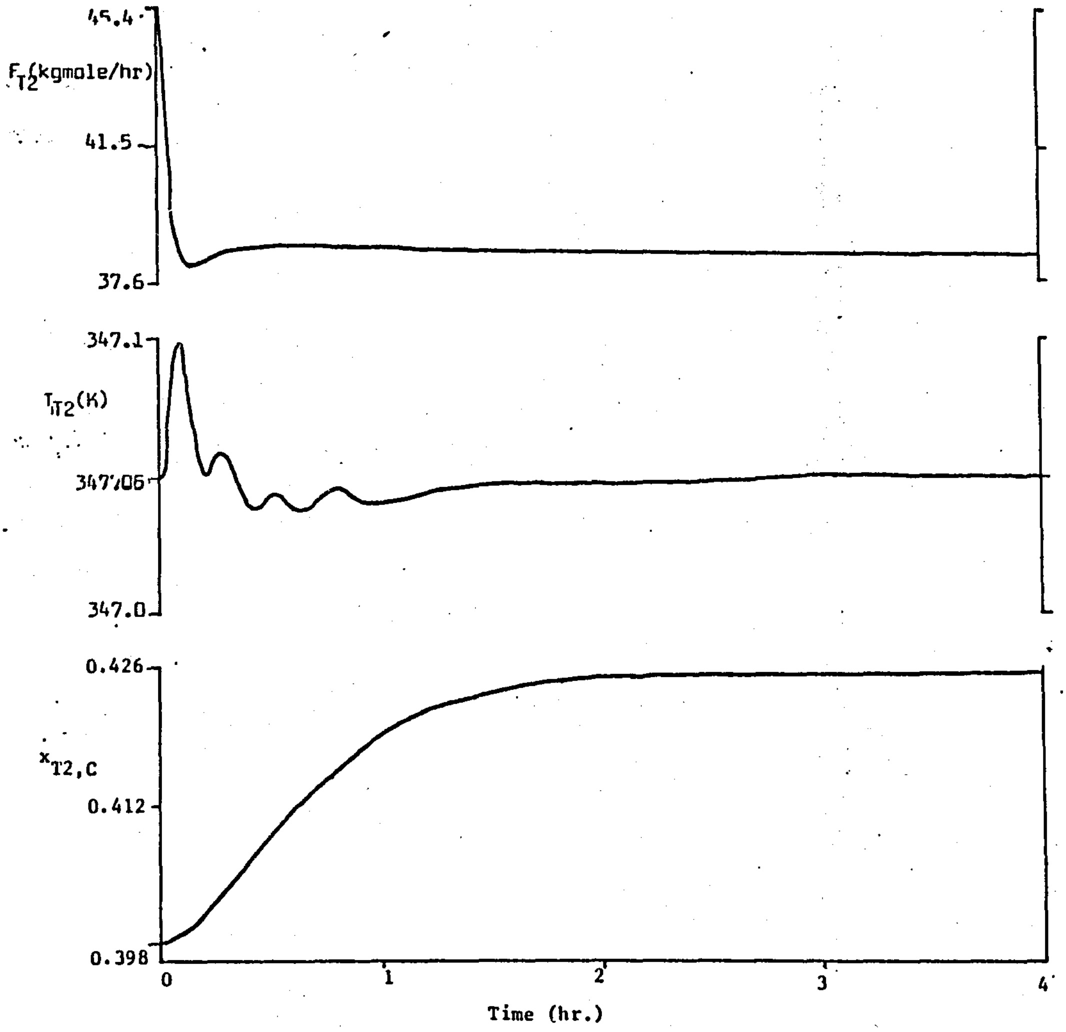


Figure 4.44 Response of tank in Example 10

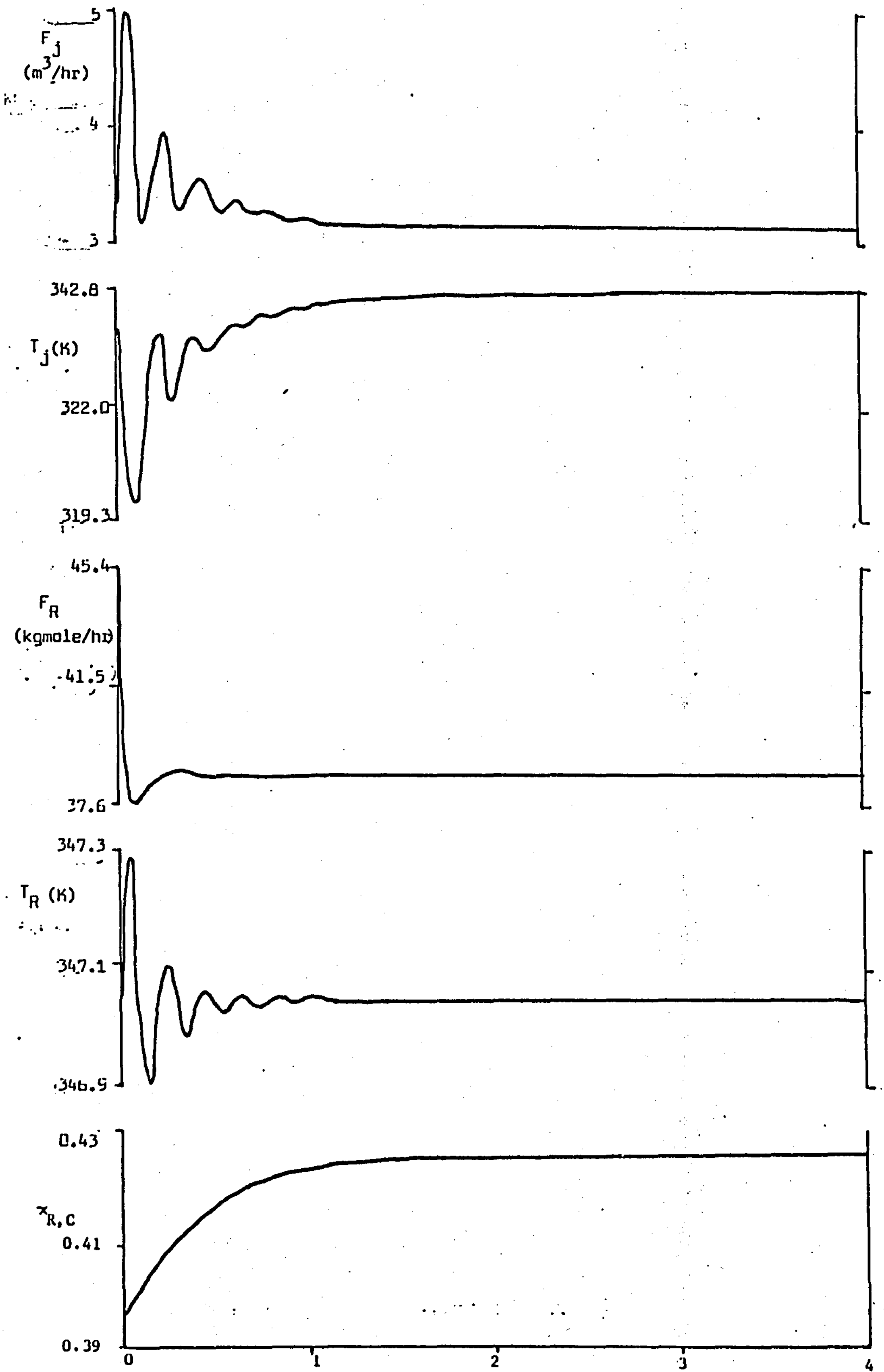


Figure 4.45 Response of the reactor in Example 10

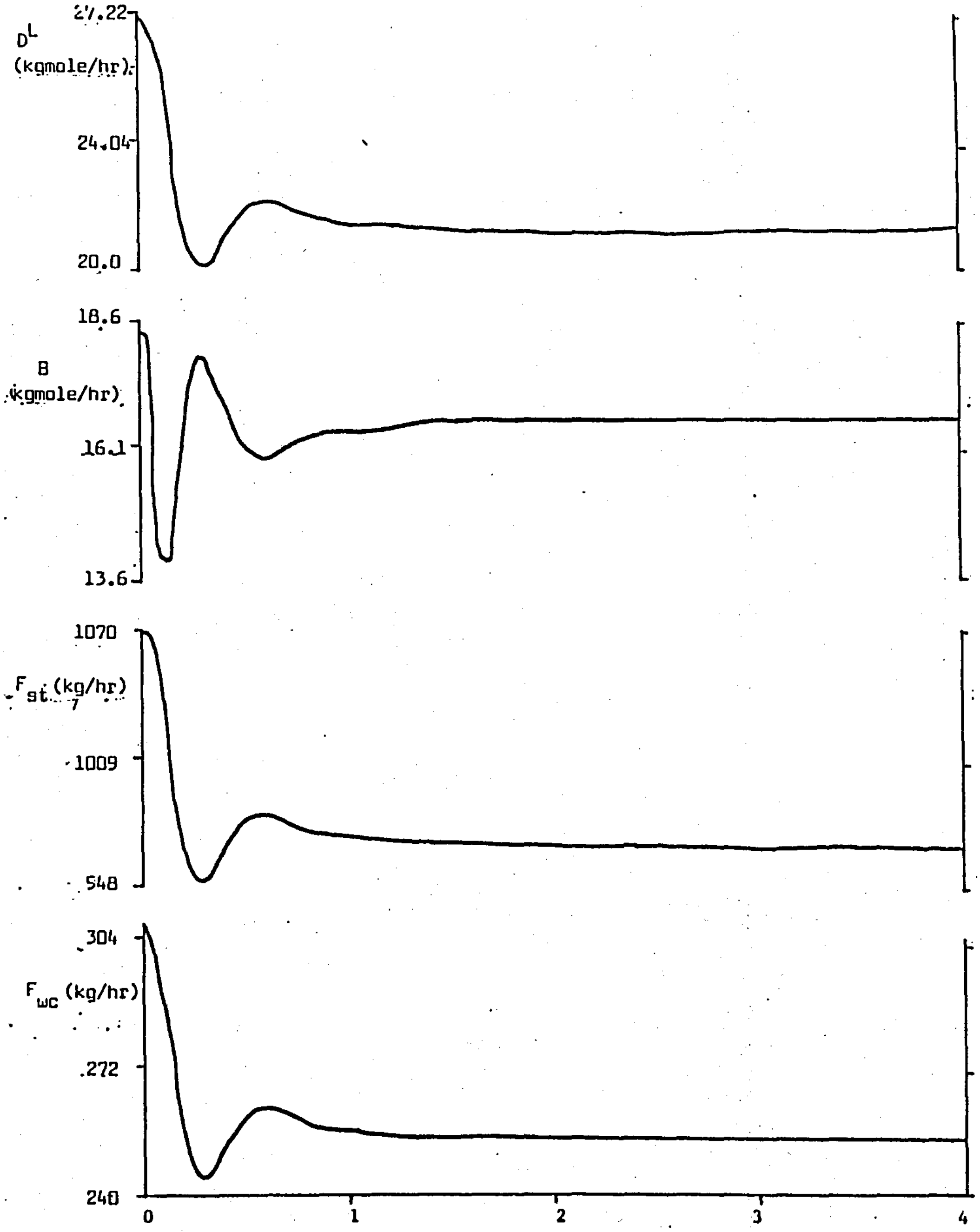


Figure 4.46 Response of the column (flows) in Example 10

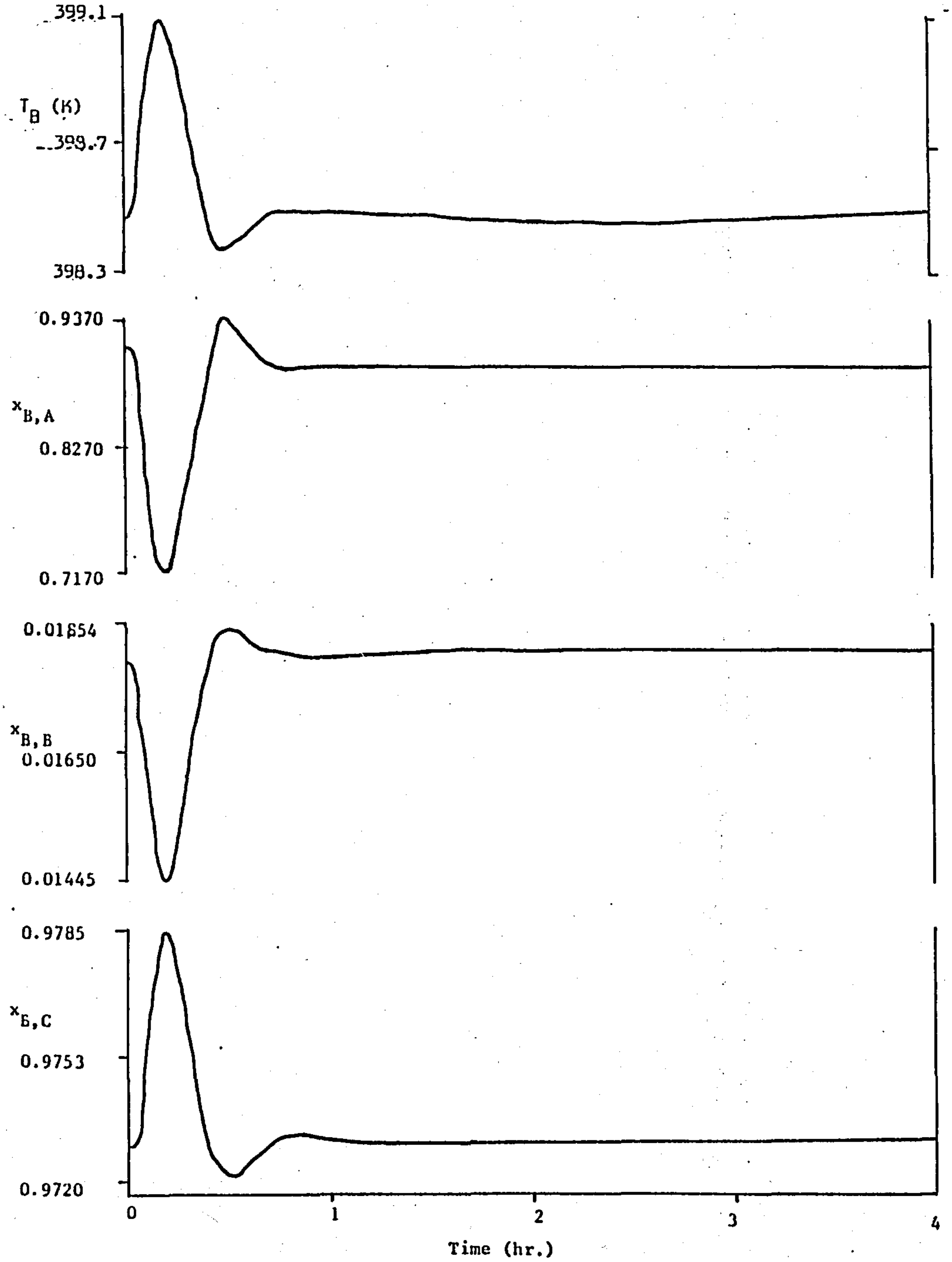


Figure 4.47. Response of the column (bottoms temperature and compositions) in Example 10

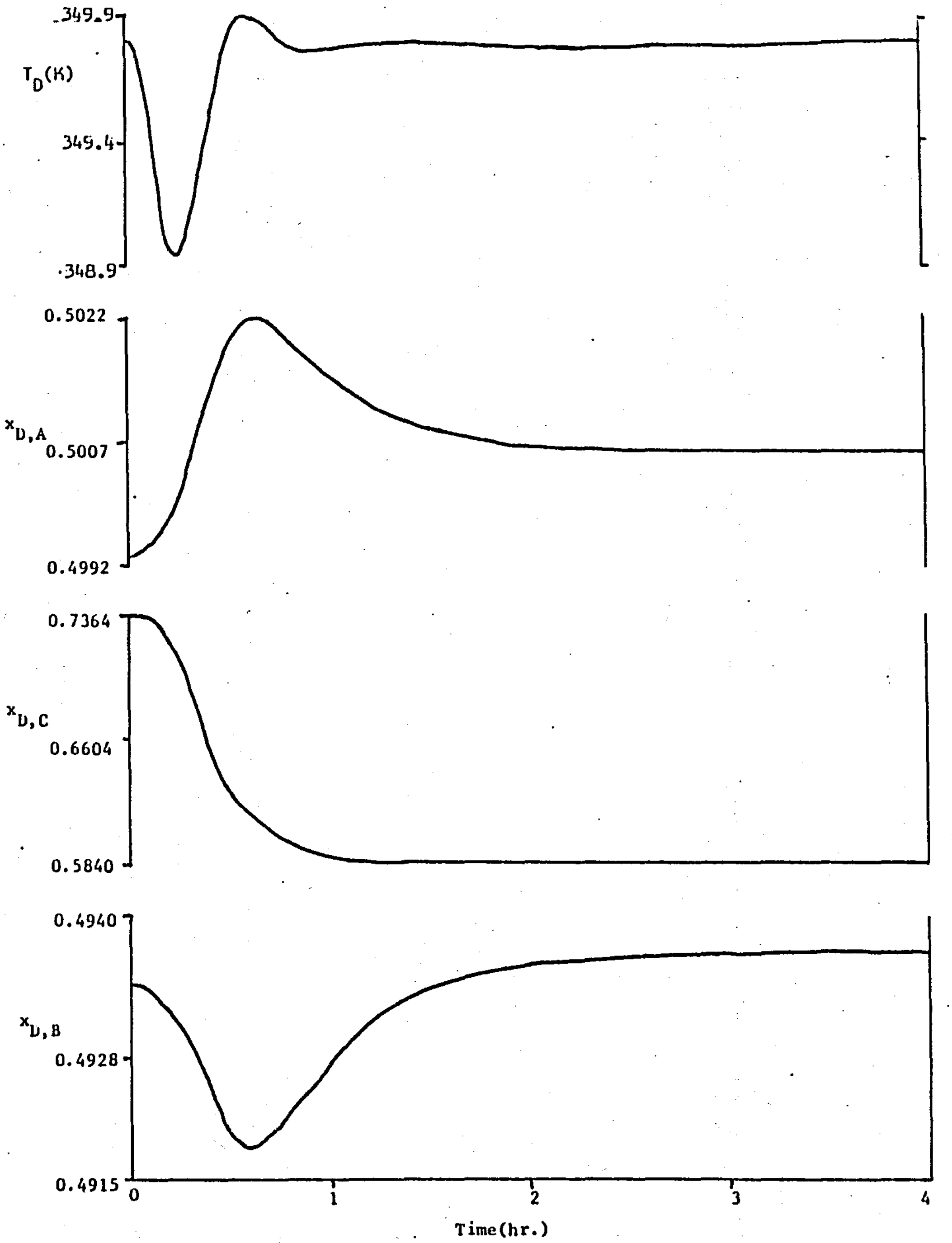


Figure 4.48 Response of the column (distillate temperature and composition in Example 10

temperature starts to increase and then return to its set value with oscillations. The responses of the reactor temperature is a typical control response as shown in Figure 4.45 . The initial increase in the temperature is due to the increase in residence time in the reactor which will cause higher heat generation and then higher conversion due to the exothermic reaction. The PID temperature controller of the reactor manipulates the flow of the cooling water in the reactor jacket. The changes in the reactor temperature and in the jacket temperature are shown in Figure 4.45 . The changes in the reactor temperature and the jacket temperature give an indication of the heat transfer between the reactor and its jacket.

When the feed flow decreases, due to the increase in reactor residence time, the mole fraction of the reaction product , $x_{FR,C}$, increases without oscillation as shown in Figure 4.45 .

When the feed flow rate decreases, the outflow rate of the intermediate tank also decreases as show in Figure 4.44 . As can be seen , the response of the tank temperature is oscillatory, but the amplitute of oscillations is much smaller than the amplitute of the oscillations in the reactor. This justifies that this intermidiate storage tank decreases the fluctuations in the temperature and provides an increase in the operability of the distillation column where the temperature is used as a secondary control variable in it.

When the feed flow decreases, the distillate, D^L, and the bottom, B, product rates of the column also decreases as shown in Figure 4.46 . A decrease in the feed flow rate results in a temporarily excessive heat input from the reboiler and this causes the temperature at the bottom of the column, T_B, to increase as shown in Figure 4.47 . Since the bottom temperature is