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COMPUTER CONTROL OF TWO CONTINUOUS
STIRRED-TANK REACTORS IN SERIES

by

NKONGHO EBOBEBANGAH, EGBEWATT, MSc

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The University of Aston in Birmingham

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1984

PhD

SUMMARY

This study is focused on reacting systems in a train of reactors and the different digital control strategies that can be developed to eliminate the effect of disturbances entering the system. A Honeywell 316 minicomputer is interfaced via HADIOS to a pilot plant containing two C.S.T.R.s connected in series and a partial simulation of a first order irreversible exothermic chemical reaction taking place in them is carried out. This control system offers only a single communication channel from the user to the output multiplexers and since all the control functions are performed by software of one digital system, the frequency with which the control functions are updated is of utmost importance. The reaction heat is provided by heaters placed in the reactors which are triggered on receipt of appropriate signals from the computer.

A judicious use of solenoids and multiplexers allows the regulation of two pneumatic process control valves using one air supply line and the scanning of eight thermocouples. Two coils, one in each reactor, provide the conduit for the independently controlled cooling water whose flow rate is used as the manipulative variable for implementing the different control schemes and a surface for heat exchange with reactors. Using differential equations to represent the plant, a total simulation of the system is achieved in a FORTRAN programme that runs interactively on the HARRIS 800 computer and the experimental runs provide data suitable for verification of the theoretical model. Based on the large axial temperature gradient in the cooling coils, the model assumes a chain of cells each of uniform temperature but necessarily different from the rest and twenty five of these are used for the total simulation.

All implemental control functions are performed by the software of the control computer in the direct digital mode. Unstable systems are stabilised using controllers and the relative stabilities of open and closed loop stable systems are established by constructing Lyapunov's function. The control strategies adopted vary from those based on absolute error of control variables, through absolute values of measured disturbances to others derived from system equations and plant parameters. The first group consists of feedback controllers centered on the first reactor and a combination of feedback and feedforward controllers in the second reactor. Invariance control of reactor and coil temperatures is attainable on both reactors by using an iterative method that updates the system parameters and calculates flow rates from the system equations. Decoupling control of the model is made possible by first establishing an axial temperature profile in the cooling coil and using piecewise decoupling to select an appropriate response constant for the system that leaves it within the stated constraints.

Keywords:- Simulation; Single channel control; Invariance and Decoupling control.

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Table of Symbols

A	Lyapunov's matrix
A_{ij}	elements of matrix A
C_a	concentration of reactant (kg/m^3)
C_p	specific heat of feed (kJ/kg K)
a_1, a_2, a_3	exponential decay constant (s)
D_s	digital signal
ΔE	activation energy (kJ/kg mole)
F	feed flow rate (m^3/s)
ΔH	heat of reaction (kJ/kg)
J	Jacobian matrix
J_{ij}	elements of Jacobian matrix J
k	reaction rate constant ($k_0 \exp(-E/RT)$)
k_0	frequency factor(s)
K_c	proportional gain (m^3/s)
R	radius of coil
R	Universal gas constant (kJ/kg mole K)
t	time (s)
T_2, T_5	reactor 1 & 2 temperatures (K)
$T_{3,i}$	coil one temperature profile (K) $i=1,2,\dots,n$
$T_{6,i}$	coil two temperature profile (K) $i=1,2,\dots,n$
UA_1, UA_2	heat transfer conductance in reactors 1&2 (kJ/s K)
X_1, X_4	dimensionless concentration of reactant in reactors 1&2 C_a/C_{a0}
X_2, X_5	dimensionless temperature in reactors 1&2 $((T_2 - T_0)/(E/RT_0))$
$X_{3,i}, X_{6,i}$	dimensionless temperature profile in coil 1&2 (K) $i=1,2,\dots,n$ $((T_{3,i} - T_0)/(E/RT_0))$
Y_1	dimensionless inlet concentration (C_a/C_{a0})
Y_2	dimensionless inlet temperature into reactors $((T_{20} - T_0)/(E/RT_0))$
Y_3	dimensionless inlet temperature into coils $((T_{\infty} - T_0)/(E/RT_0))$
π	pi

p	dimensionless heat transfer coefficient $(UA/PC_p F)$
B	dimensionless adiabatic temp. $(-^{\Delta}H)C_{ao}^{\Delta E}/(PC_p T_o^2 RT)$
κ	$RT/\Delta E$
β	$1/\kappa$
ρ	density of feed (kg/m^3)
$\lambda_1, \lambda_2, \lambda_3$	eigenvalues of matrix J
τ	residence time in reactors (s)
τ_c	residence time in coils (s)
τ_m	time constant of measuring element (s)
τ_v	time constant of control valve (s)
α_1	trigger angle
α	$(\pi - \alpha_1)$

Subscripts

ss	steady state
cal	calculated
act	actual
o	inlet condition
c	pertaining to coolant stream

Superscripts

*	sampled values
^	perturbation
.	differential with respect to time

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CHAPTER ONE

INTRODUCTION

The use of digital computers to supervise, monitor, control and simulate processes in chemical industries is receiving greater applicability due to their cheapness, ease of implementation, flexibility in operation of plants and fast speed of resolution of large and difficult mathematical problems. While mainframe computers are employed in supervisory roles or as database systems in whole plants or units thereof, microcomputers are increasingly being used as controllers in the different process units. In certain process plants the use of conventional control becomes inadequate because of large throughput, the need to regulate by-products and frequent property changes in a variety of feeds and in such circumstances more advanced control techniques are applied with the aid of the computer. Human interference is reduced to the barest minimum as the integrated computers strive to maintain the plant at some predetermined optimal state of production making the necessary adjustments if there is a change in operating parameters. The use of computers for simulating processes has become a valuable tool for monitoring and improving existing plants and for the development of new processes. The appropriateness of the simulation technique depends on the closeness in representation of the mathematical model to the actual system.

The objectives of this work are:

- (i) the study of the stability problems inherent in a series of two connected C.S.T.R.'s and ^{to compare} the partially and totally simulated results.
- (ii) the development of computer control strategies that will ensure a stable system operating under the influence of different disturbances.

The process unit in this work consists of two C.S.T.R.'s connected in series in which a first order irreversible exothermic reaction is taking place. Water is used both as reactor feed and also as cooling liquid for the reactors. The experimental rig is interfaced to a Honeywell 316 minicomputer which plays the dual role of supervisor and controller. It calculates the mass balance and sends out signals proportional to the heat of reaction to immersion heaters situated in the reactors. Flow rates and temperatures are monitored by computer and when necessary, signals are issued to flow control valves to regulate the latter. In addition to proportional controllers which are based on deviation of system variables from set values due to disturbances, noninteracting and invariance controls are implemented on the system. Due to the propagation of disturbances leaving the first reactor into the second, both feedforward and feedback controls are implemented on the latter. The system is operated at the open loop stable steady state and the effects of disturbances with and without controls are noted, simulated and experimental results being displayed on graphs plotted on the Harris 800.

There has been a greater emphasis on constructing a unit that is representative of those employed in industry rather than using one

whose mathematical model is simple and elegant but which differs in important respects from actual industrial units. In this respect stirred cooling jackets were discarded in favour of cooling coils whose velocity distribution is essentially plug flow. A residence time distribution (RTD) study of the cooling jackets, as reported in Appendix A.4.1(a-d), clearly portrayed the unsatisfactory heat distribution due to channelling and dead space.

The total simulation of the described system is achieved on the HARRIS 800, the interactive program being written in FORTRAN 66. This simulated program covers a wider range of the system steady states than is obtainable on the experimental range of heaters and liquid flows. Each of the steady states is analyzed for stability and stabilized if unstable.

Before embarking on the tasks enumerated above, the starting point was to review studies of similar systems in the literature so as to get a better perception of the need for this study; this survey is the context of the next chapter.

CHAPTER TWO
LITERATURE SURVEY

2.1 Introduction

In tackling the objectives enunciated in the introductory chapter, a literature survey encompassing the following areas was reviewed.

- a) Utilization of a single or of a multiple train of reactors in series for chemical processes.
- b) Simulation of reacting systems.
- c) Multiplicity and stability in reactors.
- d) Application of computers to control of process units.

2.2 Series C.S.T.R.s:

Since a C.S.T.R. operates at or close to uniform conditions of temperature and composition, its kinetics and product temperature can usually be predicted more accurately and controlled with greater ease, especially if a single simple reaction is taking place(2). The use of a single C.S.T.R. for the study of reacting systems is a well-trodden path both theoretically and experimentally. Semenov(4) seems to be the first who pointed out for zero order reaction that the heat generation curve can exhibit two intersections with a heat removal curve and later van Heerden(5) independently found that for first order reactions three intersections can exist. Bilous and Amundson(6) handled this case analytically. Aris and Amundson(7) studied stabilization of unsteady states by implementing different perfect control strategies and phase plane plots of the complete nonlinear reactor equations were constructed. They generated limit

cycles by varying the controller gain and extrapolating the results to cover multiple reactions and reactors. Luss and Amundson(8) investigated the behaviour of a completely segregated two phase C.S.T.R. and the effect of stirring on the various steady states and the latter author analysed a case of polymerization reactions(9,10). Hlavacek and others(11) extended the number of dependent variables in the phase-space treatment of first order exothermic consecutive reaction. They established regions of multiplicity, stability of steady states, behaviour of limit cycles and shapes of separatrices in relation to the dimensionless variables Damkohler number and the Frank-Kamenetskii temperature. Cohen and Keener(12) took this work further by using a multi-time scale perturbation technique in analysing the multiplicity and stability of oscillatory states of the system equations. Poore and Halbe(13) investigated the same system using perturbation techniques based on an extensive numerical search method. They discussed different types of jump phenomena including the classical ignition and extinction process and stated Hopf bifurcation formulae which have been successfully used in distributed parameter systems. Varma and Huang(14) gave a theoretical treatment that tied in with their experimental results on a gas-liquid system and recognised the non-existence of limit cycles in their system.

In the case of multiple highly exothermic reactions accompanied by great change of physical properties, control becomes more difficult and a slowing down of the reaction rate may become necessary. Reactors connected in series are used in industrial polymerization

processes in order to achieve the right product mix with a refinement unobtainable in a single reactor(1). Since a polymerization process is a chain of intermediate reactions (initiation, propagation and termination), inhibitors are deliberately added to the reacting monomers to prevent premature polymerization; their concentration is controlled to get the right product in each reactor. In order to reduce composition drift in product polymer particles which is apparent in usage of a single C.S.T.R., feed streams of the more reactive monomer are introduced between reactors when in cascade control. These reactors are sensitive to changes in operating parameters because highly exothermic reactions are involved and relatively minor fluctuations in the operating variable can cause difficulties due to particle nucleation, conversion oscillations leading to limit cycles and latex flocculation due to uneven heat loads(2). The industrial platforming process which is the upgrading of the octane ratings of straight chain natural and thermally cracked gasolines into aromatic compounds, represents simultaneous multiple endothermic reactions which require a fine temperature tuning in the different reactors to produce the right mixture of benzene, toluene, xylenes and other aromatic hydrocarbons(3). An inter-stage heater raises the temperature of feed into each subsequent fixed bed alumina catalyst reactor after the first.

2.3 Process simulation

The use of mathematical simulation techniques to develop new processes or improve existing ones is as old as the science of process design. The initial absence of fast calculating machines to

take the drudgery out of long mathematical calculations made simulation quite unattractive. The situation improved on the introduction of analogue computers, but these had the drawback of bulkiness and needing the scaling of some variables in order to increase their range. Digital computers offer an unlimited range and flexibility in the system variables being simulated and they are fast and efficient. Actual chemical process systems can seldom be modelled exactly by mathematical equations due to unpredictable deviations from ideal behaviour of some components like transducers, valves and others. The noise and inaccuracy of measurements all contribute to the overall nonideality of a control system and these are hardly ever accounted for in the system model. While a bench scale experimental model of the system being studied is expensive and time consuming to build, some parts could be constructed while others are represented by their mathematical analogues on a digital computer. Herein lies the idea of the partial simulation technique which has been exploited a great deal in chemical reactor studies in this department. Expensive chemicals are saved by using a digital computer to simulate the kinetics of the reaction process and to determine the mass balance of reactant and product in the experimental set-up.

Previous studies can be broadly divided into two groups: early researchers like Chao(15), Alpaz(16) and Buxton(17) who used analogue computers with conventional controllers and Farabi(18) and Mukesh(19) who used digital computers to effect more sophisticated control action. Unlike his four predecessors whose studies were based on a first order irreversible exothermic reaction, Mukesh

simulated reactions of order $-2, -1, 0, 1$ and 2 in a C.S.T.R. The present work had to revert to a first order exothermic reaction when initial surveys of a first order reversible reaction indicated constraints imposed by the experimental rig in terms of limited temperature range and heat generated.

2.4 Multiplicity and Stability of Steady States

A detailed analysis of the multiplicity and stability of the steady states of a system is necessary in the operation and control of chemical reactors as their response to control action should not lead to unpredictable patterns of behaviour. The case of a first order exothermic reaction carried out in a lumped-parameter system has been studied exhaustively both theoretically(23-27) and experimentally(22). Conditions for uniqueness and multiplicity have been established and it is well known that the system can have one or two steady states. When there are three steady states, the middle one is unstable to infinitesimal perturbations in any of system variables while the other two are stable. The situation gets more complex with simultaneous reactions in a system or complexity of the occurring reaction, as the reaction rates of the different species change with temperature of reactor or concentration of particular species. Luss and Cheri(20) have shown that multiple steady states exist when a single reactant participates in two simultaneous first order endothermic reactions, although it is well established that only a unique steady state exists for the single endothermic reaction. Pikios and Luss(21) developed criteria for multiplicity for first order consecutive or parallel reactions in a C.S.T.R. They

found that a maximum of five steady states existed when both reactions were exothermic and a maximum of three if one of the reactions was endothermic. Hlavacek et al(11) described a systematic classification of the regions of multiplicity based on dependence of system equations on Damkohler number (Da) and the dimensionless adiabatic temperature. Their study of a consecutive first order exothermic reaction identifies a maximum of five steady states and the stability status of these is established using the Routh-Hurwitz criterion(28) after constructing the characteristic polynomial. Sabo and Dranoff(29) analysed the above system and their analysis also included the estimation of the regions of asymptotic stability obtained by an application of Lyapunov's direct method. Berger and Lapidus(30) apply Lyapunov's direct method to a single and a series of three C.S.T.R.'s using the Fletcher-Powell minimization technique to develop a Krasovskii kind of Lyapunov function. Their method is criticized by Davison and Kurak(31) who point out that all points on the surface of the hypervolume formed are not rigorously tested for the differential of the function being less than zero. The latter then develop a computational procedure which involves LaSalle and Lefschetz's(32) theorem, and an optimization routine using Rosenbrock's(33) hill-climbing method. A fine grid mesh set up in n -dimensional space and a search where this grid intersects the Lyapunov's hypersurface guarantees that the hypervolume encompasses the region of asymptotic stability (RAS). In a system with multiple steady states, this RAS is local and not global and formation of the Lyapunov's function is a sufficient but not necessary condition for stability.

2.5 Feedforward and Feedback Control

The commonest controller, usually employed in chemical processes to vary the manipulative input vector in such a way that known and unknown input variations will result in minimum deviations in the process output, are feedforward and feedback controllers. The latter is used to adjust the relevant process variable following the introduction of any unknown disturbance into the system and is based on a measurement of the output deviation from the set value. There is a time lag between measurement of the deviation and application of corrective action which tends to cause over or undercompensation with increase in this lag. In addition to stabilising open loop unstable steady state systems, a variation of controller setting will cause the system response to exhibit various forms of behaviour including the generation of limit cycles as noted by Aris and Amundson(7). Feedforward controllers take remedial action in expectation of a known disturbance entering a process and thereby forestall any deviation in any of the process variables. In the case of reactors in series deviations in preceding reactors enter subsequent ones as disturbances, so an elimination of those using feedforward controllers becomes desirable. As there are other channels for unknown disturbances entering the reactors, both feedforward and feedback controllers acting in concert will counter the effects of the disturbances. While most of these controllers are linear, Chen and Ku(34) have shown in their paper that multiplicative feedback (nonlinear) controllers could effect better control of their linear system.

2.6 Noninteracting Control

Since there is usually strong interaction in a system with multi-variable inputs and outputs, there sometimes arises the need to have each output variable influenced by one input variable only. The variable thus segregated or driven to a new state by this input only is said to be noninteracting with respect to other system inputs. All the variables in the system are said to be noninteracting if for every particular input only one corresponding output is disturbed or influenced. Tokumaru and Iwai(35) treated this control problem as a variational one and derived necessary and sufficient conditions for noninteracting control of linear (time invariant and variant) multi-variable systems. Other authors obtained necessary and sufficient conditions for systems using state variable feedback. Linear time-variant systems cannot be made noninteracting by using diagonalization techniques as applied to time-invariant systems but variational methods can. Falb and Wolovich(36) introduced the concept of decoupling to multivariable systems and discussed necessary and sufficient conditions for decoupling linear time-variant systems using feedback loops. While their definition coincides with Tokumaru and Iwai's(35) concept of noninteracting control for time-invariant systems, it is inconceivable that it can be expanded to include general continuous linear and nonlinear systems. Hence we may conclude that the concept of noninteracting control is a more general one than that of decoupling. Mesarovic(37) achieved noninteraction by first transforming the linear multivariable system to the so-called V-canonical form so that the cross effects to be eliminated became internal feedback signals and these were eliminated by addition of corresponding external feedback loops. Foster and Stevens(38) used a modified form of the V-canonical structure with

inputs greater than outputs. They then developed a method by which a linear multivariable system represented by a set of first-order differential equations may be decoupled into a set of subsystems characterised by first-order transfer functions. On a study of a C.S.T.R. using an analogue computer, noninteraction is achieved by means of feedforward amplifiers and feedback proportional plus derivative controllers. Luyben(39) implemented positive feedback compensation between product composition on a simulated distillation unit to achieve noninteraction between product compositions at both ends. Tokumaru et al(40) used relays and linear compensating networks as controllers and noninteraction was obtained by the sliding motion of relays; this system was easily constructed because it did not need cross-term controllers. Most authors are concerned with a diagonalization of a closed-loop transfer function matrix which often requires complex compensators; this classical approach lacks the ability to incorporate constraints on the system variables. Liu(41) developed an algorithm for piecewise noninteracting control of linear and nonlinear systems that takes care of the system constraints.

2.7 Invariance Control

The realization of invariance requires that at least one of the system output variables remains invariant (independent) for any external disturbance, load or interference in a specified input variable. Although invariance control theory has been developed for over a quarter of a century especially in the Soviet Union, theoretical treatment has not been matched by experimental evidence

and few nonlinear systems have been studied. Linear invariance theory has been presented by Petrov(42) and Kulebakin(43) and been restated by Bollinger and Lamb(44). The classical approach they adopt is the transformation of the equations using either laplacian or differential operators. Rozonoer(45) tackled the invariance problem for linear and nonlinear systems using variational mathematics and developed theorems for necessary and sufficient conditions. He distinguished between 'weak' and 'strong' invariance in a system; the latter applying when the output variable of interest is independent of a particular external disturbance for the whole time range under consideration and the former at a particular instant only. Haskins and Sliecevich(46) applied invariance control to a C.S.T.R. in which a heat transfer process between oil and an ethylene glycol and water mixture was taking place. Both an analogue computer simulation of the system and an experimental run were tested with the designed invariance controllers being implemented.

The attainment of invariance is fundamentally based on three requirements:

- a) The mathematical model adequately describes the system behaviour, including the important process disturbances. Especially in systems where there are severe nonlinearities, an inaccurate nonlinear model may not be any better than its linearized equivalent.
- b) The control system is allowable by satisfaction of the dual channel conditions, which as stated by Petrov(42) requires that in a dynamic system there must be at least two channels for propagation of the influences between the point of application of the

external effect and the point of measurement of magnitude, whose relation to this effect must be secured.

- c) The theoretically derived controller equations can be accurately executed except where a pure dead time is encountered or controller equations based on the second derivative of a variable are involved, as these are not always reliable.

2.8 Conclusion

2.8.1 Research in the Literature

From the literature it can be seen that extensive theoretical work has been carried out on:

- 1) single C.S.T.R. units.
- 2) First order irreversible and consecutive first and mixed order exothermic reactions.
- 3) controlling single units using conventional feedforward and feedback controllers and recently greater use of computers to apply more advanced control algorithms

Most of the researchers assume a uniform temperature profile for the cooling coil and some of the cooling methods(19) are not feasible for engineering on large scale plants. An appreciable amount of experimental work has been recorded especially in this department to complement the above theoretical studies but there are no reports on series connected reactors and the inherent problems in control that are apparent due to interaction of the reactors.

2.8.2 Work covered in this study

In view of the the areas already covered by the existing literature, this work was started with the objective of using a reversible first

order reaction which would have provided more control challenges than the first order irreversible reaction used, as deviation in any of the fixed variables will cause the reaction to proceed in the favoured direction. But this was not to be as the calculations in appendix 4.2 show that for a significant change in the effective direction of reaction, a large temperature change is also required, which is unobtainable on the experimental plant due to the limited heating capabilities of the immersion heaters used.

In this study coils, whose modelled temperature profile is plug flow and are employed extensively in the chemical process industry, are used for cooling the respective reactors. Although only the inlet and outlet temperatures of the coils are measured experimentally, the intermediate temperatures are simulated for nonconventional control, like decoupling and invariance control which are applied to both reactors.

In the experimental set up described in chapter four, the existing plant scanning and control capabilities were expanded at very low cost due to a careful study of the available alternatives.

Having surveyed reported works in the literature, a description of the mathematical model and how this was derived, logically forms the contents of the next chapter.

CHAPTER THREE

MATHEMATICAL DEVELOPMENT OF MODEL

3.1 Introduction

Before embarking on writing a mathematical model for the system under study, a series of residence time distribution (RTD) experiments in cooling jackets was carried out as reported in Appendix A.4.1 so as to verify and confirm the chosen model. These experiments indicated the nonconformity of the flow pattern in the cooling jacket to either of the two standard forms of plug or completely mixed flow. The cooling jacket was replaced by a cooling coil which does conform to plug flow and because of the small radius of the copper tube of which the coil is made, it is also assumed there is complete radial mixing within the tube. The coincidence or nearness of the simulated to experimental values will be a measure of the rightness of assumptions made in formulating model equations.

3.2 System Equations

The following assumptions were made in synthesising the system equations:

- (a) The heat of reaction does not depend on the temperature or compositions in the reactors.
- (b) The volume change due to the reaction can be neglected and liquid volume in the reactors is maintained constant with large diameter drain pipes.

- (c) Heat capacities of feed and products and the heat transfer coefficient are temperature independent.
- (d) Heat loss from the system is negligible and only pure A component feed is introduced into the first reactor.
- (e) A first order irreversible exothermic reaction is taking place in the reactors with the product of the first reactor being feed to the second reactor.
- (f) Each cooling coil is divided into n equal theoretical cells for heat balance calculations and each reactor is supplied by fresh cooling liquid.

A mass balance on component A for the first reactor feed and product and energy balances on the reactor and cooling coil result in the following equations based upon the notation of fig. 3.1 (page 21):-



Component balance

$$F(C_{a0} - C_a) + V(r) = VdC_a/dt, \text{ where } r = -k_o \exp(-\Delta E/RT)$$

$$F(C_{a0} - C_a) + V(-k_o \exp(-\Delta E/RT))C_a = VdC_a/dt \tag{1}$$

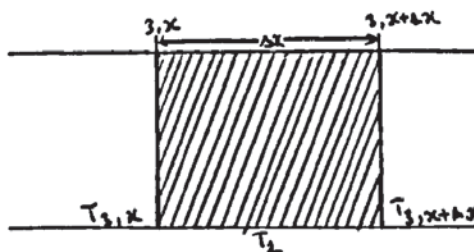
Energy balances:

Reactor

$$BC_p F(T_{2in} - T_2) + V(-\Delta H)k_o \exp(-\Delta E/RT)C_a - \sum_{i=1}^n q'(t)_i = BC_p VdT_2/dt \tag{2}$$

Single cell in coil:

$$2ZRN \Delta x (T_{3,x} - T_{3,x+\Delta x}) + 2ZRN \Delta x q'(t) = 2ZRN \Delta x BC_p dT_{3,x+\Delta x}/dt$$



where $q'(t) = U \cdot 1 \cdot (T_2 - T_{3,x+\Delta x})$

$A = 2ZRN \Delta x$ (total surface area of coil)

$V = ZRN \Delta x$ (total volume of coil)

$$BC_p F_c (T_{3,x} - T_{3,x+\Delta x}) + 2ZB\Delta x U (T_2 - T_{3,x+\Delta x}) = 2ZB\Delta x BC_p dT_{3,x+\Delta x}/dt \quad (3)$$

Converting equations (1) to (3) into dimensionless variables,

$$(Y_1 - X_1) - DaX_1 \exp(X_2/(1+X_2)) = dX_1/dt' \quad (1a)$$

$$(Y_2 - X_2) + BDaX_1 \exp(X_2/(1+X_2)) - (p/n)(nX_2 - X_{3,i}) = dX_2/dt' \quad (2a)$$

$$(X_{3,i-1} - X_{3,i}) + (p_c/n)(X_2 - X_{3,i}) = (\epsilon_c/n\epsilon) dX_{3,i}/dt' \quad (3a)$$

$$\text{where } i=1,2,\dots,n, \quad t' = t/\epsilon, \quad \epsilon = V/F$$

For the coil divided into 25 equal units the following unsteady state equations result:-

$$X_{3,1} = ((Y_3 - X_{3,1}) + (p_c/n)(X_2 - X_{3,1}))(n\epsilon/\epsilon_c) \quad (3b)$$

$$X_{3,2} = ((X_{3,1} - X_{3,2}) + (p_c/n)(X_2 - X_{3,2}))(n\epsilon/\epsilon_c) \quad (3c)$$

$$X_{3,25} = ((X_{3,24} - X_{3,25}) + (p_c/n)(X_2 - X_{3,25}))(n\epsilon/\epsilon_c) \quad (3d)$$

Total heat transferred through the coil

$$Q'(t) = \sum_{i=1}^n q'_i(t) = 2ZB\Delta x \sum_{i=1}^n (T_2 - T_{3,i}) \quad (4)$$

Similar equations are written for the second reactor and its corresponding cooling coil. These equations describe the dynamic state of the system at any particular time and the trajectory of the variables as the system moves from one initial state to another can be obtained by integrating the equations. The method of numerical integration used in this study is the Runge-Kutta(47) fourth-order method and the variables are plotted in pairs to give a phase plane profile of the system behaviour for these initial conditions.

3.3 Steady state

If the system is at a steady state, the right hand sides of equations (1a) to (3d) are equated to zero and the resultant

equations are solved simultaneously to obtain the steady state values of the variables employing the Newton-Raphson method. A correct choice of starting values for the iterations in this method is necessary in order to discover all the steady states of this system.

Thus at steady state equations (1a) to (3d) become:

$$(Y_1 - X_1) - DaX_1 \exp(X_2 / (1 + \epsilon X_2)) = 0 \quad (5)$$

$$(Y_2 - X_2) + BDaX_1 \exp(X_2 / (1 + \epsilon X_2)) - (p/n) (nX_2 - \sum_{i=1}^n X_{3,i}) = 0 \quad (6)$$

$$(X_{3,i-1} - X_{3,i}) + (p_c/n) (X_2 - X_{3,i}) = 0 \quad i=1, 2, \dots, n \quad (7)$$

$$X_{3,1} = (n / (n + p_c)) Y_3 + p_c X_2 (1 / (n + p_c) + n / (n + p_c)) \quad (7a)$$

$$X_{3,2} = (n / (n + p_c))^2 Y_3 + p_c X_2 (1 / (n + p_c) + n / (n + p_c)^2) \quad (7b)$$

$$X_{3,25} = (n / (n + p_c))^{25} Y_3 + p_c X_2 (n^{24} / (n + p_c)^{25} + n^{23} / (n + p_c)^{24} + \dots + 1 / (n + p_c)) \quad (7c)$$

It is already known that at steady state the heat removed from the reactor and that absorbed by the cooling liquid equals the heat generated by reacting system. A heat balance of these two streams over the first reactor will also give the steady state values of the variables (since the treatment of both tanks follows the same pattern, we will concern ourselves with equations 1a-3d only). The heat generation expression is

$$V(-\Delta H)k_1 C_a \quad (8)$$

and the heat removal expression is

$$PC_p F (T_2 - T_{2in}) + \sum_{i=1}^n q'(t)_i \quad (9)$$

These two expressions are the components of the energy balance equation(2) over the reactor at steady state. A plot of expressions(8) and (9) versus the reactor temperature will indicate the steady state tank and coil temperature distribution at intersections of the two curves, and substitution of this resultant value into equation(5) will yield the concentration of reactant in the reactor.

Integration of the set of equations(1a-3a), describing the dynamic state of the system, will ultimately end at one of the stable steady states; so a judicious choice of the initial starting values is necessary to identify all the stable steady states. It is not easy to identify the unstable steady state with this method, even when a backward (in time) integration is carried out. For each of the steady states in the first reactor, there is a maximum of three steady states that can be attained in the second reactor by a manipulation of the cooling liquid flow rate or temperature in this reactor. Actual steady states obtained in this reactor during experimental runs depend on equipment constraints.

A modification of assumption (f) in the above mathematical development allows counter-current cooling of the reactors, with the cooling liquid entering the coil in the second reactor and on exit being fed into the coil of the first reactor. Thus there is only one cooling stream and it can be manipulated by one control valve. From the contacting arrangement illustrated in the diagram (fig. 3.1,pg 21), a heat balance on the cooling coils for this single coolant stream results in the following dimensionless equations:

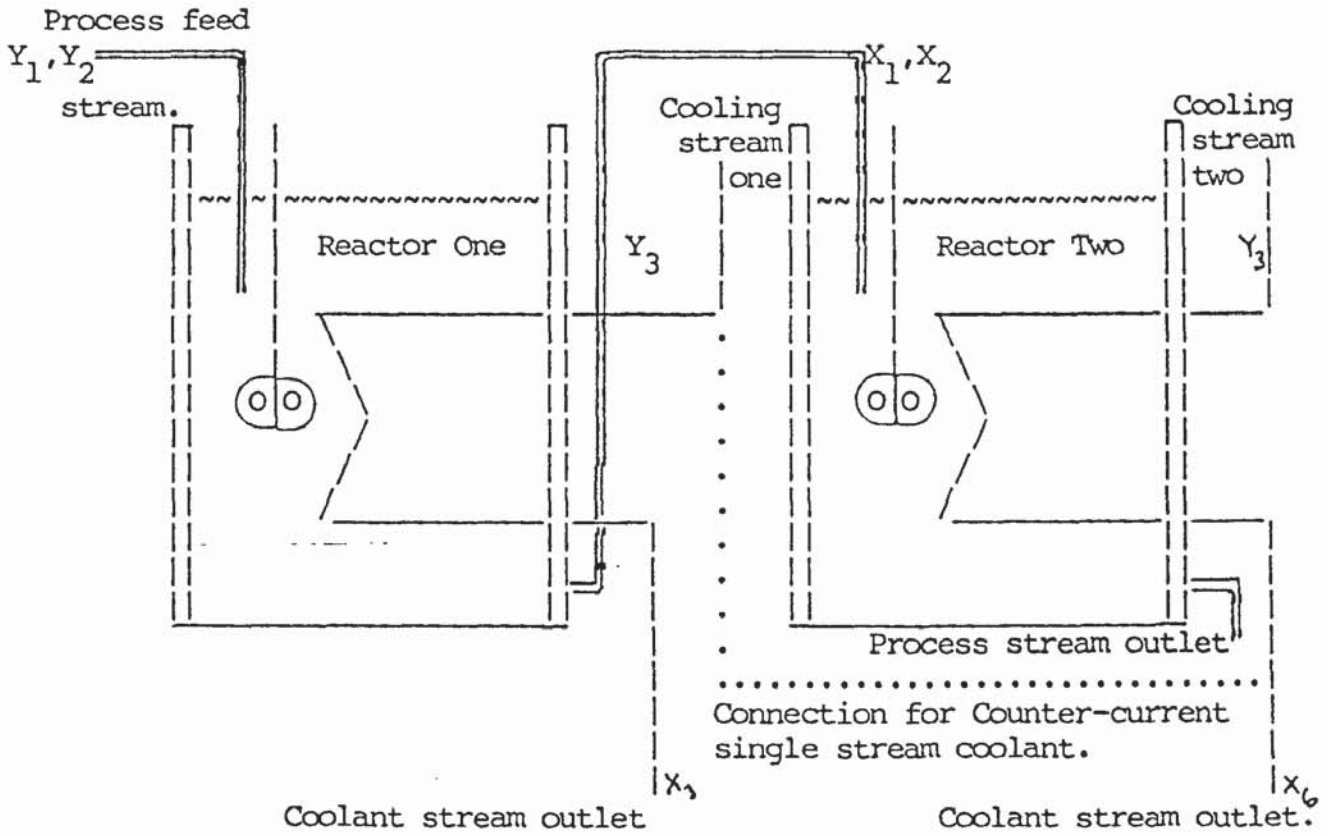


Fig. 3.1 Diagram of Reactors and Cooling Coils.

Tank One

$$\dot{X}_{3,1} = (nX_{3,0} - (n+p_c)X_{3,1} + p_c X_2) \epsilon / \epsilon_c = (nX_{6,n} - (n+p_c)X_{3,1} + p_c X_2) \epsilon / \epsilon_c \quad (10a)$$

$$\dot{X}_{3,2} = (nX_{3,1} - (n+p_c)X_{3,2} + p_c X_2) \epsilon / \epsilon_c \quad (10b)$$

$$\dot{X}_{3,n} = (nX_{3,n-1} - (n+p_c)X_{3,n} + p_c X_2) \epsilon / \epsilon_c \quad (10c)$$

Tank Two

$$\dot{X}_{6,1} = (nX_{6,0} - (n+p_c)X_{6,1} + p_c X_5) \epsilon / \epsilon_c = (nY_3 - (n+p_c)X_{6,1} + p_c X_5) \epsilon / \epsilon_c \quad (11a)$$

$$\dot{X}_{6,2} = (nX_{6,1} - (n+p_c)X_{6,2} + p_c X_5) \epsilon / \epsilon_c \quad (11b)$$

$$\dot{X}_{6,n} = (nX_{6,n-1} - (n+p_c)X_{6,n} + p_c X_5) \epsilon / \epsilon_c \quad (11c)$$

At steady state equations (10a) to (11c) are equal to zero. These are solved simultaneously together with the reactor mass and heat balance equations (5) and (6) to obtain the steady state values. An iterative Newton-Raphson method is used and since there are four equations to be solved, derivation of the iterative method is included in Appendix A.4.3

3.4 Stability

The stability of the particular steady state is tested by finding the eigenvalues of the Jacobian matrix formed by differentiating the system equations at steady state with respect to the state variables. If all the eigenvalues are real and negative, then at that steady state the system is asymptotically stable and will return to the particular steady state if it is slightly disturbed from its state of rest. If any of the eigenvalues is positive, it implies that the system is unstable and if slightly disturbed from that particular steady state will move to a new steady state which

will be more stable than the previous one. If the eigenvalues turn out to be complex, the system oscillates with decreasing or increasing amplitude depending on whether the real part of the complex roots is negative or positive. In the case of purely imaginary eigenvalues, cyclic motions at fixed amplitude ensue.

Three steady states have been identified for the first reactor using the heat balance expressions and Newton-Raphson method for solving autonomous equations. The topmost and the lowest of these are stable, while the intermediate is unstable. While local stability of each steady state of the second reactor is determined using the above method, the global stability of the system is determined by considering the effect of the first reactor on the second, knowing that products of the former are feed to the latter.

With several dimensionless groups in the state equations, the influence of each on the stability of the system can be explored by varying the particular dimensionless group while keeping the others constant. This approach will result in a myriad of diagrams whose value may not match the effort. Rather, a verification of a collection of dimensionless groups at a time (as some of them are interrelated) is carried out and the effect of this change is analysed in terms of the number of steady states available and their stability. While the eigenvalues of the Jacobian matrix at steady state give an indication of the system, they do not define the extent in phase space of the stability. A method that determines the area or volume of the region of asymptotic stability like the Lyapunov function is employed to get a feel of how far the system could be displaced from its steady state and still remain stable.

3.5 Lyapunov Function

The actual extent of the region of asymptotic stability (RAS) can be determined by integrating the dynamic equations (1a-3d) and similar ones for the second reactor starting from different initial conditions. From a phase space display of the trajectories, the RAS can be calculated. This is a rather tedious task and a way round it would be the construction of a Lyapunov function $V(X)$ which has the following characteristics(31):

(a) $V(X) > 0 \quad X \neq X_{ss}$ where X_{ss} is the steady state value of the variable

(b) $V(X_{ss}) = 0$

(c) $\dot{V}(X) = F'(X)\text{grad } V(X) < 0 \quad X \neq X_{ss}$

(d) $\dot{V}(X_{ss}) = 0$

This function will define a region within which the system $X = F(X)$ is asymptotically stable. While this function is not unique for a particular system and does not necessarily mark the boundary between asymptotically stable and unstable regions as it does not always include all the region of asymptotic stability, its advantage lies in the ease of application.

In constructing the quadratic Lyapunov function $V(X)=X'AX$, the following algorithm as suggested by Davison and Kurak(31) was used.

(i) Evaluate the Jacobian ($J = (dF/dX)_{X=X_{ss}}$) and solve for A_0 in the expression $J'A_0 + A_0J = -I$

(ii) Maximize function $X'AX = \lambda$

subject to the following constraint

$$F' \left\{ \frac{Y_i}{/Y'_i (A_0 / \epsilon) Y_i} \right\} A_0 Y_i < \emptyset$$

where X is the vector of control variables,

A_0 is a matrix of constant coefficients,

Y_i are mesh of unit vectors spanning the phase space and

ϵ is a small constant.

(iii) Find \bar{A} so as to minimize $\lambda_{\max}(\bar{A})$ subject to the constraint

$$\lambda_{\min}(\bar{A}) > \emptyset$$

$$F' \left\{ \frac{Y_i}{/Y'_i (\bar{A}) Y_i} \right\} A_0 Y_i < \emptyset$$

where \bar{A} is the matrix of constants after first optimization.

(iv) Using \bar{A} as initial value, find A so as to minimize $\prod_{i=1}^n \lambda_i(A)$

subject to constraints

$$\min \lambda_i(A) > \emptyset$$

$$\max F' \left\{ \frac{Y_i}{/Y'_i A Y_i} \right\} A_0 Y_i < \emptyset \quad i=1, 2, \dots, n$$

The volume of the Lyapunov function is considered to be directly proportional to the product of the eigenvalues of A , the matrix of constant coefficients. The ratio defined by expressing the volume of constructed Lyapunov function with different control schemes gives an indication of the enlargement or reduction in the stability region achieved on using different control schemes. The above method which the authors found to be superior to several other techniques, is conveniently implemented in the LYAPON section of the total

simulation programme on the fast speed and large memory Harris 800 mainframe computer.