controlled by a PID cotroller which manipulates the rate of steam flow, the response of bottom temperature is a typical controlled response. The changes in the flow of steam, F_{st}, are shown in Figure 4.46 . Since the boiling points of components A and B are lower than the boiling point of component C, as the bottoms temperature increases, their mole fraction in the bottom decreases.

The response in the distillate temperature, T_D, and the mole fractions of the components in the distillate stream $x_{D,A}$, $x_{D,B}$, and $x_{D,C}$ are shown in Figure 4.48 . Contrary to the situation at the bottom of the column, these responses do not closely follow each other. The behaviour of the distillate temperature is strongly related to the condenser temperature which is controlled by the manipulations of the condenser cooling water flow rate. Since the condenser temperature is controlled by a PI controller, the response in the reflux drum temperature is a typical controlled response. The changes in the flow rate of cooling water, F_{wc}, is shown in Figure 4.46 . The boiling point of component B is closer to the boiling point of component C than the boiling point of component A. Then, as distillate temperature decreases the mole fraction of B decreases.

When this example is compared with the fourth example in Akman's work,it can be said that; the fluctuations in the variables of the distillation column are smoother in this example. This is due to the intermediate storage tank which is replaced between the reactor and the column, as expected.

EXAMPLE 11

This example is also different than the Example 4 in Akman's thesis. The technical specifications of the equipment, initial conditions, and the controller settings are the same as in that example. The only difference this example from Akman's Example 4 is the level controller of the reflux drum which in this example manipulates the reflux flow rate.

The product stream of the process is the bottom stream of the distillation column which is rich in component C.

The flowsheeting parameters, integration step size

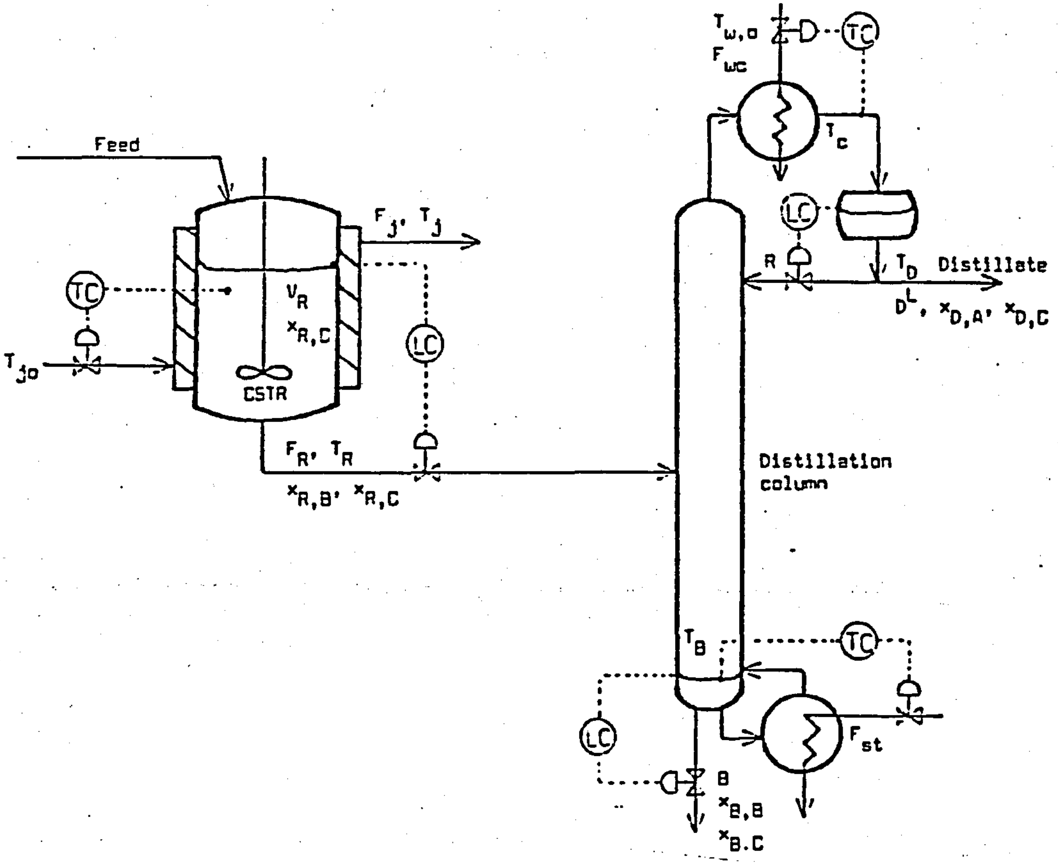


Figure 4.49 Flowsheet of the plant in Example 11.

and the physical properties of the components are as given in Table A.17. The initial conditions and the technical specifications of the equipments are given in Tables A.15, A.18 .

The upset given is a -5 % step change from 45.36 kgmole/hr. in the flowrate of fresh feed to the reactor.

The various terminal variables are plotted as functions of time in Figures 4.50 through 4.53 to follow the response of time.

After the upset, the outflow rate of the reactor, F_{R}, decreases as shown in Figure 4.50 . The response is nonoscillatory.

After the upset, the liquid level in the reflux drum of the distillation column decreses. Since the distillate flow rate is kept constant, the level controller of reflux drum manipulates the reflux flow rate. When the feed flow rate decreases, the reflux flow rate and the bottoms flow rate decraeses shown in Figure 4.51 . As can be seen from the graphs, the response of the reflux flow rate is not oscillatory and decreases continuously, but the flow rate of bottoms has an initial oscillation and then decreases continuously. These initial oscillations occur due to the excessive boil-up rate as explained in the previous example.

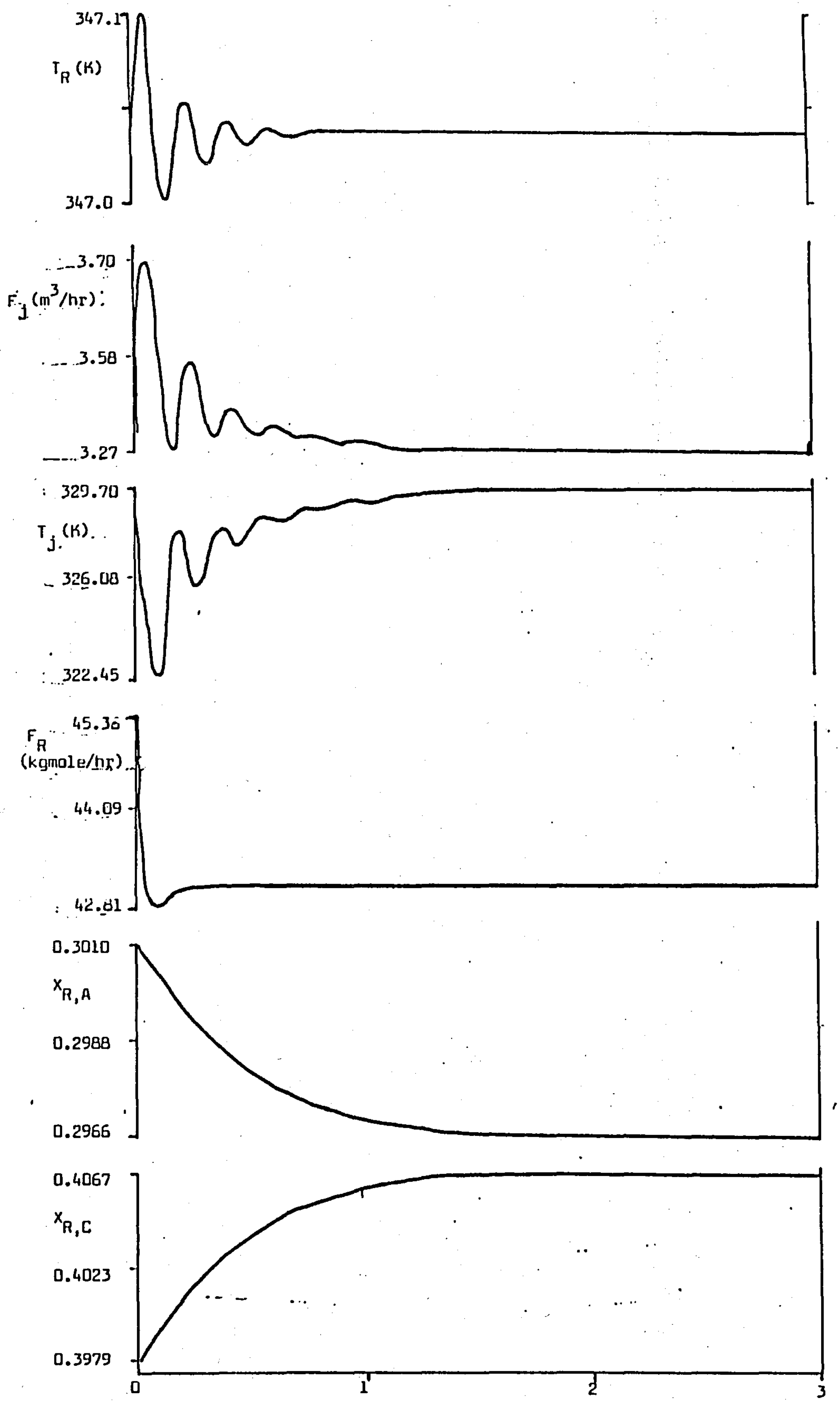


Figure 4.50 Response of the reactor in Example 11

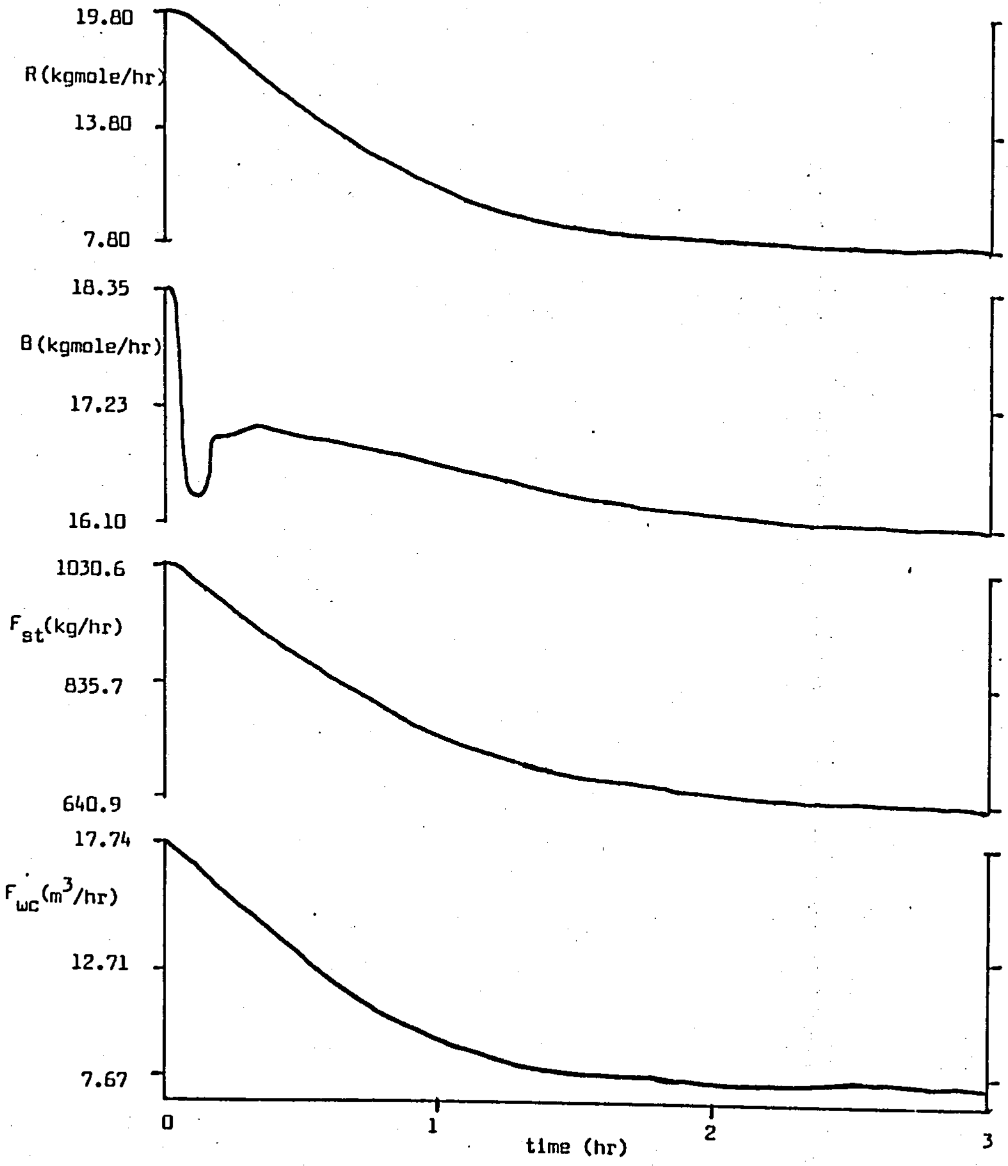


Figure 4.51 Response of the column (flows) in Example 11

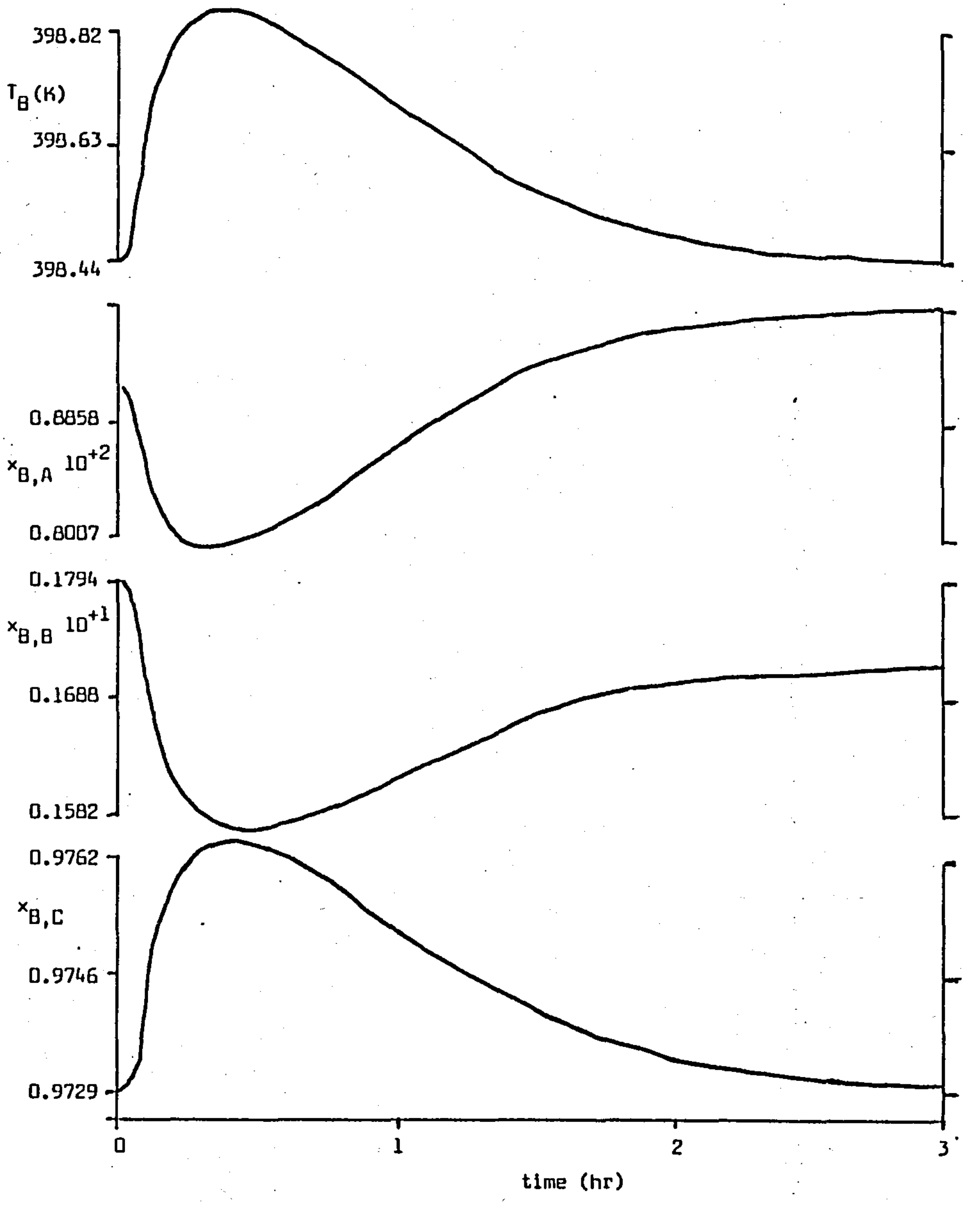


Figure 4.52 Response of the column (bottoms temperature and compositions) in Example 11