3.6 Control

Systems where control presents difficulties because the static and dynamic properties of the system depend on certain operational ratings which vary over a considerable range are frequently encountered. In such situations the often used control method, which is based on the operating controller rating being a function of control deviation only was not capable of adapting to the new state of the system as the controller parameters were unalterably adjusted. Systems that are supervised and controlled by large memory and fast speed mainframe computers do not suffer this disadvantage as the parameter values can be re-evaluated quickly and the controller settings adjusted. Any system with more than one steady state will have both stable and unstable steady states. Within the immediate neighbourhood of the stable steady state, the system will return to the same state if slightly disturbed. In the vicinity of the unstable state, the system will need control action to maintain it at the stated steady state, otherwise it will drift to a stable steady state whose position is different from the former unstable state. The system is said to have local and not global stability at or near each of the steady states. The system under consideration has five manipulable variables(52) and these will each be considered in turn, either singly or in combination, for the types of control action that are possible. Each of these manipulable variables (T_{2in} , C_{a0} , T_{c0} , F_c , F) can be directly or indirectly made a function of

the controlled variables (T_2, C_a, T_3) and a feedforward or feedback control system output.

While theoretically it is possible to use any of the said five manipulable variables, effecting actual control is difficult for some of them. The convenient ones that can be employed are the flow rates as a process control valve is provided which responds to pneumatic signals which in turn are generated from a combination of D/V, V/I and I/P converters.

3.6.1 Feedforward and Feedback

The stabilization of the open loop unstable steady state and increase of the RAS of stable steady state can be effected using conventional feedforward and feedback perfect controllers. While the latter controller relies on the actual deviation of variables from their set values, the former takes remedial action based upon the measured value of a disturbance. If the deviation of the controlled variables (\hat{X}_i) from the steady state values are chosen as functions of the operating controllers and the cooling liquid as manipulable variable, the following feedback proportional control law consequently evolves:-

$$\hat{F}_c = -K_c \hat{X}_i \quad (12)$$

$$\text{where } \hat{F}_c = F_c - F_{css}$$

$$\hat{X}_i = X_i - X_{iss} \quad i=1,2,\dots,m$$

m is the number of state variables

K_c is the controller gain and

$\hat{}$ denotes perturbation variable

Rewriting the dynamic equations (1a-3a) in perturbation form and noting that changes in inlet concentration of reactant from values established at steady state constitute forcing disturbances into the system, these equations become:

$$Y_{1ss} + \hat{Y}_1 - X_{1ss} - \hat{X}_1 - Da(X_{1ss} + \hat{X}_1) \exp((X_{2ss} + \hat{X}_2)/(1 + (X_{2ss} + \hat{X}_2))) = d(X_{1ss} + \hat{X}_1)/dt' \quad (13)$$

$$Y_{2ss} + \hat{Y}_2 - X_{2ss} - \hat{X}_2 + BDa(X_{1ss} + \hat{X}_1) \exp((X_{2ss} + \hat{X}_2)/(1 + (X_{2ss} + \hat{X}_2))) - (p/n)(n(X_{2ss} + \hat{X}_2) - (X_{3,iss} + \hat{X}_{3,i})) = d(X_{2ss} + \hat{X}_2)/dt' \quad (14)$$

$$((X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,iss} - \hat{X}_{3,i}) + (F_c/F_{css})(X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,i} - X_{3,iss} - \hat{X}_{3,i})) + (p_c/n)(X_{2ss} + \hat{X}_2 - X_{3,iss} - \hat{X}_{3,i}) = \epsilon_c d(X_{3,iss} + \hat{X}_{3,i})/n dt' \quad (15)$$

$i=1, 2, \dots, n$

If the manipulable variable is made a function of reactor temperature and the proportional control law (equation 12) is applied to equation(15) which implicitly contains the cooling liquid flow rate, the following equation results:

$$((X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,iss} - \hat{X}_{3,i}) - K_c(\hat{X}_2/F_{css})(X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,i} - X_{3,iss} - \hat{X}_{3,i})) + (p_c/n)(X_{2ss} + \hat{X}_2 - X_{3,iss} - \hat{X}_{3,i}) = \epsilon_c d(X_{3,iss} + \hat{X}_{3,i})/n dt' \quad (16)$$

$i=1, 2, \dots, n$

The following equations are realised when the manipulable variable is made a function of the reactant concentration(17) or the coil temperature(18) and the proportional control law (equation 12) is applied to equation (15):

$$\begin{aligned} & ((X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,iss} - \hat{X}_{3,i}) - K_c (\hat{X}_1 / F_{css})) (X_{3,i-1ss} + \hat{X}_{3,i-1} - \hat{X}_{3,i} - \\ & X_{3,iss}) + (p_c/n) (X_{2ss} + \hat{X}_2 - X_{3,iss} - \hat{X}_{3,i}) = n \frac{d(X_{3,iss} + \hat{X}_{3,i})}{dt} \end{aligned} \quad (17)$$

$$\begin{aligned} & ((X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,iss} - \hat{X}_{3,i}) - K_c (\hat{X}_{3,i} / F_{css})) (X_{3,i-1ss} + \hat{X}_{3,i-1} - \hat{X}_{3,i} - \\ & X_{3,iss}) + (p_c/n) (X_{2ss} + \hat{X}_2 - X_{3,iss} - \hat{X}_{3,i}) = n \frac{d(X_{3,iss} + \hat{X}_{3,i})}{dt} \end{aligned} \quad (18)$$

$$i=1, 2, \dots, n$$

The proportional control law encompassing feedforward and feedback control analogous to equation (12) as applicable to the second reactor will be

$$\hat{F}_c = -K_c (\hat{X}_i + \hat{Y}_i) \quad (19)$$

where \hat{X}_i is the error signal expected (disturbance)

from the first reactor and \hat{Y}_i is actual error

signal in reactor two.

The use of the combination of feedforward and feedback controllers in the second reactor is due to the source of disturbances into it, viz a carry over from the first reactor and disturbances in cooling liquid inlet temperature.

3.6.2 Invariance

The general criterion of complete invariance of a multivariable system is the development of relationships based on fixed or variable system parameters between measured external disturbances or loads and controlled variables, such that one or more of the latter become independent of one or several of the former.

Its practical realization requires(46) that the following conditions be fulfilled:-

- i) the mathematical relation developed adequately describes the system.
- ii) the control system is allowable by satisfaction of the dual channel conditions.
- iii) the derived controller equations can be implemented.

In the well-ordered system represented by equations(1a-3d), complete invariance is achieved if the following relationships apply to the controlled variables for their steady state values

$$\hat{X}_1 = d\hat{X}_1/dt' = 0 \quad (20)$$

$$\hat{X}_2 = d\hat{X}_2/dt' = 0 \quad (21)$$

$$\hat{X}_{3,i} = d\hat{X}_{3,i}/dt' = 0 \quad i=1,2,\dots,n \quad (22)$$

Only partial invariance is attained in this work as the feed is not made invariant with respect to load disturbances of the feed. This is due to the fact that the manipulable variable cannot be related to the feed and also, since the feed is computer simulated, it is not possible to monitor its value without simulation. Substituting equations (13-15) results in the following equations:

$$Y_{1ss} + \hat{Y}_1 - X_{1ss} - \hat{X}_1 - Da(X_{1ss} + \hat{X}_1) \exp(X_{2ss}/(1+X_{2ss})) = d(X_{1ss} + \hat{X}_1)/dt' \quad (23)$$

$$Y_{2ss} + \hat{Y}_2 - X_{2ss} + BDa(X_{1ss} + \hat{X}_1) \exp(X_{2ss}/(1+X_{2ss})) = (p/n) (nX_{2ss} - \sum_{i=1}^n X_{3,iss}) = 0 \quad (24)$$

$$(X_{3,i-1ss} - X_{3,iss}) + (\hat{F}_c/F_{css}) (X_{3,i-1ss} - X_{3,iss}) +$$

$$(p_c/n)(X_{2ss} - X_{3,iss}) = 0 \quad i=1,2,\dots,n \quad (25)$$

Noting that $X_{3,0} = Y_{3ss} + \hat{Y}_3$, substituting to replace the unmeasurable

intermediate temperatures in equations (24) and (25), combining and rearranging these two equations results in

$$Y_{2ss} + Y_2 - X_{2ss} + BDa(X_{1ss} + \hat{X}_1) \exp(X_{2ss}/(1 + X_{2ss})) - (p_c/n)(nX_{2ss} - ((A^{n-1}D + A^{n-2}D^2 + \dots + A^0D^0)(Y_{3ss} + \hat{Y}_3) + (p_c/n)(nA^{n-1}D^0 + (n-1)A^{n-2}D + \dots + A^0D^{n-1})X_{2ss})/A^n) = 0 \quad (26)$$

$$\text{where } A = (1 + (F_c/F_{css})) + p_c/n \quad \text{and } D = (A - p_c/n)$$

The above is a nonlinear polynomial relating the cooling liquid flow rate, and the reactor and cooling coil temperature responses to disturbances in reactor and cooling coil inlet temperatures. An iterative Newton-Raphson method is used in calculating the flow rate required to annul the effect of any of these disturbances, having first integrated equation (23) for the perturbation in concentration (\hat{X}_i). If disturbances through the feed are eliminated, then total invariance can be attained in the system. While it is not easily discernable from equation (26) whether the inlet reactor temperature disturbance or inlet coil temperature disturbance has greater adverse effect on the system, experimental runs with disturbances of equal magnitude are carried out to ascertain this. The maximum magnitude of acceptable disturbance is limited by the difference between the steady state flow rate and the maximum attainable from the cooling pump.

As there is no time element involved in equation (26), it is theoretically assumed that inlet temperature disturbances can be eliminated instantaneously, while those involving feed concentration disturbance will not lead to temperature rise, but their annulment is time dependent. In actual practice, it needs to be stressed that valve settings and temperature scanners have in-built dead times and these must be taken into consideration.

3.6.3 Noninteracting

In multivariable completely interacting systems a change in one system input variable affects the output of all the variables. The need to maintain certain system output variables noninteracting with respect to input variables other than their own is of paramount importance when the system outputs are tailored to certain physical characteristics. For instance, an increase in feed rate may change the conversion rate, which in itself will not change the physical characteristics of the product if a change in the reactor temperature can be prevented. Noninteracting control is said to be attained in a system if a change of any one reference input quantity causes only the one corresponding controlled output variable to change. For the system under consideration, complete decoupling is achieved if the nonlinear mathematical model equations can be resolved into the following linear dynamic(41) equations:

$$\hat{X}_1 = \hat{Y}_1 - a_1 \hat{X}_1 \quad (27)$$

$$\hat{X}_2 = \hat{Y}_2 - a_2 \hat{X}_2 \quad (28)$$

$$\hat{X}_3 = \hat{Y}_3 - a_3 \hat{X}_3 \quad (29)$$

where a_i are positive constants whose values are dependent on the system parameters, \hat{X}_i are the perturbation variables and \hat{Y}_i are load disturbances. With the cooling liquid being the only manipulative variable, it is possible to decouple only one of two state variables at a time and in this study, the reactor temperature was singled out for decoupling. If the total disturbances entering the system are restricted to feed and coolant temperatures, equations (13-15) can be rewritten as:-

$$\hat{X}_1 = \hat{X}_1 - Da((X_{1ss} + \hat{X}_1) \exp((X_{2ss} + \hat{X}_2)/(1 + \epsilon(X_{2ss} + \hat{X}_2))) - X_{1ss} \exp(X_{2ss}/(1 + \epsilon X_{2ss}))) \quad (30)$$

$$\hat{X}_2 = \hat{Y}_2 - \hat{X}_2 + BDa(X_{1ss} + \hat{X}_1) \exp((X_{2ss} + \hat{X}_2)/(1 + \epsilon(X_{2ss} + \hat{X}_2))) - X_{1ss} \exp(X_{2ss}/(1 + \epsilon X_{2ss})) - (p/n)(n\hat{X}_2 - \sum_{i=1}^{n\wedge} X_{3,i}) \quad (31)$$

$$\hat{X}_{3,i} = ((p_c/n)(\hat{X}_2 - \hat{X}_{3,i}) + (X_{3,i-1ss} + \hat{X}_{3,i-1} - X_{3,iss} - \hat{X}_{3,i}))n\epsilon/\epsilon_c \quad (32)$$

On decoupling coil temperature from the other two state variables, equations (29) and (32) will therefore represent the same state. Equating and manipulating these two equations results in

$$\hat{F}_c = ((\epsilon_c a_3/n) \hat{X}_{3,i} + (p_c/n)(\hat{X}_2 - \hat{X}_{3,i}) + (X_{3,i-1} - \hat{X}_{3,i}))F_{css} / (X_{3,iss} + \hat{X}_{3,i} - X_{3,i-1ss} - \hat{X}_{3,i-1}) \quad (33)$$

$$\hat{X}_{3,1} = \hat{Y}_3 - a_3 \hat{X}_{3,1} \quad (34a)$$

$$\hat{X}_{3,2} = \hat{X}_{3,1} - a_3 \hat{X}_{3,2} \quad (34b)$$

$$\hat{X}_{3,n} = \hat{X}_{3,n-1} - a_3 \hat{X}_{3,n} \quad (34y)$$

In order to make the system described by equations (30), (31) and (34a-y) stable, a_3 the exponential decay constant must be positive. Its value determines the speed of response of the system to a disturbance. The larger the value, the faster the response and hence a large adjustment flow rate, but an excessively large value will introduce oscillations and instead increase the settling time. A reasonable practical approach is to have a small value of a_3 when the error is large and gradually increase this value as the error decreases. There are physical limitations to the maximum value of \hat{F}_c attainable on the experimental rig based on the cooling pump maximum capacity. While there are several values of a_3 that can be used, an acceptable value is one whose flow rate adjustment still falls short of the maximum cooling liquid flow rate. If for a particular value of a_3 , the flow adjustment exceeds maximum flow, a lower value is adopted and a new flow rate adjustment (\hat{F}_c) is calculated. With the digital computer as controller, an algorithm that automatically selects new values of a_3 when the flow rate constraint is breached, is employed and this procedure known as piecewise decoupling is as follows:

- (a) Select a large value for a_3 (a_{3max})
- (b) Integrate equations (30), (31) and (34a-y)
- (c) Solve for \hat{F}_c in equation (33)
- (d) Check whether $F_{cmax} - F_{css} > \hat{F}_c > -F_{css}$. If F_c is acceptable,

set the flow rate, else reduce a_3 by 10% say, and go to step (b).

Decoupling of reactor temperature has the advantage of leaving feed load disturbances independent of the coil temperature and cooling liquid disturbances independent of the reactor concentration as the equations consequential to this decoupling are:

$$\hat{X}_1 = \hat{Y}_1 - \hat{X}_1 - Da((X_{1ss} + \hat{X}_1) \exp((X_{2ss} + \hat{X}_2)/(1 + (X_{2ss} + \hat{X}_2) - X_{1ss} \exp(X_{2ss}/(1 + X_{2ss})))) \quad (35)$$

$$\hat{X}_2 = \hat{Y}_2 - a_2 \hat{X}_2 \quad (36)$$

$$\hat{X}_{3,i} = ((p_c/n)(\hat{X}_2 - \hat{X}_{3,i}) + (\hat{X}_{3,i-1} - \hat{X}_{3,i})n\epsilon_c) \quad (37)$$

Substituting for the different cell temperatures, summing and manipulating equation (15), the flow adjustment (\hat{F}_c) becomes

$$\hat{F}_c = ((\epsilon_c/n) \sum_{i=1}^n \hat{X}_{3,i} - (p_c/n)(n\hat{X}_2 - \sum_{i=1}^n \hat{X}_{3,i}) + \hat{X}_{3,n} - \hat{Y}_3) F_{css} / (Y_{3ss} + \hat{Y}_3 - X_{3,nss} - \hat{X}_{3,n}) \quad (38)$$

Equating equations (31) and (36) results in

$$\sum_{i=1}^n \hat{X}_{3,i} = ((1 + -a_2)\hat{X}_2 - BDa((X_{1ss} + \hat{X}_1) \exp((X_{2ss} + \hat{X}_2)/(1 + (X_{2ss} + \hat{X}_2) - X_{1ss} \exp(X_{2ss}/(1 + X_{2ss})))) - X_{1ss} \exp(X_{2ss}/(1 + X_{2ss})))n/p \quad (39)$$

Differentiating equation (39) with respect to time

$$\sum_{i=1}^n \dot{\hat{X}}_{3,i} = ((1 + -a_2)\dot{\hat{X}}_2 - BDa((\dot{\hat{X}}_1 + (X_{1ss} + \hat{X}_1)/(1 + (X_{2ss} + \hat{X}_2) - X_{1ss} \exp(X_{2ss}/(1 + X_{2ss})))) - X_{1ss} \exp(X_{2ss}/(1 + X_{2ss}))))n/p \quad (40)$$

Substituting equations (39) and (40) into equation (38), \hat{F}_c is then calculated with $\hat{X}_{3,n}$ being the value obtained from equation (37). A more accurate value for $\hat{X}_{3,n}$ can be obtained from equation (31) if an empirical relation is evolved for the temperature profile along the cooling coil for the dynamic state, in which case the summation equations can be decomposed into their individual units.

3.7 Effect of controller Gain

The properly controlled system responds to and eliminates the effects of any disturbances entering it, thus ensuring its stability. The effect the various control strategies have in enhancing this stability can be studied by applying Krasovskii's theorem(30) to the system equations. This states that for a system defined by $\dot{X}=F(X)$ where $F(X)$ is a linear or nonlinear continuous function with partial derivatives, if a quadratic function of the form $V=F'AF$ could be defined with the following characteristics:

- (i) A is a positive definite symmetric matrix
- (ii) $V = 0$ at $X=0$
- (iii) $V \rightarrow \infty$ as $X \rightarrow \infty$

then the region of asymptotic stability extends to the surface where $\dot{V} < 0$. A notational representation of the Jacobian matrix for the uncontrolled system at steady state is

$$J = \begin{vmatrix} J_{11} & J_{12} & 0 \\ J_{21} & J_{22} & J_{23} \\ 0 & J_{32} & J_{33} \end{vmatrix}$$

where the reactant concentration and reactor and cooling coil temperatures are respectively stated as

$$(i) \quad J = \begin{vmatrix} J_{11} & J_{12} & \emptyset \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{vmatrix} \quad (ii) \quad J = \begin{vmatrix} J_{11} & J_{12} & \emptyset \\ J_{21} & J_{22} & J_{23} \\ \emptyset & J_{32} & J_{33} \end{vmatrix}$$

where $J_{3,1}$, $J_{3,2}$ and $J_{3,3}$ are derived from equations 17,16 and 18.

Considering a general symmetric matrix A and applying Sylvester's theorem for positive definiteness to the matrix $-(J^T A + A J)$, the following relationships ensure the asymptotic stability of the system.

$$S_1 = -2(J_{11}A_{11} + J_{21}A_{12} + J_{31}A_{13}) > \emptyset \quad (41)$$

$$S_2 = -2(J_{12}A_{12} + J_{22}A_{22} + J_{32}A_{23}) > \emptyset \quad (42)$$

$$S_3 = -2(J_{23}A_{23} + J_{33}A_{33}) > \emptyset \quad (43)$$

$$S_4 = S_1 S_2 - S_7^2 > \emptyset \quad (44)$$

$$S_5 = S_3 S_4 + 2S_7 S_8 S_9 - S_2 S_8^2 - S_1 S_9^2 > \emptyset \quad (45)$$

$$S_6 = S_2 S_3 - S_9^2 > \emptyset \quad (46)$$

$$\text{where } S_7 = A_{12}(J_{11} + J_{22}) + J_{21}A_{22} + J_{31}A_{23} + J_{12}A_{11} + J_{32}A_{13}$$

$$S_8 = A_{13}(J_{11} + J_{33}) + J_{21}A_{23} + J_{31}A_{33} + J_{23}A_{12}$$

$$S_9 = A_{23}(J_{22} + J_{33}) + J_{12}A_{13} + J_{23}A_{22} + J_{32}A_{33}$$

Examining the six equations (41-46) for the qualitative effect of large controller gains, it can be seen that the control laws do not affect equations (41) and (42). For proportional control of the reactant concentration, $J_{31} = (-K_c/F_{css})(Y_1 - X_1)$ which is always positive for values of $K_c > \emptyset$. Equation (42) is weakened by a large J_{31} especially as this increases the value of S_7 . Equation (45) is strengthened by a large J_{31} , so that the overall effect is that the

condition for asymptotic stability is reinforced for certain values of the controller gain and weakened for others. J_{31} is increased for large controller gain for the control law of equation (16) and J_{31} is reduced to zero. This has a mixed effect on S_7 and increases values of S_9 while reducing that of S_8 . Since equations (44), (45) and (46) are off the principal diagonal of the matrix $-(J'A+AJ)$, large increases need to take place in order to influence the eigenvalues of this matrix. A range of gains for stabilizing unstable systems for different control laws is given in Table 3.1. These clearly confirm the fact that control laws 16 and 17 need smaller controller gains than control law 18. A quantitative expression of the relative areas of stability for different controls are given in Table 3.2 with the upper half of the symmetric matrix A constructed using Lyapunov's functions. Having evolved the required mathematical representation for the system under study, the next stage will be a review of the tools that will be employed for both the experimental and theoretical study and this is the basis for the next chapter.

TABLE 3.1 STABILITY OF SYSTEM FOR VARIOUS GAIN VALUES FOR DIFFERENT CONTROLLER EQUATIONS.

CONTROL equation	REACTOR number	STABILITY of Steady state	MAGNITUDE OF CONTROLLER GAIN and effect on stability.
16	1	unstable	unstable for all range of values.
16	2	unstable	unstable stable unstable $0 \longrightarrow 3E-05 \longrightarrow 3.61E-05 \longrightarrow$
17	1	unstable	unstable stable & oscillates. $0 \longrightarrow 3.75E-06 \longrightarrow 2.0$
17	2	unstable	unstable stable & oscillates. $0 \longrightarrow 2.29E-06 \longrightarrow 2.0$

TABLE 3.2 REGION OF ASYMPTOTIC STABILITY FOR DIFFERENT CONTROLLER EQUATIONS AND VARIOUS GAIN VALUES.

REACTOR number	STEADY state number	CONTROLLER gain(Kc) & equation	MATRIX	VOLUME enclosed	RATIO OF controlled/uncontrolled
1	1	0.0	0.0902 0.0380 0.0243 0.0829 0.0471 0.0504	1.42E-04	1.0
2	1	0.0	0.3252 0.1850 0.1015 0.1811 0.0923 0.0740	6.55E-04	1.0
1	1	5.0E-05 18	0.1888 0.0357 0.0057 0.1120 0.01735 0.0772	3.49E-04	2.46
1	1	5.0E-05 16	0.2168 0.0341 0.0086 0.1755 -0.0190 0.0597	2.1E-03	14.8
1	1	5.0E-05 17	0.2566 0.0578 0.01357 0.4119 -0.0368 0.0585	5.5E-04	3.87
2	1	1.0E-04 16	0.5619 0.2397 0.0491 1.8453 -0.0782 0.1092	9.72E-04	1.49
2	1	5.0E-05 18	0.1989 0.3499 0.0037 0.1129 0.0121 0.0219	2.76E-04	0.421
2	1	4.0E-04 16	0.2000 0.0277 0.0078 0.1345 -0.0119 0.0589	1.5E-03	2.29
1	1	1.0E-04 18	0.2028 0.0578 0.0136 0.1755 -0.0190 0.0597	2.36E-04	1.67
1	1	2.0E-04 17	0.2440 0.0687 0.0167 0.7991 -0.0499 0.0489	8.6E-03	6.05

CHAPTER FOUR
EQUIPMENT AND COMPUTER SYSTEM

4.1 Introduction

The experimental assembly consists essentially of two modular units. The plant module wherein the actual experiment is taking place and the supervisory and control module which is the Honeywell 316 computer. These two are interfaced through the Honeywell Analogue Digital Input Output System (HADIOS).

In modifying and expanding the plant which was used in the research thesis as described by Mukesh(19), two essential factors were taken into consideration:-

- i) equipment set-up and operation were to reflect actual industrial plant application and
- ii) cost of additional hardware was to be minimized without sacrificing the appropriate operational technique or accuracy of results obtained.

In keeping the cost of this research low, water was used as reactant and product medium and its characteristics were used for modelling reacting species; the actual reaction kinetics and the mass balance were therefore part of the software in all the experiments. While flow rates and temperatures were monitored on the plant which is schematically displayed in figure 4.1, the values were conditioned and relayed to the Honeywell which after executing some correlations or algorithms for the mass balance and required controller setting

in turn sent out digital values which were converted to analogue signals for heat of reaction generation or control of flow rate.

4.2 Description of Equipment

The prominent features of the experimental plant were two cylindrical copper reactors connected in series in which the reactions took place. Each of these reactors had a concentric copper insulating jacket enclosing it. The reactors were supplied with water from one of two feed tanks and a solenoid valve arrangement in the pipe line controlled the flow from either tank, with the discharge from the first reactor being feed to the second. An overflow pipe in each reactor maintained a constant volume of 0.0173m^3 and stirrers within them ensured uniform temperature and concentration. Heat losses were minimized by having insulating material between the concentric walls of each reactor and its jacket and wrapped on the outside of each reactor and connecting piping. Immersion heaters fitted to each of the reactors simulated reaction heat, each set being controlled by a unique analogue output channel. Water from two large feed tanks was pumped through a copper cooling coil in each reactor, the flow rate being manipulated through a process control valve. Temperatures of liquid into and out of the reactors and cooling coils were monitored by eight Comark thermocouples arranged in two groups, readings being taken via the Thermocouple Interchange Box by addressing one of two analogue output channels. Rotameters placed strategically along the flow path of the liquid streams indicated flow rates which were fed manually into the computer as the need arose. A switch panel on the plant offered control of individual or groups of similar electrical

items and a 'sudden death' switch for shut-down in case of an emergency. While the operation of some of the equipment was self-evident, a detailed description of some other parts and their operational ranges is necessary.

4.3.1 Process Control Valve(47)

The two pneumatic control valves were manipulated by the same air supply lines and arrangement of D/A, V/I and I/P converters. This was made possible by the attachment of a solenoid valve to the instrument air supply line of each of the control valves, and the loading and unloading of the latter was preceded by the excitation of the former through one of two analogue output channels. The control valves were fitted with valve positioners to reduce the reset time and hysteresis. Digital signals from the computer in the range 0-32767 were converted by D/A converters to analogue signals in the range 0-10volts. A V/I converter then translated this signal to current in the range 0-20mA DC and the latter was subsequently converted to a pressure signal in the range 0-15psia by the I/P converter and a flapper-nozzle mechanism provided the means of controlling the pneumatic output which was applied to the top of the diaphragm. A correlation was developed between the voltage range and the rotameter range $(0-1.67) \times 10^{-4} \text{ m}^3/\text{s}$ and this had to be recalibrated often to forestall any drift in the settings. The valve position had to be calibrated using the following procedure:-

- i) Shut off the supply pressure to the positioner. Connect the necessary tubing from the positioner output to the actuator

pressure connection. Connect instrument pressure to the positioner and set the instrument pressure at midrange.

- ii) Move the flapper to approximately position 6 in the proper operating quadrant and apply supply pressure to the positioner. The actuator should move close to its mid-travel position. If it does not, first check for loose linkage or improper cam installation.
- iii) Apply an instrument signal equal to the low value of the instrument pressure range. Adjust the nozzle until the actuator strokes to the proper end of its travel.
- iv) Apply an instrument signal equal to the high value of the instrument pressure range and observe the actuator stroke. If the actuator does not stroke to the opposite end of its travel, increase the travel by moving the flapper towards a higher number.
- v) Repeat steps (iii) and (iv) until the correct travel is achieved.

4.3.2 Immersion Heaters

Three 3kw immersion heaters in each reactor were controlled by a thyristor assembly and two analogue output channels. The thyristor unit consisted of two thyristors arranged in inverse parallel form and sent current pulses to the immersion heaters when triggered. The power emanating from the heaters was inversely proportional to the trigger angle which was related to the voltage supply and heater

resistance by
$$P = V_s^2 (\frac{Z - \cos\alpha}{Z + \cos\alpha} \sin 2\alpha) / (ZR_1)$$

The digital signal output by the computer was related to the trigger angle as

$$D_s = 32767(z - \alpha_k) / z$$

4.3.3 Thermocouples and Interchange Box

The thermocouples were connected to eight anchors on the Thermocouples Interchange Box (TIB) arranged in two groups, the box containing wetted reed relays facilitating alternating contact between the two groups, switching from one group to another by addressing either of the analogue output channels which connect that set to the A/D converter. The analogue signal from the thermocouple was amplified five-fold to a signal in the range 0-5v and then converted by the A/D converter to a number in the range 0-1023. A linear correlation was developed between measured temperature and its digital equivalent. Regular recalibration of the thermocouples was necessary if used over long periods as errors accumulated due to thermal emf and noise in the relays.

4.4 The Honeywell 316 and the Hadius Data Acquisition System

The data acquisition and manipulation system was comprised of the following three hardware units:

- i) A Honeywell 316 digital computer and its associated peripherals
- ii) A Honeywell 316 Analogue Digital Input Output System (HADIOS)
- iii) A remote signal conditioning box

4.4.1 Computer and its Peripherals (48,49,50)

The basic Honeywell 316 minicomputer includes a main frame and a control panel mounted on a rack cabinet. Integrated circuits are

used in its construction for system reliability and dense packaging and the computer is a stored programme, parallel binary type using a two's complement machine code to shorten computation time. The system memory of size 32k is a high speed, digital storage device capable of storing a maximum of 16 bits of information in 8k of randomly accessible locations. Some of its characteristics include a powerful 72 instruction repertoire, high speed arithmetic unit option, indexing, multilevel indirect addressing, a real time clock, interrupt line and interface logic for communication with peripheral devices. The computer system is designed for real time systems applications involving on-line control, data logging and formatting, process monitoring and message switching. The system software available makes it possible to run source programmes in BASIC-16, FORTRAN IV, DAP-16 or any mixture of these in separate subroutines on the computer. In addition to its standard devices, the following additional peripheral devices were used:-

- i) A High-Speed Paper-Tape Reader operating at 200 characters per second.
- ii) A High-Speed Paper-Tape Punch operating at 75 characters per second.
- iii) A Magnetic Tape cassette unit for input and output of 375 bytes per second.
- iv) A Newbury 8006 computer terminal operating at a baud rate of 9600. This VDU has four different modes of display, ranging from standard characters display to graphics modes. Some keys on the VDU console are programmable and depending on which are set, any of the four display modes is accessed.

4.4.2 Honeywell Analogue Digital Input Output System (HADIOS)

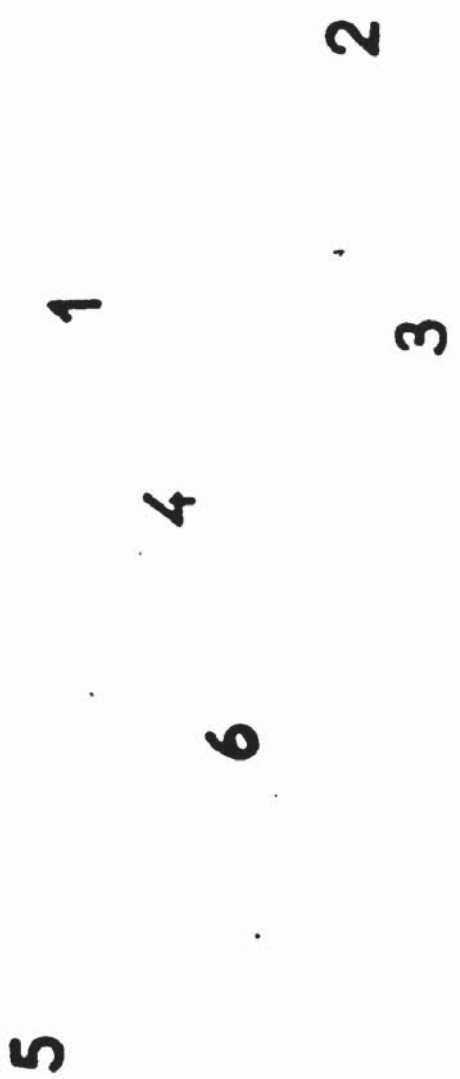
The Honeywell Analogue Digital Input Output System which consists basically of a controller connected to input-output data highway and control lines of a computer is an extremely economic and flexible method of interfacing the computer to a wide range of input-output devices on-line. The controller generates subsidiary data, addresses and controls up to fifteen analogue or digital sub-interfaces, and the latter can be increased by addition of as many as seven extra controllers. The highway controller contains interrupt mask circuits which enable the system to operate under interrupt control. From the several standard subinterfaces included in the HADIOS system, the following two only were used:-

(i) High Level analogue inputs:

This subinterface consists of a single channel analogue to digital converter (A/D) with 10-bit resolution, that is connected to two sixteen channel multiplexers which individually enable uni-polar analogue signals to be converted to decimal numbers in the range 0-1023.

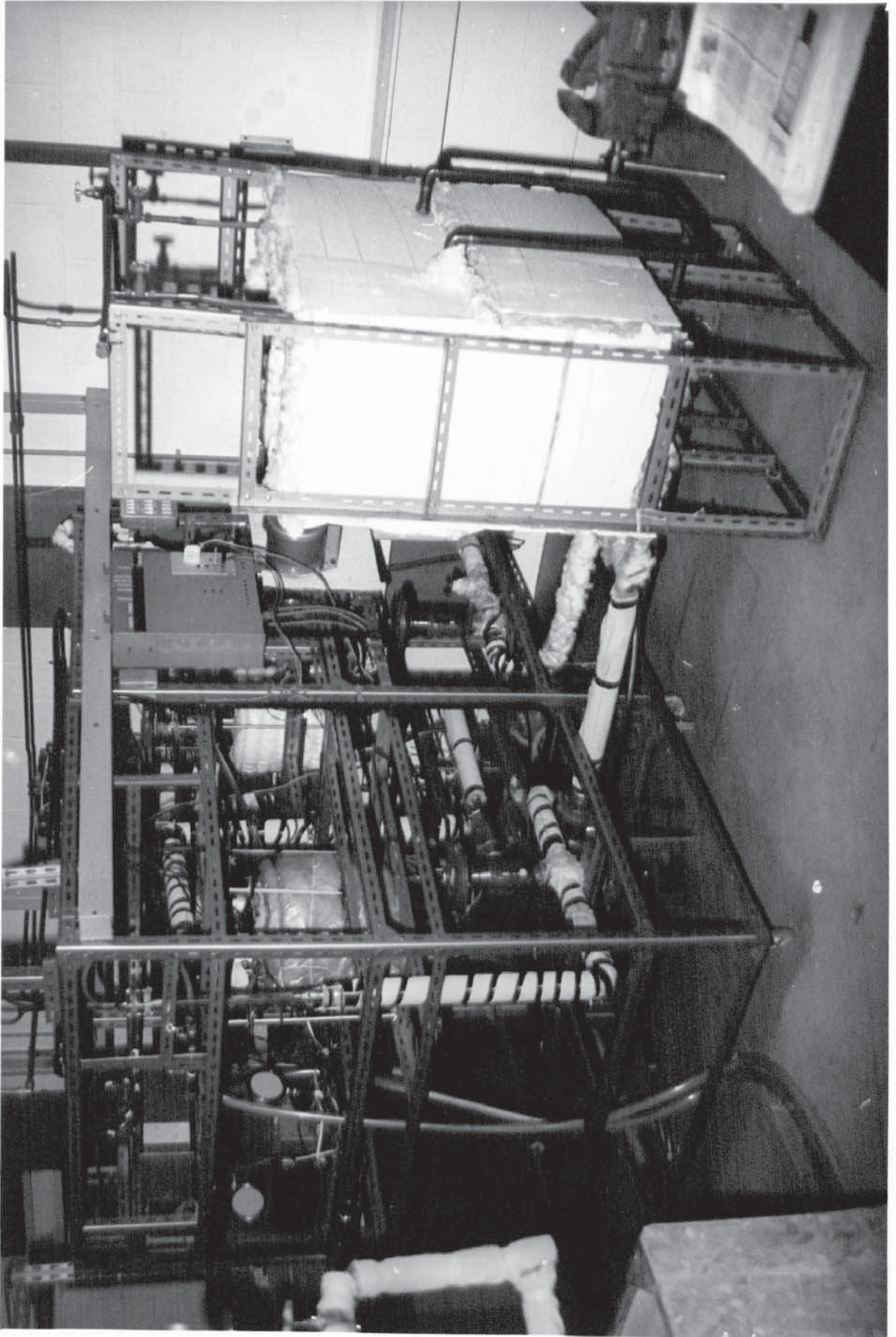
(ii) Digital Output:

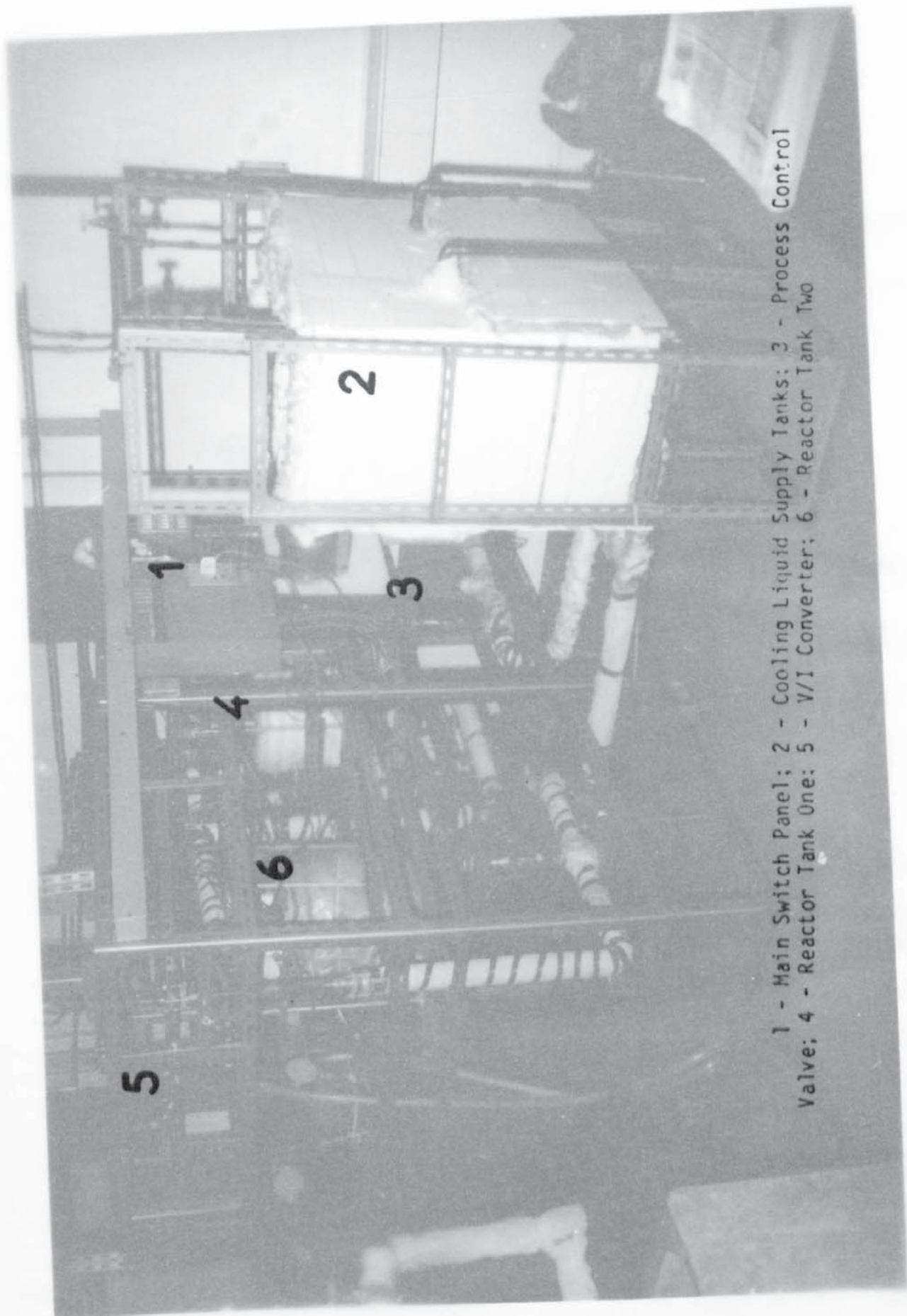
This subinterface has sixteen parallel output lines and analogue signals can be sent to an equivalent number of analogue channels via a digital to analogue (D/A) converter which utilizes twelve of the sixteen-bits for data transmission and the other four for analogue channel identification. The digital output corresponding to the range 0-32767 is converted to analogue signals in the range 0-10v. Using a multiplexer, sixteen analogue channels (0-15) are provided on



1 - Main Switch Panel; 2 - Cooling Liquid Supply Tanks; 3 - Process Control Valve; 4 - Reactor Tank One; 5 - V/I Converter; 6 - Reactor Tank Two

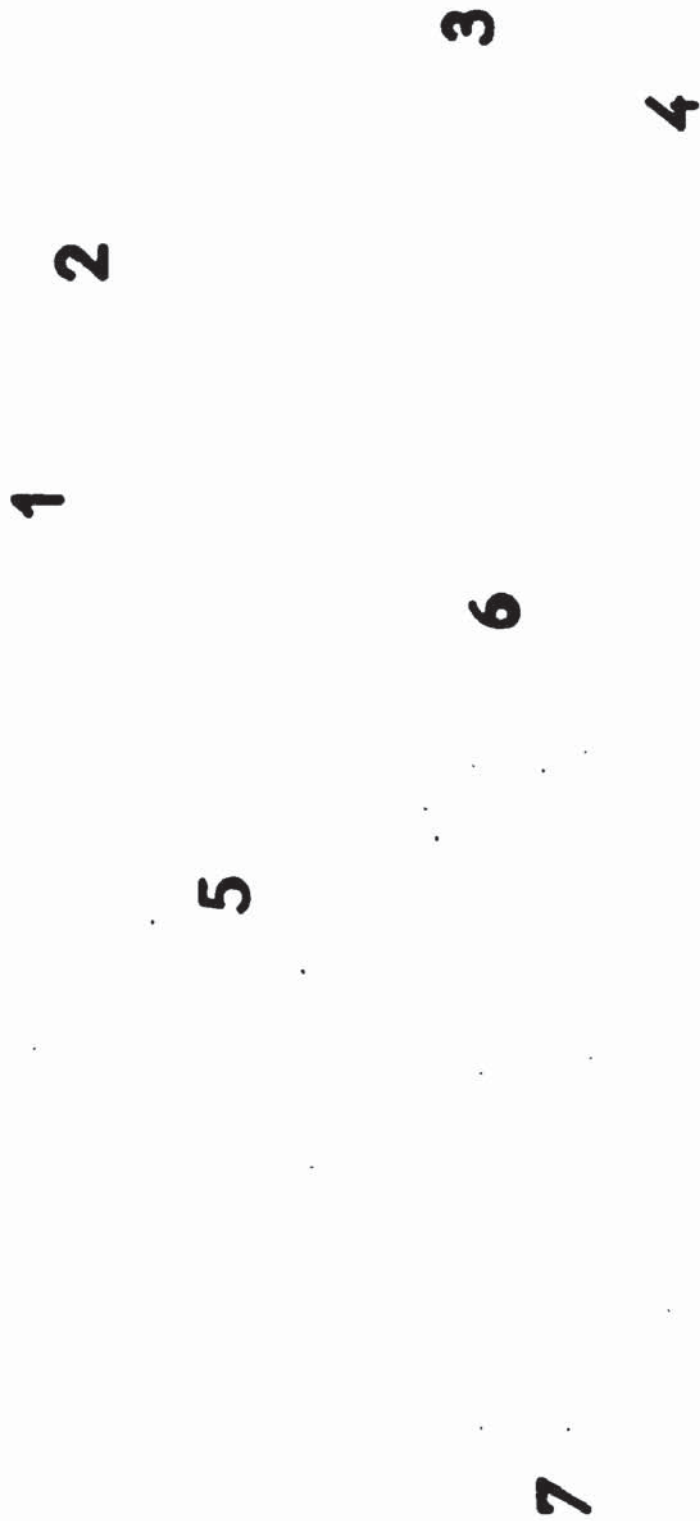
PLATE 4.1 The Experimental Plant





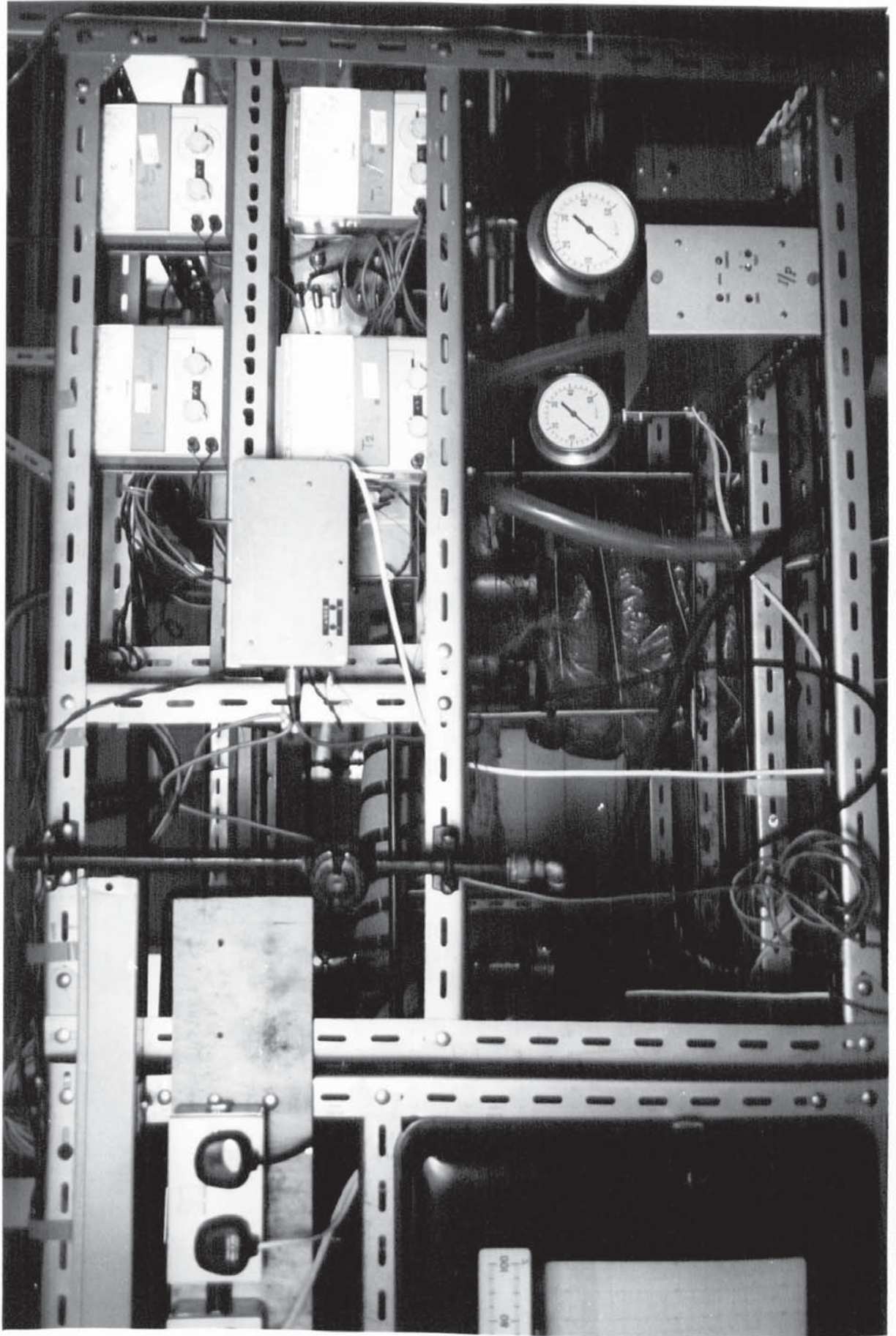
1 - Main Switch Panel; 2 - Cooling Liquid Supply Tanks; 3 - Process Control Valve; 4 - Reactor Tank One; 5 - V/I Converter; 6 - Reactor Tank Two

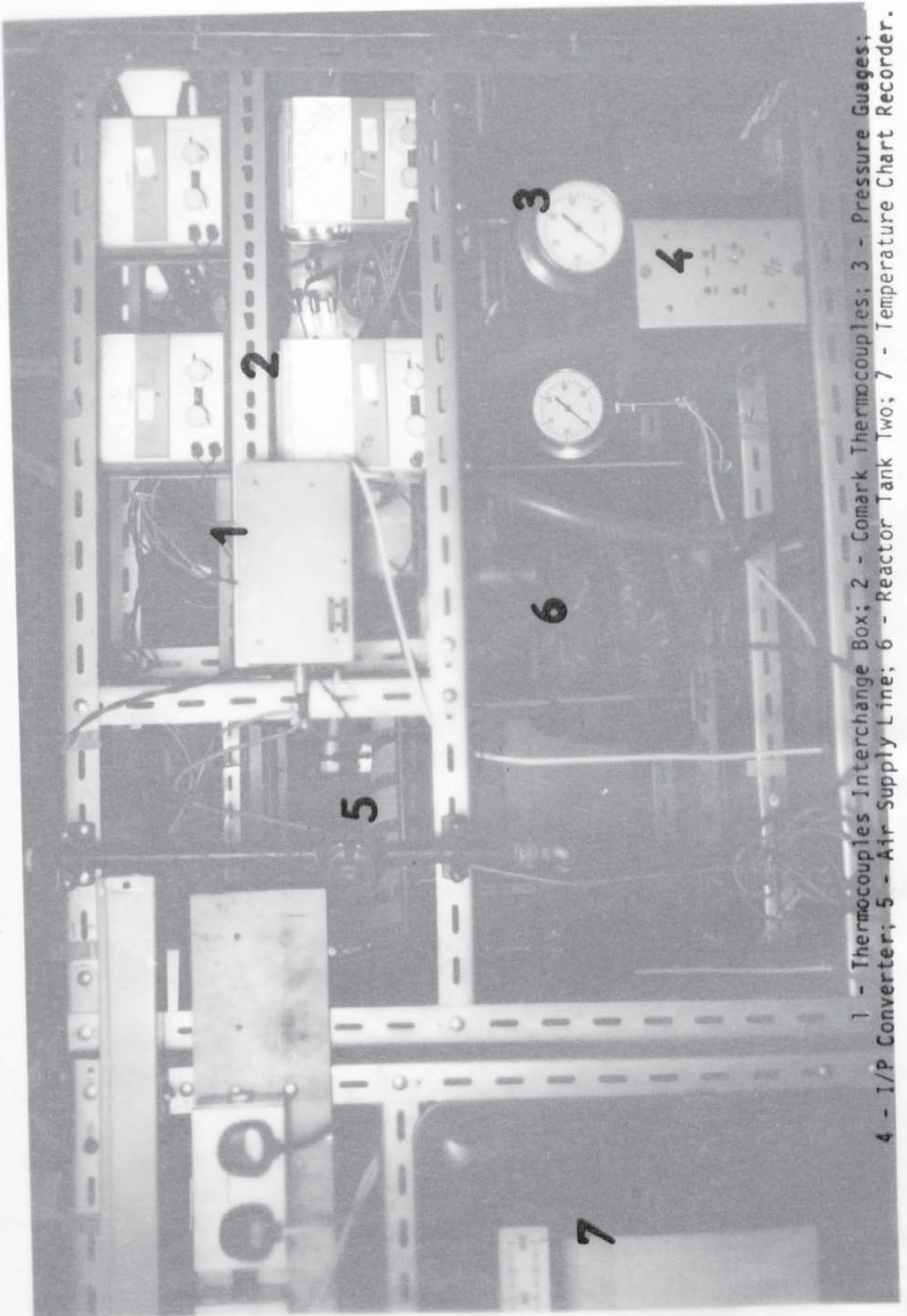
PLATE 4.1 The Experimental Plant



- 1 - Thermocouples Interchange Box; 2 - Comark Thermocouples; 3 - Pressure Guages;
- 4 - I/P Converter; 5 - Air Supply Line; 6 - Reactor Tank Two; 7 - Temperature Chart Recorder.

PLATE 4.2 The Experimental Plant





1 - Thermocouples Interchange Box; 2 - Comark Thermocouples; 3 - Pressure Gauges;
4 - I/P Converter; 5 - Air Supply Line; 6 - Reactor Tank Two; 7 - Temperature Chart Recorder.

PLATE 4.2 The Experimental Plant

1

2

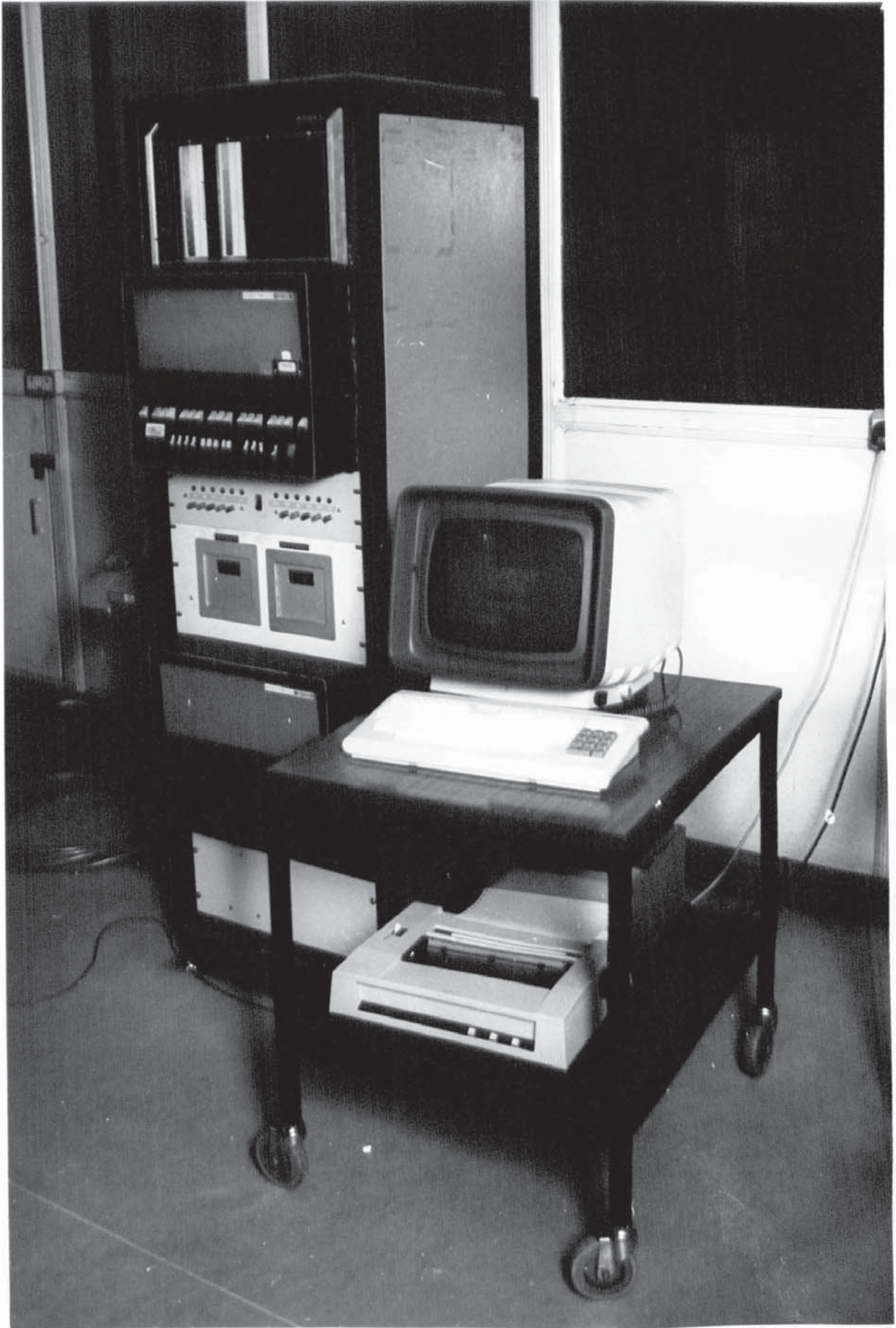
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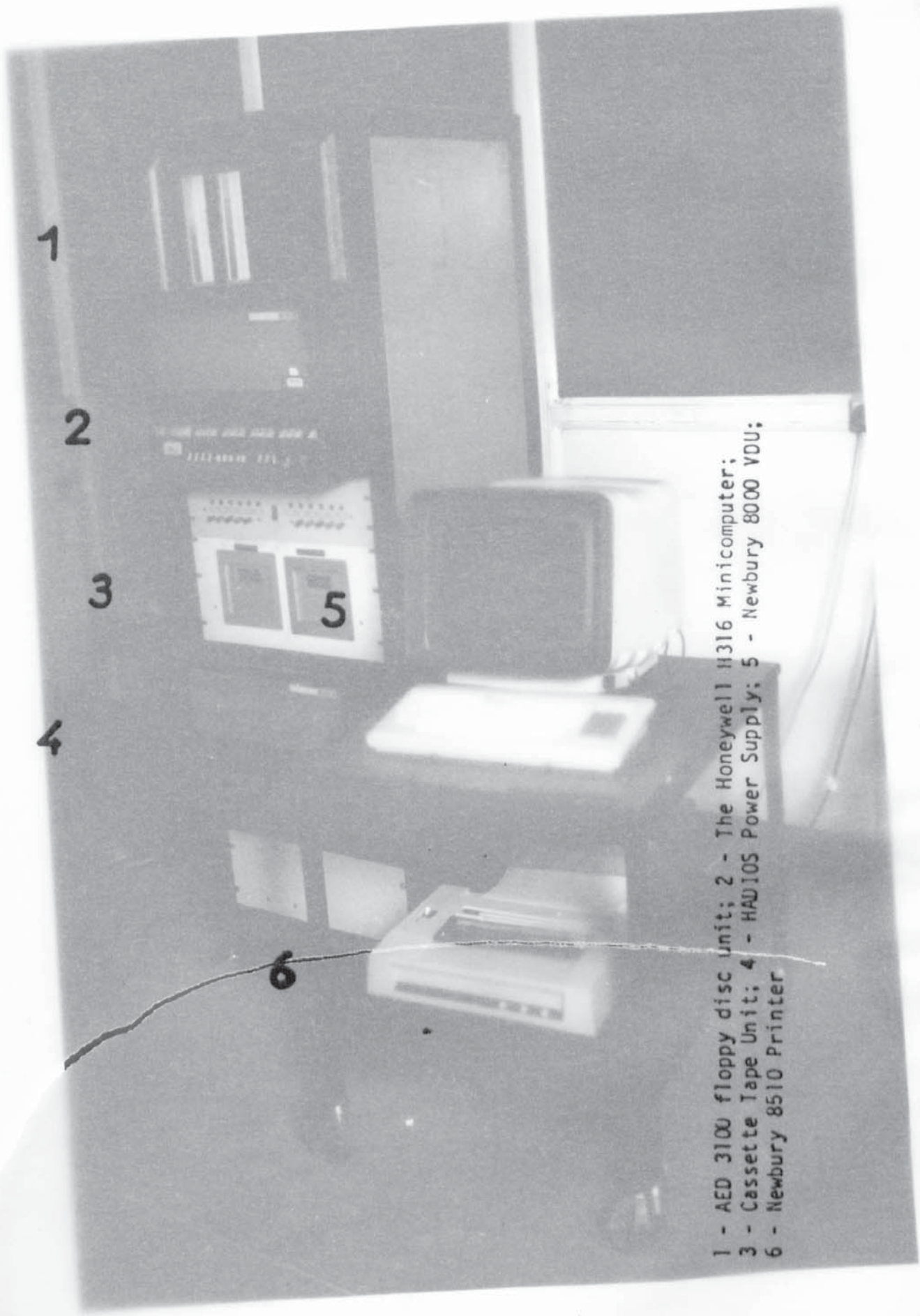
5

4

6

1 - AED 3100 floppy disc unit; 2 - The Honeywell H316 Minicomputer;
3 - Cassette Tape Unit; 4 - HAU10S Power Supply; 5 - Newbury 8000 VDU;
6 - Newbury 8510 Printer





1 - AED 3100 floppy disc unit; 2 - The Honeywell H316 Minicomputer;
3 - Cassette Tape Unit; 4 - HAD105 Power Supply; 5 - Newbury 8000 VDU;
6 - Newbury 8510 Printer

PLATE 4.3 The Honeywell H316 Minicomputer System
and Peripherals

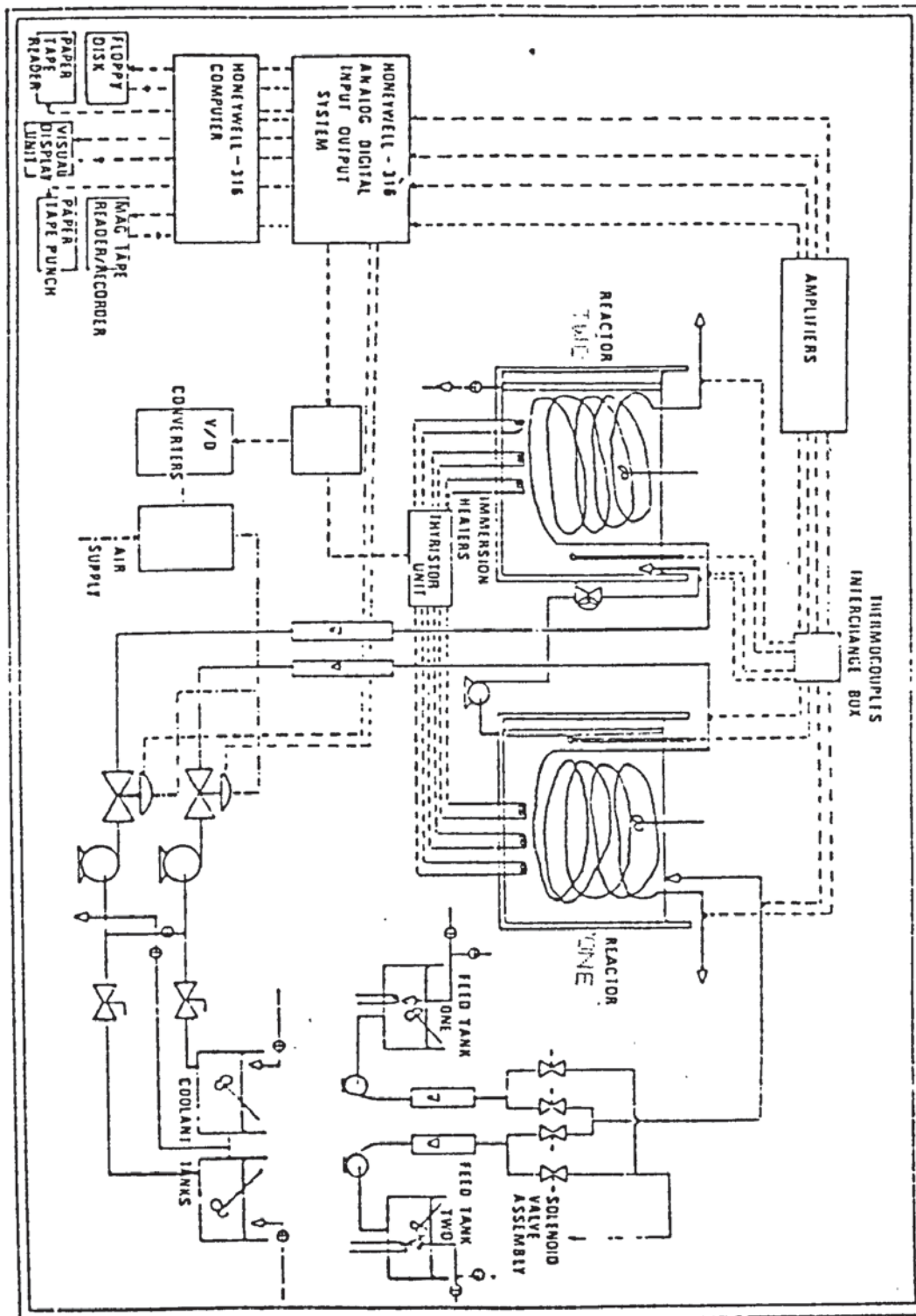


FIG. 4.1 SCHEMATIC DIAGRAM OF PLANT & COMPUTER SYSTEM INTERACTION

CHAPTER FIVE

ON-LINE SOFTWARE DEVELOPMENT

5.1 Introduction

The development of software for interfacing and controlling the experimental plant from the Honeywell 316 computer was the most intricate and time-consuming aspect of this research. Different problems were encountered which did not exist in off-line computing, the least of which was understanding the DAP-16 command repertoire. In off-line computing where total simulation of the system was involved, the digital range of the Harris 800 computer is very large and not easy to breach while the same cannot be said of the Honeywell computer, and this led to corruption of core resident programme in the Honeywell and needed reloading. It was necessary and mandatory that the control computer should have the ability to communicate effectively and efficiently with the process instrumentation and control equipment and have the capability to operate upon data fast enough to provide effective control action and, as explained in the preceding chapter, the Honeywell 316 fulfilled these requirements adequately. Since the control process involved many interrelated variables and required extensive data reduction and logging, complex calculations for advanced control algorithms or models, the first requirement in building up the operating programme was to set up a logical hierarchical structure for programming these stages. The Honeywell 316 has a maximum memory size of 32k words for loading the core resident programme and working storage and this required a streamlining of the numerous subroutines to occupy as small

a memory space as possible. While there was enough provision for swapping of part of the core resident programmes at any time of plant operation for programmes from other storage devices like floppy disks and magnetic tape, problems associated with overwriting core resident programmes do arise, the most prominent of these being the waste of time.

Subroutines with numerous calculation steps had to be executed in the shortest time possible, with the input and output of data being accomplished in like fashion, so that the scanning of the different measuring equipment was done with the same regularity. The need for the central processing unit to communicate with several devices at once, and also to perform computations at the same time required it to be capable of simultaneous or essentially parallel operation, which the Honeywell 316 is incapable of. In order to reduce execution times of these large subroutines, they were written in a high level language, viz FORTRAN or Assembly language (DAP-16 is Honeywell 316 dependent), and compiled before loading into memory, and they could then be accessed from the BASIC executive. The BASIC executive shared some of its library subroutines with the compiled subroutines so as to minimize storage memory. The BASIC executive needed a core resident interpreter and this comparatively slowed down the execution of the BASIC programme.

Input and output operations were reduced to the barest essential minimum as the peripheral devices like the paper tape punch normally operate at slower speeds than the CPU and made a significant contribution to the lengthening of intervals between scans. The

interval or dead time between sending out successive analogue signals to control valves had to depend more on their reset times and this was taken care of in the form of executing dummy routines, as too fast emission of these signals without due regard to the waiting time would have resulted in muddled settings for the different valves.

The essential software consisted of seven subroutines written in DAP 16 and FORTRAN and accessed from the BASIC main programme. These subroutines performed various tasks like input and output signals, simulation, graph plotting and other house-keeping tasks for the smooth execution of the programme.

5.2 HADIOS Executive

The first three subroutines which are in Assembly Language (DAP 16), are the embodiment of the HADIOS executive, which as used in this research is a modification of the one listed in Webb's thesis(51). Subroutines 1 and 2 which indicate the initiation, execution and termination of the scanning of the various analogue input channels and are always used in tandem, retain their original form. These subroutines make use of the computer clock to maintain a fixed scanning interval which is user specified. Subroutine 2 causes the programme to wait for the next clock interrupt if all scans requested have not been successfully completed or else the scanning process is terminated and the programme continues execution of subsequent instructions. Subroutines 4 and 5 of HADIOS EXEC 02 were deleted to create more memory space for other programmes as these were not needed and subroutine 5 became subroutine 3 of the present

version of HADIOS EXEC 03. Subroutine 3 sends out digital input to the specified analogue output channels without waiting for a clock interrupt. The address table was modified to reflect the above changes and the HADIOS executive was compiled and loaded into memory location '25000 and extended to address '26777. In the event the computer interrupt facility was not used as the turbine flow meter became faulty and was therefore removed from the plant.

5.3 Utility Subroutines

The next two subroutines (4 and 5) in the software package were also written in assembly language and these regulated the communication of the computer with the peripheral devices. Both subroutines appear in Mukesh's thesis(19) and only slight changes were made so as to provide compact loading into computer memory. These subroutines performed the following functions:-

- i) Sent output data to the visual display unit or high speed paper tape punch or magnetic cassette by setting or resetting sense switch 4.
- ii) Punched leaders on paper tape to separate different sets of results.
- iii) Started and stopped the computer clock after execution of certain instructions and gave the elapsed time of each stop.

5.4 Simulation Subroutines

There are four FORTRAN subroutines, three of which represent the reactant and product concentration in the system at unsteady states. The first of these subroutines is the precursor of the other three and acts as the control subroutine with options from the main BASIC

programme for accessing any of the other three. This subroutine only is represented on the Basic CALL address Table and transfer of variables between Basic and this control subroutine is facilitated by the argument transfer subroutine FFAT, the latter being loaded from FORTRAN library subroutines. Unlike in Basic where declared variables are available to both the main programme and its several GOSUB routines, a COMMON BLOCK statement is needed in Fortran for the same variables to be made available to each of the subroutines. A Fourth order Runge-Kutta method is used in integrating the differential equations and the integrating step is the time elapsed between two successive calculations, the recorded temperatures and flow rates being made available through the CALL arguments. Since all the compiled Fortran subroutines did not fit into one sector of computer memory, enough space (Base) had to be provided for intersector linkage and this was a tedious trial and error job.

5.5 Graphical Subroutines

The graphical subroutine as called from Basic is a combination of several Fortran subroutines grouped together to produce patterns on the screen. As the Newbury screens do have different character and graphical display options, auxiliary subroutines were needed to programme the keyboard to effect a change to the right display mode before characters or pictures were drawn. Digital and graphical display of some results alternated with each other on the screen. Labelling of screen pictures was not included as this would have needed loading more subroutines in computer memory and an increase in execution time and since the pictures were used merely to monitor the overall progress of each experiment.

5.6 On-line Basic Programme

The Basic On-line programme co-ordinated to the Basic Executive, HADIOS and the other aforementioned Fortran subroutines to achieve a smooth control of the experimental plant. Having set the relevant HADIOS parameters, the programme scanned the analogue input channels and using flow values input manually from keyboard calculated the dimensionless variables in the model equations. Correlations developed for flow rates and control valve scale were used in setting the latter. The computer clock was started and the following cyclic operations were executed as the reactions progressed through the unsteady state in search of a steady state.

1. Scanning the input channels and calculating temperatures.
2. Integrating the mass balance equations.
3. Calculating the reaction heat release and sending appropriate signals to the immersion heaters.
4. Outputting results to paper tape punch or display on VDU.
5. Plotting reactor temperatures and concentration against time.

The above process was terminated when the temperatures and concentration of masses were constant over a period and these steady state values were recorded. The next stage dealt with the introduction of disturbances into the system and its transient response to different control strategies. A control strategy was selected from the control menu and a disturbance was input from the keyboard if it was a mass disturbance or else the heaters in feed tanks were set for heat disturbances. The following tasks were then performed:-

1. Scanning the input channels and calculating of temperatures.
2. Integrating the transient response mass balance equations.

3. Calculating reaction heat release and sending of signals to immersion heaters.
4. Calculating coolant flow rates for the control strategy on each reactor and setting control valves to reflect new flow rates.
5. Outputting results to paper tape punch.
6. Plotting reactor temperatures and concentration against time.

The above steps were executed repeatedly until constant temperatures and concentrations were attained before the programme stopped. In cases where the coolant flow rates required for a particular control strategy exceeded the maximum flow rate available on the plant, the programme printed an error message on leaving and could only be rerun from the unsteady state. While every effort was made to reduce the time between successive scans in the transient response section of the programme, the setting of the control valves used up substantial time as the following execution times show:

a) Scanning of channels	1 sec
b) Executing simulation routines	2 secs
c) Executing graphics routines	3 secs
d) Outputting results to paper tape	2 secs
e) Setting of one control valve	4 secs
f) Setting of both control valves	7.7 secs

In setting both control valves in succession a time delay was needed in order that the analogue signals did not get mixed up and produce

inaccurate settings. This time delay, which was the minimum permissible by the electrical arrangement, was more than the total time for simulation, scanning and executing of graphics routines.

5.7 Basic Interpreter

The Basic-16 Interpreter is the Honeywell version of Basic for series 16 machines and is an interactive High-level language with a simple command repertoire. The compiler is interactive and all constants are stored as floating points. When used with FORTRAN subroutines in which a distinction has to be made between real and integer variables, conversion has to be made in the FORTRAN subroutine. In addition to the usual GOSUB routines, there is provision for CALL statements which enable FORTRAN or DAP-16 subroutines to be accessed from the main BASIC programme. The general form of the CALL statement is:

$$\text{CALL } (L, S_1, S_2, \dots, S_n, V(\emptyset))$$

where L is the subroutine reference number

and $S_1, S_2, \dots, S_n, V(\emptyset)$ are arguments to be passed to the subroutines called.

A maximum of ten subroutines can be accessed with the starting address of each being loaded into a reference table that occupies location '516-'530. When subscripted variables are passed as arguments to FORTRAN subroutines, the first subscript in Basic is numbered as zero while in Fortran the first member of an array is one. Special care is taken when these arrays are dimensioned in both Fortran and Basic.

In the Basic on-line programme for this research, the different sub-routines called and their arguments are described in Appendix 2.

5.8 Preparation of Software Tapes

The writing of subprogrammes in languages other than Basic is the first stage in preparing subroutines accessible from Basic. The source Fortran (DAP-16) tapes have to be compiled (assembled). The compiler (assembler) is a system programme that converts High-Level (symbolic assembly) language into machine code. The compiling (assembling) process involves setting of the A-register for selected Input/Output bit pattern and sense switches and the compiler is able to detect coding, typing or printing errors and send out diagnostic messages whenever these are encountered. Using OBJCHOP, another system programme, the object Honeywell 316 subprogrammes are selectively grouped for easy subsequent loading into any of 32 memory sectors. Self-loading system tapes (SLST) or ones which can be loaded using the key-in loader and a two-part self-contained loader have to be prepared for the core resident programmes; this reduces the subsequent loading of memory to a case of merely entering of 1 in P-register and pressing the START pushbutton. All the object tapes are loaded into memory by a relocating loader (LDR-APM) and then punched out of memory by the punch and load (PAL-AP) programme. After PAL-AP has been directed to an output device and the limits of memory to be dumped have been set, it dumps the two-part self-contained loader that is used to supplement the key-in bootstrap at programme load time and whatever is contained in computer memory within the set limits. In between loading and dumping

onto tapes a memory map of the loaded programme is obtained and is recorded in Appendix A.1.8.

5.9 Conclusion

A review of the Honeywell 316 software relevant to this research was discussed together with a summary of the user constructed package for running the plant on-line. A detailed description of the loading procedure and the making of SLST tapes was left out as these can be obtained from several of the referenced user booklets. Although this was not described as a separate subroutine since it was not accessible from Basic like other CALLABLE routines, there was a pointer subroutine whose main function was to make available to the Fortran programmes the addresses of certain functional routines common to both Fortran and Basic. This eliminated the need for loading these routines from the Fortran library. The final, compact package assembled was versatile enough to accommodate the different sophisticated control strategies applied to the system and how the experiments were carried out is the subject of the next chapter.