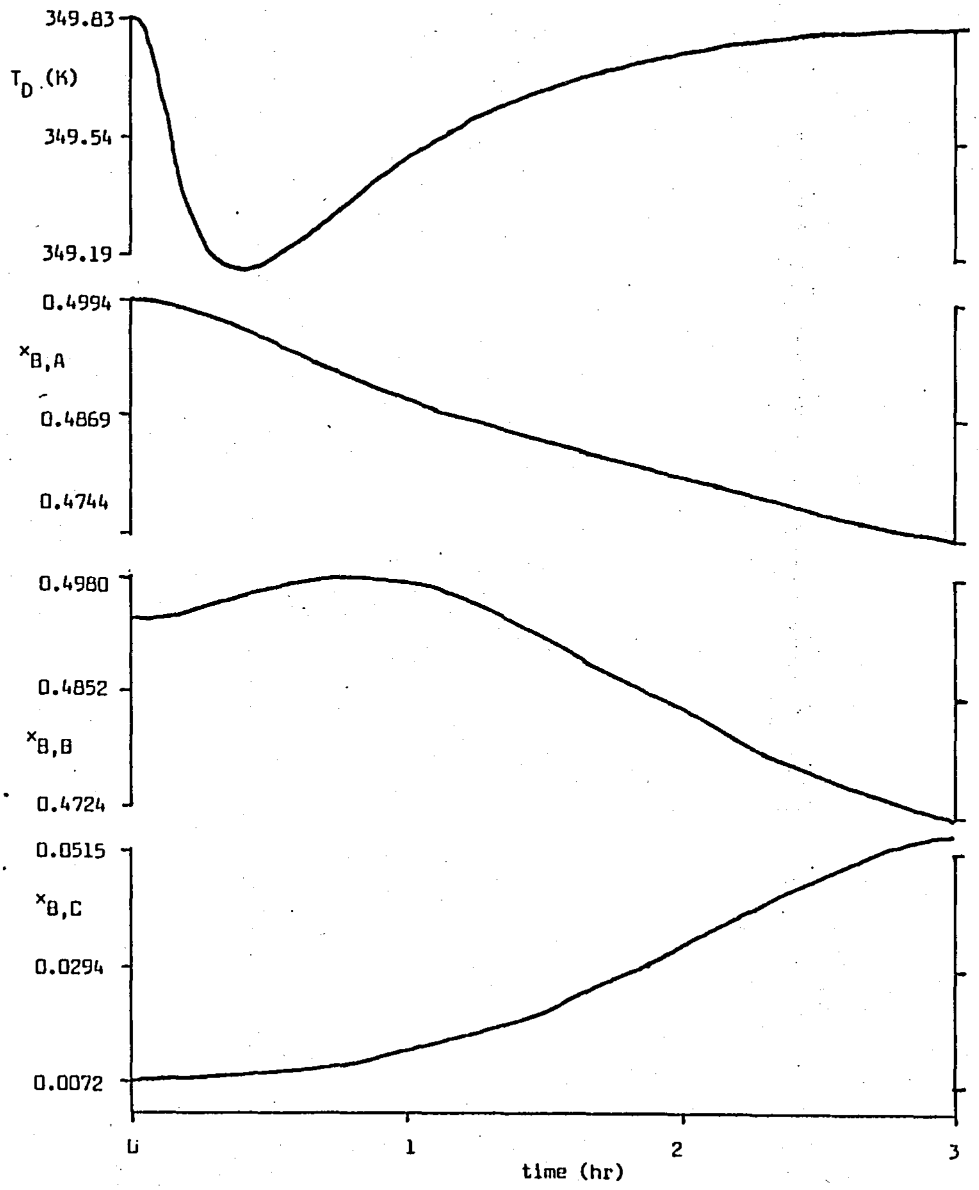


Figure 4.53 Response of the column (distillate temperature and compositions) in Example 11

When the feed flow rate to the reactor decreases, the temperature of the reactor oscillates as shown in Figure 4.50 .This is due to the increasing residence time in the reactor which causes higher conversion and hence higher heat generation due to the exothermic reaction. The changes in the flow rate of cooling water, F_J, and in the jacket temperature, T_J, also oscillates until the reactor reach their new steady-state condition. The response in the reactor temperature, T_R, and the jacket temperature, T_J, are indicators of the heat trnsfered between the reactor and its cooling jacket.

The responses of the mole fractions of the components A and C in the reactor is shown in Figure 4.50. The mole fraction of component C increases continuously. This is due to the increase in residence time in the reactor as explained above.

The changes in the variables of the distillation column are primarily due to the change in feed flow rate. A decrease in feed flow rate results in a temporary heat input from the reboiler and causes the temperature the bottom of the column, T_B, to increase. The temperature of the bottom increases initialy and then decreases continuouly as shown in Figure 4.52 .

Since the boiling point of C (heaviest component) is close to the set point of bottoms temperature, the response of the mole fraction of component C in the bottom stream is similar to the bottoms temperature. This justifies that the temperature can be used as a controlled variable to control the bottom composition.

The responses of the distillate temperature, T_D, and the mole fraction of component A (volatile component) in the distillate stream $x_{D,A}$ are shown in Figure 4.53 . Response of the distillate temperature is affected by the continuous reflux flow coupled with the changes in feed composition. Mole fraction of volatile component (A), slowly decreases without oscillations. This is due to the decrease in reflux flow which disturbs the energy balance throughout the column and causes the temnperature on the upper section of the column to increase.

As can be seen from Figure 4.51 , the flow rate of the condenser cooling water is uniform and decreases continuously.

EXAMPLE 12

Flowsheet for this example is given in Figure 4.54. The flowsheeting parameters, integration step size and the physical properties of the components are given in Table A.13 . The initial conditions and the technical spesifications of the equipments are as given in Tables A.14, A.15, A.18.

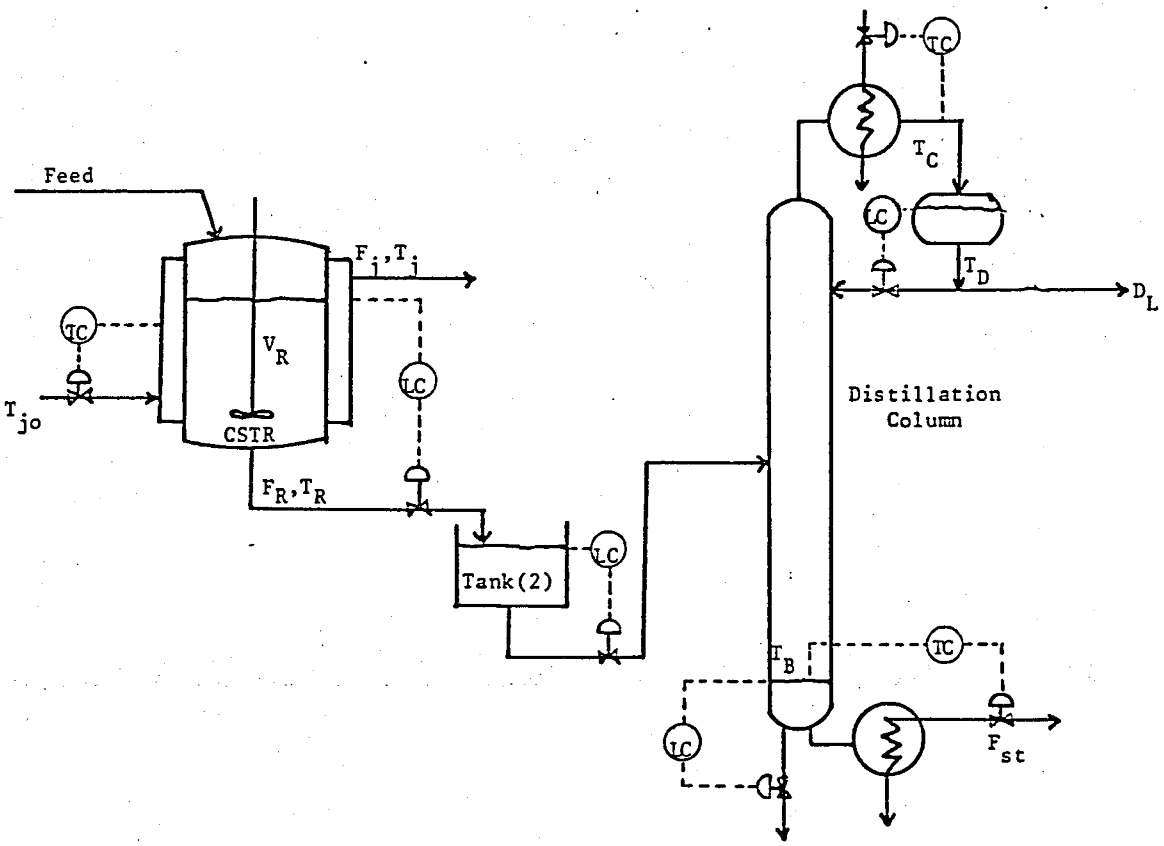


Figure 4.54 Flowsheet of the plant in Example 12.

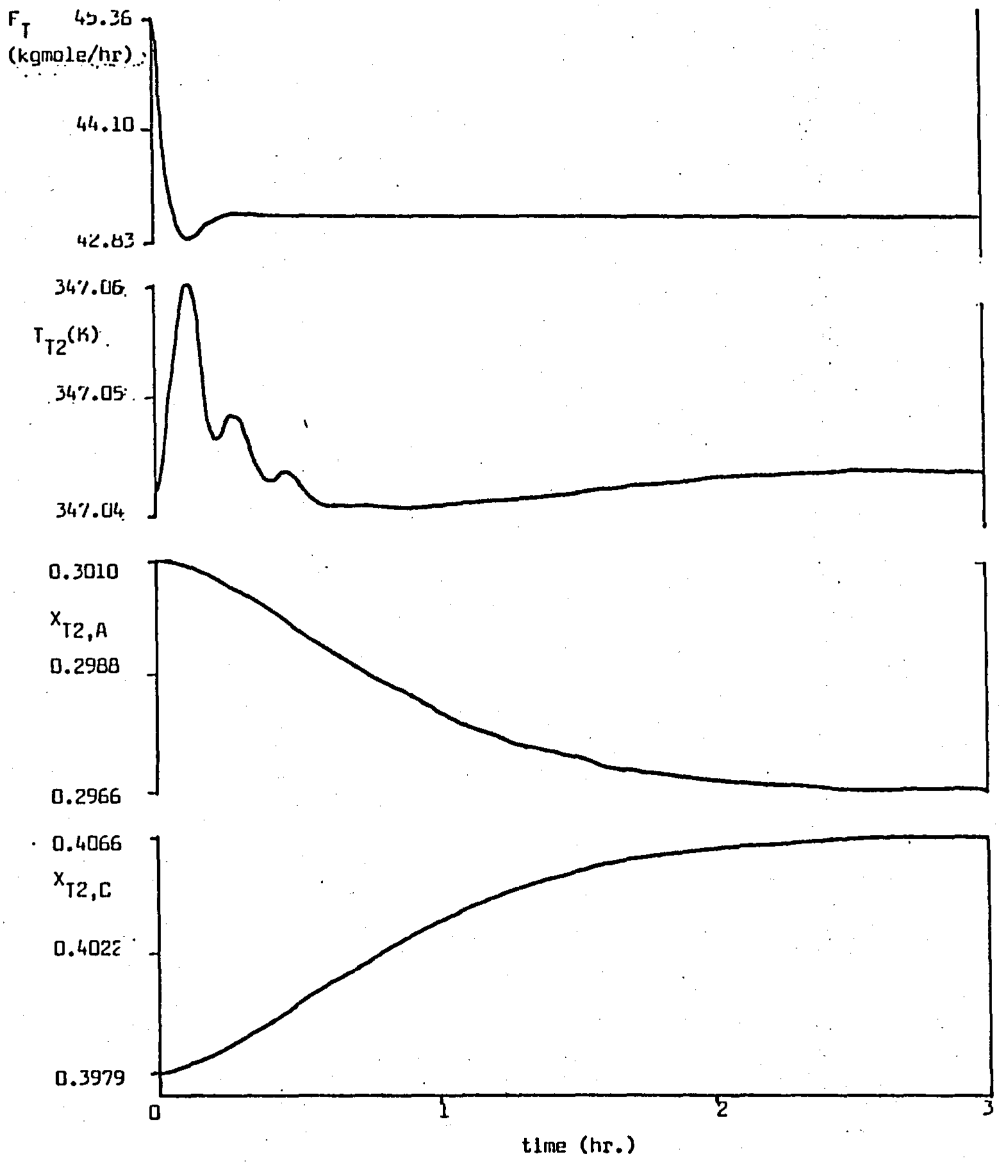


Figure 4.55 Response of tank in Example 12

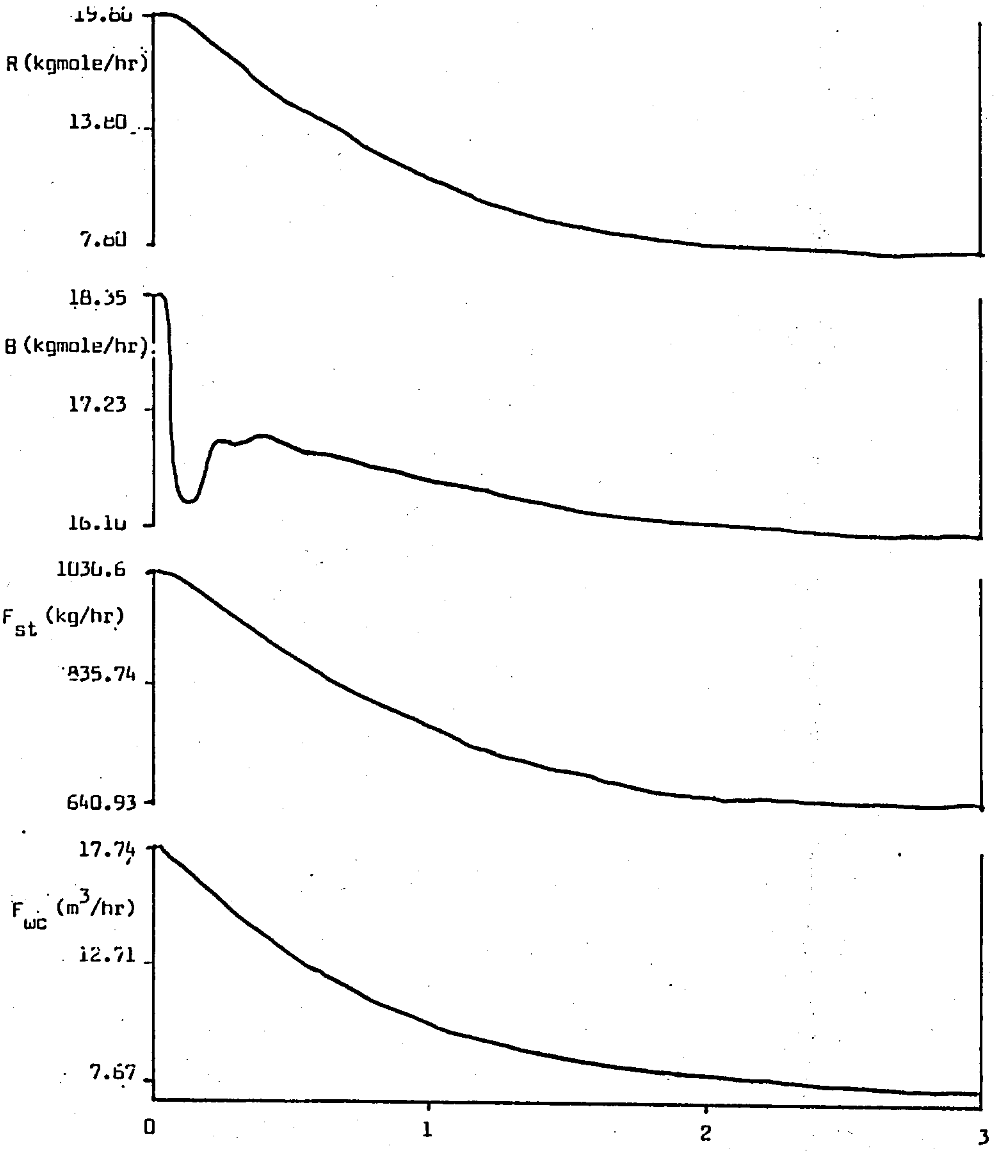


Figure 4.56 Response of the column (flows) in Example 12

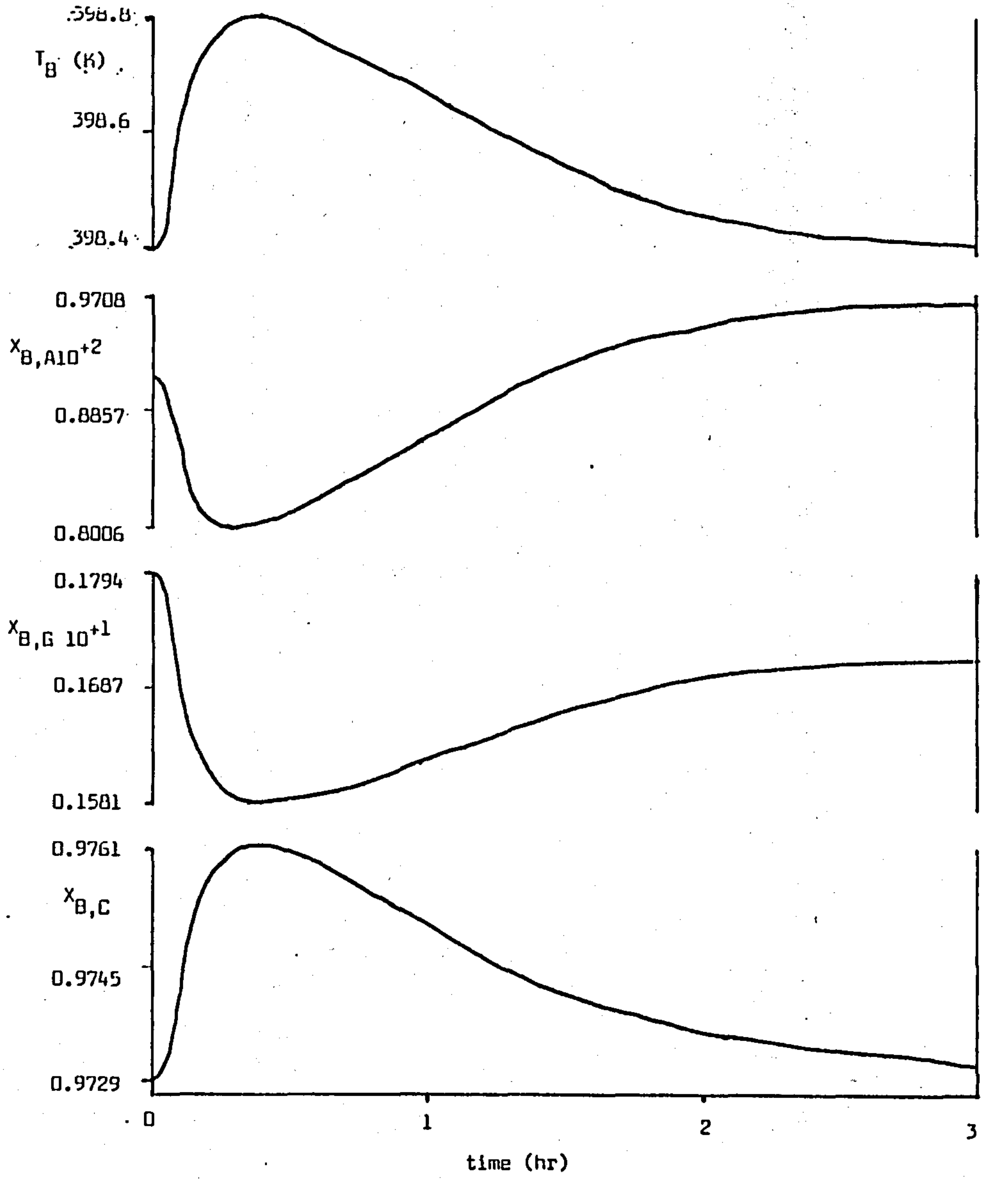


Figure 4.57. Response of the column (bottoms temperature and compositions) in Example 12

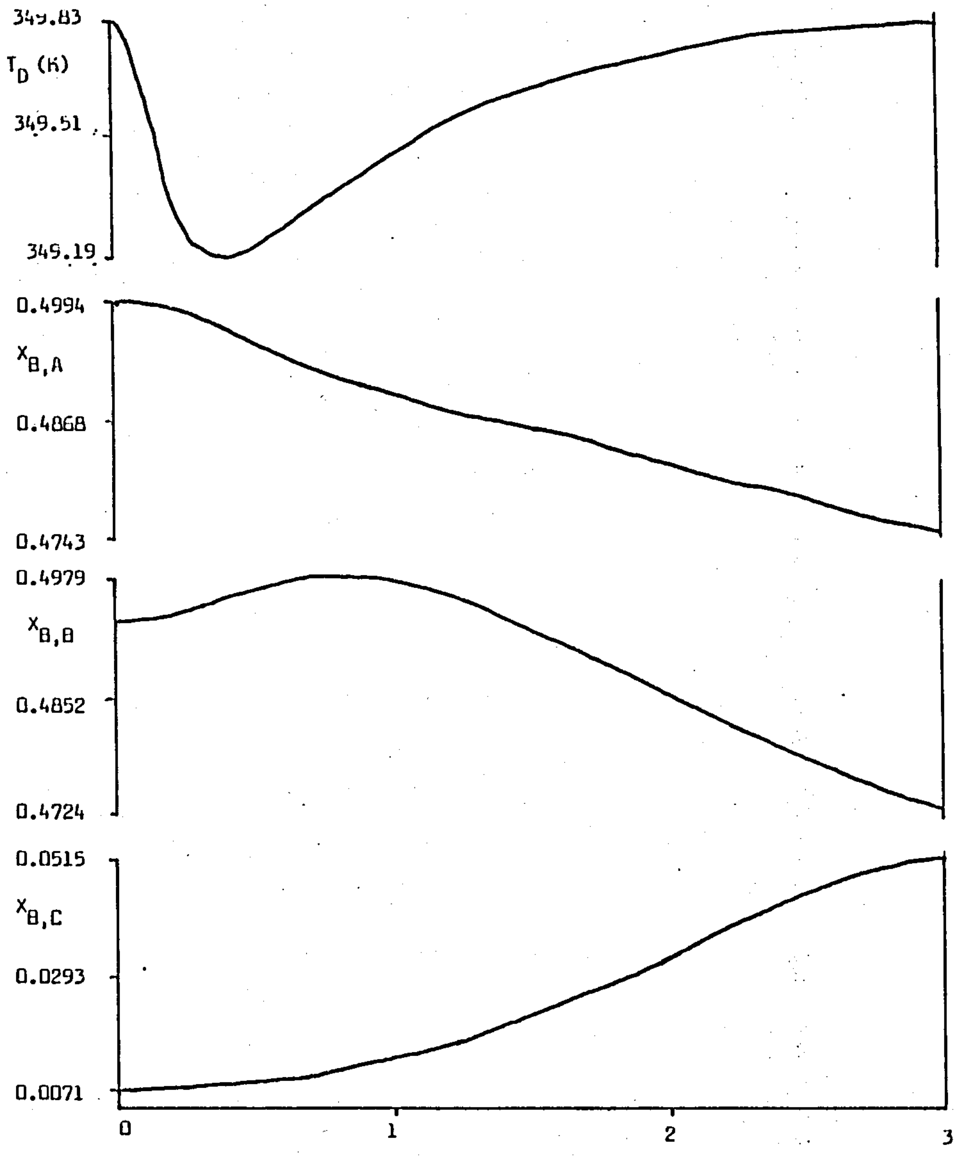


Figure 4.58 Response of the column (distillate temperature and compositions) in Example 12

It can be noted that the difference in this example from the previous one, is the presence of an intermidiate tank between the reactor and the column.

The response of the reactor is same as in previous example. (Figure 4.50).

The responses in the terminal variables of the tank is given in Figure 4.55 . It can be noted that the tank reduces the fluctuations in temperature.

The responses in various terminal variables of the column are plotted in Figures 4.55 to 4.58.

Comparing this example with the previous one, it is concluded that the tank makes the responses in the column a little smoother by eliminating the fluctuations in temperature. But the main affects on column are changes in feed flow rate and in the composition.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

In this work, firstly, a precursor simulation package was extented so that the developed package, CHPDSC, can simulate a chemical plant which may have a reactor, a distillation column, a heat exchanger and two mixing tanks. The chemical plant may have two, three or four components, and the chemical reaction may be first or second order with respect to any componet in the system. The reaction may be in the form of in equal molar balance.

Secondly, various examples are applied to CHPDSC for the investigation of the performance of a controlled multi-purpose chemical plant. When doing this, different types of flowsheets (process structures), control structures, and controller gains are tried for different types of physical systems.