CHAPTER SIX

EXPERIMENTAL STUDIES

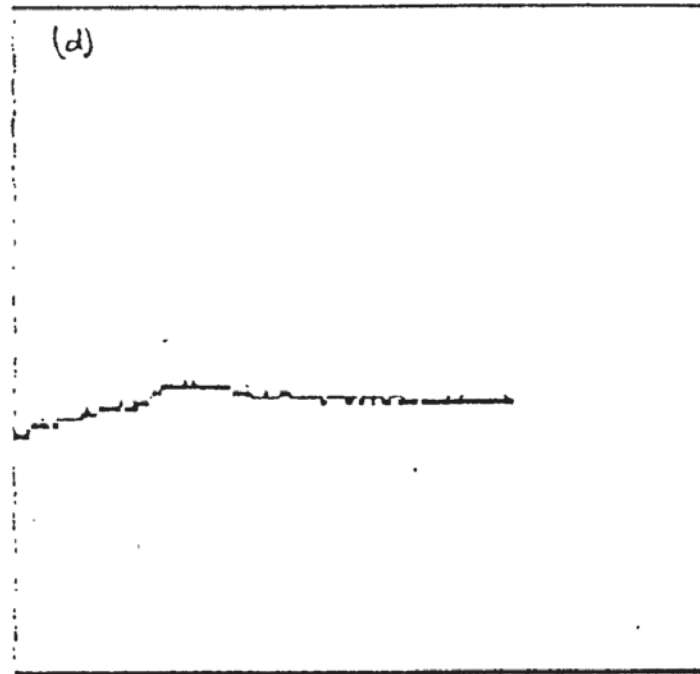
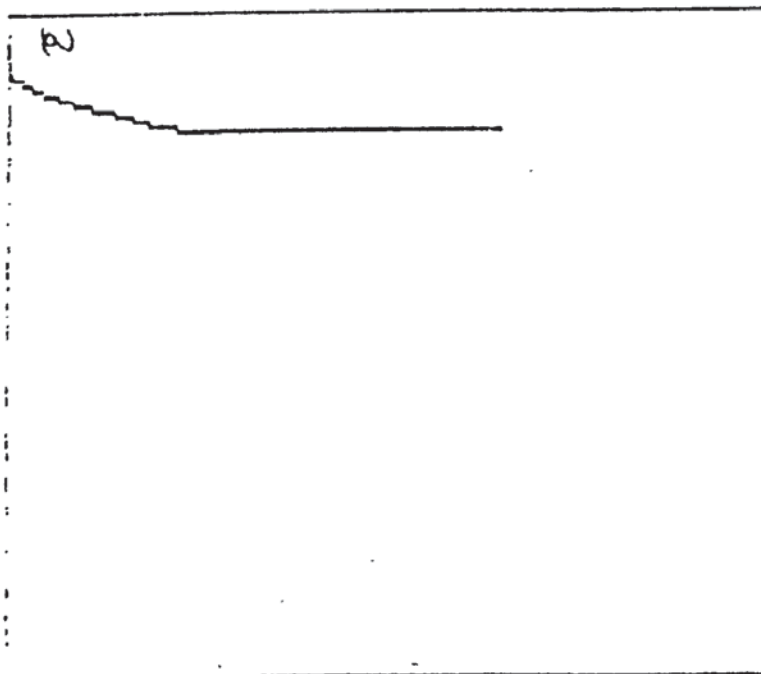
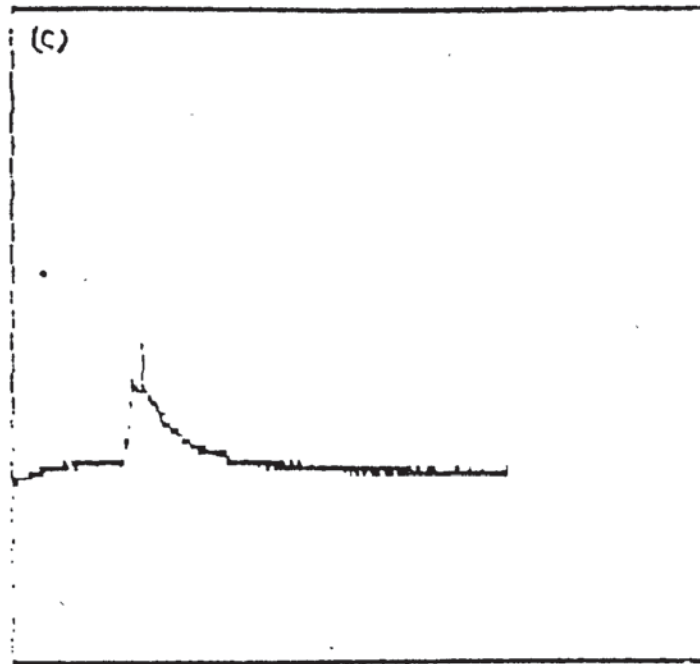
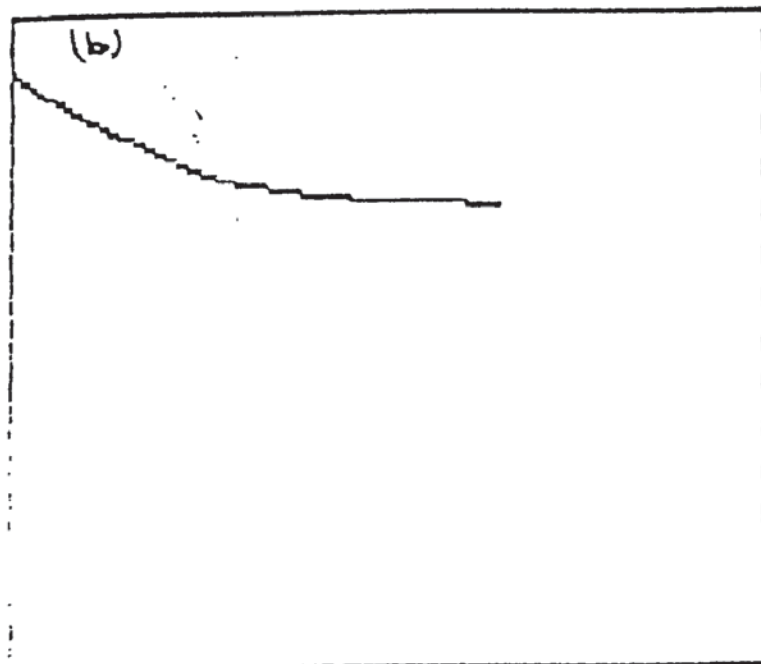
6.1 Introduction

The experimental studies on the plant were the means of verifying the applicability or otherwise of the total simulation of the system implemented on the Harris 800 mainframe computer and also to make a qualitative comparison of experimental and simulated results.

Though this in itself was not totally experimental as the mass of reactant and product components had to be simulated on the Honeywell minicomputer, the reaction heats released, flow rates and monitored temperatures were as real as would be found on any scaled down industrial equipment. Each experimental run consisted of two sections, a run up to the steady state and transient response to disturbances applied to the steady state of the system under different control strategies.

While most of the experiments were carried out with each reactor having an independently controlled coolant stream, the advantage or otherwise of using a single cooling stream flowing counter-currently to the process feed stream was also investigated. The stability implications to each of the reactors were also studied for the various control strategies and coolant flow arrangements. This chapter outlines the type and range of experiments conducted. The details of the individual experiments are set out in chapter 8 and Appendix 6.2

6.2 Run Up to the Steady State



- a = Concentration of reactant versus time graph in Reactor 1
- b = Concentration of reactant versus time graph in Reactor 2
- c = Temperature versus time graph in Reactor 1
- d = Temperature versus time graph in Reactor 2

Sample output of experimental run from start-up to steady state.

Fig. 6.1

Depending on the existing tap water temperature, different process feed flow rates were set manually and with a fixed feed concentration the experiment was run to its steady state value, the latter being attained when the concentration of product in the second reactor changed in two successive scannings by less than 2×10^{-5} % of the final product which was at an operating level of the order of 0.5 kg/m^3 . For counter-current cooling of both reactors, a change in the flow path of the cooling liquid was made by closing and opening certain flow valves, but change in location of thermocouples was not made as these were strategically placed to monitor temperatures in flow routes. The process feed rate had to be observed throughout the run to make sure it was constant and slight manual modifications were made to maintain it at the required value. The cooling liquid flow rates were intermittently reset to arrest any drifts in their values. The reactors' reactant concentrations and temperatures were displayed on the VDU between scans, a copy of a typical run being shown in figure 6.1 (page 63). Two methods were used to reach the steady state. In one case the system was allowed to run its course, the only heating coming from the reaction heat; this took a long time (on average 50 minutes). In the second method, which on average, took 15 minutes, hot water was introduced into the reactor before reaction started and this high temperature accelerated the reaction rate. For such 'quickie' runs, the criterion for attainment of steady state was tightened to a tolerance half the value of a normal run. In a normal run using the first method, reactor one usually got to its steady state before reactor two, but for a 'quickie' run a careful observation was made such that the second reactor did not

satisfy the stated tolerance for steady state before the first reactor. It was observed that in cases of liquid hotter than the steady state temperature of the first reactor being introduced into it, a higher conversion than the steady state value was obtained for some time. This overshoot was then eliminated as the reactor cooled to its steady state, thereby taking a longer time than usual. The temperatures of the process feed and coolant streams for most of the experiments was below 14°C . On warm days when the tap water temperature was above this figure, a high flow rate of cooling water was needed to get a steady state temperature of reactor one below 20°C ; this in turn reduced the range of cooling liquid available to implement control on either reactor if, say, a step increase in temperature were introduced. Such runs for inlet flow temperatures far in excess of this value were unsuccessful and were consequently discarded.

6.3 Transient Response of Controlled System

The input of temperature load disturbances was done manually by turning on the heaters in the feed tanks and adjusting the rheostats for the appropriate heating rates or sending a hot water stream into the feed tanks.

The disturbances introduced into the steady state were:

- (i) Step change in feed temperatures by switching on heating coils in feed tanks.
- (ii) Step in coil temperature by sending hot water into supply tanks.

(iii) Perturbation in reactor or coil temperature by the addition of hot water to the appropriate feed tanks.

(iv) Step or perturbation in reactor concentration by feeding the disturbance value into the computer programme.

On days when there were freak weather conditions, changes in tap water temperatures were utilized as load disturbances. Step increases in feed temperature and concentration were applied only to reactor one as the second reactor took its feed from the first and its inlet was inaccessible. While step changes in feed reactant concentration were instantaneous, it took 1-2 minutes for changes in temperature to reach the maximum values. Whenever step changes in feed temperatures were implemented, the process flow rate had to be kept constant by manually adjusting the flow valves.

The flexibility of the digital computer as a controller was exploited to generate different control strategies, which is not possible with analogue controllers. These latter would have needed part or total replacement as different strategies are implemented. Due to the trial and error nature of tuning PID controllers and the sensitivity of the derivative mode to process or measurement noise, only ideal proportional controllers were used in the experimental runs.

The control schemes implemented for these disturbances by manipulation of coolants rates were as follows and are shown in block diagram on page 347:

- (i) Proportional feedback control in reactor one of:
 - a) reactor temperature at outlet
 - b) coil temperature at outlet
 - c) reactant concentration at outlet.

(ii) Combined proportional feedback and feedforward control in reactor two of:

- a) reactor temperature at outlet
- b) coil temperature at outlet
- c) reactant concentration at outlet

Also simultaneous invariance type control in reactors one and two of reactors' temperature at outlet:

The disturbances applied to reactor one for this control scheme were:

- a) step in reactor inlet temperature
- b) step in coil inlet temperature
- c) step in reactor inlet concentration
- d) steps in reactor and coil inlet temperature

Only disturbance (b) was applicable to the second reactor as it received disturbances in the other variables from reactor one.

Block diagram representations of these control arrangements are given on page 346.

Responses of transient studies were punched on paper tape for subsequent transfer to the Harris computer for plotting of graphs and on-line displays of both reactors' concentrations and temperatures were done simultaneously. The calculations and display of results were reduced to the barest minimum so as to reduce time between scans. The resetting of process control valves was the major time-consuming routine between scans, taking up about 50% of the 16 seconds interval. Sampling of responses was carried on for over 30 minutes in each experimental run. In runs where the cooling water demand exceeded the valve's maximum, the computer printed an error message and the run was aborted. This was found more likely to occur



when large load disturbances were introduced or large controller gains were applied.

6.4 Stability of Open and Closed Loop System

The stability of each of the controlled and uncontrolled reactors was established by applying step disturbances to the steady state or by starting from an unsteady state and observing the direction of movement of the response, that is, whether this was towards an open-loop stable state, a closed-loop stable state or an unstable steady state. In cases where the reactor was moving away from a particular steady state, the demand for control action became obvious and how easily it was restored to its initial steady state depended on the type of control applied, the controller gain and the parameters for the system. The controller gains and other parameters for the experimental runs, were chosen as far as possible, to be the same values as used for the total simulation so as to have a common basis for comparing the results of the two methods later, and also the need to keep the system in a controllable range.

6.5 Conclusion

The above documentation has described the control schemes implemented on each of the reactors experimentally and the disturbances whose adverse effects these controllers were supposed to minimize. With the description of the total simulation being the object of the next chapter, the stage will then be set for the comparison of both results.

CHAPTER SEVEN
TOTAL SIMULATION OF THE PLANT

7.1 Introduction

The total simulation of the plant was carried out on the Harris 800 mainframe computer with no constraints on allotted user memory space, a large library of subroutines and through an interactive FORTRAN 66 programme described in much detail later. This simulation provided the testing ground for some of the control strategies which were later applied on the plant. Some of the control modes like decoupling control, though not implemented on plant due to the need to know the temperature profile of the cooling coil, were easily applied in this simulation due to the ease of calculating the intermediate temperature values. As mathematical instabilities in the calculations were encountered when the system of differential equations was numerically integrated using long step lengths of time corresponding to scanning intervals, short step lengths which do not correspond to intervals between two successive scans on the plant were used in the total simulation. This mathematical instability is a consequence of the large difference in residence time constants in the reactor and the cooling coils, resulting in one component of the solution decaying much faster (a feature of stiff system) than the other two. Thus the eigenvalues of the Jacobian matrix show one of the three values to be more than twice the sum of the other two. The complete model includes the chemical process, the measuring elements and the final control element, the time lags associated with

measuring elements in their transfer functions, the transfer functions of control valves and the characteristics of P/I, A/D and D/A converters. Thus the model equations used for the total simulation are a modification of the component mass balance transient equations and the heat balance transient equations for the reactors and cooling coils as set out in chapter 3 plus additional dynamic equations representing the thermocouples and control valves. Parameters like volumes of vessels, flow rates, heat transfer coefficients and others were taken from the experimental plant after averaging values of several readings or measurements. The following assumptions in addition to those stated in section 3.2 were made in formulating the complete plant model equations:

- (a) The temperature of products from first reactor is the same as the inlet feed temperature into the second reactor, emphasizing the negligible heat losses from the system.
- (b) The time lag between products leaving the first reactor and entering the second is neglected due to the small diameter ($\emptyset.0022\text{m}$) and short length (2m) of the connecting tube and the high flow rate through this tube (about $4 \times 10^{-4} \text{ m}^3/\text{sec}$).
- (c) The transfer functions for the thermocouples and control valves are first order with the time constants given in Appendix 4.5.(page 127). The gains of V/I and I/P converters are combined into the valve transfer functions.
- (d) The time delay in the release of reaction heat was neglected.
- (e) Sampling time during each run was constant.
- (f) Noises entering the system via A/D and D/A conversions and due to drifts in electronic components were neglected because these

were small. Their effect was minimized by taking several readings during each scan and averaging these for the actual reading. Installation of analogue and digital filters would have reduced the noise but this would have added to the equipment cost. At zero scale reading on the rotameter some liquid still seeps through the control valve into the cooling coil and this is also neglected in the simulation.

7.2 Model Equations of the Plant

The schematic representation of the plant given in figure 4.1 is represented by the following nondimensional equations as applied to the first reactor :

Component balance

$$(Y_1 - X_1 - DaX_1 \exp(X_2^*/(1+KX_2^*))) = dX_1/dt' \quad (41)$$

Energy balance

Reactor

$$(Y_2^* - X_2^*) + BDaX_1 \exp(X_2^*/(1+KX_2^*)) - (p/n)(nX_2^* - \sum_{i=1}^n X_{3,i}) = dX_2/dt' \quad (42)$$

Cooling coil

$$\dot{X}_{3,1} = ((Y_3^* - X_{3,1}) + (p_c/n)(X_2^* - X_{3,1}))n\epsilon/\epsilon_c \quad (43a)$$

$$\dot{X}_{3,2} = ((X_{3,1} - X_{3,2}) + (p_c/n)(X_2^* - X_{3,2}))n\epsilon/\epsilon_c \quad (43b)$$

$$\dot{X}_{3,n}^* = ((X_{3,n-1} - X_{3,n}^*) + (p_c/n)(X_2^* - X_{3,n}^*))n\epsilon/\epsilon_c \quad (43c)$$

Measuring elements

$$t_m (dY_2^*/dt') + Y_2^* = Y_2 \quad (44a)$$

$$t_m (dY_3^*/dt') + Y_3^* = Y_3 \quad (44b)$$

$$t_m (dx_2^*/dt') + X_2^* = X_2 \quad (44c)$$

$$t_m (dx_{3,n}^*/dt') + X_{3,n}^* = X_{3,n} \quad (44d)$$

Control valve

$$t_v (dF_{cact}/dt') + F_{cact} = F_{ccal} \quad (45)$$

At steady state, equations (44a-45) combined with equations (41-43c) will be equivalent to equations (5-7c).

A set of similar equations applies to the transient state of the second reactor.

7.3 Computer Programme

The user-friendly computer programme written in FORTRAN was run interactively and not only simulated the plant but entailed sections for calculating steady state values and determining their stability, calculating of Lyapunov's functions and plotting of both simulated and experimental results. The constraints imposed on the system by its parameters are taken care of in the writing of the programme with error traps inserted to stop any ridiculous results being output due to input and acceptance of faulty data. These error traps are especially useful as it was experienced that for bulky programmes some undefined variables or parameters often obtain default values and the error analysis software of the operating computer system does not spot the undefined arrays. The initialization of values was from the VDU terminal and the different options of calculations provided a flexibility which could have been lost if the programme was run batchwise and data was read from files. The only data read from files was that from experimental runs which had

to be read into the 1904S computer from paper tapes and subsequently transferred to the Harris system. Most of the VDU terminals have graphics capabilities and, though not of very high resolution, allowed the user to plot results on the screen and only produced hard copies when he was satisfied with these. On the system being heavily loaded, execution of jobs slowed down considerably and running of programmes as background jobs (batchwise) would have saved user time. Interactive computing during such periods was time wasting and boring but still provided greater flexibility in inputting of data which influenced subsequent calculations performed. In most cases the choice of calculations depended on the results of the preceding sections and since the user followed closely the execution of the programme, he had the opportunity of making judgments and alterations that batch processing would not have provided. The dynamic differential equations describing the controlled and uncontrolled system were integrated numerically using a fourth-order Runge-Kutta method with a fixed step. Solution of the steady state equations was by the Newton-Raphson method, and since this required an initial guess which is near the solution, a plot of the heat generation and removal for the system preceded this iterative method so as to set a good initial guess. The commands for compiling and running the programme were as follows:-

```
FO.MEWND MANX
VU.R KNOX
LIB *NAG10D *GINO-F *LIBERY
BE
AS 8=*
KNOX
```


An alternate method of determining the steady state values was to integrate the equations of the dynamic state from some initial state, until constant values of the state variables were obtained. This invariably ended up at one of the two stable steady states and gave no indication as to the position of the intermediate unstable steady state. A typical result for the uncontrolled system starting from different initial values in both reactors is displayed in figures 7.1 and 7.2 (pages 76&77); in each case the integration ends at the stable steady state. These trajectories are seen to criss-cross each other, introducing more critical points than do actually exist. This is because the displays are in two dimensional space; this would not happen if three dimensional space is used. The results of the total simulation are given in tables 8.1 and 8.2 and the graphs depicting responses to different disturbances and control schemes applied to the system are shown in Appendix A.6 (Figs. A.6.1.1-A.6.1.59). The programme listing and the corresponding flow chart are given in Appendices A.4.6 and A.4.7 respectively.

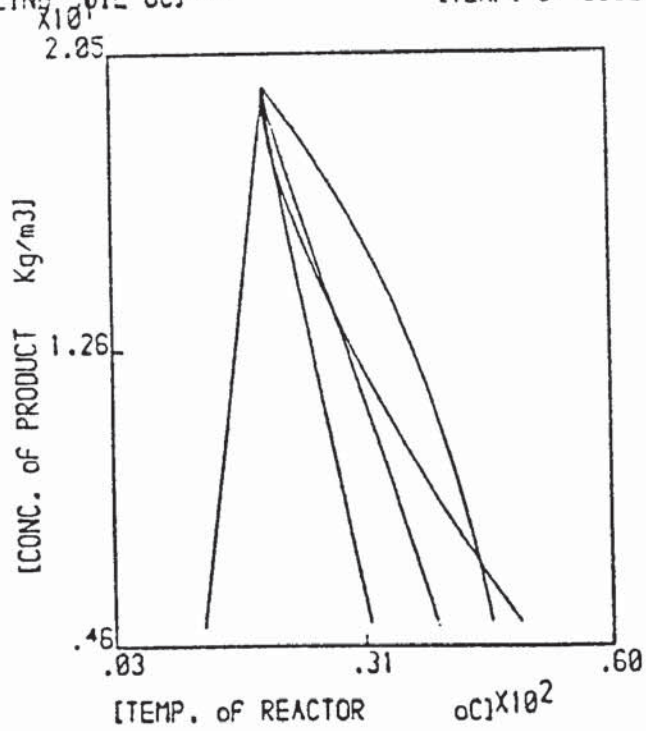
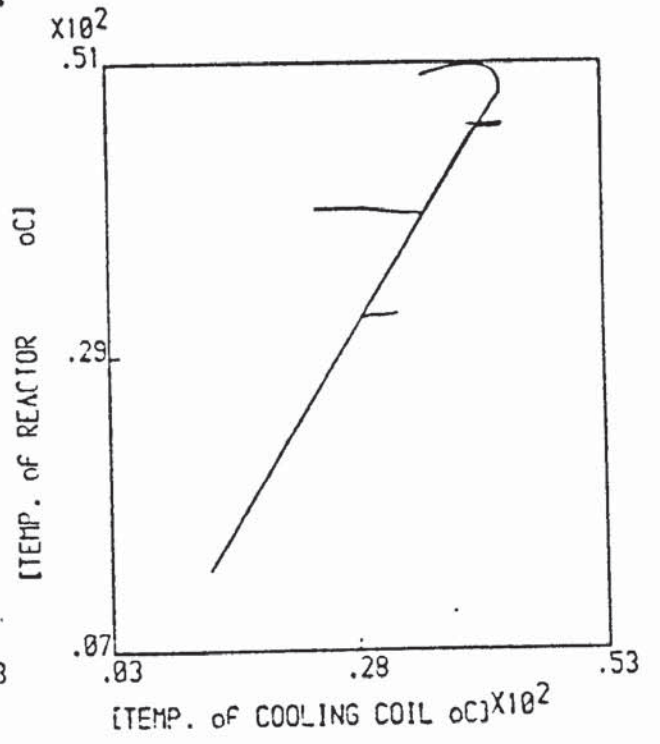
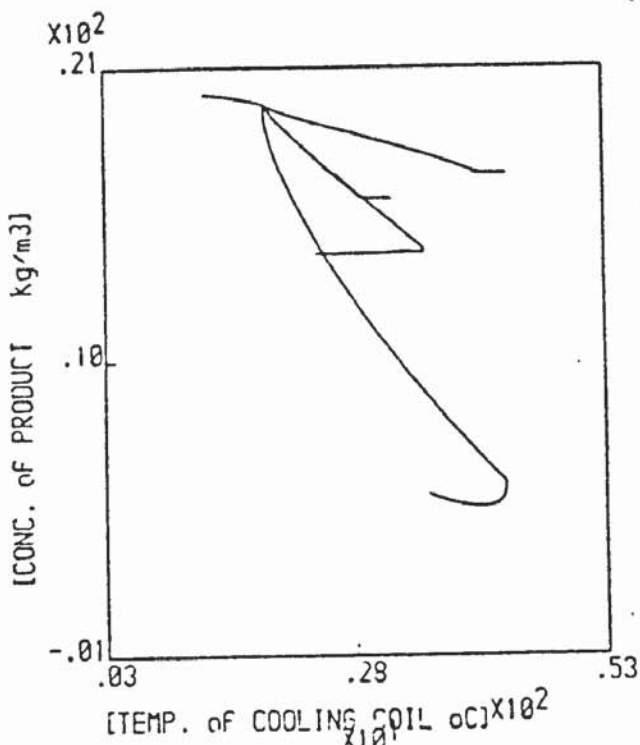
7.4 Control Schemes and Disturbances

In addition to the control schemes and disturbances enumerated in chapter 6.3 which were all achieved in this simulation package, non-interacting control (page 346) of each reactor's temperature at outlet was attained using the mathematical derivations as set out in chapter 3.; the disturbances being the same as referred to above. There were no time delays involved in implementing the temperature load disturbances as only digital values were involved. All load disturbances into either of the reactors or coils were implemented at the beginning of the integration of the transient equations and

were fixed in magnitude until the end of a particular simulation. In cases where there was a large divergence between calculated and experimental temperature values out of the first reactor, the experimental values were used as inlet temperatures for the second reactor in the total simulation.

7.5 Conclusion

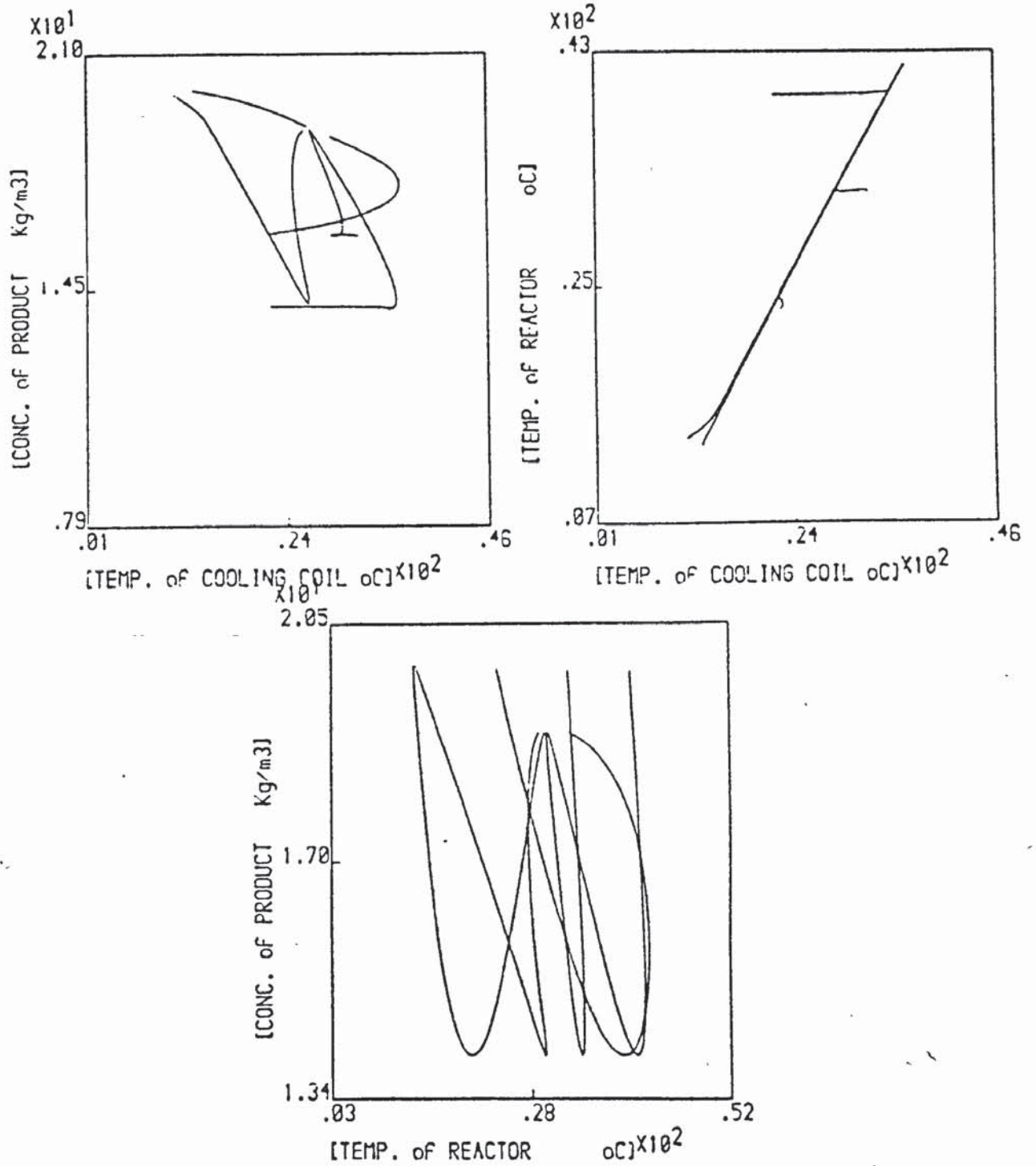
In addition to applying all the proportional control and invariance control schemes enumerated in chapter six, noninteracting control is attained in this total simulation package. Both experimental and simulated results are brought together in the graphical section of the package for a qualitative comparison of the results. The programme contains a section for implementing PID control on both reactors. This lacked the right values for the derivative and integral time constants in the controllers and these could not be obtained experimentally because other more important tasks had to be tackled and the time available was limited.



PHASE-SPACE For REACTOR ONE.

NO CONTROL of SYSTEM VARIABLES.

Fig. 7.1



PHASE-SPACE For REACTOR TWO.
NO CONTROL of SYSTEM VARIABLES.

Fig. 7-2

CHAPTER EIGHT

ANALYSIS AND DISCUSSION OF SIMULATED AND EXPERIMENTAL RESULTS

8.1 Introduction

An account of the results of extensive simulations and experiments which have been done will give a complete picture of the evolved control strategies implemented and develop an understanding of the quantitative accuracy of the model in total simulation by comparing its predictions with the experimental values. In this work comparisons between schemes are based upon qualitative observations of the output variables since a considerable proportion of the available time went in the development of the software needed to operate the system. Results of some of the studies are presented in table 8.1 and the different control strategies applied to various load disturbances and initial perturbations are given in table 8.2. In all experimental runs load disturbances were applied to the system at a stable steady state but attempts to drive it to the next unstable steady state were futile due to the large temperature differences (about 30K) between the two. In experiment 1 the difference in simulated temperature for reactor one between stable and unstable steady states is 30.21K. Transient responses to disturbances are displayed in diagrams in Appendices 6.1 and 6.2. Stabilization of the disturbed system at unstable steady state was done on reactor two in the total simulation studies only as in figures A.6.1.(32,38,39,40,41,45,51,52 and 53). All figures cited hereafter in this chapter without a prefix refer to those with the prefix A.6.1 which are the results of the total simulation. The experimental results are shown in figures prefixed A.6.2 in

discontinuous heavy typed lines, while the simulated results are superimposed on these figures in fine continuous lines. Also in the diagrams in A.6.1. and A.6.2. the product concentration refers to the residual reactant concentration as the mass balance equation is based on it. The experiment numbers refer to those listed in tables 8.1 and 8.2. In some cases the state of only one of the reactors is shown diagrammatically as the situation in the other reactor may not have been changed; as it appeared in an earlier diagram and for lack of space, this was not repeated. Additional disturbances into the experimental set-up could not be avoided as this had much to do with the prevailing weather conditions. Section 8.2 surveys the degree of accuracy of the experimental measurements as these were the basis of the values used in total simulation runs. The remaining sections give an in-depth discussion of the system steady states and of the various control strategies.

8.2 Calibration and Accuracy of Measurements

The calibration of measuring devices was broadly grouped into two. The first consisted of those that needed only a single calibration before the start of the first experiment and these remained unalterable throughout the rest of the study. These included calibration of flow meters (rotameters), developing correlations between heat released and voltage applied to heaters, conductance through the cooling coils, measurements of volumes of reactors and cooling coils and the graduation of thermocouples. Since the rotameter float measures a mass flow, a modest temperature variation (about 5K), as occurred in the experiments when hot water was introduced into reactors or cooling coils, did not affect the accuracy of the readings. The average of several readings was taken to represent the heat

transfer coefficients between reactors and cooling coils since the extreme values varied from the average by 7% or less. Inserting a temperature dependent heat transfer coefficient in the model equations could only have made their numerical solutions unnecessarily difficult and especially as the temperature range involved was less than 20K, the effort could not be justified. Some error was introduced into the thermocouple readings with the inclusion of the switch box (TIB). While the manufacturer's accuracy specification for the Ni-Cr/Ni-Al thermocouple is 0.5K (at 23°C), a noticeable shift to lower readings was realised when there was a to and fro switch of the set. To reduce the impact of this switching, the mains supply to the system was turned off after each experiment and the number of such to and fro switchings was reduced to the barest needed minimum.

The second group of measuring devices which needed recalibration before each day's operation consisted solely of the two pneumatic control valves. While these two produced the same settings for signals of the same magnitude on a particular day, the same could not be necessarily true for subsequent days. It was also noticed that signals of the same magnitude produced slightly different readings depending on whether the rotameter flow was higher or lower than the new settings, and hence average values were used.

8.3 Steady State Operation (simulated and experimental)

The experimental steady state values as recorded in table 8.1 varied with the inlet conditions into the reactors and coils and were much dependent on the weather conditions on the particular day. This table also contains corresponding simulated values. A diagrammatic

representation for all the possible steady state values of both reactors for the specific inlet conditions of experiment 31 is given in figure 8.1 (page 101), which is a plot of the heat generated by the reacting process and the heat removed from the system by flowing liquid streams. While most of the experimental steady state temperatures in the first reactor and coil were within one degree of the corresponding simulated values, those for the second reactor and coil were much less coincidental. High temperatures in the first reactor will normally produce a high temperature gradient for heat loss from the connecting pipe to the environment and could be partly responsible for the large difference between experimental and simulated values in the second reactor. The experimental temperatures in both reactor and coil outlet in the first reactor are slightly higher than their corresponding simulated values. The situation is reversed in the second reactor and coil and the differences between simulated and experimental values are higher than in the first reactor and coil. A comparison of the inlet feed temperature into reactor two and the outlet temperature from reactor one showed the former to be often slightly lower.

Experimental product concentrations in the second reactor varied from 109% to 126% of those in the first reactor. The inlet temperature and flow rates into reactors ranged from 283.7 to 289.8K and from 3.66×10^{-5} to $5 \times 10^{-5} \text{ m}^3/\text{sec}$ respectively, while the cooling flow rates covered a wider span from 5.73×10^{-5} to $1.3 \times 10^{-4} \text{ m}^3/\text{sec}$. For the same cooling liquid flow rate through the coils, the unstable state temperature in the second reactor and coil was always lower than that of the first reactor. Lower inlet temperatures into the first reactor and coil resulted in temperatures and concentrations having

low values at steady state in both reactors and the converse was equally true. Comparison of the simulated steady state values for figures 25,26,27 and 28 with those of 1,2,16 and 20 clearly illustrates this point. Increase in feed flow rate resulted in lower steady state values for both reactor and coil temperatures and reactant conversion as shown by comparison of experiments 3 and 8A.

8.4 Transient Response (simulated and experimental)

The system at steady state was subjected to different kinds of disturbance to study its response and to evaluate how large these disturbances need be in order to destabilise it; that is, how large the region of absolute stability extended within this zone with the system returning to the same steady state value if transient disturbances were applied to it. Both open and closed loop responses were noted and the disturbances at times were a combination of load and initial perturbations like in figures (18-20). Step disturbances in feed temperatures into reactor one and both cooling coils varied from -2.0 to 3.4K while initial perturbations in state variable temperatures ranged from -2.71 to 13.4K. The load disturbances in reactant concentration into reactor one spanned from 1.25 to 7.5% of the initial feed reactant concentration which was fixed at 20kg/m^3 . In the total simulation load disturbances were applied at the start of integration of the transient response equation while in the experimental run unannounced disturbances appeared at random for a short duration as depicted by the response of figures A.6.2. (21,25,26 and 27). Each of these shows disjointed bands of cooling liquid flow rates responding in time to different load temperature disturbances.

8.4.1 Open Loop

When starting from an initial unsteady state, open loop systems were found to drift gradually to settle at the steady state value (figure 34) and for load disturbances new stable steady states resulted which are a constant deviation from the initial steady state as shown in figures 1,2 and 3. While the state variables in the first reactor were rather monotonically declining, in the second reactor a tortuous path interspaced with increases and decreases of state variables was followed as the effects from the first reactor were carried over into the second, and these fluctuations easily resulted in the breaching of the RAS in the second reactor. In figure 35, reactor two was operated at unstable steady state and the continuous drift away from the initial steady state is well exemplified. For steps in feed concentration of 0.5 to 1.0kg/m^3 , the conversion and temperature rise in the reactors are not very significant as shown in figures 1 and 3, though higher in the second reactor than the first. The combined effect of a step in feed reactor concentration and temperature is studied in figure 2 and the 0.9K feed temperature fall increases the conversion in reactor one by 0.044kg/m^3 above reactor one's conversion in figure 1.

8.4.2 Controlled Loop Stability

The need to control both stable and unstable systems arises when the magnitude of the disturbances entering the systems cannot be easily predicted and the probability of systems staying in the region of absolute stability especially in the latter case is not assured. While the requirement to control some of the state variables, like the coil outlet temperature, may not be obvious in many chemical

processes, this becomes necessary if this cooling stream is a feed to another process and it needs preheating; it can absorb heat from the reactor.

Thus the responses to the following control strategies were studied:

- i) Ideal or perfect proportional control of reactors outlet temperatures.
- ii) Proportional control of cooling coils outlet temperatures.
- iii) Proportional control of reactant outlet concentration.
- iv) Combination of the above three controllers.
- v) Noninteracting control of reactors outlet temperatures.

8.4.2.1 Proportional Control of Reactant Concentration in Reactor

Figures 4,5,36,37 and 29 showed the effect of the use of feedback control of reactant concentration in reactors with increasing gains ranging from $1.0E-06$ to $3.0E-04$. In figures 36 and 37 where the disturbances entering reactor one are of the same magnitude, the off-set in product concentration for this reactor was greater in figure 36 (0.44kg/m^3) in which the controller gain is smaller ($5E-05$), than in figure 37 (0.32kg/m^3) where the controller gain was twice as large. The overshoot which is just discernable in figure 37, becomes very conspicuous in figure 29, the controller gain having been increased threefold. Each of these figures depicted a decrease in the effect of the disturbances. An excessively large value of gain, however, as in figure 13, only introduced instability into the first reactor with an ever increasing off-set which is carried over to the second. Figures 32 and 52 showed that it was not possible to control the second reactor with the assigned parameters at unstable steady state by deploying proportional controllers based on reactant

concentration. A modest load disturbance in reactant concentration in each case caused the second reactor to become uncontrollable. Increasing controller gain only made the system more unstable. Adding feedforward controllers to the second reactor effectively minimized the effects of disturbances and for stable states performed as well as feedback controllers with larger gains without incurring the oscillatory tendencies the latter induces. It did not fundamentally change the state of the system as shown in figures 38 and 39. In figures A.6.2.(4,5 and 10) where the experimental results of the control of the first reactor using proportional controllers based on reactant concentration are displayed, the unsatisfactory control action is depicted by the monotonically increasing coolant rate which in all three cases exceeds the valve maximum. Although the error in reactant concentration was minimized, the reactor and coil temperatures' maximum off-set was large, at about 4K.

8.4.2.2 Proportional Control of Reactor Temperature

With the control law based on reactor temperature, it was possible to stabilize the unstable steady state with a large gain value as portrayed in figures 40 and 45 although in figure 41 this value was not large enough. Oscillatory but decreasing values of some of the state variables were encountered when large gains were applied to the stable steady states as depicted in figure 48. The gain used to effect the same control was smaller than for either reactant concentration or cooling coil temperature controllers, this being due to its being the lynchpin of all the system model equations and as such exerting the greatest influence on the eigenvalues of the system matrix at steady state. It was observed to be the most effective of all the proportional controllers. Comparison of figures 16 and 23

with figures 44 and 47 showed that addition of a feedforward controller with same gain on the second reactor did not make a difference to the response in these particular cases. Oscillatory behaviour in state variables was also observed in most of the experimental runs using this controller. This as noted earlier was partly due to the long time intervals involved in the scanning of temperatures and resetting of control valves. With controller gains equal to or below $2.0E-06$, these oscillations gradually died down to steady state values as shown in figures A.6.2.(19,20,22 and 14). Gains larger than $3.0E-06$ caused the oscillations to grow bigger until the cooling liquid demand exceeded valve maximum as in figures A.6.2.(12 and 11).

8.4.2.3 Proportional Control of Cooling Coil outlet Temperature

The effects of increasing controller gains from $2.0E-06$ to $8.0E-04$ in the control of the temperature of the cooling coil in reactor one are shown in figures 15,7 and 43. Larger controller gains compared to controllers based on reactor temperature were needed to accomplish the reduction or elimination of the effects of disturbances using this control law. In figures 7 and 40 where controllers with equal gains($3.0E-05$) were applied to reactor one to control similar load disturbances, the perturbations in state variables are less in figure 40 where reactor temperature is controlled variable. An unstable system could not be stabilized using proportional controllers based on this law as shown in figure 51. Oscillatory behaviour in some of the state variables was noticeable in several of the experimental results with this controller; this being expected as the coil temperature is directly coupled to the manipulative variable.