In the previous work [1], firstly control structures for a reactor, a distillation column, a heat exchanger and two mixing tanks, is developed and then for eliminating the overspesifications between control loops, two possible control structure is offered for the hypothetical plant. In one structure which is offered, the distillate flow is kept constant and the liquid in the reflux drum of the column is controlled by manipulating the reflux flow. In the other control structure, the reflux flow is kept constant and the liquid level in the reflux drum is controlled by manipulating the distillate stream.

In this work, two diffrerent control structures have been tried which are explained above. Comparing these two control strategies in various models, it is seen that when the distillate flow is kept constant, the terminal variables give non-oscillatory but much slower responses. Hence the time required to reach the process to the new steady-state condition takes much more operation time. Additionally, if the distillate stream is recycled it is determined that the response of the cooling water in the condenser has high frequency oscillation.

In this work, it determined that the tank between the reactor and the column, primarily reduces the fluctuations in the response of temperature. This makes a little affect to the column temperature. The column is primarily affected by the flow rate and composition changes.

When comparing of Examples 7,8 and 9 (Chapter 4.2), the tank used affects the terminal variables of the process and the responses become overdamped and slow.

The tank also reduces the heating liquid consumption for the reactor and also reduces the steam consumption when the process goes to the new steady-state condition.

Another conclusion is that temperature can be used as a secondary control variable when the set point for the bottom of the column is adjusted close to the boiling point of the heaviest component. In the examples, the main product was the heaviest component and it is observed that the response of the heaviest component composition follows the bottoms temperature.

It is also concluded that the response of the composition of the reactor effluent stream is strongly affected by the residence time in the reactor. Although the reactor temperature is controlled at desired set points, the product concentration is changed with the residence time. In Examles 8, 9, & 10, the composition of the reactor effluent is strongly affected by the concentration changes in the feed stream to the reactor. The effects of residence time and the changes in feed concentration shows that it is difficult to select a suitable measured variable to keep the operational objectives in a chemical plant.

Investigating the phthalic anhydride production, it is seen that, different type of process structures change the dynamic behaviour of the process. Different flowsheets for the same production prosess may changes the easiness of the operability of the production. The different flowsheets models will change the fixed capital investment and change the operational costs. Hence it must be noted that a detailed optimization analysis has to be done depending on the operational objectives when selecting the flowsheet model. This conclusion justifies Buckley's work for the control of chemical processes.

RECOMMENDATIONS FOR FURTHER WORK

In the view of this work, it can be commended ; i) CHPDSC may be extended so that package can also consider the economic variables under different control and process structures. ii) Utilizing the simulation analysis which can be obtained by the CHPDSC , an expert system may be developed which interacts the results of package and search the best control structure and also the controller gains.

APPENDIX

DATA FILES FOR THE EXAMPLES

TABLE A. 1 Data file INSYST for Examples 1, 3 to 5.

```
                  DATA FILE : INSYST

                 Flow-sheeting Parameters
                 ________________________

$SYST            NJ= 4,
                 IFCSTR=  1 , IFDIST=  1 ,
                 IFTANK1= 0 , IFTANK2= 0 ,
                 IFHEX=   0 ,

                 IFTOTRC= 0 ,
                 IFRCDR=  0 , IFRCDT1= 0 ,
                 IFRCBR=  0 , IFRCBT1= 0 $

                 Integration Parameters
                 ______________________

$NPRPLOT         IFPLOTR= 1 , IFPLOTD= 1 ,
                 IFPLTT1= 0 , IFPLTT2= 0 ,

                 DTPLOT= 0.025000 , DTPRINT= 0.02500 ,
                 HSTEP = 0.000200 , TSTOP  = 4.00000 $

                 Physical properties of components
                 _________________________________

 MW       DENS     HVAP     BPT       HVAP     HCAPL     BVP      AVP       CVP
_______  ______   _______  _______   _______  _______   _______  ________  _______

 74.123,  810.  , 43124. ,390.86  , 1963.6 , 2876.3  , 17.216, 3137.02, -94.43
222.232, 1527.  , 49614. ,571.16  , 1256.0 , 1863.1  , 15.998, 4467.01, -83.15
278.340, 1045.  , 79131. ,607.96  , 1256.0 , 1946.8  , 16.954, 4852.47,-138.10
 18.015, 1000.  , 40683. ,373.16  , 1925.9 , 4186.8  , 18.954, 3816.44, -46.13
```

TABLE A. 2 Data file for the reactors in Examples 1 to 5.

```
                DATA FILE : INCSTR

             Initial steady-state conditions
             _______________________________

$RCSET       RX(1)=  0.887490 ,RX(2)=    0.06897  ,RX(3)= 0.02177  ,RX(4)=0.02177,
             RX0(1)= 0.90926  ,RX0(2)=   0.09074  ,RX0(3)=0.00000 ,RX0(4)=0.0,
             RT=     373.159 ,RT0=       297.048 ,
             RTJAVG= 422.570 ,RTJ0=     427.603  ,
             RFS=     45.359 ,RF0S=      45.359  ,
             RFJS=    72.169 ,RV=         2.832  ,RVSET=  2.832 ,
             RTSET=  373.159 ,
             FRCYCS=    .000  $

             System parameters
             _________________

$NRDATA      AHS=       7.9   ,ARRHEN= 2.6101E+08 ,EACTIV= 86546.3   ,
             UR=      567.8   ,VJ=       0.283    ,HRXN=     -205.3   ,
             DENSJL= 997.0    ,CPJL=   2202.3     ,RGC=       8.314   $

$NDRXN       MTRXN=    1,   MORDRXN=       3   $

             Controller Settings
             ___________________

$CSTRCON     KV=  1600.0 ,TAUIV=  0.08000 ,TAUDV=  0.00000 ,
             KJ=    25.5 ,TAUIJ=  0.08500 ,TAUDJ=  0.00000  $
```

TABLE A. 3 Data file for the columns in Examples 1 to 5.

DATA FILE : INDIST

Initial steady-state conditions

```
$DISCSET
         BS=        0.926  ,RS=       23.587  ,DLS=     44.433 ,
         FSTS=   5252.768  ,FWCS=     25.330  ,DVS=      0.000  ,
         TWC=     336.916  ,TST=     627.095  ,TC=     375.590  ,
         PDSET=   101.350  ,MDSET=     0.283  ,MBSET=    0.500  ,
         TCSET=   375.590  ,TNTSET= 465.820  ,TBSET= 606.232  ,
```

System parameters

```
$DISSYST
         NT= 10,
         UB=   1135.0  ,UC=     567.8   ,
         AB=     51.0  ,AC=      37.2   ,
         PB=    110.32 ,PD=     101.35  ,
         MVB=     0.50 ,MVD=      0.28  ,
         VOLRDR=  1.00 ,VSTB=     0.35  ,VWC=  0.28 ,
         TWC0=  297.05 ,DENSWC=1000.0   ,CPWC= 4186.8 ,RG=8.314 $
```

Controller settings

```
$DISTCON
         KB=  1600.0 ,TAUIB=   99.999E+99 ,TAUDB=   0.00000  ,
         KR=      .0 ,TAUIR=   99.999E+99 ,TAUDR=   0.00000  ,
         KDL= 1600.0 ,TAUIDL=  99.999E+99 ,TAUDDL=  0.00000  ,
         KDV=     .0 ,TAUIDV=  99.999E+99 ,TAUDDV=  0.00000  ,
         KST=   77.5 ,TAUIFST= 0.09500    ,TAUDFST=0.01000   ,
         KFWC=   3.8 ,TAUIFWC= 0.08500    ,TAUDFWC=0.00000   ,
```

no. of liq. feed	no. of vap. feed	no. of liq. sidestream	no. of vap. sidestream	no. of heat removals
1,	0,	0,	0,	0

feed stage	feed temp.	feed flowrate	feed composition
5,	373.159	45.359 ,	.88749, .06897, .02177, .02177

Initial temperatures, liquid rates, compositions

tray no.	T	L	x(I)
bottoms	606.232,	0.926,	.00000, .09278, .90720, .00000
1	600.059,	154.911,	.00000, .20094, .79905, .00000
2	594.206,	155.135,	.00000, .32191, .67808, .00000
3	588.290,	155.493,	.00002, .46462, .53534, .00000
4	579.613,	155.065,	.00126, .60382, .39488, .00001
5	490.810,	39.353,	.06103, .66849, .26937, .00109
6	532.067,	18.348,	.02156, .68890, .28911, .00041
7	532.597,	12.433,	.02061, .76430, .21468, .00039
8	530.656,	12.396,	.02120, .83562, .14275, .00040
9	523.616,	12.340,	.02542, .88537, .08872, .00047
10	465.820,	10.761,	.10634, .84329, .04855, .00179
distil.	375.589,	23.586,	.90598, .06847, .00331, .02222
		44.433,	.00000, .00000, .00000, .00000

TABLE A. 4 Data file INSYST for Example 2.

```
                  DATA FILE : INSYST

                 Flow-sheeting Parameters
                 ------------------------
$SYST            NJ= 4,
                 IFCSTR=  1 , IFDIST=  1 ,
                 IFTANK1= 0 , IFTANK2= 1 ,
                 IFHEX=   0 ,

                 IFTOTRC= 0 ,
                 IFRCDR=  0 , IFRCDT1= 0 ,
                 IFRCBR=  0 , IFRCBT1= 0 $

                 Integration Parameters
                 ----------------------
$NPRPLOT         IFPLOTR= 1 , IFPLOTD= 1 ,
                 IFPLTT1= 0 , IFPLTT2= 0 ,

                 DTPLOT= 0.025000 , DTPRINT= 0.02500 ,
                 HSTEP = 0.000200 , TSTOP   = 4.00000 $

                 Physical properties of components
                 ---------------------------------
 MW       DENS    HVAP     BPT      HVAP     HCAPL    BVP     AVP      CVP
-------  ----    ------   ------   ------   ------   ------  -------  -------
 74.123,  810. , 43124. ,390.86 , 1963.6 , 2876.3 , 17.216, 3137.02, -94.43
222.232, 1527. , 49614. ,571.16 , 1256.0 , 1863.1 , 15.998, 4467.01, -83.15
278.340, 1045. , 79131. ,607.96 , 1256.0 , 1946.8 , 16.954, 4852.47,-138.10
 18.015, 1000. , 40683. ,373.16 , 1925.9 , 4186.8 , 18.954, 3816.44, -46.13
```

TABLE A. 5 Data file for the tank in Example 2.

DATA FILE : INTANK2

Initial steady-state conditions

```
$T2CSET   T2X(1)=  0.88749 ,T2X(2)=  0.06897 ,
          T2X(3)=  0.02177 ,T2X(4)=  0.02177 ,
          T2T=    373.159  ,T2T0=  373.159   ,
          T2V=      0.780  ,T2VSET=  0.780   ,
          T2FS=    45.359   $
```

Controller Setting

```
$T2CON    KVT2=  400.0  $
```

TABLE A. 6 Data file INSYST for Examples 6 to 8.

```
                 DATA FILE : INSYST

                Flow-sheeting Parameters
                ________________________
$SYST           NJ= 4,
                IFCSTR=  1 , IFDIST=  1 ,
                IFTANK1= 0 , IFTANK2= 0 ,
                IFHEX=   0 ,

                IFTOTRC= 0 ,
                IFRCDR=  0 , IFRCDT1= 0 ,
                IFRCBR=  0 , IFRCBT1= 0 $

                Integration Parameters
                ______________________
$NPRPLOT        IFPLOTR= 1 , IFPLOTD= 1 ,
                IFPLTT1= 1 , IFPLTT2= 1 ,

                DTPLOT= 0.025000 , DTPRINT= 0.02500 ,
                HSTEP = 0.000200 , TSTOP  = 4.00000 $

                Physical properties of components
                _________________________________
 MW       DENS     HVAP    BPT      HVAP     HCAPL    BVP     AVP      CVP
_______  ______   ______  ______   ______   ______   ______  _______  ______

 74.123,  810. , 43124. ,390.86 , 1963.6 , 2876.3 , 17.216, 3137.02, -94.43
148.118, 1527. , 49614.. ,559.96 , 1256.0 , 1863.1 , 15.998, 4467.01, -83.15
278.340, 1045. , 79131. ,607.96 , 1256.0 , 1946.8 , 16.954, 4852.47,-138.10
 18.015, 1000. , 40683. ,373.16 , 1925.9 , 4186.8 , 18.954, 3816.44, -46.13
```

TABLE A. 7 Data file for the reactors in Examples 6,7 & 8

```
               DATA FILE : INCSTR

            Initial steady-state conditions
            -------------------------------
$RCSET      RX(1)=  0.88027  ,RX(2)=    0.06657  ,RX(3)= 0.02658  ,RX(4)=0.02658,
            RX0(1)= 0.90926  ,RX0(2)=   0.09074  ,RX0(3)=0.00000  ,RX0(4)=0.0,
            RT=     374.826  ,RT0=      297.048  ,
            RTJAVG= 421.911  ,RTJ0=     427.603  ,
            RFS=     44.184  ,RF0S=      45.359  ,
            RFJS=    60.812  ,RV=         2.832  ,RVSET=  2.832 ,
            RTSET=  374.826  ,
            FRCYCS=    .000  $

            System parameters
            -----------------
$NRDATA     AHS=       7.9  ,ARRHEN= 2.6101E+08 ,EACTIV= 86546.3  ,
            UR=      567.8  ,VJ=       0.283    ,HRXN=    -205.3  ,
            DENSJL= 997.0   ,CPJL=   2202.3     ,RGC=       8.314 $

$NDRXN       MTRXN=     1,  MORDRXN=       3  $

             Controller Settings
             -------------------
$CSTRCON     KV=  1600.0 ,TAUIV=  0.08000 ,TAUDV=  0.00000 ,
             KJ=    25.5 ,TAUIJ=  0.08000 ,TAUDJ=  0.01000  $
```

TABLE A. 8 Data file for the columns in Examples 6 and 7.

```
                DATA FILE : INDIST

            Initial steady-state conditions

$DISCSET
            BS=          1.232  ,RS=        23.587  ,DLS=      42.952  ,
            FSTS=     4027.458  ,FWCS=      16.767  ,DVS=       0.000  ,
            TWC=       346.538  ,TST=      622.697  ,TC=      374.825  ,
            PDSET=     101.350  ,MDSET=      0.283  ,MBSET=     0.500  ,
            TCSET=     374.825  ,TNTSET=  399.586  ,TBSET=  605.381   ,

            System parameters

$DISSYST
            NT= 10,
            UB=    1135.0  ,UC=     567.8    ,
            AB=      51.0  ,AC=      37.2    ,
            PB=     110.32 ,PD=     101.35   ,
            MVB=      0.50 ,MVD=      0.28   ,
            VOLRDR=  1.00  ,VSTB=     0.35   ,VWC=  0.28 ,
            TWC0=   297.05 ,DENSWC=1000.0    ,CPWC= 4186.8 ,RG=8.314 $

            Controller settings

$DISTCON
            KB=   1600.0 ,TAUIB=   99.999E+99 ,TAUDB=   0.00000  ,
            KR=       .0 ,TAUIR=   99.999E+99 ,TAUDR=   0.00000  ,
            KDL=  1600.0 ,TAUIDL=  99.999E+99 ,TAUDDL=  0.00000  ,
            KDV=      .0 ,TAUIDV=  99.999E+99 ,TAUDDV=  0.00000  ,
            KST=   200.0 ,TAUIFST= 0.09500    ,TAUDFST=0.01000   ,
            KFWC=    3.8 ,TAUIFWC= 0.08500    ,TAUDFWC=0.00000   ,

no. of      no. of      no. of liq.   no. of vap.   no. of heat
liq. feed   vap. feed   sidestream    sidestream    removals

1,          0,          0,            0,            0

feed     feed      feed
stage    temp.     flowrate     feed composition

5,       374.825,   44.1840,  .88025, .06655, .02660, .02660

Initial temperatures, liquid rates, compositions

tray no.    T          L                    x(I)

bottom    605.381,     1.232,   .00000, .04807, .95192, .00000
   1      589.410,   145.537,   .00000, .17562, .82438, .00000
   2      568.856,   147.686,   .00000, .39089, .60910, .00000
   3      551.040,   153.675,   .00019, .64349, .35630, .00000
   4      531.943,   157.978,   .00597, .81318, .18073, .00009
   5      454.785,   148.563,   .13399, .77263, .09062, .00275
   6      485.839,    19.236,   .05150, .87568, .07169, .00111
   7      485.819,    14.442,   .04998, .92244, .02648, .00108
   8      483.284,    14.500,   .05337, .93722, .00825, .00114
   9      470.159,    14.204,   .08022, .91569, .00249, .00158
  10      399.587,    14.514,   .36779, .62479, .00058, .00681
distil.   374.825,    23.586,   .90550, .06708, .00004, .02736
                      42.9516,  .00000, .00000, .00000, .00000
```

TABLE A. 9 Data file for the reactor in Example 8 and 9.

```
               DATA FILE : INCSTR

          Initial steady-state conditions

$RCSET    RX(1)=  0.88027  ,RX(2)=    0.06657  ,RX(3)= 0.02658  ,RX(4)=0.02658,
          RX0(1)= 0.90926  ,RX0(2)=   0.09074  ,RX0(3)=0.00000 ,RX0(4)=0.0,
          RT=     374.826  ,RT0=      297.048  ,
          RTJAVG= 421.911  ,RTJ0=     427.603  ,
          RFS=     41.184  ,RF0S=      43.091  ,
          RFJS=    60.812  ,RV=         2.832  ,RVSET=  2.832 ,
          RTSET=  374.826  ,
          FRCYCS=    .000  $

          System parameters

$NRDATA   AHS=       7.9  ,ARRHEN= 2.6101E+08 ,EACTIV= 86546.3  ,
          UR=      567.8  ,VJ=      0.283      ,HRXN=    -205.3  ,
          DENSJL= 997.0   ,CPJL=   2202.3      ,RGC=      8.314  $

$NDRXN    MTRXN=     1,  MORDRXN=      3  $

          Controller Settings

$CSTRCON  KV=  800.0  ,TAUIV=  0.08000 ,TAUDV=  0.00000 ,
          KJ=    5.0  ,TAUIJ=  0.08500 ,TAUDJ=  0.00000  $
```

TABLE A.10 Data file for the column in Example 8 and 9.

```
                 DATA FILE : INDIST

          Initial steady-state conditions
          -------------------------------
 $DISCSET
          BS=         1.232  ,RS=       23.587  ,DLS=     42.952  ,
          FSTS=    4027.458  ,FWCS=     16.767  ,DVS=      0.000  ,
          TWC=      346.538  ,TST=     622.697  ,TC=     374.825  ,
          PDSET=    101.350  ,MDSET=     0.283  ,MBSET=    0.500  ,
          TCSET=    374.825  ,TNTSET= 399.586  ,TBSET= 605.381  ,

          System parameters
          -----------------
 $DISSYST
          NT= 10,
          UB=    1135.0  ,UC=     567.8    ,
          AB=      51.0  ,AC=      37.2    ,
          PB=     110.32 ,PD=     101.35   ,
          MVB=      0.50 ,MVD=      0.28   ,
          VOLRDR=  1.00  ,VSTB=     0.35   ,VWC=  0.28 ,
          TWC0=   297.05 ,DENSWC=1000.0    ,CPWC= 4186.8 ,RG=8.314 $

          Controller settings
          -------------------
 $DISTCON
          KB=    720.0 ,TAUIB=  99.999E+99 ,TAUDB=  0.00000  ,
          KR=       .0 ,TAUIR=  99.999E+99 ,TAUDR=  0.00000  ,
          KDL=   720.0 ,TAUIDL= 99.999E+99 ,TAUDDL= 0.00000  ,
          KDV=      .0 ,TAUIDV= 99.999E+99 ,TAUDDV= 0.00000  ,
          KST=    77.5 ,TAUIFST= 0.09500   ,TAUDFST=0.01000  ,
          KFWC=    1.3 ,TAUIFWC= 0.08500   ,TAUDFWC=0.00000  ,

 no. of      no. of      no. of liq.   no. of vap.   no. of heat
 liq. feed   vap. feed   sidestream    sidestream    removals
 ---------   ---------   -----------   -----------   -----------
 1,          0,          0,            0,            0

 feed    feed      feed
 stage   temp.     flowrate     feed composition
 -----   -------   --------     ------------------------------
 5,      374.825,   44.1840,  .88025, .06655, .02660, .02660

 Initial temperatures, liquid rates, compositions
 ------------------------------------------------
 tray no.     T          L                  x(I)
 --------  -------    -------    ------------------------------
 bottom    605.381,     1.232,  .00000, .04807, .95192, .00000
    1      589.410,   145.537,  .00000, .17562, .82438, .00000
    2      568.856,   147.686,  .00000, .39089, .60910, .00000
    3      551.040,   153.675,  .00019, .64349, .35630, .00000
    4      531.943,   157.978,  .00597, .81318, .18073, .00009
    5      454.785,   148.563,  .13399, .77263, .09062, .00275
    6      485.839,    19.236,  .05150, .87568, .07169, .00111
    7      485.819,    14.442,  .04998, .92244, .02648, .00108
    8      483.284,    14.500,  .05337, .93722, .00825, .00114
    9      470.159,    14.204,  .08022, .91569, .00249, .00158
   10      399.587,    14.514,  .36779, .62479, .00058, .00681
 distil.   374.825,    23.586,  .90550, .06708, .00004, .02736
                       42.951, .00000, .00000, .00000, .00000
```

TABLE A.11 Data file INSYST for Example 9.

```
                DATA FILE : INSYST

               Flow-sheeting Parameters

$SYST          NJ= 4,
               IFCSTR=  1 , IFDIST=  1 ,
               IFTANK1= 1 , IFTANK2= 0 ,
               IFHEX=   0 ,

               IFTOTRC= 0 ,
               IFRCDR=  0 , IFRCDT1= 0 ,
               IFRCBR=  0 , IFRCBT1= 0 $

               Integration Parameters

$NPRPLOT       IFPLOTR= 1 , IFPLOTD= 1 ,
               IFPLTT1= 1 , IFPLTT2= 1 ,

               DTPLOT= 0.025000 , DTPRINT= 0.02500 ,
               HSTEP = 0.000200 , TSTOP   = 4.00000 $

               Physical properties of components

 MW       DENS     HVAP     BPT       HVAP     HCAPL     BVP     AVP       CVP

 74.123,  810. , 43124. ,390.86 , 1963.6 , 2876.3 , 17.216, 3137.02, -94.43
148.118, 1527. , 49614. ,559.96 , 1256.0 , 1863.1 , 15.998, 4467.01, -83.15
278.340, 1045. , 79131. ,607.96 , 1256.0 , 1946.8 , 16.954, 4852.47,-138.10
 18.015, 1000. , 40683. ,373.16 , 1925.9 , 4186.8 , 18.954, 3816.44, -46.13
```

TABLE A.12 Data file for the tank in Example 9.

```
                DATA FILE : INTANK1

             Initial steady-state conditions
             -------------------------------
$T1CSET      T1X(1)=  0.90926 ,T1X(2)=  0.09074 ,
             T1X(3)=  0.00000 ,T1X(4)=  0.00000 ,
             T1T=   297.048   ,T1T0=  297.048   ,
             T1V=      2.12   ,T1VSET=   2.12   ,
             T1FS=   45.359  $

             Controller setting
             ------------------
$T2CON       KVT1=  400.0  $
```

TABLE A.13 Data file INSYST for Example 10 and 12.

```
                 DATA FILE : INSYST

                Flow-sheeting Parameters

$SYST           NJ= 3,
                IFCSTR=  1 , IFDIST=  1 ,
                IFTANK1= 0 , IFTANK2= 1 ,
                IFHEX=   0 ,

                IFTOTRC= 0 ,
                IFRCDR=  0 , IFRCDT1= 0 ,
                IFRCBR=  0 , IFRCBT1= 0 $

                Integration Parameters

$NPRPLOT        IFPLOTR= 1 , IFPLOTD= 1 ,
                IFPLTT1= 1 , IFPLTT2= 1 ,

                DTPLOT= 0.02500 , DTPRINT= 0.02500 ,
                HSTEP = 0.00015 , TSTOP   = 5.00000 $

                Physical properties of components

MW      DENS    HVAP     BPT      HVAP     HCAPL    BVP      AVP      CVP

46.07 , 789. , 38769. ,351.46 , 1603.5 , 2847.0 , 13.912 , 3804.0 , -41.68
60.09 , 786. , 39857. ,355.36 , 1720.8 , 2595.8 , 18.693 , 3640.2 , -53.54
53.08 , 850. , 16453. ,399.16 , 1687.3 , 1913.4 , 15.494 , 3151.1 , -69.15
```

TABLE A.14 Data file for the tanks in Examples 10 and 12.

```
                DATA FILE : INTANK2

            Initial steady-state conditions
            -------------------------------
$T2CSET     T2X(1)=  0.30104 ,T2X(2)=  0.30104 , T2X(3)= 0.39792,
            T2T=   347.048   ,T2T0=  347.048   ,
            T2V=     0.708   ,T2VSET=  0.708   ,
            T2FS=   45.359   $

            Controller Setting
            ------------------
$T2CON      KVT2=  400.0  $
```