In many instances like in figures A.6.2.(16,23 and 24) these oscillations died down with time; the step disturbance in feed reactor temperature of 2.8K was too large for the controller on reactor one of figure A.6.2.15. It soon exceeded the valve maximum as the oscillations increased in amplitude. A combined feedforward and feedback controller on the second reactor did not improve its stability potential, as the effects of disturbances carried over from the first reactor appeared in it although in diminished strength as in figure 48.

8.4.2.4 Mixture of Controlled Variables

In figures 14,15,19 and others the reactor temperature was used as controlled variable in reactor one and coil temperature as controlled variable in reactor two. In figure 49 the effectiveness of this joint application of control laws was portrayed. Compared to figure 4, figure 49 applied control laws to the variables with the greatest potential for causing instability, viz temperature in reactor one and outlet temperature in coil in reactor two. In the use of a mixture of control laws in both reactors, it was necessary to identify the most potent of disturbances and try eliminating it. In applying control to figure 4, control of the 'wrong' variable, viz reactant concentration in the reactor, was studied instead of either reactor temperature or cooling coil outlet temperature. The control of reactor temperature or reactant concentration in the first reactor is advantageous since disturbances in feed reactant concentration and temperature enter the second reactor only as carry over disturbances from the first reactor. The interchange of the control laws applied to reactor and coil temperatures and the resulting effects are documented in figures 15 and 49. The oscillatory tendencies in the state

variables in the experimental results as documented in the two preceding sections above are repeated in this control arrangement as is evident in figures A.6.2. (14,15,16 and others).

8.5 Invariance Control

Experimental results depicted in figures A.6.2.(21,25,26 and 27) were carried out to study invariance control of reactor and cooling coil temperature due to load disturbances in feed concentration and temperatures. In each case where the step disturbances involved were only in temperature, the minimization of the effects of these was instantaneous following the adjustment of the flow rate as in figure A.6.2.25 and no lingering deviations in state variables were noticed. The addition of a step in feed reactant concentration in figures A.6.2.26 and 27 resulted in a gradual increase in coolant rate to reduce the creeping effect of the ever increasing reactant concentration in the reactor. Since invariance control was achieved for disturbances in reactor and coil inlet temperatures, the disturbance in feed reactant concentration could not be annulled. This control scheme proved to be quite superior to proportional control schemes in its elimination of the effects of disturbances introduced through feed temperatures; its only disadvantage in this study being the absence of a second manipulative variable with which invariance control for disturbances in feed reactant concentration could be accomplished. As in proportional control, another constraint to eliminate the effects of temperature disturbances was the limit imposed on the maximum coolant rate by the valve.

8.6 Noninteracting Control of Reactor Temperature

In this control scheme, the temperature of the reactor was the controlled variable and disturbances entering the reacting system through feed concentration and temperature of inlet liquid into the cooling coil, did not affect the reactor temperature. In each reactor, its temperature had been made independent of the cooling coil temperature and the reactant concentration. A step in feed reactant concentration as in figure 54 affected neither the reactor nor the cooling coil temperature and an additional step in temperature of liquid into the cooling coil as in figure 55 still left the reactor temperature unaffected. Larger controller gains were applicable in this control method compared to any of the aforementioned methods without necessarily giving rise to oscillatory behaviour. With a wide range of controller settings (0.5-2.0) used, the cooling liquid flow rate was still within the obtainable flow range on the experimental plant. This may have been due to the unsatisfactory value of the coil temperature used in equation (38) in calculating the flow rate, as was noted earlier. Open loop unstable systems are easily stabilized for load disturbances and initial perturbation as can be seen from an observation of the response of reactor two in figures 53 and 58. The temperature of the cooling coil responded almost instantaneously to load disturbances in temperature of liquid flowing into the coil, this being partly due to the smallness in volume of the coil compared to volume of reactor. The region of asymptotic stability was greatly enhanced by this control scheme as shown in table 3.2. Thus this control method was superior to proportional control.

8.7 Comparison of Simulated and Experimental Results

A comparison of the totally simulated and experimental runs will naturally start with a look at the values of the state variables at steady state as these are expected to be coincidental regardless of the path taken to attain this state. The values in table 8.1 portray the differences in temperatures in the first reactor for most of the runs between simulated and experimental as varying from 0.04 to 0.6K of each other except for a few cases like 1,15,16,17 and 20 where this was in excess of 1K. In the second reactor the difference was noted to be greater with the experimental reactor temperatures being higher than simulated values. Corresponding variations were noted in the cooling coil temperatures and reactant concentration. The broad band of values resulting from some of the transient temperature measurements showed the susceptibility of the thermocouples to noise in the system as the mixing, especially in the reactors, was good enough to eliminate any localized temperature gradients. The simulation model did not take into consideration the heat loss in the connecting tubing between the reactors or the churning action of the supply pump to the second reactor which may have resulted in heat being generated. In spite of the above observations, many of the uncontrolled transient responses showed similar patterns but displaced by a margin of error reflecting the coincidence or not of the steady state values. The situation differed when controlled transient responses were concerned. The integrating step for system equations using the fourth order Runge-Kutta method varied between 0.15 to 0.27 second while in the cases where both process control valves needed setting for proportional control action, the time interval was a staggering 12 seconds. This long lapse caused the conspicuously present oscillations in the experimental results which at times led to systems becoming unstable as in figures

A.6.2.(8,11,12,16 and 17). In addition to lengthy times due to the resetting of valves, the iterative method used in calculating the flow rates for invariance control implied uneven sampling times and hence longer periods between two successive remedial control actions. The mitigating aspect in the latter case is the fact that the starting values for the iteration are close to the final results as disturbances are not too large and rapid convergence of the solution is assured. There is an initial offset in the second reactor for each of the invariance control responses which could be due to an initial drift in the steady state temperatures or error incurred from the heat transfer coefficient. From figures A.6.2 (7d,25d,26d and 27d) it was noticed that load disturbances in temperature entered the system randomly and the corresponding simulation considered these values to be input at the beginning of the integration, resulting in the flow rates being lower than in the former case. In relation to invariance control, a more liberal use of both thermocouple access channels was exercised in attempts to monitor temperature load disturbances into the system, thereby incurring the earlier noted measuring error inherent in the TIB arrangement.

TABLE 8.1 EXPERIMENTAL AND SIMULATED STEADY STATE CONDITIONS.

EXPT. No	OPERATING INLET CONDITIONS				EXPERIMENTAL VALUES(ONE STEADY STATE)										SIMULATED TEMPERATURES(TWO STEADY STATES)									
	F m /s	FC1	Tb1	Tco1	REACTOR ONE		REACTOR TWO		REACTOR ONE		REACTOR TWO		REACTOR ONE		REACTOR TWO		REACTOR ONE		REACTOR TWO					
	-5	-5	(K)	(K)	Css (kg/m)	ss (K)	T	Css (kg/m)	ss (K)	T	Css (kg/m)	ss (K)	T	Css (kg/m)	ss (K)	T	ss (K)	T	ss (K)	T				
1	3.66	5.85	287.79	286.71	19.27	298.32	295.34	18.39	302.27	296.90	296.42	293.48	307.21	299.80										
		6.14	296.40	286.33	-	-	-	-	-	-	326.63	314.20	317.65	306.54										
2	3.66	5.73	287.30	286.15	19.35	296.58	293.51	18.55	301.06	295.35	295.47	292.72	304.28	297.81										
		6.02	295.64	285.66	-	-	-	-	-	-	326.62	314.67	320.00	308.07										
3	3.92	6.72	284.10	283.35	19.58	289.91	287.91	19.11	292.76	289.24	289.49	287.33	293.81	289.70										
		6.83	290.09	283.35	-	-	-	-	-	-	334.22	316.30	330.69	312.09										
4	3.66	6.89	285.62	285.64	19.44	293.38	290.61	18.81	296.82	292.01	292.84	290.24	298.78	293.33										
		6.89	292.24	285.03	-	-	-	-	-	-	331.03	314.63	326.06	309.80										
5	3.66	7.36	286.73	286.14	19.41	294.31	291.40	18.72	298.30	292.97	293.98	290.97	300.36	294.21										
		7.36	293.83	285.72	-	-	-	-	-	-	330.92	313.68	325.53	308.82										
6	3.66	7.58	284.79	284.55	19.51	291.64	288.78	18.95	294.49	290.07	290.99	288.45	295.36	290.82										
		7.58	291.94	284.29	-	-	-	-	-	-	333.60	314.19	329.41	309.99										
7	3.66	8.05	286.46	286.60	19.41	294.38	291.46	18.72	298.30	293.03	293.98	290.91	299.92	293.57										
		7.93	293.97	285.69	-	-	-	-	-	-	331.96	313.04	326.68	308.38										
8	3.66	6.25	286.66	286.64	19.36	296.19	292.81	18.56	303.95	295.35	296.00	292.27	304.57	298.05										
		6.25	295.64	286.10	-	-	-	-	-	-	328.13	314.59	320.14	308.00										
8A	3.66	6.89	284.52	284.48	19.53	290.56	288.08	19.00	293.43	289.43	290.96	288.63	296.38	291.67										
		6.89	290.96	284.48	-	-	-	-	-	-	332.48	315.14	327.89	310.69										
9	3.66	6.83	285.93	285.76	19.43	293.79	290.68	18.74	297.71	292.76	293.22	290.55	299.51	293.91										
		6.83	293.79	285.26	-	-	-	-	-	-	330.63	314.56	325.38	309.61										
10	3.66	7.48	286.17	286.34	19.42	294.01	291.07	18.74	298.09	292.76	293.69	290.82	300.07	294.12										
		7.18	293.79	285.60	-	-	-	-	-	-	328.29	314.84	322.68	309.05										

TABLE 8.1 continued

EXPT. No	OPERATING INLET CONDITIONS				EXPERIMENTAL VALUES (ONE STEADY STATE)				SIMULATED TEMPERATURES (TWO STEADY STATES)								
	F m /s	FC1	T ₀₁	T ₀₂	T ₀₁	T ₀₂	C _{ss}	C _{ss}	REACTOR ONE	REACTOR TWO	REACTOR ONE	REACTOR TWO	REACTOR ONE	REACTOR TWO	REACTOR ONE	REACTOR TWO	
	x10	x10 m /s	(K)	(K)	(kg/m)	(kg/m)	(kg/m)	ss (K)	ss (K)	T	T	ss (K)	ss (K)	T	T	ss (K)	ss (K)
11	3.66	6.25	285.93	287.07	19.40	18.67	-	294.55	291.81	299.15	293.68	294.79	292.27	301.80	295.71		
		6.25	294.90	284.94	-	-	-	-	-	-	-	328.29	314.84	322.68	309.05		
12	3.66	7.48	287.00	286.91	19.38	18.62	19.38	295.30	292.27	300.11	294.42	294.91	291.79	300.46	293.94		
		7.48	294.40	285.13	-	-	-	-	-	-	-	330.37	313.39	325.70	308.43		
13	3.66	6.89	285.11	285.31	19.48	18.90	19.48	292.29	289.22	295.15	290.69	292.14	289.67	296.72	291.60		
		6.89	292.20	283.79	-	-	-	-	-	-	-	331.57	314.86	327.70	310.30		
14	3.66	6.95	285.41	284.92	19.45	18.85	19.45	292.50	289.22	295.87	290.69	291.99	289.42	297.76	292.64		
		6.95	291.90	284.73	-	-	-	-	-	-	-	331.80	314.72	326.93	310.15		
15	3.66	7.01	287.61	287.63	19.25	18.41	19.25	298.54	295.32	302.24	295.57	296.41	293.18	305.55	297.50		
		7.99	296.41	287.63	-	-	-	-	-	-	-	328.40	313.43	322.07	306.60		
16	3.66	6.43	287.44	286.99	19.25	18.38	19.25	298.54	294.88	302.75	296.69	295.94	292.93	309.33	301.52		
		6.30	295.94	286.82	-	-	-	-	-	-	-	327.72	314.02	315.32	304.95		
17	3.66	5.79	287.18	286.77	19.72	18.37	19.72	298.11	294.44	301.34	295.76	295.94	293.20	307.29	302.01		
		6.14	295.94	286.77	-	-	-	-	-	-	-	326.38	314.54	317.52	306.62		
18	3.66	6.31	287.35	287.08	19.21	18.32	19.21	298.54	295.21	303.18	296.07	296.03	293.08	305.53	298.13		
		6.91	297.13	286.92	-	-	-	-	-	-	-	327.41	314.12	320.33	307.06		
19	3.66	5.73	287.06	286.70	19.33	18.46	19.33	295.95	293.14	300.63	294.42	295.81	293.13	301.40	296.19		
		6.25	295.17	285.16	-	-	-	-	-	-	-	326.35	314.64	322.10	308.75		
20	3.74	5.85	287.74	287.07	19.21	18.28	19.21	299.59	296.62	304.24	297.52	296.58	293.30	306.86	299.20		
		6.66	296.58	286.91	-	-	-	-	-	-	-	326.33	314.45	319.25	306.83		
21	3.66	5.79	286.56	285.62	19.34	18.61	19.34	294.66	291.40	299.15	293.38	294.21	291.64	301.18	295.57		
		5.91	294.16	284.71	-	-	-	-	-	-	-	327.37	315.17	322.39	309.55		

TABLE 8.1 continued

EXPT. No	OPERATING INLET CONDITIONS				EXPERIMENTAL VALUES (ONE STEADY STATE)				SIMULATED TEMPERATURES (TWO STEADY STATES)							
	F m /s	FC1	To1	Tco1	REACTOR ONE		REACTOR TWO		REACTOR ONE		REACTOR ONE		REACTOR TWO		REACTOR TWO	
	-5	-5	(K)	(K)	Css (kg/m)	T ss (K)	Css (kg/m)	T ss (K)	T ss (K)	T ss (K)	T ss (K)	T ss (K)	T ss (K)	T ss (K)	T ss (K)	T ss (K)
22	3.79	5.79	287.47	286.94	19.27	297.16	18.44	302.33	295.97	296.12	293.38	307.54	300.14			
		5.91	296.00	286.63	-	-	-	-	-	326.78	314.86	317.41	306.92			
23	3.92	6.14	287.35	287.08	19.30	296.81	18.55	300.63	294.01	295.65	292.96	302.69	295.51			
		8.05	296.19	286.87	-	-	-	-	-	328.41	315.19	325.53	308.06			
24	3.92	5.73	286.42	286.15	19.36	294.10	18.71	298.30	292.35	294.18	291.81	301.04	295.03			
		7.01	294.16	286.11	-	-	-	-	-	328.71	316.14	325.42	309.60			
25	3.66	6.02	283.41	283.36	19.56	289.48	19.25	293.43	290.07	289.54	287.60	294.59	290.67			
		6.02	289.17	283.31	19.56	-	-	-	-	331.88	316.70	327.72	312.28			
26	3.66	5.85	283.75	283.56	19.55	289.91	19.01	294.01	290.90	290.02	288.07	295.43	291.43			
		5.85	290.23	283.56	-	-	-	-	-	331.14	316.74	326.74	312.18			
27	3.66	6.31	283.72	282.53	19.58	288.62	19.09	292.37	288.83	288.95	286.83	293.23	289.40			
		6.20	289.20	282.55	-	-	-	-	-	332.92	316.13	329.09	312.42			
28	3.79	6.78	288.38	282.66	19.61	287.97	19.15	291.53	287.79	288.38	286.36	292.42	288.61			
		6.78	288.38	282.66	-	-	-	-	-	334.69	316.21	331.15	312.22			
29	3.79	13.10	287.15	287.12	18.89	304.57	17.93	306.14	294.62	303.38	-	308.94	-			
		13.10	298.87	-	-	-	-	-	-	298.87	-	295.63	-			
30	3.66	6.89	284.52	284.48	19.53	290.56	19.07	293.43	289.66	290.96	288.62	296.38	291.67			
		6.89	291.04	284.48	-	-	-	-	-	332.48	315.14	327.89	310.69			
31	5.00	4.00	287.00	287.00	-	-	-	-	-	293.60	292.09	302.72	299.28			
		4.00	293.60	287.00	-	-	-	-	-	329.48	321.78	322.35	314.84			
32	4.06	9.72	283.91	284.00	19.43	295.95	18.85	296.93	290.48	294.47	-	297.19	-			
		9.72	292.54	-	-	-	-	-	-	292.53	-	290.37	-			

TABLE 8.1 continued

EXPT. No	OPERATING INLET CONDITIONS			EXPERIMENTAL VALUES (ONE STEADY STATE)						SIMULATED TEMPERATURES (TWO STEADY STATES)						
	F m /s	FC1	To1	Tco1	REACTOR ONE		REACTOR TWO		REACTOR ONE		REACTOR TWO		REACTOR ONE		REACTOR TWO	
	-5	FC2	To2	Tco2	Css (kg/m)	T ss (K)	Css (kg/m)	T ss (K)	ss (K)	T ss (K)	ss (K)	T ss (K)	ss (K)	T ss (K)	ss (K)	T ss (K)
	x10	x10 m /s	(K)	(K)												
	11.40	284.20	284.00	284.00	19.43	295.09	289.22	289.97	295.97	289.28	293.57	295.93	293.57	295.93	295.93	295.93
33	4.06	11.40	291.21	-	-	-	-	-	-	-	-	-	291.21	-	289.19	-

TABLE 8.2 DISTURBANCES AND CONTROL SCHEMES IMPLEMENTED

Fig. no. A.6	Experiment no.	CONTROL STRATEGY	INITIAL PERIURBATION		LOAD CHANGES		
			T(K)	T(K)	T(K)	C(kg/m)	T(K)
1	1	1*	-	-	-	0.5	-
		1	-	-	-		-
2	2	1	-	-	-0.9	0.5	-
		1	-	-	-		-0.2
3	3	1	-	-	-	1.0	-
		1	-	-	-		-
4	4	2 Kc=0.1E-05	-	-	-1.3	0.5	-1.26
		1	-	-	-		-1.23
5	5	2 Kc=0.3E-05	-	-	-2.125	0.5	-1.934
		1	-	-	-		-1.84
6	6	3 Kc=0.3E-05	-	-	-0.2	0.5	-
		1	-	-	-		-
7	7	4 Kc=0.3E-04	-	-	-	0.5	-1.5
		1	-	-	-		-0.5
8	8A	3 Kc=0.5E-04	-	-	-0.4632	0.5	-
		1	-	-	-		-
9	9	2 Kc=0.3E-04	-	-	-	1.5	-
		2 Kc=0.3E-04	-	-	-		-
10	10	2 Kc=0.5E-06	-	-	-0.579	0.5	-
		3 Kc=0.5E-06	-	-	-		-
11	11	3 Kc=0.5E-05	-	-	1.014	-	-0.58
		3 Kc=0.5E-05	-	-	-		-0.61
12	12	3 Kc=0.3E-05	-	-	1.614	-	-0.65
		3 Kc=0.3E-05	-	-	-		-0.652

* See page 100 for key.

TABLE 8.2 continued

Fig. no. A.6	Experi- ment no:	CONTROL STRATEGY	INITIAL PERTURBATION		LOAD CHANGES		
			T(K)	T(K)	T(K)	C(kg/m)	T(K)
13	9	2 Kc=0.5E-03	-	-	-	1.5	-
		2 Kc=0.5E-04	-	-	-		-
14	14	3 Kc=0.2E-05	-	-	0.79	-	-0.3485
		4 Kc=0.2E-05	-	-			-
15	15	4 Kc=0.2E-05	-	-	2.7599	-	-1.23
		3 Kc=0.2E-05	-	-			-0.582
16	16	4 Kc=0.23E-5	-	-	3.3775	-	-0.1025
		6 Kc=0.15E-5	-	-			-0.6576
17	17	4 Kc=0.3E-05	-	-	-0.56	0.1	0.65
		6 Kc=0.2E-05	-	-			-0.56
18	18	1	4.31	3.61	0.0579	-	-0.41
		1	-0.22	-0.83			-0.188
19	19	3 Kc=0.1E-06	8.99	7.21	-0.3667	-	-0.902
		4 Kc=0.1E-06	0.00	0.12			-0.113
20	20	3 Kc=0.5E-06	7.57	5.67	-0.6755	-	-0.984
		4 Kc=0.5E-05	0.21	0.00			-0.226
21	28	8	-	-	0.772	-	-0.41
		8	-	-			-0.75
22	21	3 Kc=0.1E-05	5.69	4.77	-0.444	-	-0.246
		4 Kc=0.5E-06	-1.70	-1.97			-0.113
23	22	4 Kc=0.3E-05	6.90	5.23	-0.676	-	-0.82
		6 Kc=0.1E-05	-2.71	-2.06			-0.075
24	24	4 Kc=0.35E-5			0.1	-	-
		3 Kc=0.1E-05					0.489

TABLE 8.2 continued

Fig. no. A.6	Experiment no.	CONTROL STRATEGY	INITIAL PERTURBATION		LOAD CHANGES		
			T(K)	T(K)	T(K)	C(kg/m)	T(K)
25	25	8	-	-	-1.062	-	-1.64
		8	-	-			-1.5
26	26	8	-	-	-	0.2	-0.82
		8	-	-			-0.75
27	27	8	-	-	-0.193	0.2	-
		8	-	-			-0.75
28	28	9	-	-	2.5	-	-
		9	-	-			-
29	5	2 Kc=.3E-03	-	-	-	0.25	-
		2 Kc=.3E-03	-	-			-
30	32	1	7.76	0.632	-0.212	-	-
		3 Kc=.5E-04	0.414	0.43			-0.53
31	29	1	-	-	-0.39	0.5	-
		3 Kc=.2E-04	-	-			-0.47
32	5	2 Kc=.1E-04	-	-	-	0.25	-
		2 Kc=.15E-04	-	-			-
33	33	1	-	-	3.09	-	-
		3 Kc=.3E-05	-	-			-
34	1	1	2.5	2.5	-	0.5	-
		1	2.5	2.5			(I.P)
35	1	1	2.5	2.5	-	0.5	-
		1	2.5	2.5			(I.P)
36	4	2 Kc=0.5E-04	-	-	-	0.5	-
		2 Kc=0.5E-04	-	-			-

TABLE 8.2 continued

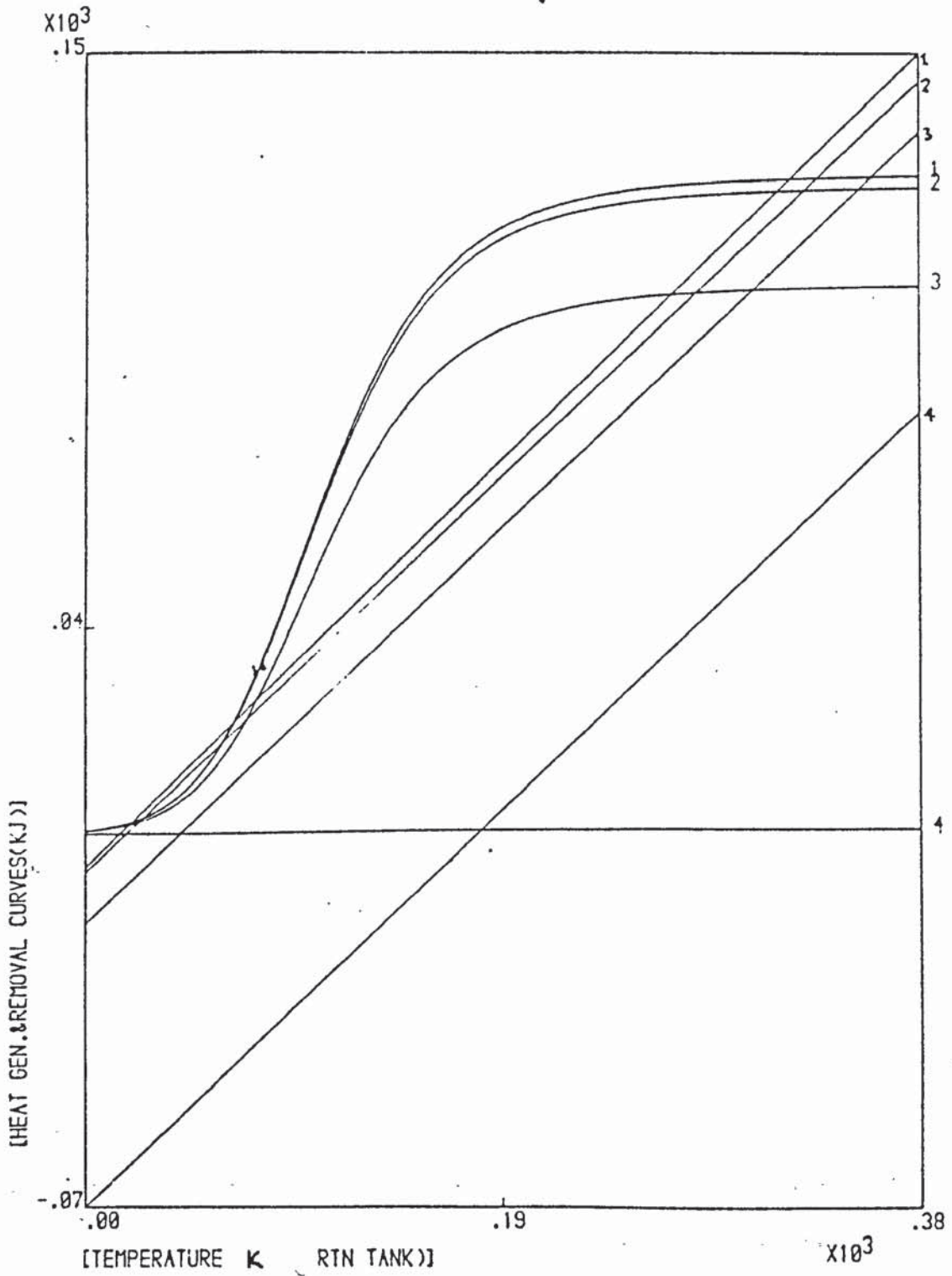
Fig. no. A.6	Experiment no:	CONTROL STRATEGY	INITIAL PERTURBATION		LOAD CHANGES		
			T(K)	T(K)	T(K)	T(kg/m)	T(K)
37	4	2 Kc=0.1E-03 2 Kc=0.1E-03	-	-	-	0.5	
38	5	2 Kc=.1E-05 5 Kc=.75E-06	-	-	-	0.25	-
39	5	2 Kc=0.1E-04 5 Kc=.15E-04	-	-	-	0.25	-
40	31	3 Kc=0.3E-04 3 Kc=0.3E-04	-	-	-	0.25	-
41	31	3 Kc=0.3E-04 4 Kc=.22E-05	-	-	-	0.25	-
42	31	9 a2=0.5 9 a2=0.5	3.5	2.5	-	-	-
43	31	4 Kc=0.8E-03 6 Kc=0.4E-03	-	-	2.0	-	-
44	16	4 Kc=0.23E-5 3 Kc=0.5E-05	-	-	3.3775	-	-0.1025 -0.6576
45	31	1 3 Kc=0.1E-02	-	-	2.0	-	-
46	4	3 Kc=0.1E-05 1	-	-	-1.3	0.5	-1.26 -1.23
47	22	4 Kc=0.3E-05 3 Kc=0.1E-05	6.9	5.23	-0.676	-	-0.82 -0.075
48	31	3 Kc=.15E-04 7 Kc=0.5E-04	-	-	2.0	-	-
49	15	3 Kc=0.2E-05 4 Kc=0.2E-05	-	-	2.76	-	-1.23 -0.582

TABLE 8.2 continued

Fig. no.	Experiment no:	CONTROL STRATEGY	INITIAL PERTURBATION		LOAD CHANGES		
			T(K)	T(K)	T(K)	C(kg/m)	T(K)
50	7	4	-	-	-	0.5	-1.5
		Kc=.3E-03	-	-	-	0.5	-0.5
51	7	4	-	-	-	0.5	-1.5
		Kc=0.3E-02	-	-	-	0.5	-0.5
52	31	2	-	-	-	0.25	-
		Kc=0.1E-04	-	-	-	0.25	-
53	31	9	13.36	11.02	-	-	-
		a2=0.5	13.36	11.02	-	-	-
54	4	9	-	-	-	1.5	-
		a2=0.05	-	-	-	1.5	-
55	5	9	-	-	-	-1.0	1.5
		a2=0.05	-	-	-	-1.0	1.5
56	31	9	-	-	2.0	-	-
		a2=1.0	-	-	2.0	-	-
57	31	9	-	-	2.0	-1.0	0.5
		a2=2.0	-	-	2.0	-1.0	0.5
58	31	9	-	-	2.0	1.0	0.5
		a2=2.0	-	-	2.0	1.0	0.5

Key to table

- 1 = No control of state variables
 2 = Proportional feedback control of reactant concentration.
 3 = Proportional feedback control of reactor temperature.
 4 = Proportional feedback control of coil temperature.
 5 = Proportional feedback & feedforward control of reactant conc.
 6 = Proportional feedback & feedforward control of reactor temp.
 7 = Proportional feedback & feedforward control of coil temp.
 8 = Invariance control. 9= Noninteracting control



1- Heat generation and removal in Reactor 1
 2-4 Heat generation and removal in Reactor 2

Fig. 8.1

CHAPTER NINE

CONCLUSIONS AND RECOMMENDATIONS

This research has highlighted some of the opportunities available in the application of digital computers to effect control of chemical process units and the problems or limitations imposed by the computer software and hardware being used. While it can be conceded that more powerful and versatile generations of computers are now available on the market for use on pilot plant models, some kind of limitation on hardware and software would often be encountered for each digital computing system chosen. Except for well-known and used chemical processes where specially tailored packages may be readily available, the user has in many instances to develop the programmes to modify the existing software to suit the reacting system and this requires a mastering of one or several of the programming languages, which in itself is time consuming. Once the software package has been developed, the total simulation technique offers the chance of exploring the available system parameters far in excess of the range that can be obtained on an experimental plant, as well as being relatively cheap and fast.

9.1 CONCLUSIONS:

9.1.1 Simulation Studies.

The theoretical work came first and its purpose was to determine the applicability of the experimental work for the system parameters.

The following conclusions could be deduced from it:

- (i) The stability of each of the C.S.T.R.s in the open loop system can be enhanced by employing proportional feedback control of the temperature state variable, but depending on the controller gain this can induce oscillations. The values of gain showing the combinations of stability and oscillation/non-oscillations are recorded in Table 3.1.
- (ii) The operation of the first reactor at the lowest stable steady state can give rise to as many as three steady states in the second reactor. The other two steady states in the first reactor each produce only one steady state in the second reactor.
- (iii) Control of different state variables in both C.S.T.R.s permits the elimination of the divergent tendency on the most sensitive state variable in each reactor. In figures 15 and 49 identical disturbances are applied to the reactors. Although the controllers which are based on different variables have gains of same magnitude, the resultant responses are different, that of figure 49 being less stable than the former.
- (iv) Invariance control is more effective than proportional control in counteracting the effects of load disturbances in feed coolant temperatures.
- (v) Noninteracting type control of reactor temperature is very effective for reducing the effect of load disturbances in the feed inlet temperature and for stabilizing open loop unstable steady states. It makes the reactor temperature invariant to load disturbances in the feed concentration and the coolant inlet temperature.
- (vi) The mathematical model representing the coil temperature results in an axial temperature profile and although a higher number of cells, than the 25 used, would have reduced the error incurred, this error was smaller than the margin of error of the thermocouples.

- (viii) Counter-current flow to the feed of a single cooling liquid stream is not very successful, especially if the first reactor is to be operated at its unstable steady state and control is based on state variables in the second reactor.
- (ix) The method used for determining RAS was found to be efficient and showed large volumes to exist for the system under consideration.

9.1.2 Experimental Studies

The full capabilities of the Honeywell 316 computer are exploited in its use as a calculating tool and controller. In the latter role its adaptability is equally stretched with the application of several control strategies. Some of the observations of the limitation of the computer and equipment on plant were:-

- a) Unimodal operation of computer which excluded continuous scanning of temperatures throughout an experimental run and imposed long intervals between successive scans.
- b) The unsuitable arrangement of using one air supply line and set of P/I, I/V and V/D converters for control of two pneumatic valves.

The usefulness of the partial simulation technique is well illustrated by the use of water as both reactant and product and the generation of heat which is a realistic feature of a reacting chemical process.

The following inferences could be made from the several experiments performed:-

- (i) Proportional feedback controllers are employed effectively in stabilizing open loop unstable systems. Feedforward controllers do not enhance system stability but ameliorate the effect of disturbances. Reactor temperatures are more easily controlled than product concentration or coil temperature.
- (ii) Oscillation in the closed loop system response is not only due to large controller gains but can also be a result of long scanning intervals or reset times.
- (iii) Confirms the theoretical assertion that a series connected C.S.T.R. system produces a higher conversion at lower temperature than a single C.S.T.R. of equivalent volume. Disturbances from the first reactor introduce control problems into the second reactor in addition to the local disturbances.
- (iv) The versatility of the computer as a controller is well illustrated with the opportunities of changing the controlled state variable from the control menu.
- (v) Experimental runs sometimes cannot be fully reproduced in theoretical simulations, especially when the load disturbances appear randomly, except when these are treated stochastically as they deserve.
- (vi) The use of a single cooling stream flowing counter-currently to the feed direction in order to eliminate effects of disturbances is not a viable option, especially if one of the reactors is unstable or the disturbances are large.
- (vii) Invariance control is certainly superior to proportional feedback control schemes although drifts in set-points or parameter variation may need redress by adding the feedback control.

9.2 Suggestions for Further Research

This research, though extensive in its application of different control arrangements on this system, is not exhaustive and some of its shortcomings as noted earlier could be remedied by carrying out further research in line with the following suggestions:-

- (a) Use of variable volume reactors by replacing the fixed drain tube in each reactor with a detachable one of different height. High temperatures can then be obtained with the same set of heaters and a reversible first order reacting system could be studied experimentally.
- (b) An experimental verification of the temperature profile of the cooling coil will provide intermediate temperature values which are necessary for implementing noninteracting control experimentally.
- (c) Elimination of the long reset times for the process control valves by providing separate P/I converters for each of the valves and using different air supply lines.
- (d) Adding of a process control valve on the feed line. The feed flow rate can then be treated as a second manipulative variable. Invariance control for step in feed concentration and temperature can then be accomplished together with noninteracting type control of feed concentration.
- (e) Tuning for the constants in the integral and derivative components in a P+I+D three term controller could be carried out and a comparison made of these results with the invariance plus proportional control scheme.
- (f) Use of reversible reacting systems of mixed orders.

- (g) The use of parallel access system will enable the continuous monitoring of feed temperature and temperature of coolant into the coil without interrupting the execution of the other sections of the on-line programme. These temperatures are needed to get the right simulation response to the invariance control strategy.
- (h) Perform a quantitative analysis of the system for the various control schemes applied and evaluate their performance numerically, in the form of integrated error or integrated square error. This would allow the various schemes to be ranked and would identify marginal or significant improvements between them.

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APPENDICES

APPENDIX A

A.1.1 ON-LINE PROGRAMME FOR CONTROL OF EXPERIMENTAL PLANT

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10 REM          MAIN BASIC ON-LINE PROGRAMME.
20 DIM A(13),B(135),Z(12)
30 A(0)=7:A(1)=3:A(2)=2:A(3)=30:A(4)=33:A(5)=5
40 A(6),A(7),A(8),A(9),A(10),A(11)=0
50 A(12),B(10)=1:A(13),B(0),B(1),B(5),B(8)=0
60 B(4)=460:B(9)=380:B(2),B(3)=500:B(6),B(7)=400
70 D,Q1=0:N=1: GOSUB 2040:N=2: GOSUB 2040: GOSUB 2670
80 PRINT "TANK FLOW RATE.(CM)";: INPUT F3
90 PRINT "LIQUID FLOW RATE IN COIL ONE.(M3/SEC)";: INPUT F1
100 PRINT "LIQUID FLOW RATE IN COIL(2). F2)5CM";: INPUT F2
110 PRINT "CONCENTRATION OF REACTANT.C1 (KG/M3)";: INPUT C1
120 GOSUB 2770: GOSUB 1600:N=6:J=0: GOSUB 2110:J=1:N=5: GOSUB 2110
160 GOSUB 1680: PRINT T,B(18),B(19),F1:B(20),S3,W1,H1,X1=0:S1=.2E-03
190 N=4: GOSUB 1750:N=6:J=0: GOSUB 2110:A(0)=1:N=3: GOSUB 1880
240 PRINT "STARTING CONCENTRATION FOR RUN";: INPUT B(24):B(95)=C1/C1
250 B(24)=B(24)/C1:B(98)=1:T9,L,B(26),B(27)=0:B(25)=B(24): GOSUB 2080
330 B(90),B(91),B(92),B(93)=0: GOSUB 2730:F5=F1:F6=F2
340 H1,H2=0:N=6:J=0: GOSUB 2740: GOSUB 2110:X1=2: GOSUB 2220:X1=0
350 J1=1:T9=T9+A(0): GOSUB 2730: GOSUB 2600:N=1: GOSUB 2220:N=2
360 GOSUB 2310: GOSUB 2550:B(133)=B(25):B(134)=B(26):B(135)=B(10)
370 GOSUB 1450:S2=ABS(B(25)-S3): IF S2>S1 THEN S3=B(25)
440 L=L+1: IF L=100 THEN GOTO 450
445 N=3: GOSUB 1680:A(0)=5: GOSUB 2680:N=4: GOSUB 1750
450 IF L=100 THEN L=0
460 REM          IF B(10)=101 THEN GOTO 490
470 IF S2>S1 THEN 340
480 GOTO 500
490 PRINT "RUNOUT OF COUNTER"
500 B(93)=2: GOSUB 2550:N=5:J=1:A(0)=5: GOSUB 2740: GOSUB 2110
510 PRINT "INLET TEMPS":B(114);B(115);B(116);B(117):N=6:J=0: GOSUB 2110
520 A(0),B(10)=1:J1=B(114):J2=B(115):J3=B(116): GOSUB 1730
540 D=2: GOSUB 2530:B(80)=B(84)
550 B(90)=B(96):B(91)=B(24):B(92)=B(97):B(93)=B(25):B(82)=B(87)
560 PRINT "STEADY STATE VALUES":B(110);B(91);B(113);B(93)
570 PRINT TAB(20);B(111);B(112):B(24),B(25),B(26),B(27),W1,S3,T9=0: GOSUB 2670
580 PRINT "TANK 1 & 2 CONTROL CONSTANTS Z(0),Z(1)";: INPUT Z(0),Z(1)
590 PRINT "CONTROL OPTION";TAB(30);"PROP CONTROL FB(1)"
600 PRINT TAB(30);"PROP CONTROL FE&FF(2)": PRINT TAB(30);"INVARNO CNTRL(3)"
610 PRINT TAB(30);"NON-INTERACTING CONTROL(4)": INPUT K3
620 PRINT "CONTROLLED VARIABLE(K1 K2)";TAB(30);"CONCENTRATION(1)"
630 PRINT TAB(30);"TANK TEMP(2)": PRINT TAB(30);"COIL TEMP(3)": INPUT K4,K2
640 PRINT "STEP INCREASE IN CONC.FIRST TANK ONLY";: INPUT B(95)
650 B(95)=B(95)/C1:S1=.1E-10: GOSUB 2080: GOSUB 2730:L,L9=0
660 H1,H2=0:L=L+1:N=6:J=0: GOSUB 2740: GOSUB 2110
670 N=5:J=1: GOSUB 2020:T9=T9+A(0):L9=L9+1
680 IF L9=15 THEN L9=0
690 ON K3 GOTO 700,700,940,1080
700 ON K4 GOTO 710,720,730
710 P2=Z(0)*B(24)*C1: GOTO 738
720 P2=Z(0)*(B(96)-B(90))*T0+B(89): GOTO 738
730 P2=Z(0)*(B(86)-B(80))*T0+B(89)
738 IF K3=2 THEN GOTO 772
740 ON P2 GOTO 750,760,770
750 P3=Z(1)*B(26)*C1: GOTO 780
760 P3=Z(1)*(B(97)-B(92))*T0+B(89): GOTO 780
770 P3=Z(1)*(B(87)-B(82))*T0+B(89): GOTO 780
772 ON K2 GOTO 774,776,778
774 P3=Z(1)*(B(24)+B(26))*C1: GOTO 780
776 P3=Z(1)*(B(96)-B(90))*(B(97)-B(92))*T0+B(89): GOTO 780
778 P3=Z(1)*(B(86)-B(80))*(B(87)-B(82))*T0+B(89)
780 IF Z(0)=0 THEN 850
790 F1=F1+P2: IF F1>.1826E-03 THEN GOTO 930
800 N=3: GOSUB 1880: IF Z(1)>0 THEN GOTO 840
810 IF Z(1)=0 THEN IF L<50 THEN GOTO 850
820 A(0)=3: GOSUB 2880:N=4:L=0: GOSUB 1750: GOTO 850
840 A(0)=4.2: GOSUB 2880
850 IF B(10)=200 THEN GOTO 1180
860 IF Z(1)=0 THEN GOTO 880
870 F2=F2+P3:N=4: GOSUB 1750: IF F2>.1826E-03 THEN 930
880 A(0)=1.2: GOSUB 2880
890 X1=2: GOSUB 2220:X1=0:N=5:J=1: GOSUB 2600:N=1: GOSUB 2220
900 N=2: GOSUB 2310: GOSUB 2550: GOSUB 2060:B(133)=B(26):B(134)=F1
910 B(135)=F2: GOSUB 1450: GOSUB 2090: IF B(10)=90 THEN 1180
920 GOTO 660
930 PRINT "RUNOUT OF COOLING LIQUID RANGE";F1,F2: GOTO 1180
940 A1,B(105),J=0:X1=3:B(98)=1:N=6: GOSUB 2740: GOSUB 2110
950 J=1:T9=T9+A(0): IF L9<1 THEN GOTO 970
960 A(0)=2:N=5: GOSUB 2110: GOSUB 1730:T9=T9+A(0)
970 N=6: GOSUB 2040:A(0)=1: GOSUB 2730
1000 GOSUB 2600:B(24)=B(24)+B(91):B(25)=B(25)+B(93):N=1: GOSUB 2220
1010 N=2: GOSUB 2310:B(24)=B(24)-B(91):B(25)=B(25)-B(93)
1020 GOSUB 1210:N=3: GOSUB 1880:A(0)=4.5: GOSUB 2880
1030 N=4: GOSUB 1750: GOSUB 2550: GOSUB 2060:B(133)=B(25)
1040 B(134)=F1:B(135)=F2: GOSUB 1450: GOSUB 2090
1060 IF B(10)=90 THEN GOTO 1180
1070 GOTO 660

```



```

2110 REM FOR CHANGING OF SCANNING CHANNELS.
2115 M3,Q1=0: GOSUB 2040
2120 CALL (1,A(0),B(0)): IF M3=0 THEN 2200
2130 IF N=5 THEN 2170
2140 B(110)=B(30)*.10778:B(111)=B(31)*.1089
2150 B(112)=B(32)*.10347:B(113)=B(33)*.1059
2160 IF N=6 THEN 2200
2170 B(114)=B(30)*.965E-01:B(115)=B(31)*.1025
2180 B(116)=B(32)*.9394E-01:B(117)=B(33)*.9236E-01
2190 IF M3=A(2)-1 THEN M3=0
2200 M3=M3+1: CALL (2)
2210 RETURN
2220 REM SUBROUTINE TO SET HEATERS ON, HTR1
2230 B(96)=(B(110)+273.1-T0)/(B(89)*T0): IF X1=2 THEN 2310
2240 B(14)=B(110): IF Y1=3 THEN B(96)=B(90)
2250 B3=EXP(B(96)/(1+B(89)*B(96))): B(S6)=(B(111)+273.1-T0)/(B(89)*T0)
2260 IF B(98)=2 THEN 2290
2270 Q2=B3*B(99)*B(24)*B(94)*B(89)*F*R1*C2*T0
2280 IF B(98)=1 THEN 2300
2290 Q2=B3*B(99)*(B(91)+B(25)+B(24))*B(94)*B(89)*F*R1*C2*T0
2300 GOTO 2380
2310 B(97)=(B(113)+273.1-T0)/(B(89)*T0): IF X1=2 THEN 2840
2320 B(15)=B(113): IF X1=3 THEN B(97)=B(92)
2330 B5=EXP(B(97)/(1+B(89)*B(97))): B(87)=(B(112)+273.1-T0)/(B(89)*T0)
2340 IF B(98)=2 THEN 2370
2350 Q2=B5*B(99)*B(25)*B(94)*B(89)*F*R1*C2*T0
2360 IF B(98)=1 THEN 2390
2370 Q2=B5*B(99)*(B(93)+B(26))*B(94)*B(89)*F*R1*C2*T0
2380 Q2=2*1000/3
2390 IF Q2>50 THEN 2420
2400 Z(9)=-.1188E-01:Z(10)=-.7057E-01:Z(11)=-.6037E-02:Z(12)=-.1463E-03
2410 GOTO 2520
2420 IF Q2>1000 THEN 2450
2430 Z(9)=-.3254:Z(10)=-.2318E-02:Z(11)=-.2781E-05:Z(12)=-.1509E-08
2440 GOTO 2530
2450 IF Q2>2500 THEN 2480
2460 Z(9)=-.564:Z(10)=-.9691E-03:Z(11)=-.2965E-06:Z(12)=-.6528E-10
2470 GOTO 2520
2480 IF Q2>2900 THEN 2510
2490 Z(9)=7.49:Z(10)=-.4859E-02:Z(11)=-.1091E-05:Z(12)=0
2500 GOTO 2520
2510 Z(9)=972:Z(10)=-.6602:Z(11)=-.1124E-03:Z(12)=0
2520 G1=(Z(9)+Z(10)*Q2+Z(11)*Q2^2+Z(12)*Q2^3)
2530 Q1=Q1+.32767E05/3.1415
2540 GOTO 2040
2550 REM GRAPHICAL SUBROUTINE!!!
2560 CALL (7,T9,B(0),B(4),B(5),B(9),B(12),B(10),B(11),Z(3))
2570 Q=1
2580 CALL (7,T9,B(0),B(4),B(5),B(9),B(12),B(10),Q,Z(3))
2590 RETURN
2600 REM INTERGRATION ROUTINE.
2610 H1=(T9-U1)/T:H2=T9:H2=(T9/T)-H1: CALL (6,H2,B(24),H1,B(89))
2620 IF B(98)=2 THEN 2650
2630 B(12)=B(24)*C1:B(13)=B(25)*C1
2640 IF B(98)=1 THEN 2660
2650 B(12)=(B(24)+B(91))*C1:B(13)=(B(26)+B(93))*C1
2660 RETURN
2670 REM SUBROUTINE FOR SCALING OF AXIS.
2680 PRINT "MINIMUM & MAXIMUM X-AXIS": INPUT Z(7),Z(6)
2690 PRINT "MINIMUM Y-AXIS(CONC) & MINIMUM Y-AXIS(TEMP)": INPUT Z(3),Z(8)
2700 PRINT "MAXIMUM Y-AXIS(CONC) & MAXIMUM Y-AXIS(TEMP)": INPUT Z(4),Z(5)
2710 PRINT "COUNTER(R)": INPUT B(11): PRINT "ACCEPT(0) OR REJECT(1)"
2715 INPUT A(13): IF A(13)>0 THEN 2670
2720 RETURN
2730 M2=0: GOTO 2750
2740 M2=1
2750 P1=0: CALL (4,M2,P1): IF M2=0 THEN RETURN
2760 T9=T9+P1/50: RETURN
2770 IF F3<0 THEN F=.8333
2780 IF F3=0 THEN IF F3<4 THEN F=(.8333+.2396*F3)
2790 IF F3=>4 THEN IF F3<9 THEN F=(1.7917+.2663*(F3-4))
2800 IF F3=9 THEN IF F3<13 THEN F=(3.1232+.2666*(F3-9))
2810 IF F3=13 THEN IF F3<18 THEN F=(4.1896+.3*(F3-13))
2820 IF F3=18 THEN IF F3<26 THEN F=(5.6875+.3307*(F3-18))
2830 RETURN
2840 B(96)=B(96)-B(90):B(97)=B(97)-B(92): RETURN
2880 N=0: GOSUB 2740: GOSUB 2110: GOSUB 2730:T9=T9+A(0):A(0)=1: RETURN

```



```

1080 REM                                     MAYBE FOR NON-INTERACTING CONTROL.
1180 N=5;J=1;A(0)=5; GOSUB 2740; GOSUB 2110;J1=B(114)-J1
1190 J2=B(115)-J2;J3=B(116)-J3; PRINT "INLET REACTOR & COILS TEMP. CHANGE";
1200 PRINT J1,J2,J3; END ; STOP
1210 IF A1=1 THEN GOTO 1225
1215 B(122)=B(120);B(128)=B(16);B(129)=B(91);B(130)=B(90);B(127)=B(119)
1220 B(126)=B(118);B(132)=B(24);B(100)=F1;F4=F5; GOTO 1235
1225 B(122)=B(121);B(123)=B(17);B(129)=B(93);B(130)=B(92);B(127)=B(125)
1230 B(126)=B(131);B(132)=B(25);B(100)=F2;F4=F6
1235 S4=EXP(B(130)/(1+B(130)*B(87)))
1240 I2,I3,I4,I5,I6,I7,I8,I9=0;B(101)=(B(100)/F4)+(B(128)/B(103))
1250 B(102)=B(100)/F4;B(104)=B(102)/B(101)
1260 FOR J4=1 TO B(103);I2=I2+J4*(B(104)^J4)
1270 I3=I3+J4*(B(103)+1-J4)*(B(104)^J4); NEXT J4
1280 I2=I2*((B(101)-B(102))/(B(101)*B(102)))*(B(127)/F4)
1290 I3=(I3*B(122)+B(130))/(B(101)*B(102)*B(103)*F4)
1300 FOR J4=1 TO B(103)-1;I4=I4+J4*(B(103)-J4)*(B(104)^J4); NEXT J4
1310 I4=(I4*B(128)+B(130))/(B(101)*B(102)*B(103)*F4)
1320 I5=(I2+I4-I3)*(B(122)/B(103))
1330 FOR J4=1 TO B(103);I6=I6+(B(104)^J4);I7=I7+(B(103)+1-J4)*(B(104)^J4)
1340 NEXT J4;I8=I8+B(127)+((B(128)/(B(103)+B(102)))*I7*B(130))
1350 I9=(B(99)+B(94)*(B(129)+B(132))*S4)+((B(122)/B(103))*I8)
1355 I9=I9+B(126)-I1+B(122)+B(130);B(100)=B(100)-(I9/I5)
1360 PRINT B(101),B(100),B(105); IF ABS(B(100)-B(105))=5 THEN 1410
1370 IF A1=0 THEN GOTO 1400
1380 F2=B(100); RETURN
1400 B(105)=0;A1=1;F1=B(100); GOTO 1210
1410 B(105)=B(100); GOTO 1210
1450 PRINT TAB(2);T9
1460 PRINT TAB(2);B(110);TAB(12);B(111);TAB(22);B(112);TAB(32);B(113)
1470 PRINT TAB(2);B(24);TAB(12);B(133);TAB(22);B(134);TAB(32);B(135)
1480 RETURN
1600 REM                                     REACTION & EQUIPMENT PARAMETERS.
1610 U=.1623E-01;V1=.4E-03;V2=.53E-03;U=.5429;U1=.2721
1620 R=.31441;R1=1000;C2=4.1868;T0=273.1
1630 K1=2000;E1=.421192E05;D1=-.125604E06;B(103)=25
1640 F=F+.1E-04;F1=F*.1E-04;F2=F2+.1E-04; RETURN
1680 PEM                                     DIMENSIONLESS QUANTITIES.
1690 T=U/F1;B(16)=U/(F1*R1*C2);B(17)=U1/(F2*R1*C2)
1700 B(18)=U1/F1;B(19)=V2/F2;B(89)=(R+T0)/E1
1710 B(94)=K1*T*EXP(-E1/(R+T0));B(97)=-D1*C1/(B(89)*C2*R1*T0)
1715 B(120)=U/(F*R1*C2);B(121)=U1/(F2*R1*C2)
1720 RETURN
1730 B(118)=(B(114)+273.1-T0)/(B(89)*T0);B(119)=(B(115)+273.1-T0)/(B(89)*T0)
1740 B(125)=(B(116)+273.1-T0)/(B(89)*T0);B(131)=(B(117)+273.1-T0)/(B(89)*T0)
1745 RETURN
1750 REM                                     SETS FLOW RATES IN COILS.
1755 IF F2>.16667E-04 THEN 1760
1760 Q1=.9
1770 IF F2>.35E-04 THEN 1780
1780 Q1=.9-.8197E-01*((F2*.1E06)-1.6667); GOTO 1870
1790 IF F2>.614E-04 THEN 1800
1790 Q1=.75-.473E-01*((F2*.1E06)-3.5); GOTO 1870
1800 IF F2>.942E-04 THEN 1820
1810 Q1=.625-.35E-01*((F2*.1E06)-6.14); GOTO 1870
1820 IF F2>.1181E-03 THEN 1840
1830 Q1=.5-.315E-01*((F2*.1E06)-9.43); GOTO 1870
1840 IF F2>.1705E-03 THEN 1860
1850 Q1=.425-.334E-01*((F2*.1E06)-11.81); GOTO 1870
1860 IF F2>.1826E-03 THEN 1864
1864 Q1=.25-.124*((F2*.1E06)-17.05); GOTO 1870
1870 Q1=2
1880 IF F1>.16667E-04 THEN 1900
1890 Q1=1; GOTO 1990
1900 IF F1>.3644E-04 THEN 1920
1910 Q1=.975-.895E-01*((F1*.1E06)-1.6667); GOTO 1990
1920 IF F1>.13303E-03 THEN 1940
1930 Q1=.8-.466E-01*((F1*.1E06)-3.644); GOTO 1990
1940 IF F1>.15902E-03 THEN 1960
1950 Q1=.35-.673E-01*((F1*.1E06)-13.303); GOTO 1990
1960 IF F1>.1826E-03 THEN 1980
1970 Q1=.175-.144*((F1*.1E06)-15.902); GOTO 1990
1980 Q1=2
1990 Q1=Q1*.32767E05
2000 REM                                     T1 IS REACTOR OUTLET TEMP(B(30))
2040 REM                                     DIGITAL VALUES TO ANALOGUE SIGNALS.
2042 IF Q1>.32767E05 THEN PRINT Q1
2045 IF Q1>.32767E05 THEN PRINT "EXCEEDS MAXIMUM DIGITAL VALUE"
2047 IF Q1>.32767E05 THEN GOTO 1180
2050 CALL (3,D,N,Q1); RETURN
2060 B(22)=0;B(23)=1; GOTO 2100
2070 B(2),B(23)=1; GOTO 2100
2080 B(22)=2;B(23)=0; GOTO 2100
2090 B(22),B(23)=0
2100 CALL (5,B(22),B(23)); RETURN

```

A.2 ON-LINE SOFTWARE PACKAGE

The functions and calling procedure of various FORTRAN and DAPI6 subroutines loaded with the BASIC interpreter to form the ONLINE SIMULATION PACKAGE are described in detail.

A.2.1

Subroutines 1 and 2 jointly form the scanning routines and are always called together, routine 1 initiating and routine 2 terminating the scanning procedure.

Subroutine 1

CALL(1,A(0),B(0))

A and B are dimensioned 13 and 135 respectively in the basic on line programme.

Inputs - A(0) = scanning interval, secs

A(1) = Device required
= 1 Analogue inputs
= 2 Counter 1
= 4 Counter 2
= 8 Counter 3
= 16 digital input A
= 32 digital input B
= 64 digital output A
= 128 digital output B

A(2) = number of scans required including the initial scan

A(3) = first analogue channel to be scanned

A(4) = last analogue channel to be scanned

A(5) = number of samples of each analogue channels per scan

A(6) = counter 1 scan type
= 0 no counter interrupt
= 1 enable counter interrupt

A(7) = counter 1 present value

A(8) and A(9) = counter 2 scan and preset values

A(10) and A(11) = counter 2 scan and preset values

A(12) = digital output A mode
= 0 from 16 bit array at Basic level
= 1 from subroutine 3
= 2 from user supplied

A(13) = digital output B mode

Outputs

B(0) - B(47) = analogue input channels

B(48) = counter 1 interrupt time

B(49) = counter 1 contents at scanning time

B(50) = number of interrupts by the counter 1 during last scanning interval

B(51) - B(53) = counter 2

B(54) - B(56) = counter 3

B(57) - B(72) = value read on bits 1 to 16 of digital input A

B(73) - B(88) = digital input B

B(89) - B(104) = values output on digital output A

B(105) - B(120) = for digital output B

Subroutine 2

CALL(2)

A call to this routine discontinues clock and counter interrupt when all scans requested have been done. In the Basic on line programme a call to routine 4 occurs before and after the scanning pair.

Subroutine 3

CALL(3,D,N,Q)

to send digital signals to various devices during scanning

D = 0 digital output A

= 1 digital output B

N = analogue output channel

= 1 and 2 for thyristor unit

= 3 and 4 valve drives

= 5 set of thermocouples monitoring temperatures of reactor and cooling coils.

= 6 set of thermocouples monitoring temperatures of inlet liquids into reactors and cooling coils.

Q = digital signal to be output

0 x 32767

When called, this routine sends signals to the devices almost instantaneously.

Subroutine 4

CALL(4,M2,P1)

Input M2 = 0 start the clock

= 1 stop the clock

Output On exit when the clock is stopped, the time elapsed for

executing a set of programme commands is given by
 $T9 = P1/50$ secs.

Subroutine 5

CALL(5,I,J)

Input I = 0 set or reset SNSW4

J = 0 reset SNSW4

J = 1 set SNSW4, so output will be directed to paper tape

punch

I = 0 to perform other tasks

J = 0 output few frames of blank tape

J = 1 HALT the computer until the START button is pressed

Subroutine 6

CALL(6,X,XS,HS,Z)

Input X = starting time for integration

Z(10) = 1

XS(1) = reactor 1 dimensionless product concentration before integration

XS(2) = reactor 2 dimensionless product concentration before integration

XS(3) = 0.0

XS(4) = 0.0

Z(10) = 2

XS(1) = same as above

XS(2) = integral of absolute error of concentration

in

reactor 1 before integration
 XS(3) = same as XS(2) above
 XS(4) = integral of absolute error of concentration
 in
 reactor 2 before integration
 HS = step length of integration
 Z(1) = G1
 Z(2) = TS steady state temperature in reactor 1
 Z(3) = CS steady state concentration in reactor 1
 Z(4) = TY steady state temperature in reactor 2
 Z(5) = CY steady state concentration in reactor 2
 Z(6) = D1
 Z(7) = PV
 Z(8) = temperature in reactor 1
 Z(9) = temperature in reactor 2
 Z(10) = 1 calls routine MEX which simulates for
 steady state conditions
 = 2 calls routine MAXI which simulates for
 transient response
 Z(11) = B

Output

X time at end of integration
 XS(1) = concentration in reactor 1 at end of integration step
 XS(3) = concentration in reactor 2 at end of integration step
 This routine uses a fixed step fourth order Runge-Kutta method to
 integrate the differential equations describing the mass balance in
 the two chemical reactors.

Subroutine 7

CALL(7,T,C,D,E,F,G,X,Q,R,V)

Inputs

T = is the cumulative time for the graph plot
 C(1)-C(4) = Minimum screen X-coordinate of the screen window
 D = Extent of the screen window in the X-direction
 E(1)-E(4) = Minimum screen Y-coordinate of the screen window
 G = Extent of the screen window in the Y-direction
 X(1)-X(2) = Virtual Y-coordinate of the points (concentrations
 in
 reactors 1 and 2)
 X(3)-X(4) = Virtual Y-coordinate of the points (temperatures in
 reactors 1 and 2)
 Q = Controls initial entry values taken from Basic
 R = Total number of points to be plotted
 V(1)&V(6) = Minimum virtual Y-axis (concentration in reactors 1
 and 2)
 V(2)&V(3) = is the extent of the Y-axis
 V(4) = is the total scanning time
 V(5) = Initial time (origin for X-axis)

Outputs

Q = indicates number of points plotted

A.3 Changes in BASIC Interpreter

A.3.1 PATCHING of CALL table

The BASIC Interpreter maintains a table occupying locations '516 to '527 into which are patched the starting addresses of a maximum of ten subroutines in FORTRAN and DAP16 callable from the BASIC executive programme. In the software package for this research, the following subroutines addresses were placed in the CALL table:

Location	Address	Comment
'520	'25433	Beginning address of subroutine 3
'521	'26710	Starting address of subroutine 4
'522	'25742	Starting address of subroutine 5
'523	'27000	Starting address of subroutine 6
'524	'32000	Beginning address of subroutine 7

A.3.2 Other Modifications

Changes are made to locations '166 through '203 so that on initialization of programme, the following message is printed on the VDU 'HADIOS EXEC 03 NEE 82'. Certain changes are implemented to correct bugs in interpreter and indicate limit of memory available for user programme, hence the following amendments are effected:

Location	Original	Mnemonic	Code	Comment
'7240	JST TYPE	NOP	'101000	
'7241	XAC HMAN	NOP	'101000	
'7242	IN03 JST TYPE	NOP	'101000	
'7243	XAC AYOH	NOP	'101000	
'7245	LDA C241	JMP'7301	'003301	
'7367	'37777		'24777	High address of available core
'2540			'052726	
'5425	(CR,Rubout)		'106777	
'13167		NOP	'101000	

A.3.3 ADT1-8 Table

The assembly language listed in Appendix A.1.9 has relocated the ADT1-8 table (assigned dimensional variable table) to location '757 to '766, thus allowing the use of locations '61 to '63 for real-time applications.

I/O MOD

The relocatable assembly language programme listed in Appendix A.1.7 is loaded into locations '720 through '756. Its initial locations '550 to '715 are used by the interpreter for its base requirements.

A.4.1 RESIDENCE TIME DISTRIBUTION (RTD) STUDIES IN COOLING JACKETS

This study was accomplished by injecting a known concentration of a dye (methyl blue) into the cooling jacket and monitoring its outlet concentration. A recorded constant flow rate of water into and out of the jacket was maintained, thereby flushing the dye from the jacket in the process. Samples of the outflowing solution were collected at regular intervals and these were subsequently analysed using gas-liquid chromatography. Graphs were then drawn as indicated in Fig A.4.1(a-d) comparing the measured concentration leaving the jacket and the expected concentration if the jacket was assumed to be well stirred. The results indicate a lack of defined flow pattern with various values rising and falling at random and this makes it difficult to describe the RTD mathematically. This observation confirmed the presence of dead space and channelling when the cooling liquid in the jacket was not stirred, the latter action not generally being employed industrially.

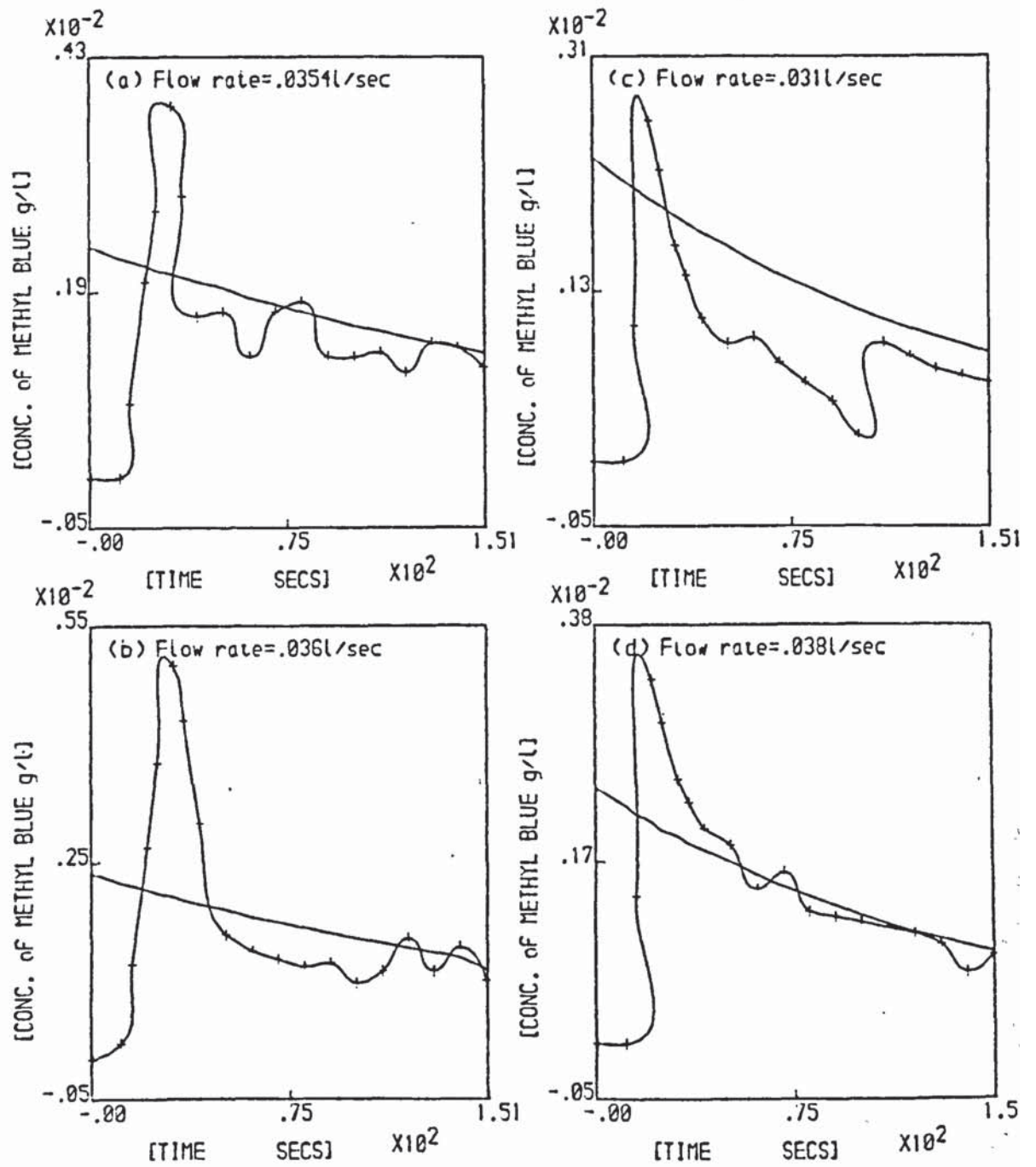


Fig A.4.1(a-d)
Residence Time Distribution
study in Cooling Jacket

A.4.2 RELATION BETWEEN $k_1, k_2, \hat{E}_1, \hat{E}_2$ and \hat{H}

It was initially intended to use one reversible reaction and this section gives the calculations which led to the rejection of this for the available plant parameters.

For a reaction whose reversibility will be easily noticeable, the ratios for the forward and backward reaction rates are fixed at two temperatures which are realisable in the reactors. Choosing the values 290K and 320K and the corresponding ratios as 2.0 and 0.5. the following equations are then fitted with the assumed values.

$$\hat{H} = \hat{E}_1 - \hat{E}_2 \quad (4.2.1)$$

Representing the ratio of forward to backward reaction rate as

$$(k_{10} \exp(-(\hat{E}_1/RT)))/(k_{20} \exp(-(\hat{E}_2/RT))) = r = \text{constant at } 290$$

and 320K, this becomes

$$r_1 = (k_{10}/k_{20}) \exp((\hat{E}_2 - \hat{E}_1)/290R) = 2.0 \quad (4.2.2)$$

$$r_2 = (k_{10}/k_{20}) \exp((\hat{E}_2 - \hat{E}_1)/320R) = 0.5 \quad (4.2.3)$$

$$k_{20} = 0.5k_{10} \exp((\hat{E}_2 - \hat{E}_1)/8.32 \times 290) \quad (4.2.2a)$$

$$k_{20} = 2.0k_{10} \exp((\hat{E}_2 - \hat{E}_1)/8.32 \times 320) \quad (4.2.3a)$$

Equating equations (4.2.2a) and (4.2.3a) and substituting for \hat{H} from equation (4.2.1)

$$\hat{H} = -8.32 \ln(r_2/r_1) (320 \times 290 / (320 - 290)) = -3.5678 \times 10^4 \text{ kJ/kg mol.}$$

Checking at 290K $k_{20} = 0.5k_{10} \exp(3.5678 \times 10^4 / 290 \times 8.32) = 1.321 \times 10^6 k_{10}$

Checking at 320K $k_{20} = 2.0k_{10} \exp(3.5678 \times 10^4 / 320 \times 8.32) = 1.321 \times 10^6 k_{10}$

With this reaction heat, multiple steady states could not be obtained with the feed and cooling flow rates ranges available. Selecting a higher heat of reaction and carrying out similar algebraic manipulations, the following results were arrived at:-

$$\hat{H} = 3.97 \times 10^5 \text{ kJ/kg mol}$$

$$-\hat{H} = \ln(r_1/r_2) 8.32 \times 290 \times 320 / 30$$

$$\ln(k_1/k_2) = -\hat{H} \times 30 / (8.32 \times 290 \times 320) = 3.97 \times 10^5 \times 30 / (8.32 \times 290 \times 320) = 15.43$$

$$r_1 = r_2 e^{15.43}$$

$$= 0.5 \exp(15.43) = 2.5 \times 10^6$$

$$r_1 = (k_{10}/k_{20}) \exp(-\hat{H}/RT_1)$$

$$k_{20} = (k_{10}/r_1) \exp(-\hat{H}/RT_1)$$

$$= 3.9968 \times 10^{-7} \times 2.875 \times 10^{71} k_{10} = 1.149 \times 10^{65} k_{10}$$

In selecting the value of \hat{E}_1 , the need to keep the ratio (\hat{E}_2/\hat{E}_1) as small as possible was appreciated as this value increases exponentially in the reactor heat balance equation. A large value of $B(-\hat{H}C_{ao}^0/pC_p T_o)$ was necessary in order to have multiple steady states for the parameters of this system and a large B implied a large \hat{H} which invariably implied a large value for \hat{E}_2/\hat{E}_1 . A compromise value of $\hat{H}(-3.97 \times 10^5 \text{ kJ/kg mol})$ was selected, barely permitting multiple steady states without making \hat{E}_2/\hat{E}_1 excessively large. The subsequent calculation as shown above led to a very large rate constant for the reverse reaction which was difficult to handle in the resulting heat balance equations. It was concluded that it is not possible to choose values of $\hat{E}_1, \hat{E}_2, k_{10}, k_{20}$ and \hat{H} which will give an appreciable first order reversible reaction over a short temperature range of 30K with the size of reactors and cooling coils as specified for this plant. Hence the reversible reaction was abandoned for an irreversible one.

A.4.3 ITERATIVE SOLUTION FOR SINGLE STREAM COOLING OF BOTH REACTORS.

Let equations representing system be

$$f=f_o+xf'_x+yf'_y+zf'_z+rf'_r = \emptyset \quad (4.3.1)$$

$$g=g_o+xg'_x+yg'_y+zg'_z+rg'_r = \emptyset \quad (4.3.2)$$

$$h=h_o+xh'_x+yh'_y+zh'_z+rh'_r = \emptyset \quad (4.3.3)$$

$$t=t_o+xt'_x+yt'_y+zt'_z+rt'_r = \emptyset \quad (4.3.4)$$

Rewriting the above equations in terms of x

$$x=-(f_o+yf'_y+zf'_z+rf'_r)/f'_x \quad (4.3.1a)$$

$$=-(g_o+yg'_y+zg'_z+rg'_r)/g'_x \quad (4.3.2a)$$

$$=-(h_o+yh'_y+zh'_z+rh'_r)/h'_x \quad (4.3.3a)$$

$$=-(t_o+yt'_y+zt'_z+rt'_r)/t'_x \quad (4.3.4a)$$

Equating equation (4.3.1a) with (4.3.2a, 4.3.3a and 4.3.4a) and re-arranging

$$f_o g'_x - f'_x g_o + y(f'_y g'_x - g'_y f'_x) + z(f'_z g'_x - g'_z f'_x) + r(f'_r g'_x - f'_x g'_r) = \emptyset \quad (4.3.2b)$$

$$f_o h'_x - f'_x h_o + y(f'_y h'_x - f'_y h'_x) + z(f'_z h'_x - f'_z h'_x) + r(f'_r h'_x - f'_x h'_r) = \emptyset \quad (4.3.3b)$$

$$f_o t'_x - f'_x t_o + y(f'_y t'_x - f'_y t'_x) + z(f'_z t'_x - f'_z t'_x) + r(f'_r t'_x - f'_x t'_r) = \emptyset \quad (4.3.4b)$$

From equations (4.3.2b), (4.3.3b) and (4.3.4b)

$$y = ((-f_o g'_x + f'_x g_o) - z(f'_z g'_x - g'_z f'_x) - r(f'_r g'_x - f'_x g'_r)) / (f'_y g'_x - g'_y f'_x) \quad (4.3.2c)$$

$$= ((f'_x h'_o - h'_x f_o) - z(f'_z h'_x - h'_z f'_x) - r(f'_r h'_x - f'_x h'_r)) / (f'_y g'_x - h'_y f'_x) \quad (4.3.3c)$$

$$= ((f'_x t'_o - f_o t'_x) - z(f'_z t'_x - f'_z t'_x) - r(f'_r t'_x - f'_x t'_r)) / (f'_y g'_x - f'_y t'_x) \quad (4.3.4c)$$

Let $S_1 = f'_z t'_x - f'_z t'_z$ $S_5 = f_o g'_x - g_o f'_x$ $S_9 = f'_r h'_x - f'_x h'_r$
 $S_2 = f'_y g'_x - f'_y g'_y$ $S_6 = f'_y h'_x - f'_y h'_y$ $S_{10} = f'_z h'_x - f'_z h'_z$
 $S_3 = f'_z g'_x - f'_z g'_z$ $S_7 = f_o h'_x - f'_x h'_o$ $S_{11} = f_o t'_x - f'_x t'_o$
 $S_4 = f'_y t'_x - f'_y t'_y$ $S_8 = f'_r g'_x - f'_x g'_r$ $S_{12} = f'_r t'_x - f'_x t'_r$
 $S_{13} = S_1 * S_2 - S_3 * S_4$ $S_{14} = S_{10} * S_2 - S_3 * S_6$

Equating equations (4.3.2c) with (4.3.3c) and (4.3.4c) and re-arranging for z

$$z = ((S_7 * S_2 - S_6 * S_5) - r(S_8 * S_6 - S_9 * S_2)) / (S_3 * S_6 - S_{10} * S_2) \quad (4.3.3d)$$

$$=((s_{11} * s_2 - s_4 * s_5) - r(s_8 * s_4 - s_{12} * s_2)) / (s_3 * s_4 - s_2 * s_1) \quad (4.3.4d)$$

Solving for r in equations (4.3.3d) and (4.3.4d) results in

$$r = ((s_2 * s_7 - s_6 * s_5) * s_{13} - (s_{11} * s_2 - s_4 * s_5) * s_{14}) / ((s_8 * s_6 - s_9 * s_2) * s_{13} - (s_8 * s_4 - s_{12} * s_2) * s_{14}) \quad (4.3.1e)$$

$$z = ((s_6 * s_5 - s_2 * s_7) + r(s_6 * s_8 - s_9 * s_2)) / (s_{14}) \quad (4.3.2e)$$

$$y = -(r * s_8 + z * s_3 + s_5) / s_2 \quad (4.3.3e)$$

$$x = -(f_o + y * f'_y + z * f'_z + r * f'_r) / f'_x \quad (4.3.4e)$$

Thus the following four equations giving the values of the variables at times (n) and (n+1) result:

$$x_{n+1} = x_n + x$$

$$y_{n+1} = y_n + y$$

$$z_{n+1} = z_n + z$$

$$r_{n+1} = r_n + r$$

where x, y, z and r have the values obtained from equations (4.3.1e) to (4.3.4e).

A.4.4 CALIBRATION EQUATIONS

FLOW VOLUME(F_c) and applied VOLTAGE(Q_s) for PROCESS CONTROL VALVES.

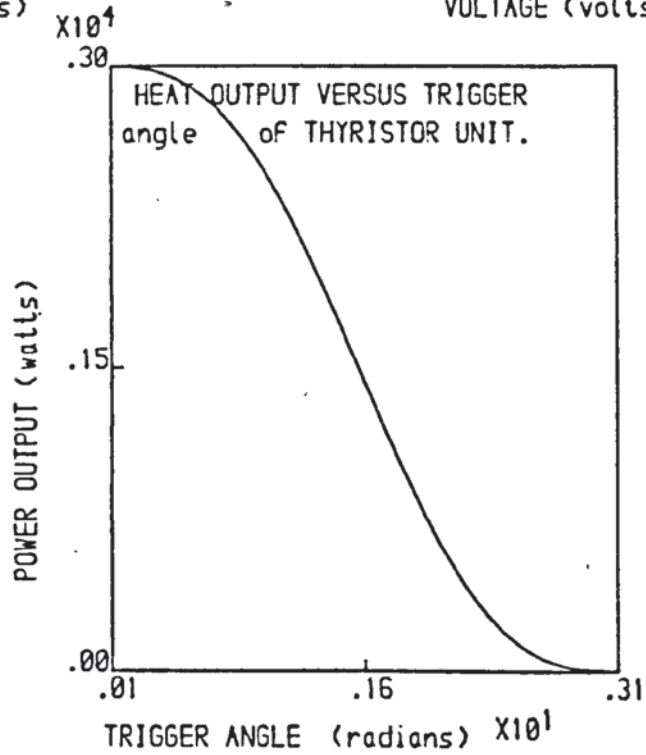
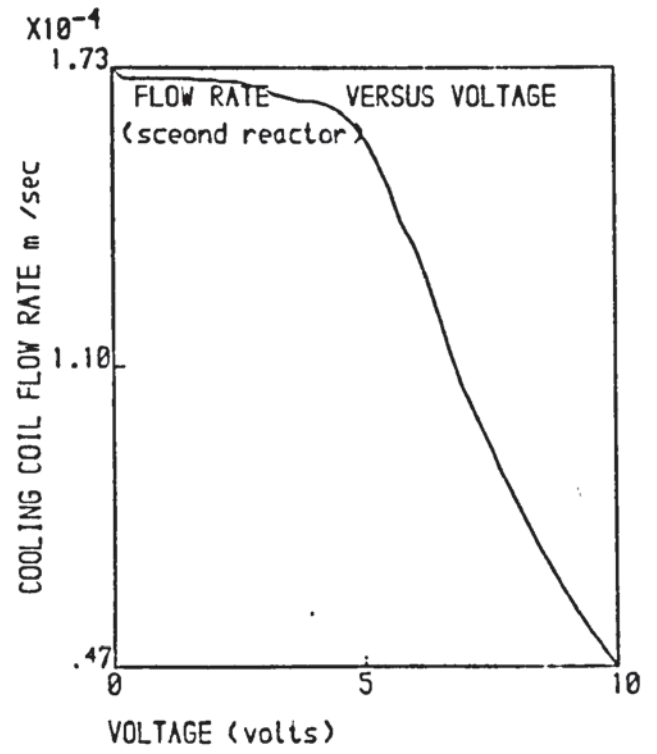
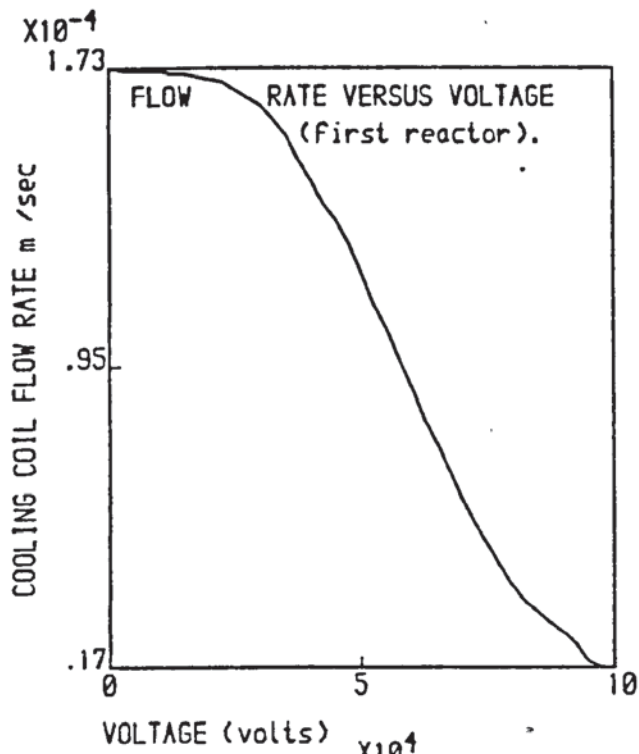
(1)	$0.0 < F_c \leq 1.6667E-05$	$Q_s = 1.0$
	$1.6667E-05 < F_c \leq 3.6444E-05$	$Q_s = 0.975 - 0.0885(F_c \times 1.0E06 - 1.6670)$
	$3.644E-05 < F_c \leq 1.3303E-04$	$Q_s = 0.8 - 0.0466(F_c \times 1.0E06 - 3.6440)$
	$1.33E-04 < F_c \leq 1.59E-04$	$Q_s = 0.35 - 0.0673(F_c \times 1.0E06 - 13.303)$
	$1.59E-04 < F_c \leq 1.826E-04$	$Q_s = 0.175 - 0.1440(F_c \times 1.0E06 - 15.902)$
(2)	$0.0 < F_c \leq 1.6667E-05$	$Q_s = 0.9$
	$1.6667E-05 < F_c \leq 3.5E-05$	$Q_s = 0.9 - 0.0820(F_c \times 1.0E06 - 1.6667)$
	$3.5E-05 < F_c \leq 6.14E-05$	$Q_s = 0.75 - 0.0473(F_c \times 1.0E06 - 3.5000)$
	$6.14E-05 < F_c \leq 9.43E-05$	$Q_s = 0.625 - 0.0380(F_c \times 1.0E06 - 6.1400)$
	$9.43E-05 < F_c \leq 1.181E-04$	$Q_s = 0.5 - 0.0315(F_c \times 1.0E06 - 9.4300)$
	$1.181E-04 < F_c \leq 1.705E-04$	$Q_s = 0.425 - 0.0334(F_c \times 1.0E06 - 11.810)$
	$1.705E-04 < F_c \leq 1.826E-04$	$Q_s = 0.25 - 0.1240(F_c \times 1.0E06 - 17.050)$

HEAT GENERATED(H) and TRIGGER ANGLE(α_1)

$$\alpha_1 = Z_1 + Z_2 H + Z_3 H^2 + Z_4 H^3$$

where Z_1, Z_2, Z_3 and Z_4 are constants of correlation.

$0 < H \leq 50$	$Z_1 = 1.880E-02$	$Z_2 = 7.057E-02$
	$Z_3 = -6.037E-03$	$Z_4 = 1.463E-04$
$50 < H \leq 1000$	$Z_1 = 3.540E-01$	$Z_2 = 2.318E-03$
	$Z_3 = -2.781E-06$	$Z_4 = 1.509E-09$
$1000 < H \leq 2500$	$Z_1 = 5.640E-01$	$Z_2 = 9.691E-04$
	$Z_3 = -2.965E-07$	$Z_4 = 6.528E-11$



CALIBRATION CURVES For HEATERS
and PROCESS CONTROL VALVES.

Fig. A.4.4

2500 < H <= 2900	$Z_1 = 7.490E-00$	$Z_2 = -4.859E-03$
	$Z_3 = 1.091E-06$	$Z_4 = 0.000E-00$
2900 < H	$Z_1 = 9.720E+02$	$Z_2 = -6.602E-01$
	$Z_3 = 1.124E-04$	$Z_4 = 0.000E-00$

A.4.5 PARAMETER VALUES USED

V_1, V_2	$= 1.62 \times 10^{-2} \text{ m}^3$
V_{C1}	$= 4.0 \times 10^{-4} \text{ m}^3$
V_{C2}	$= 5.3 \times 10^{-4} \text{ m}^3$
B, B_C	$= 1.0 \times 10^3 \text{ kg/m}^3$
C_p, C_{pc}	$= 4.1868 \text{ kJ/kg K}$
UA_1	$= 0.2998 \text{ kJ/kg K}$
UA_2	$= 0.2721 \text{ kJ/kg K}$
t_m	$= 2.0 \text{ secs}$
t_v	$= 2.0 \text{ secs}$
t_s	$= 1.0 \text{ sec}$
ΔE_1	$= 4.212 \times 10^4 \text{ kJ/kg mole K}$
ΔH	$= 1.256 \times 10^5 \text{ kJ/kg}$
C_{ao}	$= 20 \text{ kg/m}^3$
R	$= 8.314 \text{ kJ/kg mole K}$
k_o	$= 2 \times 10^3 \text{ sec}^{-1}$
F	$= 5 \times 10^{-5} \text{ m}^3/\text{sec}$
F_c	$= 8 \times 10^{-5} \text{ m}^3/\text{sec}$

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*TOTAL SIMULATION OF FIRST ORDER IRREVERSIBLE *
EXOTHERMIC REACTION IN TWO (SERIES) CONTINUOUS
*STIRRED TANK REACTORS (CSTRS). *

* MAIN PROGRAM *