TABLE A.15 Data file for the reactor in Examples 10 to 12.

```
                 DATA FILE : INCSTR

            Initial steady-state conditions

$RCSET      RX(1)=  0.30104  ,RX(2)=    0.30104  ,RX(3)= 0.39792 ,
            RX0(1)= 0.50000  ,RX0(2)=   0.50000  ,RX0(3)=0.00000 ,
            RT=     347.048  ,RT0=      297.048  ,
            RTJAVG= 323.901  ,RTJ0=     297.048  ,
            RFS=     45.359  ,RF0S=      45.359  ,
            RFJS=     3.330  ,RV=         2.283  ,RVSET=  2.832 ,
            RTSET=  347.048  ,
            FRCYCS=    .000  $

            System parameters

$NRDATA     AHS=        7.9  ,ARRHEN= 437.948 ,  EACTIV= 46519.3  ,
            UR=       567.8  ,VJ=     0.283,     HRXN=  -69778.9  ,
            DENSJL= 1000.0   ,CPJL= 4186.8,      RGC=       8.314 $

             Controller Settings

$CSTRCON     KV=    801.0 ,TAUIV=  0.08500 ,TAUDV=  0.00000 ,
             KJ=      4.8 ,TAUIJ=  0.09000 ,TAUDJ=  0.01000 ,
```

TABLE A.16 Data file for the column in Example 10.

```
                 DATA FILE : INDIST

            Initial steady-state conditions
            _______________________________

$DISCSET
            BS=        18.347  ,RS=        28.350  ,DLS=     27.012  ,
            FSTS=    1069.518  ,FWCS=      19.176  ,DVS=      0.000  ,
            TWC=      324.473  ,TST=      409.471  ,TC=     349.825  ,
            PDSET=    101.350  ,MDSET=    409.471  ,MBSET=    0.500  ,
            TCSET=    349.826  ,TNTSET=   353.826  ,TBSET=  398.437  ,

            System parameters
            _________________

$DISSYST
            NT= 10,
            UB=    1135.0  ,UC=     567.8   ,
            AB=      51.0  ,AC=      37.2   ,
            PB=    110.32  ,PD=    101.35   ,
            MVB=     0.50  ,MVD=     0.28   ,
            VOLRDR=  1.00  ,VSTB=    0.35   ,VWC=  0.28 ,
            TWC0=  297.05  ,DENSWC=1000.0   ,CPWC= 4186.8 ,RG=8.314 $

            Controller settings
            ___________________

$DISTCON
            KB=    881.0 ,TAUIB=   99.999E+99 ,TAUDB=   0.00000  ,
            KR=       .0 ,TAUIR=   99.999E+99 ,TAUDR=   0.00000  ,
            KDL=   881.0 ,TAUIDL=  99.999E+99 ,TAUDDL=  0.00000  ,
            KDV=      .0 ,TAUIDV=  99.999E+99 ,TAUDDV=  0.00000  ,
            KST=    77.5 ,TAUIFST= 0.09500    ,TAUDFST=0.00000   ,
            KFWC=    1.3 ,TAUIFWC= 0.08500    ,TAUDFWC=0.00000   ,

no. of       no. of       no. of liq.    no. of vap.    no. of heat
liq. feed    vap. feed    sidestream     sidestream     removals
_________    _________    ___________    ___________    ___________

1,           0,           0,             0,             0

feed    feed      feed
stage   temp.     flowrate     feed composition
_____   _______   ________   ______________________

5,      347.048,  45.3593,   .30104, .30104, .39792

Initial temperatures, liquid rates, compositions
________________________________________________

tray no.    T          L                 x(I)
________  _______   _______    ______________________

bottom    398.436,   18.346,   .00913, .01792, .97293
   1      390.354,  134.383,   .03767, .06701, .89530
   2      380.496,  114.898,   .09111, .14803, .76085
   3      371.903,   98.149,   .16401, .24290, .59307
   4      366.587,   88.313,   .23023, .31081, .45895
   5      363.938,   83.276,   .27902, .34372, .37725
   6      360.219,   32.781,   .32385, .41690, .25923
   7      357.549,   30.945,   .36889, .47179, .15930
   8      355.187,   29.860,   .40336, .50560, .09102
   9      354.624,   29.228,   .43188, .52007, .04804
  10      353.812,   28.876,   .46111, .51657, .02230
distil.   349.825,   28.349,   .49930, .49333, .00736
                     27.012,   .00000  .00000, .00000
```

TABLE A.17 Data file INSYST for Example 11.

```
                    DATA FILE : INSYST

                   Flow-sheeting Parameters

$SYST              NJ= 3,
                   IFCSTR=  1 , IFDIST=  1 ,
                   IFTANK1= 0 , IFTANK2= 0 ,
                   IFHEX=   0 ,

                   IFTOTRC= 0 ,
                   IFRCDR=  0 , IFRCDT1= 0 ,
                   IFRCBR=  0 , IFRCBT1= 0 $

                   Integration Parameters

$NPRPLOT           IFPLOTR= 1 , IFPLOTD= 1 ,
                   IFPLTT1= 1 , IFPLTT2= 1 ,

                   DTPLOT= 0.02500 , DTPRINT= 0.02500 ,
                   HSTEP = 0.00015 , TSTOP   = 4.00000 $

                   Physical properties of components

MW      DENS    HVAP     BPT      HVAP     HCAPL    BVP      AVP      CVP

46.07 , 789. , 38769. ,351.46 , 1603.5 , 2847.0 , 13.912 , 3804.0 , -41.68
60.09 , 786. , 39857. ,355.36 , 1720.8 , 2595.8 , 18.693 , 3640.2 , -53.54
53.08 , 850. , 16453. ,399.16 , 1687.3 , 1913.4 , 15.494 , 3151.1 , -69.15
```

TABLE A.18 Data file for the columns in Examples 11 and 12.

DATA FILE : INDIST

Initial steady-state conditions

```
$DISCSET
          BS=        18.347   ,RS=       28.350  ,DLS=     27.012   ,
          FSTS=    1069.518   ,FWCS=     19.176  ,DVS=      0.000   ,
          TWC=      324.473   ,TST=     409.471  ,TC=     349.825   ,
          PDSET=    101.350   ,MDSET=   409.471  ,MBSET=    0.500   ,
          TCSET=    349.826   ,TNTSET= 353.826   ,TBSET= 398.437    ,
```

System parameters

```
$DISSYST
          NT= 10,
          UB=    1135.0  ,UC=     567.8    ,
          AB=      51.0  ,AC=      37.2    ,
          PB=    110.32  ,PD=    101.35    ,
          MVB=     0.50  ,MVD=     0.28    ,
          VOLRDR=  1.00  ,VSTB=    0.35    ,VWC=  0.28 ,
          TWCO=  297.05  ,DENSWC=1000.0    ,CPWC= 4186.8 ,RG=8.314 $
```

Controller settings

```
$DISTCON
          KB=    881.0 ,TAUIB=   99.999E+99 ,TAUDB=   0.00000   ,
          KR=   1201.0 ,TAUIR=   99.999E+99 ,TAUDR=   0.00000   ,
          KDL=      .0 ,TAUIDL= 99.999E+99 ,TAUDDL= 0.00000    ,
          KDV=      .0 ,TAUIDV= 99.999E+99 ,TAUDDV= 0.00000    ,
          KST=    77.5 ,TAUIFST= 0.09500    ,TAUDFST=0.00000    ,
          KFWC=    1.3 ,TAUIFWC= 0.08500    ,TAUDFWC=0.00000    ,
```

no. of liq. feed	no. of vap. feed	no. of liq. sidestream	no. of vap. sidestream	no. of heat removals
1,	0,	0,	0,	0

feed stage	feed temp.	feed flowrate	feed composition
5,	347.048,	45.359,	.30104, .30104, .39792

Initial temperatures, liquid rates, compositions

tray no.	T	L	x(I)
bottom	398.436,	18.346,	.009135, .01792, .97293
1	390.354,	134.383,	.037677, .06701, .89530
2	380.496,	114.898,	.091115, .14803, .76085
3	371.903,	98.149,	.164015, .24290, .59307
4	366.587,	88.313,	.230236, .31081, .45895
5	363.938,	83.276,	.279021, .34372, .37725
6	360.219,	32.781,	.323854, .41690, .25923
7	357.549,	30.945,	.368897, .47179, .15930
8	355.187,	29.860,	.403367, .50560, .09102
9	354.624,	29.228,	.431885, .52007, .04804
10	353.812,	28.876,	.461111, .51657, .02230
distil.	349.825,	28.349,	.499303, .49333, .00736
		27.012,	.000000 .00000, .00000

REFERENCES

1. Akman Uğur , "Dynamic Simulation of a Multi-purpose Chemical Plant", M.S. Thesis, Boğaziçi University. (1987).

2. Berman S., Andrew A. Melnychuk, and Donald F. Othmer, "Dibutyl Phthalate, Reaction Rate of Catalitic Esterification",*Industrial and Engineerig Chemistry*, Vol 40, NO 7, p 1312, 1948.

3. Buckley P. S., *Tecniques of Process Control*, Wiley & Sons, New York (1964).

4. Foss A. S., "Critique of Chemical Process Control Theory", *AIChe J.*, 18, p 209 (1973).

5. Govind R. and G.J. Powers, "Control System Synthesis Strategies", *AIChe J.*, 28, p 60 (1982).

6. Gould L. A., W. Kipiak ," Dynamic Optimization and Control of a Stirred-Tank Chemical Reactor",

7. Groggings P. H. , " Unit Processes in Organic Synthesis", 2nd ed., New York, Mc Graw Hill Co., 1938.

8. Kestenbaum A., R. Shinnar and F. E. Thau, "Design Concepts for Process Control", *Ind. Eng. Chem. Process Des. Dev.*, Vol 15, No 1, p 2 (1976).

9. Lee Wooyoung and Vern W. Weekman, "Advanced Control Practice in the Chemical Process Industry : A View from Industry", *AIChe J.*, 22, p 27 (1976).

10. Luyben, W. L., *Process Modelling, Simulation and Control for Chemical Engineers*, McGraw Hill, New York, 1973.

11. Morari M, Y. Arkun and G.Stephanopoulos, "Studies in the Synthesis of Control Structures for Chemical Processes", *AIChe J.*, 26, p 220 (1980).

12. Stephanopoulos, G., "Synthesis of Control Systems for Chemical Plants : A Challenge for Creativity", *Computers and Chemical Engineering*,Vol. 7, No 4, p 331, (1983).

13. Williams, T. J., R. E, Otto, "A Generalized Chemical Processing Model for the Investigation of Computer Control",*Trans. Am. Inst. Electr. Eng.*,Vol. 26, p. 1101, (1971).

REFERENCES NOT CITED

Adelman Alvin and William F. Stewens, "Process Optimization by the Complex Method", *AIChe J.*, 18, p 20 (1972).

Brambilla A., A. Carracciolo Di Forino, R. Celati, J. H. Kordesz and G. Nardini, "Study of Dynamic Behaviour of Chemical Plants by Digital Simulation", *Chem. Eng. Sci.*, Vol 26, p 1101 (1971).

Bristol E. H., "On a New Measure of Interaction for Multivariable Process Control", *Trans. IEEE*, p 133 (January 1966).

Douglas J. M., *Process Dynamics and Control*, Vol: 2, Prentice-Hall, N.J., 1972 .

Di bella Carlos W. and William F. Stevens, "Process Optimization by Nonlinear Programing", *Ind. Eng. Chem. Process Des. Dev.*, Vol 4, No 1, p 42 (1965).

Himmelblau D. M. and Bishoff K. B., *Process Analysis and Simulation*, Wiley, 1968.

Hodgman, C. D., "Handbook of Chemistry and Physics", 23rd ed., Cleveland Chemical Rubber Pub. Co., 1939.

Jensen K. F. and L. Henry, "Evaluation of Changeover Control Policies by Singular Value Analysis - Effects of Scaling", *AIChe J.*, 31, p 135 (1985).

McAvoy Thomas, "Some Results on Dynamic Interaction Analysis of Complex Control Systems", *Ind. Eng. Chem. Process Des. Dev.*, Vol 22, No 1, p 42 (1983).

Perry , R.H., D. Green, *Chemical Engineers' Handbook*, 6 th. Edition, 1986.

Stephanopoulos, G., *Chemical Procees Control*, Prentice Hall Inc., New Jersey, 1984.