```
PROGRAM STABVS
INTEGER *3 MX,MY
REAL K10,E1,C(4),NAMEIT(4,7)
SPECIAL COMMON IBR,ZZ,XT,FX,SV,XP,WX,VB,JP,WP
1,BZ,SX,SK,SD,MYX
COMMON /MYX/ MX(10),MY(10)
COMMON /SK/ X(6),E(6,6),S(2,6),Z1(6),AB(3,3)
COMMON /SD/ SA(6,6),B9(6,6),AO(3,3),AM(3,3),RQ(3)
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /WP/ BK(801),BM(801),YI(801)
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
COMMON /SX/ AS1(451,2,2),AS2(451,2,2),
1AS3(451,2,2),AST(451,2,2),AS4(451,2,2)
DATA NAMEIT/6HOPEN F,6HILE & ,6HINPUT ,6HDATA ,
16HSTEADY,6H STATE,6H CALCU,6HLATION,6HHEAT G,
26HEN &RE,6HMOVAL ,6HVALUES,6HUNSTEA,6HDY STA,
36HTE RES,6HPONSE ,6HGRAPHI,6HCAL DI,6HSPRAY ,
46H ,6HEXPERI,6HMENTAL,6H VALU,6HES ,
56HEND IT,6H ALL &,6H CLOSE,6H FILE /
DATA NI,K10/7,.2E04/
WRITE(NS,4)
GO TO 6
2 CONTINUE
WRITE(NS,3)
CALL RADS(C,4)
C DEL IS HEAT OF REACTION.
C TH IS TIME CONSTANT FOR REACTOR.
C Y1,Y2 &Y3 ARE INPUT VARIABLES.
TCO=C(1)+273.1
TP=C(2)+273.1
F=C(3)
FC(1)=C(4)
DEL=-1.25604E05
BY(1)=U(1)/(F*R1*CP)
TH=V1/F
GAY=E1/(R*TQ)
G1=(R*TQ)/E1
Y1(1)=CAO/CAO
Y2(1)=(TCO-TQ)*GAY/TQ
Y3(1)=(TP-TQ)*GAY/TQ
D1=K10*TH*EXP(-GAY)
B=(-DEL)*CAO*GAY/(R1*CP*TQ)
WRITE(NS,8) D1,G1,B
```



```

WRITE(NS,9) Y1(1),Y2(1),Y3(1)
WRITE(NS,10) DEL,BY(1),GAY
3  FORMAT(5X,' TCO Tin oC F FC ',/)
4  FORMAT(/,10X,'*****',/,10X,
1      '* [INTERACTIVE SIMULATION PROGRAM] *',/,10X,
1      '*****',/)
6  CALL SESAME(NAMEIT,NI,I)
8  FORMAT(5X,'D1=',F8.4,5X,'G1=',F8.4,5X,'B=',F8.4)
9  FORMAT(5X,'Y1(1)=',F8.4,2X,'Y2(1)=',F8.4,2X,'Y3(1)=',F8.4)
10 FORMAT(5X,'DEL=',E10.4,2X,'BY(1)=',E10.4,2X,'GAY=',E10.4)
GO TO (2,12,14,16,18,20,22),I
12 CALL SSTE
GO TO 6
14 CALL HRGT
GO TO 6
16 CALL UNCODY
GO TO 6
18 CALL GRAPHS
GO TO 6
20 CALL EXPMNT
GO TO 6
22 STOP
END

C          *****
C          * SUBROUTINE SESAME.          *
C          * SELECTS SUBROUTINES        *
C          * AND VARIOUS PRINT OPTIONS.*
C          *****

SUBROUTINE SESAME(NAMEIT,NI,I)
REAL NAMEIT(4,8)
SPECIAL COMMON JP
COMMON /JP/ JQ,IQ,LQ,LX,NS,NC,NP,NB
WRITE(NS,24)
24  FORMAT(/,10X,'ALTERNATIVES ARE',/)
DO 26 J=1,NI
26  WRITE(NS,28) J,(NAMEIT(K,J),K=1,4)
28  FORMAT(I4,5X,4A6,/)
WRITE(NS,30)
30  FORMAT(10X,'INPUT CONTROL INTEGER',/)
READ(NS,32,ERR=34) I
WRITE(NS,32) I
32  FORMAT(I3)
RETURN
34  WRITE(NS,36) I
I=NI
36  FORMAT(10X,'I IS IN ERROR=',I3,/)
RETURN
END

BLOCK DATA
SPECIAL COMMON ZZ,XT,SV,WX,JP,BZ
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
DATA TVS/312*0.0/,CAO,E1/20.,.4211921E05/
DATA R1,CP,R,TQ/1.0E3,4.1868,8.31441,273.1/
DATA VC/0.4E-03,3*.53E-03/,V1/0.0162/
DATA NS,NC,NP,NB/8,25,3,6/,U/.2998,3*.2721/
END

```

C
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* SUBROUTINE SSTE *
* SUBROUTINE TO FIND STEADY *
* STATE VALUES OF VARIABLES*

```

SUBROUTINE SSTE
REAL CIO(3),TIO(3),BID,BIX,TSV(25),SM
SPECIAL COMMON ZZ,XT,SV,XP,WX,JP,BZ,SK,SD
COMMON /SK/ X(6),E(6,6),S(2,6),Z1(6),AB(3,3)
COMMON /SD/ SA(6,6),B9(6,6),AO(3,3),AM(3,3),RQ(3)
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /JP/ JQ,IQ,LQ,LX,NS,NC,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
SM=FLOAT(NC)
TOL=1.0E-13
WRITE(NS,94)
WRITE(NS,112)
READ(NS,98) NIB
IF(NIB.NE.2) GO TO 58
FC(2)=FC(1)
Y3(2)=Y3(1)
WRITE(NS,114)
37 FORMAT(5X,'INITIALIZE CONCENTRATION (CIO(2)) VALUES',/)
38 CONTINUE
39 FORMAT(5X,'INITIALIZE TEMPERATURE (TIO(2)) VALUES',/)
WRITE(NS,37)
CALL RADS(CIO,2)
WRITE(NS,39)
CALL RADS(TIO,2)
DO 40 JF=1,2
TK(JF)=VC(JF)/FC(1)
BY(JF+1)=U(JF+1)/(F*R1*CP)
BC(JF)=U(JF)/(FC(1)*R1*CP)
40 WRITE(NS,66) JF,TK(JF),JF,BC(JF),JF,BY(JF)
LX=2
43 WRITE(NS,96)
READ(NS,98,ERR=118) LM
GO TO (41,118),LM
41 NX=0
X1=CIO(1)
X2=TIO(1)
X4=CIO(2)
X5=TIO(2)
42 CONTINUE
CALL BIXT(DTX,X61T,BAS,X31T)
CALL BIXT(TVS(26,1,1),TVS(26,1,2),BID,BIX)
CALL BIXT(DFZ,DFV,DGZ,DHY)
X60=Y3(1)
DO 44 IA=1,NC
X61=(SM*X60+BC(2)*X5)/(SM+BC(2))
X61T=X61T+X61
X60=X61
TVS(IA,1,2)=X61
TSV(IA)=TQ*(1.+(TVS(IA,1,2)*G1))-273.1
44 TVS(NC+1,1,2)=TVS(NC+1,1,2)+X61
X30=X61
DO 46 IA=1,NC
X31=(SM*X30+BC(1)*X2)/(SM+BC(1))

```

```

X31T=X31T+X31
X30=X31
TVS(IA,1,1)=X31
TSV(IA)=TQ*(1.+(TVS(IA,1,1)*G1))-273.1
46 TVS(NC+1,1,1)=TVS(NC+1,1,1)+X31
DOS=(1.+G1*X2)**2.
DDS=(1.+G1*X5)**2.
DFX=-(1.+D1*CE(X2,0.0,G1))
DFY=-D1*X1*CE(X2,0.0,G1)/DOS
DGX=B*D1*CE(X2,0.0,G1)
S1P=SM/(SM+BC(2))
S2P=SM/(SM+BC(1))
S1T=BC(1)/(SM+BC(1))
S2T=BC(2)/(SM+BC(2))
DO 48 IA=2,NC
BIX=BIX+(S1P**IA)
BID=BID+(SM-IA)*(S2P**IA)
BAS=BAS+(SM-IA)*(S1P**IA)
48 CONTINUE
BIX=(1.+BIX)*S2T
BID=S1T*(SM+BID)
BAS=S2T*(SM+BAS)
DGY=-(1.+BY(1))+(B*D1*X1*CE(X2,0.0,G1)/DOS)+(BY(1)/SM)*BID
DGV=(BY(1)/SM)*BIX
DHX=1.0
DHZ=-(1.+D1*CE(X5,0.0,G1))
DHV=-D1*X4*CE(X5,0.0,G1)/DDS
DTY=1.0
DTZ=B*D1*CE(X5,0.0,G1)
DTV=-(1.+BY(2))+(B*D1*X4*CE(X5,0.0,G1)/DDS)+(BY(2)/SM)*BAS
FD=Y1(1)-X1-D1*X1*CE(X2,0.0,G1)
GD=Y2(1)-X2+B*D1*X1*CE(X2,0.0,G1)-(BY(1)/SM)*(SM*X2-TVS(NC+1,1,1))
HD=X1-X4-D1*X4*CE(X5,0.0,G1)
TD=X2-X5+B*D1*X4*CE(X5,0.0,G1)-(BY(2)/SM)*(SM*X5-TVS(NC+1,1,2))
S1=DFZ*DTX-DTZ*DFX
S2=DFY*DGX-DFX*DGX
S3=DFZ*DGX-DFX*DGZ
S4=DFY*DTX-DFX*DTY
S5=FD*DGX-GD*DFX
S6=DFY*DHX-DFX*DHX
S7=FD*DHX-HD*DFX
S8=DFV*DGX-DFX*DGX
S9=DFV*DHX-DFX*DHV
S10=DFZ*DHX-DHZ*DFX
S11=FD*DTX-TD*DFX
S12=DFV*DTX-DFX*DTV
S13=S1*S2-S3*S4
S14=S10*S2-S3*S6
VX5=((S7*S2-S5*S6)*S13-(S11*S2-S5*S4)*S1
14)/((S2*S12-S8*S4)*S14-(S9*S2-S8*S6)*S13)
ZX4=((S7*S2-S6*S5)+VX5*(S9*S2-S8*S6))/(-S14)
YX2=-(VX5*S8+ZX4*S3+S5)/S2
XX1=-(FD+YX2*DFY+ZX4*DFZ+VX5*DFV)/DFX
BX1=X1+XX1
BX2=X2+YX2
BX4=X4+ZX4
BX5=X5+VX5
NX=NX+1
X1B=ABS(BX1-X1)
X2B=ABS(BX2-X2)
X4B=ABS(BX4-X4)
X5B=ABS(BX5-X5)

```



```

IF(X1B.LT.TOL.AND.X2B.LT.TOL.AND.X4B.LT.
1TOL.AND.X5B.LT.TOL.OR.NX.GT.50) GO TO 54
X1=BX1
X2=BX2
X4=BX4
X5=BX5
GO TO 42
54 CONTINUE
IF(X1B.GT.TOL.OR.X2B.GT.TOL.OR.X4B.GT.TOL.
1OR.X5B.GT.TOL.AND.NX.GT.50) WRITE(NS,82) X1B,X2B
WRITE(NS,88) NX
N=1
CIS(1,1)=BX1
TIS(1,1)=BX2
TCS(1,1)=TVS(NC,N,1)
CIS(1,2)=BX4
TIS(1,2)=BX5
TCS(1,2)=TVS(NC,N,2)
DO 56 LB=1,2
CA=CAO*CIS(1,LB)
T=TQ*(1.+(TIS(1,LB)*G1))-273.1
TC=TQ*(1.+(TCS(1,LB)*G1))-273.1
WRITE(NS,55) CA,T,TC
WRITE(NS,90) N,LB,CIS(N,LB)
WRITE(NS,92) N,LB,TIS(N,LB),N,LB,TCS(N,LB)
55 FORMAT(5X,'CA=',F10.4,5X,'T=',F10.4,5X,'TC=',F10.4)
56 CONTINUE
57 FORMAT(5X,'Y1(',I1,')=',F10.5,5X,'Y2(',I1,')=',F10.4,5X,
1'Y3(',I1,')=',F10.4)
GO TO 43
58 CALL BIXT(TCI,TI,CA,BIX)
WRITE(NS,116)
LX=0
60 FORMAT(4(E9.4,/))
62 FORMAT(2X,11F7.3)
64 LX=LX+1
IF(FC(LX).EQ.0.0) WRITE(NS,86)
IF(FC(LX).EQ.0.0.OR.LX.EQ.5) RETURN
N=0
TK(LX)=VC(LX)/FC(LX)
BY(LX)=U(LX)/(F*R1*CP)
BC(LX)=U(LX)/(FC(LX)*R1*CP)
WRITE(NS,67)
CALL RADS(CIO,3)
WRITE(NS,69)
CALL RADS(TIO,3)
66 FORMAT(5X,'TK(',I1,')=',F10.4,5X,'BC(',I1,')=',F10.4,5X,
1'BY(',I1,')=',F10.4)
67 FORMAT(5X,'INITIALIZE CONCENTRATION (CIO(3)) VALUES',/)
68 WRITE(NS,96)
69 FORMAT(5X,'INITIALIZE TEMPERATURE (TIO(3)). VALUES',/)
WRITE(NS,66) LX,TK(LX),LX,BC(LX),LX,BY(LX)
IF(LX.EQ.1) GO TO 70
Y1(LX)=CA/CAO
Y2(LX)=(TI-TQ)*E1/(R*(TQ**2))
Y3(LX)=(TCI-TQ)*E1/(R*(TQ**2))
WRITE(NS,57) LX,Y1(LX),LX,Y2(LX),LX,Y3(LX)
70 CONTINUE
READ(NS,98,ERR=118) IM
GO TO (72,118),LM
72 X1=CIO(N+1)
X2=TIO(N+1)

```

```

NX=0
74 BP=(1.+G1*X2)
PRE=-(1.+D1*CE(X2,0.0,G1))
PRT=-D1*X1*CE(X2,0.0,G1)/(BP**2.)
DRY=B*D1*CE(X2,0.0,G1)
TVS(NC+1,N+1,LX)=0.0
SNI=(SM+BC(LX))
BID=0.0
DO 78 IA=1,NC
BIX=0.0
DO 76 JA=1,IA
PSS=(SM)**(JA-1)
BIX=BIX+(SNI-SM)*(PSS/(SNI**JA))
76 CONTINUE
TVS(IA,N+1,LX)=BIX*X2+Y3(LX)*((SM/SNI)**IA)
BID=BID+BIX
78 CONTINUE
WRITE(NS,62) BID,(TVS(IA,N+1,LX),IA=1,NC)
DO 80 IA=1,NC
80 TVS(NC+1,N+1,LX)=TVS(NC+1,N+1,LX)+TVS(IA,N+1,LX)
DRX=B*D1*X1*CE(X2,0.0,G1)/(BP**2.)
DRS=DRX-1.-BY(LX)+((BID*BY(LX))/SM)
BIS=Y2(LX)-X2+B*D1*X1*CE(X2,0.0,G1)
GIT=BIS-(BY(LX)/SM)*(SM*X2-TVS(NC+1,N+1,LX))
GIS=Y1(LX)-X1-D1*X1*CE(X2,0.0,G1)
NX=NX+1
CISX=X1-(GIS*DRS-PRT*GIT)/(PRE*DRS-DRY*PRT)
TISX=X2-(GIT*PRE-DRY*GIS)/(PRE*DRS-DRY*PRT)
XC=ABS(CISX-X1)
XZ=ABS(TISX-X2)
82 FORMAT(5X,'N-R DOES NOT CONVERGE',/,2(3X,E9.4,3X),/)
IF(XC.LT.TOL.AND.XZ.LT.TOL) GO TO 84
IF(NX.GT.50) GO TO 84
X1=CISX
X2=TISX
GO TO 74
84 CONTINUE
IF(XC.GT.TOL.OR.XZ.GT.TOL.AND.NX.GT.50)
1WRITE(NS,82) XC,XZ
WRITE(NS,88) NX
86 FORMAT(5X,'NO DATA PROVIDED',/)
88 FORMAT(5X,' NUMBER OF ITERATIONS IS=',I3,/)
N=N+1
DO 89 IA=1,NC
89 TSV(IA)=TQ*(1.+(TVS(IA,N,LX)*G1))-273.1
WRITE(NS,62) (TSV(IA),IA=1,NC)
CIS(N,LX)=CISX
TIS(N,LX)=TISX
TCS(N,LX)=TVS(NC,N,LX)
IF(LX.LT.4) CA=CAO*CIS(LX,1)
IF(LX.LT.4) T=TQ*(1.+(TIS(LX,1)*G1))-273.1
IF(LX.LT.4) TC=TQ*(1.+(TCS(LX,1)*G1))-273.1
ZCA=CAO*CIS(N,LX)
ZT=TQ*(1.+(TIS(N,LX)*G1))
ZTC=TQ*(1.+(TCS(N,LX)*G1))
WRITE(NS,55) ZCA,ZT,ZTC
WRITE(NS,90) N,LX,CIS(N,LX)
WRITE(NS,92) N,LX,TIS(N,LX),N,LX,TCS(N,LX)
90 FORMAT(5X,'CIS(',I1,',',I1,')=',E12.4)
92 FORMAT(5X,'TIS(',I1,',',I1,')=',E12.4,/,5X,'TCS('
1,I1,',',I1,')=',E12.4,/)
94 FORMAT(10X,' *CALCULATION OF STEADY STATE VALUES*',/)

```

```

IF(N+1.LT.4) GO TO 72
96  FORMAT(5X,'*S.S. CALC(1) OR RETURN(2)',/)
98  FORMAT(I3)
100 WRITE(NS,102)
102  FORMAT(5X,'second reactor CALC(1) OR RETURN(2)',/)
    READ(NS,98,ERR=118) ML
    GO TO (104,118),ML
C   SELECTION OF INPUT PARAMS FOR SECOND REACTOR.
104  WRITE(NS,117)
    CALL RADS(TCI,1)
    TCI=TCI+273.1
    WRITE(NS,106)
106  FORMAT(4X,'change of PARAMS reactor(2) YES(1) OR NO(2)',/)
    READ(NS,98,ERR=118) MT
    WRITE(NS,98) MT
    IF(MT.EQ.1) GO TO 108
    TI=T+273.1
    FC(LX+1)=FC(LX)
    GO TO 64
108  WRITE(NS,110)
110  FORMAT(5X,' NEW PARAMS: TI oC FC ',/)
112  FORMAT(14X,'CO(1) OR COUNTER(2) CURRENT ',/,16X,
1'FLOW OF COOLING LIQUID?'/)
114  FORMAT(10X,'COUNTER CURRENT FLOW. ONE STREAM ONLY.'/)
116  FORMAT(10X,'CO-CURRENT FLOW. TWO COOLING STREAMS.'/)
117  FORMAT(5X,'INPUT INLET TEMP. OF SECOND JACKET(oC)',/)
    READ(NS,60) TI,FC(LX+1)
    TI=TI+273.1
    GO TO 64
118  RETURN
    END

SUBROUTINE RADS(AOI,NOE)
DIMENSION AOI(10)
SPECIAL COMMON JP
COMMON /JP/ J,IQ,IQ,LX,NS,NC,NP,NB
120  FORMAT(4(E15.5,/)
    READ(NS,120) (AOI(I),I=1,NOE)
    WRITE(NS,120) (AOI(I),I=1,NOE)
    RETURN
    END
C
SUBROUTINE HRGT
C   VALUES FOR HEAT GENERATION AND REMOVAL CURVES
SPECIAL COMMON IBR,ZZ,XT,FX,SV,WX,JP,BZ
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /JP/ JQ,IQ,IQ,LX,NS,NC,NP,NB
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
    WRITE(NS,142)
    IF(LX.EQ.0) WRITE(NS,150)
    IF(LX.EQ.0) RETURN
    IH=0
130  DO 140 IM=1,LX
    WRITE(NS,144)
    READ(NS,146) NST,STL
    DO 138 I=1,NST

```



```

X2=STL*(I-5)
IF(NST.GT.999) GO TO 148
AXT(I,1,IM)=TQ*(1.+X2*G1)-273.1
X1=Y1(IM)/(1.+D1*CE(X2,0.0,G1))
SNI=(SM+BC(IM))
BID=0.0
BIX=0.0
DO 134 IA=1,NC
IF(IA.EQ.1) VIX=Y3(IM)
IF(IA.NE.1) VIX=BIX
BIX=(SM*VIX+BC(IM)*X2)/SNI
BID=BID+BIX
134 CONTINUE
X3=TQ*(1.+BIX*G1)-273.1
AX1(I,1,IM)=(-DEL)*CAO*F*D1*X1*CE(X2,0.0,G1)
AX2(I,1,IM)=R1*CP*F*TQ*G1*((X2-Y2(IM))+BY(IM)/SM)*(SM*X2-BID))
WRITE(NS,136) AX1(I,1,IM),AX2(I,1,IM),AXT(I,1,IM),X1,X2,X3
136 FORMAT(3X,6F10.2)
138 CONTINUE
IH=IH+1
140 NZ(IH)=NST
142 FORMAT(/,10X,'*HEAT GENERATION AND REMOVAL VALUES*',/)
144 FORMAT(/,10X,'STEPS STEPLENGTH',/)
146 FORMAT(I3,F5.3)
RETURN
148 WRITE(NS,152) NST
GO TO 130
150 FORMAT(5X,' NO DATA STORED',/)
152 FORMAT(/,10X,'ERROR IN NSTEP=',A3,/)
END

```

C Forms Jacobian matrix, calculates eigenvalues
C and determines Stability status of steady state.

```

SUBROUTINE JANSS(NM,NN,NAS,NAD)
REAL RR(3),RI(3)
SPECIAL COMMON ZZ,XT,SV,XP,WX,VB,JP,BZ,SK,SD
COMMON /SK/ X(6),E(6,6),S(2,6),Z1(6),AB(3,3)
COMMON /SD/ SA(6,6),B9(6,6),AO(3,3),AM(3,3),RQ(3)
COMMON /ZZ/ TCI,TL,CA,VC(4),FC(4),V1,E1
COMMON /JP/ JQ,IQ,LQ,LX,NS,NI,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
INTEGER I,IA,IN,IFAIL,INTEG(3),NM,NN
DATA IN,IA,IFAIL/2*3,1/
NAD=2
X1=CIS(NM,NN)
X2=TIS(NM,NN)
AM(1,1)=-1.-D1*CE(X2,0.0,G1)
AA1=(1.+G1*X2)**2.
AM(1,2)=-D1*X1*CE(X2,0.0,G1)/AA1
AM(1,3)=0.0
AM(2,1)=B*D1*CE(X2,0.0,G1)
AM(2,2)=-1.-BY(NN)+(B*D1*X1*CE(X2,0.0,G1)/AA1)
AM(2,3)=BY(NN)
AM(3,1)=0.0
AM(3,2)=BC(NN)
AM(3,3)=-1.+BC(NN)
IF(NN.EQ.1) ZS1=S1

```

```

      IF(NN.GE.2) ZS1=S4
      GO TO (8,6,4,2,10),NAS
2     AM(3,1)=-ZS1*(Y3(NN)-TCS(NM,NN))*(CAO/FC(NN))
      GO TO 8
4     AM(3,2)=BC(NN)+ZS1*((Y3(NN)-TCS(NM,NN))*(TQ*G1/FC(NN)))
      GO TO 8
6     AM(3,3)=-1.-BC(NN)+ZS1*((Y3(NN)-TCS(NM,NN))*(TQ*G1/FC(NN)))
      GO TO 8
10    AM(2,1)=0.0
      AM(2,2)=-ZS1
      AM(2,3)=0.0
8     CONTINUE
      DO 155 I=1,IN
      DO 154 J=1,IN
154   AB(I,J)=AM(I,J)
      WRITE(NS,172) (AM(I,JIL),JIL=1,IN)
155   CONTINUE
      CALL F02AFF(AM,IA,IN,RR,RI,INTEG,IFAIL)
      IF(IFAIL.EQ.0) GO TO 156
      WRITE(NS,174) IFAIL
      RETURN
156   WRITE(NS,176)
      WRITE(NS,178) (RR(I),RI(I),I=1,IN)
      DO 158 I=1,IN
      DO 157 JIL=1,IN
157   AM(I,JIL)=AB(I,JIL)
      IF(RR(I).GE.0) NAD=1
158   IF(RR(I).GT.0.) GO TO 166
      DO 160 I=1,IN
160   IF(RI(I).NE.0.) GO TO 162
      WRITE(NS,180)
      RETURN
162   WRITE(NS,184)
      RETURN
164   FORMAT(10X,'*JACOBIAN MATRIX AT S.S.*',/)
166   DO 168 I=1,IN
168   IF(RI(I).NE.0.) GO TO 170
      WRITE(NS,182)
      RETURN
170   WRITE(NS,186)
      RETURN
172   FORMAT(4(3X,F12.4,3X),/)
174   FORMAT(5X,'ERROR IN IFAIL=',I3)
176   FORMAT(5X,'EIGENVALUES OF MATRIX',/)
178   FORMAT(2(7X,E10.2,7X),/)
180   FORMAT(5X,' SYSTEM COMPLETELY STABLE',/)
182   FORMAT(5X,' SYSTEM UNSTABLE',/)
184   FORMAT(5X,' SYSTEM OSCILLATES AND IS STABLE',/)
186   FORMAT(5X,' SYSTEM OSCILLATES AND IS UNSTABLE',/)
      RETURN
      END

```

C Graph plotting subroutines.

```

SUBROUTINE GRAPHS
REAL NAMEIT(4,3)
SPECIAL COMMON MXY,IBR,ZZ,XT,FX,SV,JP,WP,SX
COMMON /MXY/ MX(10),MY(10)
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /WP/ BX(801),BM(801),YI(801)

```

```

COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
COMMON /SX/ AS1(451,2,2),AS2(451,2,2),
1AS3(451,2,2),AST(451,2,2),AS4(451,2,2)
DATA NAMEIT/6HHGNG ,6H ,6H ,6H ,
16HNKWOH ,6H ,6H ,6H ,6HRETURN,
26H ,6H ,6H /,NI/3/
192 CALL SESAME(NAMEIT,NI,I)
GO TO (194,196,201),I
194 CALL HGNG
GO TO 192
196 CALL NKWOH
GO TO 192
201 CALL DEVEND
CLOSE 15
RETURN
END

```

C Calculates Heat Generation and Removal values.

```

SUBROUTINE HGNG
INTEGER *3 MJX(10),MJY(10)
SPECIAL COMMON MXY,IBR,FX,JP,WP
COMMON /MXY/ MX(10),MY(10)
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /WP/ BX(801),BM(801),YI(801)
COMMON /JP/ JQ,IQ,LQ,LX,NS,NC,NP,NB
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
DATA MJX/"[TEMPERATURE K(RTN TANK)]"/
DATA MJY/"[HEAT GEN.&REMOVAL CURVES(KJ)]"/
WRITE(NS,216)
READ(NS,218) IQX
WRITE(NS,222) IH
DO 202 IO=1,IH
202 WRITE(NS,224) IO,NZ(IO)
XX=30.0
YY=XX*(4/3)
NOS=0
CALL FIXT(XM,YM,X,Y,NOS)
DO 204 IX=1,IH
IP=NZ(IX)
DO 204 IM=1,IP
CALL SELECT(IM,1,IX,YI,BM,AXT,AX2,XM,YM,X,Y)
XMS=XM
YMS=YM
XS=X
YS=Y
CALL SELECT(IM,1,IX,BX,BM,AXT,AX1,XM,YM,X,Y)
IF(XMS.LE.XM) XM=XMS
IF(YMS.LE.YM) YM=YMS
IF(XS.GE.X) X=XS
IF(YS.GE.Y) Y=YS
204 CONTINUE
ENCODE(30,206,MX) (MJX(IZ),IZ=1,10)
ENCODE(30,206,MY) (MJY(IZ),IZ=1,10)
206 FORMAT(10A3)
GO TO (208,210),IQX
208 CALL T4010
PP=YY*2.
GO TO 212
210 CALL OPEN

```



```

PP=YY*(3.5)
212 PA=1.4*PP
NIT=1
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
LN=0
DO 220 IX=1,IH
IP=NZ(IX)
DO 214 IM=1,IP
BM(IM)=AXT(IM,1,IX)
BX(IM)=AX1(IM,1,IX)
214 YI(IM)=AX2(IM,1,IX)
LN=LN+1
VS=BM(IP)+0.1*LN
VZ=BX(IP)-0.25*(LN-1)
CALL GRACUR(BM,BX,IP)
CALL GRAMOV(VS,VZ)
CALL CHAINT(LN,2)
216 FORMAT(10X,'INPUT GRAPH OUTPUT. SCREEN(1) OR PAPER(2)',/)
218 FORMAT(I3)
220 CALL GRAPOL(BM,YI,IP)
222 FORMAT(5X,'NUMBER OF PHASES TO BE PLOTTED ',I3,/)
224 FORMAT(5X,'PHASE NUMBER ',I3,' NUMBER OF POINTS ',I3,/)
CALL BIXT(XX,YY,X,Y)
NIT=2
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
RETURN
END

```

C Control routine for transient response subroutines.

```

SUBROUTINE UNCODY
REAL PS(105),SGX(105,4),NAMEIT(4,8)
SPECIAL COMMON IBR,ZZ,XT,FX,SV,XP,WX,VB,JP,BZ
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /JP/ J,IQ,IQ,LX,NS,LZ,NP,NB
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
EXTERNAL MEX,PIDLIN,NONINT,INVART
DATA NAMEIT/6HPHASE ,6HSPACE ,6HCO-CUR,6HRENT(1,
26HPHASE ,6HSPACE ,6HCOUNTE,6HR CT(2,6HCOIL T,
C 26HEMPERA,6HTURE(3,6H) ,6HREACTO,6HR TEMP,
26HEMPERA,6HTURE(3,6H2) ,6HREACTO,6HR TEMP,
C 36HERATUR,6HE(4) ,6HREACTO,6HR CONC,6HENTRAT,
36HERATUR,6HE(23) ,6HREACTO,6HR CONC,6HENTRAT,
46HION(5),6HNON-IN,6HTERACT,6HING (6,6H) ,
56HINVARI,6HANCE C,6HONTROL,6H(7) ,6HRETURN,
66H(8) ,6H ,6H /,NI/8/
NFI=2*(2+LZ)
NIM=4*(1+LZ)
NIT=2*(3+LZ)
C NIT=5+3*LZ
NIY=2
CALL SESAME(NAMEIT,NI,I)
GO TO (230,230,232,234,234,236,242,244),I
C GO TO (230,230,234,234,232,236,242,244),I
230 CALL LINASS(MEX,NFI,SGX,PS,I)

```

```

GO TO 244
232 CALL LINASS(PIDLIN,NIM,SGX,PS,I)
GO TO 244
234 CALL LINASS(PIDLIN,NIT,SGX,PS,I)
GO TO 244
236 CALL LINASS(NONINT,NFI,SGX,PS,I)
GO TO 244
242 CALL LINASS(INVART,NIY,SGX,PS,I)
244 RETURN
END

SUBROUTINE LINASS(BONES,NIS,SGX,PS,NIB)
REAL X,HS,PS(105),SGX(105,4),X1,X2,X3,X21,X22,X23
REAL NAMEIT(4,6),K1,K2,K3,K4,K5,K6,K7
SPECIAL COMMON IBR,ZZ,XT,FX,SV,XP,WX,VB,JP,BZ
COMMON /JP/ J,IQ,LQ,LX,NS,LZ,NP,NB
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /VB/ K1,K2,K3,K4,K5,K6,K7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
INTEGER NIS,M,NF,J,I,LQ,IQ
EXTERNAL BONES
DATA NAMEIT/6HNO CON,6HTROL(1,6H) ,6H ,
16HPROP C,6HONTROL,6H(2) ,6H ,6HP&I CO,
26HNTROL(,6H3) ,6H ,6HP&D CO,6HNTROL(,
36H4) ,6H ,6HP&I&D ,6HCONTRL,6H(5) ,
46H ,6HRETURN,6H(6) ,6H ,6H /
DATA THS,NIX/3.0,6/
246 FORMAT(5X,'INVARIANCE CONTROL',/)
252 CONTINUE
NM=1
CALL BIXT(K1,K2,K3,YIM)
CALL BIXT(K4,K5,K6,K7)
IF(NIB.GE.3) GO TO 254
WRITE(NS,304)
READ(NS,318) J
IF(LX.LT.2.OR.J.GT.LX) GO TO 372
GO TO 300
254 WRITE(NS,306)
READ(NS,318) IQ,J,LQ
IF(J.GT.LX.OR.LX.LT.2) GO TO 372
M=0
NPAX=0
IF(NIB.EQ.7) WRITE(NS,246)
IF(NIB.GE.7) GO TO 296
IF(NIB.EQ.6) WRITE(NS,256)
IF(NIB.EQ.6) GO TO 267
WRITE(NS,366)
WRITE(NS,262)
CALL SESAME(NAMEIT,NIX,IL)
GO TO (260,266,272,276,280,354),IL
256 FORMAT(5X,'NON-INTERACTING CONTROL ON REACTOR ONE',/)
257 FORMAT(5X,'NON-INTERACTING CONTROL ON REACTOR TWO',/)
258 FORMAT(10X,'FOR REACTOR TWO'/)
260 WRITE(NS,264)
262 FORMAT(10X,' FOR REACTOR ONE.'/)

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264 FORMAT(5X,'NO CONTROL ON SYSTEM MANIPULABLES',/)
GO TO 284
266 WRITE(NS,268)
267 CALL BEES(K1)
268 FORMAT(5X,'PROPORTIONAL CONTROL APPLIED TO SYSTEM',/)
GO TO 284
272 WRITE(NS,274)
CALL BEES(K1)
K2=K1/THS
274 FORMAT(5X,'PROPORTIONAL PLUS INTERGRAL CONTROL',/)
GO TO 284
276 WRITE(NS,278)
CALL BEES(K1)
K3=K1*THS
278 FORMAT(5X,'PROPORTIONAL PLUS DIFFERENTIAL CONTROL',/)
GO TO 284
280 WRITE(NS,282)
CALL BEES(K1)
K3=K1*THS
K2=K1/THS
282 FORMAT(5X,'PROPORTIONAL PLUS INTERGRAL PLUS DIFFERENTIAL'
1' CONTROL',/)
284 CONTINUE
WRITE(NS,366)
WRITE(NS,258)
IF(NIB.EQ.6) WRITE(NS,257)
IF(NIB.EQ.6) GO TO 289
CALL SESAME(NAMEIT,NIX,IC)
GO TO (286,288,290,292,294,354),IC
286 WRITE(NS,264)
GO TO 296
288 WRITE(NS,268)
289 CALL BEES(K4)
GO TO 296
290 WRITE(NS,274)
CALL BEES(K4)
K5=K4/THS
GO TO 296
292 WRITE(NS,278)
CALL BEES(K4)
K6=K4*THS
GO TO 296
294 WRITE(NS,282)
CALL BEES(K4)
K6=K4*THS
K5=K4/THS
296 WRITE(NS,141)
IF(NIB.LE.2.OR.NIB.GE.7.OR.K1.EQ.0.0.AND.K4.EQ.0.0) NAT=1
IF(NIB.EQ.3.AND.K1.NE.0.0.OR.NIB.EQ.3.AND.K4.NE.0.0) NAT=2
IF(NIB.EQ.4.AND.K1.NE.0.0.OR.NIB.EQ.4.AND.K4.NE.0.0) NAT=3
IF(NIB.EQ.5.AND.K1.NE.0.0.OR.NIB.EQ.5.AND.K4.NE.0.0) NAT=4
IF(NIB.EQ.6.AND.K1.NE.0.0.OR.NIB.EQ.6.AND.K4.NE.0.0) NAT=5
READ(NS,318,ERR=354) IBS,LBS
CALL JANS( IBS,LBS,NAT,NAD)
IF(NAD.EQ.2) WRITE(NS,143)
IF(NAD.EQ.2) READ(NS,318,ERR=354) NOKE
IF(NAD.EQ.2.AND.NOKE.EQ.1) CALL LYAPON( IBS,LBS,NAT)
CALL BIXT(PVS(1),PVS(2),PVS(3),PVS(4))
CALL BIXT(PX1,PX2,PVS(5),PVS(6))
LS=10
IY=10
298 WRITE(NS,371)

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READ(NS,318,ERR=354) ITT
IF(ITT.EQ.3) GO TO 252
IF(IY.NE.2) GO TO 300
WRITE(NS,362)
READ(NS,318,ERR=354) LS
IF(LS.EQ.2) GO TO 332
300 WRITE(NS,302)
WRITE(NS,308)
302 FORMAT(5X,'INPUT INITIAL CONDITIONS',)
304 FORMAT(5X,'STAGE NUMBER(J) ONLY ',)
141 FORMAT(5X,'S.S. NO(IQ) & STAGE NO(J)')
143 FORMAT(5X,'CALCULATE LYAPONUV S FUNCTION. YES(1) OR NO(2)?')
306 FORMAT(5X,'S.S(1 2 3) STAGE NO (2 3 4)AND S.S(1 2 3) ')
308 FORMAT(5X,'TIME(SECS) STEPLT(SECS)[4F8.4]')
310 FORMAT(5X,' Ca(Kg/m3) TEMP(OC) TEMP(OC) ')
311 FORMAT(5X,'Initial Peturbation of System',)
312 FORMAT(5X,'Ca2(Kg/m3) TEMP(OC) TEMP(OC) ')
DO 314 NK=1,LZ
PS(2+NK)=Y3(1)
PS(LZ+4+NK)=Y3(J)
314 CONTINUE
315 FORMAT(5X,'TEMPERATURE OF REACTOR AND JACKET OC',)
READ(NS,316) STIME,HS
HS=HS/TH
316 FORMAT(4(F8.4))
318 FORMAT(3I3)
IF(NIB.GE.3.AND.NIB.LE.6) GO TO 297
WRITE(NS,299)
READ(NS,318) NF,NNF
WRITE(NS,368) NF,NNF
IF(NIB.GT.6) GO TO 324
GO TO 317
297 WRITE(NS,320)
299 FORMAT(5X,'Number of Steps & Plot Step[max 999,8]',)
320 FORMAT(5X,'Number of Steps & Plot Step[max 999,8]',/,
1' & type of disturbance.PETURBATION(1)',/,
2' or STEP(2) or BOTH(3)',)
322 FORMAT(5X,'Ca(Kg/m3) TEMP(OC) TEMP1(OC) TEMP2(OC) ')
READ(NS,318) NF,NNF,LXD
WRITE(NS,368) NF,NNF,LXD
IF(NIB.GE.3.AND.LXD.EQ.2) GO TO 324
IF(LXD.NE.2) WRITE(NS,311)
317 WRITE(NS,310)
READ(NS,316)SX1,SX2,SX3
X1=SX1/CAO
X2=(SX2-TQ+273.1)/(TQ*G1)
X3=(SX3-TQ+273.1)/(TQ*G1)
WRITE(NS,312)
READ(NS,316) SX21,SX22,SX23
X21=SX21/CAO
X22=(SX22-TQ+273.1)/(TQ*G1)
X23=(SX23-TQ+273.1)/(TQ*G1)
975 PS(1)=X1
PS(2)=X2
DO 323 NK=1,LZ
PS(2+NK)=X3
PS(4+LZ+NK)=X23
IF(NIB.EQ.2) PS(LZ+4+NK)=Y3(1)
323 CONTINUE
PS(LZ+3)=X21
PS(LZ+4)=X22
IF(NIB.LE.2) GO TO 108
IF(LXD.EQ.2) GO TO 324

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GO TO (321,321,303,305,305,321,324),NIB
303 PS(3+2*LZ)=X21
    PS(4+2*LZ)=X22
    DO 309 NK=1,LZ
309 PS(4+2*LZ+NK)=X23
    GO TO 321
305 PS(4+LZ)=X21
    PS(5+LZ)=X22
    DO 307 NK=1,LZ
307 PS(5+LZ+NK)=X23
321 IF(LXD.EQ.3) GO TO 998
108 CONTINUE
    WRITE(NS,326)
    GO TO 330
324 DO 325 NK=1,NIS
325 PS(NK)=0.0
998 CALL BIXT(FV(1),FV(2),XVP1,XVP2)
313 WRITE(NS,322)
    READ(NS,316) (PY(IU),IU=1,4)
    PY(1)=PY(1)/CAO
    PY(2)=PY(2)/(TQ*G1)
    PY(3)=PY(3)/(TQ*G1)
    PY(4)=PY(4)/(TQ*G1)
    WRITE(NS,316) (PY(IU),IU=1,4)
319 WRITE(NS,376)
326 FORMAT(1X,' TIME      X1      X2      X3      X21      X22      X23 '/')
327 FORMAT(F7.3,4(E15.6))
328 FORMAT(F8.2,9(F7.3))
330 X=STIME/TH
    XTH=X*TH
C   WRITE(NS,328) (PS(2+JH),JH=1,LZ)
C   WRITE(NS,328) (PS(4+LZ+JH),JH=1,LZ)
    IF(NIB.LE.2) WRITE(NS,328) XTH,X1,X2,X3,X21,X22,X23
    IF(NIB.EQ.3) WRITE(NS,328) XTH,PS(1),PS(2),PS(2+LZ)
    1,FC(1),(PS(2*LZ+2+ML),ML=1,2),PS(4+3*LZ),FC(J)
    IF(NIB.EQ.4.OR.NIB.EQ.5) WRITE(NS,328) XTH,PS(1),PS(2)
    1,PS(2+LZ),FC(1),(PS(3+LZ+ML),ML=1,2),PS(5+2*LZ),FC(J)
    IF(NIB.EQ.6) WRITE(NS,328) XTH,PS(1),PS(2),PS(2+LZ)
    1,FC(1),PS(3+LZ),PS(4+LZ),PS(4+2*LZ),FC(J)
    IF(NIB.EQ.7) WRITE(NS,378) XTH,PS(1),PS(2),FC(1),FC(J)
    IF(NF.GT.999) GO TO 352
332 M=M+1
    IF(M.GT.8) GO TO 356
    NAFF=0
    DO 346 I=1,NF
    CALL D0INT(X,PS,NIS,HS,SGX,BONES,NIB)
C   WRITE(NS,328) (PS(2+JH),JH=1,LZ)
C   WRITE(NS,328) (PS(4+LZ+JH),JH=1,LZ)
    XTH=X*TH
    GO TO (999,999,333,334,336,337,331),NIB
999 IF(ITT.EQ.1) WRITE(NS,328) XTH,(PS(LI),LI=1,2),PS(2+LZ)
    1,(PS(2+LZ+LI),LI=1,2),PS(4+2*LZ)
    GO TO 340
331 PZ1=PS(1)
    PZ2=PS(2)
    CALL NEFC(PZ1,PZ2,LS)
    PX1=PV(1)
    PX2=PV(2)
    CALL MOAD(X,HS,PX1,PX2,H3,H4,3)
    IF(ITT.EQ.1) WRITE(NS,378) XTH,PS(1),PS(2),H3,H4
    GO TO 340

```

```

333 DO 335 LI=1,LZ
    PS(2+LI)=PS(2+LI)
335 PS(4+2*LZ+LI)=PS(4+2*LZ+LI)
    PX1=((K1*PS(2+LZ)+K2*TH*PS(2+2*LZ)+K3*PV(1)/TH)*TQ*G1)
    PX2=((K4*PS(4+3*LZ)+K5*TH*PS(4+4*LZ)+K6*PV(2)/TH)*TQ*G1)
C   PX2=((K4*(PS(2)+PS(4+3*LZ))+K5*TH*PS(4+4*LZ)+K6*PV(2)/TH)*TQ*G1)
    CALL MOAD(X,HS,PS(2),PS(2*LZ+4),H5,H6,1)
    CALL MOAD(X,HS,PS(2+LZ),PS(3*LZ+4),H7,H8,2)
    CALL MOAD(X,HS,PX1,PX2,H3,H4,3)
    IF(ITT.EQ.1) WRITE(NS,328) XTH,PS(1),H5,H7,H3,PS(2*LZ+3)
    1,H6,H8,H4
    GO TO 340
334 DO 301 LI=1,LZ
    PS(2+LI)=PS(2+LI)
301 PS(5+LZ+LI)=PS(5+LZ+LI)
    PX1=((K1*PS(2)+K2*TH*PS(3+LZ)+K3*PV(1)/TH)*TQ*G1)
    PX2=((K4*PS(5+LZ)+K5*TH*PS(6+2*LZ)+K6*PV(2)/TH)*TQ*G1)
C   PX2=((K4*(PS(2+LZ)+PS(5+LZ))+K5*TH*PS(6+2*LZ)+K6*PV(2)/TH)*TQ*G1)
    GO TO 338
336 DO 329 LI=1,LZ
    PS(2+LI)=PS(2+LI)
329 PS(5+LZ+LI)=PS(5+LZ+LI)
    PX1=((K1*PS(1)+K2*TH*PS(3+LZ)+K3*PV(1)/TH)*CAO)
    PX2=((K4*PS(4+LZ)+K5*TH*PS(6+2*LZ)+K6*PV(2)/TH)*CAO)
C   PX2=((K4*(PS(1)+PS(4+LZ))+K5*TH*PS(6+2*LZ)+K6*PV(2)/TH)*CAO)
338 CALL MOAD(X,HS,PS(2),PS(5+LZ),H5,H6,1)
    CALL MOAD(X,HS,PS(2+LZ),PS(5+2*LZ),H7,H8,2)
    CALL MOAD(X,HS,PX1,PX2,H3,H4,3)
    IF(ITT.EQ.1) WRITE(NS,328) XTH,PS(1),H5,H7,H3,PS(4+LZ)
    1,H6,H8,H4
    GO TO 340
20 CONTINUE
337 PX1=((TK(1)/TH)*QB(SM,BY(1),K1,TV(2),B,D1,TV(1),PS(1),
1CIS(IQ,1),G1,PS(2),TIS(IQ,1))-(BY(1)/SM)*(SM*PS(2)
2-QA(SM,BY(1),K1,PS(2),B,D1,PS(1),CIS(IQ,1),TIS(IQ,1)
3,G1))+PS(2+LZ)-PY(3))*FC(1)/(Y3(1)+PY(3)-TVS(LZ,IQ,1)
4-PS(2+LZ))
    CALL CHFLCT(PX1,K1,FC(1),KNAD)
    GO TO (20,30,372),KNAD
30 CONTINUE
    PX2=((TK(J)/TH)*QB(SM,BY(J),K4,TV(4),B,D1,TV(3),PS(3+LZ),
1CIS(LQ,J),G1,PS(4+LZ),TIS(LQ,J))-(BY(J)/SM)*(SM*PS(4+LZ)
2-QA(SM,BY(J),K4,PS(4+LZ),B,D1,PS(3+LZ),CIS(LQ,J),TIS(LQ,J)
3,G1))+PS(4+2*LZ)-PY(4))*FC(J)/(Y3(J)+PY(4)-TVS(LZ,LQ,J)
4-PS(4+2*LZ))
    CALL CHFLCT(PX2,K4,FC(J),KNAD)
    GO TO (30,40,372),KNAD
40 CALL MOAD(X,HS,PS(2),PS(4+LZ),H5,H6,1)
    CALL MOAD(X,HS,PS(2+LZ),PS(4+2*LZ),H7,H8,2)
    CALL MOAD(X,HS,PX1,PX2,H3,H4,3)
    IF(ITT.EQ.1) WRITE(NS,328) XTH,PS(1),H5,H7,H3,PS(3+LZ)
    1,H6,H8,H4
340 IF(NPAX.EQ.NNF) NPAX=0
    NPAX=NPAX+1
    IF(NPAX.NE.9) GO TO 345
    NAFF=NAFF+1
    AXT(NAFF,1,M)=X*TH
    AXT(NAFF,2,M)=X*TH
    IF(NIB.GT.2) GO TO 341
    AX1(NAFF,1,M)=CAO*PS(1)
    AX2(NAFF,1,M)=TQ*(1.+G1*H5)-273.1
    AX3(NAFF,1,M)=TQ*(1.+G1*H7)-273.1

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AX1(NAFP,2,M)=CAO*PS(3+LZ)
AX2(NAFP,2,M)=TQ*(1.+G1*H6)-273.1
AX3(NAFP,2,M)=TQ*(1.+G1*H8)-273.1
IF(NIB.LE.2) GO TO 345
341 AX1(NAFP,1,M)=CAO*(PS(1)+CIS(IQ,1))
AX2(NAFP,1,M)=TQ*(1.+G1*(H5+TIS(IQ,1)))-273.1
AX3(NAFP,1,M)=TQ*(1.+G1*(H7+TCS(IQ,1)))-273.1
AX4(NAFP,1,M)=H3+FC(1)
AX4(NAFP,2,M)=H4+FC(J)
GO TO (340,340,342,399,399,343,344),NIB
399 AX1(NAFP,2,M)=CAO*(PS(4+LZ)+CIS(LQ,J))
GO TO 111
342 AX1(NAFP,2,M)=CAO*(PS(3+2*LZ)+CIS(LQ,J))
GO TO 111
343 AX1(NAFP,2,M)=CAO*(PS(3+LZ)+CIS(LQ,J))
111 AX2(NAFP,2,M)=TQ*(1.+G1*(H6+TIS(LQ,J)))-273.1
AX3(NAFP,2,M)=TQ*(1.+G1*(H8+TCS(LQ,J)))-273.1
GO TO 345
344 AX1(NAFP,1,M)=CAO*(PS(1)+CIS(IQ,1))
AX2(NAFP,1,M)=TQ*(1.+G1*TIS(IQ,1))-273.1
AX3(NAFP,1,M)=TQ*(1.+G1*TVS(LZ,IQ,1))-273.1
AX1(NAFP,2,M)=CAO*(PS(2)+CIS(LQ,J))
AX2(NAFP,2,M)=TQ*(1.+G1*TIS(LQ,J))-273.1
AX3(NAFP,2,M)=TQ*(1.+G1*TVS(LZ,LQ,J))-273.1
AX4(NAFP,1,M)=H3
AX4(NAFP,2,M)=H4
345 CONTINUE
347 CONTINUE
346 CONTINUE
MH(M,1)=NAFP
MH(M,J)=NAFP
WRITE(NS,368) M,NAFP
WRITE(NS,374)
READ(NS,318,ERR=354) INK
IF(INK.EQ.2) M=M-1
348 WRITE(NS,364)
READ(NS,318,ERR=354) IY
IF(IY.EQ.2.OR.IY.EQ.3) NZ(1)=M
IF(IY.EQ.2.OR.IY.EQ.3) NZ(J)=M
WRITE(NS,368) IY,M
GO TO (252,298,354),IY
350 CONTINUE
352 WRITE(NS,370) NF
354 RETURN
356 WRITE(NS,358)
358 FORMAT(5X,'STORE FULL FOR THIS PHASE',)
360 FORMAT(5X,'GONE INTO UNCHARTED SPACE.SYSTEM UNDEFINED',)
IF(J.LT.LX) GO TO 348
RETURN
362 FORMAT(5X,'NEW(1) OR OLD(2) INITIAL VALUES?',)
364 FORMAT(5X,'CONT(1) OR NLINE(2) OR RET(3)?',)
366 FORMAT(/,10X,'NEW PHASE',)
368 FORMAT(1X,I3,2X,I3,1X,I3)
370 FORMAT(5X,'TOO MANY STEPS',2X,'NF=',I3,)
371 FORMAT(5X,'PRINT RESULTS: YES(1) OR NO(2) OR REPEAT S.S.(3)?')
372 WRITE(NS,360)
RETURN
374 FORMAT(5X,'STORE(1) OR DISCARD(2) LINE?')
376 FORMAT(1X,' TIME X1 X2 X3 FC X21 X22 '
1' X23 FC'/)
378 FORMAT(F8.2,2(F7.3),2(E15.6))
END

```

```

SUBROUTINE CHFLCT(P1X,SKI,P1,KNAD)
SPECIAL COMMON JP
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
IF(ABS(P1X-P1).GT.0.18E-03.AND .SKI.NE.0.0) KNAD=1
IF(ABS(P1X-P1).LT.0.18E-03) KNAD=2
IF(ABS(P1X-P1).GT.0.18E-03.AND.SKI.EQ.0.0) KNAD=3
GO TO (10,30,20),KNAD
10 SKI=SKI*0.9
WRITE(NS,15) KNAD,SKI,P1X
15 FORMAT(5X,I3,2F15.9,'WATER NEED EXCEEDS SUPPLY.')
```

GO TO 30

```

20 WRITE(NS,25) KNAD,SKI,P1X
25 FORMAT(5X,I3,2F15.9,'BEYOND CONTROL')
```

30 RETURN

END

```

REAL FUNCTION CE(CE1,CE2,CE3)
CE=EXP((CE1+CE2)/(1.+CE3*(CE1+CE2)))
END
```

```

REAL FUNCTION QA(QA1,QA2,QA3,QA4,QA5,QA6,QA7,QA8,QA9,QA10)
QA=(QA1/QA2)*((1.+QA2-QA3)*QA4-QA5*QA6*((QA7+QA8)*CE(
1QA4,QA9,QA10)-QA8*CE(QA9,0.0,QA10)))
END
```

```

REAL FUNCTION QB(QB1,QB2,QB3,QB4,QB5,QB6,QB7,QB8,QB9
1,QB10,QB11,QB12)
QB=(QB1/QB2)*((1.+QB2-QB3)*QB4-QB5*QB6*(QB7+((QB8+QB9)/((1
1.+QB10*(QB11+QB12))**2.))*QB4)*CE(QB11,QB12,QB10))
END
```

```

SUBROUTINE MOAD(X,HS,H1,H2,SH3,SH4,I)
REAL PA(2),SGB(2,4),HS
SPECIAL COMMON SV,BZ
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
EXTERNAL COFC
X=X-HS
PA(1)=H1
PA(2)=H2
CALL D0INT(X,PA,2,HS,SGB,COFC,I)
SH3=PA(1)
SH4=PA(2)
GO TO(10,20,30),I
10 PVS(1)=PA(1)
PVS(2)=PA(2)
GO TO 40
20 PVS(3)=PA(1)
PVS(4)=PA(2)
GO TO 40
30 PVS(5)=PA(1)
PVS(6)=PA(2)
40 RETURN
END
```

```

SUBROUTINE BEES(SL)
SPECIAL COMMON JP
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
256 FORMAT(2X,F15.12/)
270 FORMAT(10X,' K1CTC[F15.12]positive',)
WRITE(NS,270)
READ(NS,256) SL
```

```

WRITE(NS,256) SL
RETURN
END

```

```

SUBROUTINE COFC(PAT,PA,X,IOE)
REAL PAT(2),PA(2),X
SPECIAL COMMON SV,BZ
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
GO TO (10,20,30),IOE
10 TIM=1.0/TH
PAT(1)=(PA(1)-PVS(1))/TIM
PAT(2)=(PA(2)-PVS(2))/TIM
GO TO 40
20 TIM=2.0/TH
PAT(1)=(PA(1)-PVS(3))/TIM
PAT(2)=(PA(2)-PVS(4))/TIM
GO TO 40
30 TIM=2.0/TH
PAT(1)=(PA(1)-PVS(5))/TIM
PAT(2)=(PA(2)-PVS(6))/TIM
40 RETURN
END

```

```

SUBROUTINE MEX(PT,PS,X,MP)
C This Subroutine Integrates the equations
C describing the Dynamic state of system
REAL PT(105),PS(105),X
SPECIAL COMMON ZZ,XT,SV,JP,BZ
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
TV(1)=0.0
TV(J)=0.0
PT(1)=Y1(1)-PS(1)-D1*PS(1)*CE(PS(2),0.0,G1)
DO 226 I=1,NC
226 TV(1)=TV(1)+PS(I+2)
FYE=Y2(1)-PS(2)-(BY(1)/SM)*(SM*PS(2)-TV(1))
PT(2)=FYE+B*D1*PS(1)*CE(PS(2),0.0,G1)
IF(MP.EQ.1) SAY=(Y3(1)-PS(3))
IF(MP.EQ.2) SAY=(PS(2*NC+4)-PS(3))
PT(3)=(SAY+(BC(1)/SM)*(PS(2)-PS(3)))*SM*TH/(TK(1))
DO 10 II=1,NC-1
I=II+3
10 PT(I)=((PS(I-1)-PS(I))+(BC(1)/SM)*(PS(2)
1-PS(I)))*SM*TH/(TK(1))
PT(NC+3)=(PS(1)-PS(NC+3))-D1*PS(NC+3)*CE(PS(NC+4),0.0,G1)
DO 228 I=1,NC
228 TV(J)=TV(J)+PS(NC+4+I)
ZYE=PS(2)-PS(NC+4)-(BY(J)/SM)*(SM*PS(NC+4)-TV(J))
PT(NC+4)=ZYE+B*D1*PS(NC+3)*CE(PS(NC+4),0.0,G1)
IF(MP.EQ.1) S1Y=(Y3(J)-PS(NC+5))
IF(MP.EQ.2) S1Y=(Y3(1)-PS(NC+5))
PT(NC+5)=(S1Y+(BC(J)/SM)*(PS(NC+4)-PS(NC+5)))*SM*TH/(TK(J))
DO 20 I=1,NC-1
20 PT(NC+5+I)=((PS(NC+4+I)-PS(NC+5+I))+(BC(J)/SM)*(
1PS(4+NC)-PS(NC+5+I)))*SM*TH/(TK(J))
RETURN
END

```



```

SUBROUTINE PODLIN(PT,PS,X,MP)
C   MP=9: Reactor Temp. as controlled variable
C   in reactor one & coil temp. in reactor two.
C   MP=10: Cooling coil temp. as controlled variable
C   in reactor one & reator temp. in reactor two.
REAL PT(105),PS(105),X,SP
SPECIAL COMMON ZZ,XT,SV,XP,WX,VB,JP,BZ
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /JP/ J,IQ,LQ,LX,NS,NI,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /VB/ S1,S2,S3,S4,S5,S6
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
10  CONTINUE
    CALL BIXT(TV(1),TV(2),TV(3),TV(4))
    FQ=TIS(IQ,1)
    FM=CIS(IQ,1)
    ZQ=TIS(LQ,J)
    ZM=CIS(LQ,J)
    FW=PS(2)+FQ
    ZW=PS(NI+5)+ZQ
    IF(MP.EQ.3) ZW=PS(4+2*NI)+ZQ
    PT(1)=PY(1)-PS(1)-D1*((PS(1)+FM)*CE(FW,0.0,G1)-FM*CE(FQ,0.0,G1))
    DO 20 I=1,NI
20  TV(1)=TV(1)+PS(I+2)
    PT(2)=PY(2)-PS(2)+B*D1*((PS(1)+FM)*CE(FW,0.0,G1)-FM*CE(FQ,0.0,G1))
    1-(BY(1)/SM)*(SM*PS(2)-TV(1))
    IF(MP.EQ.4) GO TO 378
    AX1=(Y3(1)+PY(3)-TVS(1,IQ,1)-PS(3))
    PT(3)=(((BC(1)/SM)*(PS(2)-PS(3)))+(PY(3)-PS(3))
    1+((S1*PS(3)+S2*TH*PS(3+NI))*AX1*TQ*(G1/FC(1))))
    2*SM*TH*(FC(1)/G1))/((VC(1)/G1)-S3*TQ*SM*AX1))
    DO 30 I=1,NI-1
    AX1=(TVS(I,IQ,1)+PS(I+2)-TVS(I+1,IQ,1)-PS(I+3))
    PT(3+I)=(((BC(1)/SM)*(PS(2)-PS(I+3)))+(PS(I+2)-PS(I+3)
    1))+((S1*PS(I+3)+S2*TH*PS(3+NI+I))*AX1*TQ*(G1/FC(1))))
    2*SM*TH*(FC(1)/G1))/((VC(1)/G1)-S3*TQ*SM*AX1))
30  CONTINUE
    DO 40 I=1,NI
    PT(2+NI+I)=PS(2+I)
40  CONTINUE
    PV(1)=PT(2+NI)
384 PT(3+2*NI)=(PS(1)-PS(3+2*NI))-D1*((PS(3+2*NI)+ZM)*
    1CE(ZW,0.0,G1)-ZM*CE(ZQ,0.0,G1))
    DO 85 I=1,NI
85  TV(J)=TV(J)+PS(4+2*NI+I)
    PT(4+2*NI)=(PS(2)-PS(4+2*NI))+B*D1*((PS(3+2*NI)+ZM)*CE
    1(ZW,0.0,G1)-ZM*CE(ZQ,0.0,G1))-(BY(J)/SM)*(SM*PS(4+2*NI)-TV(J))
    AX1=(Y3(J)+PY(4)-TVS(1,LQ,J)-PS(5+2*NI))
    AX=(S4*PS(4+2*NI)+S5*TH*PS(5+3*NI)+S6*(PT(4
    C   AX=(S4*(PS(2)+PS(4+2*NI))+S5*TH*PS(5+3*NI)+S6*(PT(4
    1+2*NI)/TH))*TQ*G1/FC(J)
    PT(5+2*NI)=((BC(J)/SM)*(PS(4+2*NI)-PS(5+2*NI)))+(PY(4)
    1-PS(5+2*NI))+(AX*AX1))*SM*(TH/(TK(1)))
    DO 90 I=1,NI-1
    AX1=(TVS(I,LQ,J)+PS(4+2*NI+I)-TVS(I+1,LQ,J)-PS(5+2*NI+I))
    PT(5+2*NI+I)=((BC(J)/SM)*(PS(4+2*NI)-PS(5+2*NI+I)))+(PS(5+
    1NI+I)-PS(5+2*NI+I))+(AX*AX1))*SM*(TH/(TK(J)))
90  CONTINUE
    PT(5+3*NI)=PS(4+2*NI)

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```

PV(2)=PT(4+2*NI)
GO TO 388
378 AX=(S1*PS(2)+S2*TH*PS(3+NI)+S3*(PT(2)/TH))
1*TQ*G1/FC(1)
PT(3)=((BC(1)/SM)*(PS(2)-PS(3)))+(PY(3)-PS(3))+(A
1X*(Y3(1)+PY(3)-TVS(1,IQ,1)-PS(3))) *SM*(TH/(TK(1)))
DO 50 I=1,NI-1
PT(3+I)=((BC(1)/SM)*(PS(2)-PS(3+I)))+(PS(I+2)-PS(I+3)
1)+AX*(TVS(I,IQ,1)+PS(2+I)-TVS(I+1,IQ,1)-PS(3+
2I)) *SM*(TH/(TK(1)))
50 CONTINUE
PT(3+NI)=PS(2)
PV(1)=PT(2)
PT(4+NI)=(PS(1)-PS(4+NI))-D1*((PS(4+NI)+ZM)
1*CE(ZW,0.0,G1)-ZM*CE(ZQ,0.0,G1))
DO 60 I=1,NI
60 TV(J)=TV(J)+PS(I+4+2*NI)
PT(5+NI)=(PS(2)-PS(5+NI))+B*D1*((PS(4+NI)+ZM)
1*CE(ZW,0.0,G1)-ZM*CE(ZQ,0.0,G1))-(BY(J)/SM)*(SM*PS(5+NI)-TV(J))
AX=(S4*PS(6+NI)+S5*TH*PS(5+3*NI))
C AX=(S4*(PS(3)+PS(6+NI))+S5*TH*PS(5+3*NI))
AX1=(Y3(J)+PY(4)-TVS(1,LQ,J)-PS(6+NI))
PT(6+NI)=(((BC(J)/SM)*(PS(5+NI)-PS(6+NI))
1+(PY(4)-PS(6+NI)))+(AX1*AX*TQ*(G1/FC(J))))*
2SM*TH*(FC(J)/G1)/((VC(J)/G1)-S6*TQ*SM*AX1)
DO 70 I=1,NI-1
AX1=(TVS(I,LQ,J)+PS(5+NI+I)-TVS(I+1,LQ,J)-PS
1(6+NI+I))
AX=(S4*PS(6+NI+I)+S5*TH*PS(5+3*NI+I))
C AX=(S4*(PS(3+I)+PS(6+NI+I))+S5*TH*PS(5+3*NI+I))
PT(6+NI+I)=(((BC(J)/SM)*(PS(5+NI)-PS(6+NI+I))
1+(PS(5+NI+I)-PS(6+NI+I)))+(AX*AX1*TQ*(G1/FC(J))))*
2SM*TH*(FC(J)/G1)/((VC(J)/G1)-S6*TQ*SM*AX1)
70 CONTINUE
DO 80 I=1,NI
80 PT(5+2*NI+I)=PS(5+NI+I)
PV(2)=PT(5+2*NI)
388 RETURN
END

```

```

SUBROUTINE PIDLIN(PT,PS,X,MP)
C Program describing Dynamic state of
C Perturbed system near steady state value
C and controlled using cooling liquid flow.
C MP=3: Coil Temp. being controlled variable.
C MP=4: Reactor Temp. as controlled variable.
C MP=5: Reactor conc. as controlled variable.
REAL PT(105),PS(105),X,FQ,FM,ZQ,ZM,FW,ZW
SPECIAL COMMON ZZ,XT,SV,XP,WX,VB,JP,BZ
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /JP/ J,IQ,LQ,LX,NS,NI,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
CALL BIXT(TV(1),TV(2),TV(3),TV(4))
FQ=TIS(IQ,1)
FM=CIS(IQ,1)
ZQ=TIS(LQ,J)
ZM=CIS(LQ,J)

```

```

FW=PS(2)+FQ
ZW=PS(NI+5)+ZQ
IF(MP.EQ.3) ZW=PS(4+2*NI)+ZQ
PT(1)=PY(1)-PS(1)-D1*((PS(1)+FM)*CE(FW,0.0,G1)-FM*CE(FQ,0.0,G1))
DO 20 I=1,NI
20 TV(1)=TV(1)+PS(I+2)
PT(2)=PY(2)-PS(2)+B*D1*((PS(1)+FM)*CE(FW,0.0,G1)-FM*CE(FQ,0.0,G1))
1-(BY(1)/SM)*(SM*PS(2)-TV(1))
IF(MP.EQ.4.OR.MP.EQ.5) GO TO 378
AX1=(Y3(1)+PY(3)-TVS(1,IQ,1)-PS(3))
C AX1=(PS(4+3*NI)-TVS(1,IQ,1)-PS(3))
PT(3)=(((BC(1)/SM)*(PS(2)-PS(3))+(PY(3)-PS(3))
1-(-(S1*PS(3)+S2*TH*PS(3+NI))*AX1*TQ*(G1/FC(1))))
2*SM*TH*(FC(1)/G1))/((VC(1)/G1)-S3*TQ*SM*AX1))
DO 30 I=1,NI-1
AX1=(TVS(I,IQ,1)+PS(I+2)-TVS(I+1,IQ,1)-PS(I+3))
PT(3+I)=(((BC(1)/SM)*(PS(2)-PS(I+3))+(PS(I+2)-PS(I+3)
1))-(-(S1*PS(I+3)+S2*TH*PS(3+NI+I))*AX1*TQ*(G1/FC(1))))
2*SM*TH*(FC(1)/G1))/((VC(1)/G1)-S3*TQ*SM*AX1))
30 CONTINUE
DO 40 I=1,NI
PT(2+NI+I)=PS(2+I)
40 CONTINUE
PV(1)=PT(2+NI)
GO TO 382
378 IF(MP.EQ.3.OR.MP.EQ.5) GO TO 380
AX=(S1*PS(2)+S2*TH*PS(3+NI)+S3*(PT(2)/TH))
1*TQ*G1/FC(1)
GO TO 381
380 IF(MP.EQ.3.OR.MP.EQ.4) GO TO 382
AX=(S1*PS(1)+S2*TH*PS(3+NI)+S3*(PT(1)/TH))
1*CAO/FC(1)
381 PT(3)=((BC(1)/SM)*(PS(2)-PS(3))+(PY(3)-PS(3))+(A
1X*(Y3(1)+PY(3)-TVS(1,IQ,1)-PS(3))))*SM*(TH/(TK(1)))
C 1X*(PS(5+2*NI)-TVS(1,IQ,1)-PS(3))))*SM*(TH/(TK(1)))
DO 50 I=1,NI-1
PT(3+I)=((BC(1)/SM)*(PS(2)-PS(3+I))+(PS(I+2)-PS(I+3)
1)+AX*(TVS(I,IQ,1)+PS(2+I)-TVS(I+1,IQ,1)-PS(3+
2I)))*SM*(TH/(TK(1)))
50 CONTINUE
IF(MP.EQ.4) PT(3+NI)=PS(2)
IF(MP.EQ.5) PT(3+NI)=PS(1)
IF(MP.EQ.4) PV(1)=PT(2)
IF(MP.EQ.5) PV(1)=PT(1)
382 IF(MP.EQ.4.OR.MP.EQ.5) GO TO 384
PT(3+2*NI)=(PS(1)-PS(3+2*NI))-D1*((PS(3+2*NI)+ZM)
1*CE(ZW,0.0,G1)-ZM*CE(ZQ,0.0,G1))
DO 60 I=1,NI
60 TV(J)=TV(J)+PS(I+4+2*NI)
PT(4+2*NI)=(PS(2)-PS(4+2*NI))+B*D1*((PS(3+2*NI)+ZM)
1*CE(ZW,0.0,G1)-ZM*CE(ZQ,0.0,G1))-(BY(J)/SM)*(SM*PS(4+2*NI)-TV(J))
C AX=(S4*(PS(2)+PS(5+2*NI))+S5*TH*PS(5+3*NI))
AX=(S4*PS(5+2*NI)+S5*TH*PS(5+3*NI))
AX1=(Y3(J)+PY(4)-TVS(1,LQ,J)-PS(5+2*NI))
PT(5+2*NI)=(((BC(J)/SM)*(PS(4+2*NI)-PS(5+2*NI))
1+(PY(4)-PS(5+2*NI)))+(AX1*AX*TQ*(G1/FC(J))))*
2SM*TH*(FC(J)/G1))/((VC(J)/G1)-S6*TQ*SM*AX1))
DO 70 I=1,NI-1
AX1=(TVS(I,LQ,J)+PS(4+2*NI+I)-TVS(I+1,LQ,J)-PS
1(5+2*NI+I))
C AX=(S4*(PS(2)+PS(5+2*NI+I))+S5*TH*PS(5+3*NI+I))
AX=(S4*PS(5+2*NI+I)+S5*TH*PS(5+3*NI+I))

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```

PT(5+2*NI+I)=(((BC(J)/SM)*(PS(4+2*NI)-PS(5+2*NI+I))
1+(PS(4+2*NI+I)-PS(5+2*NI+I)))+(AX*AX1*TQ*(G1/FC(J))))*
2SM*TH*(FC(J)/G1)/((VC(J)/G1)-S6*TQ*SM*AX1))
70 CONTINUE
DO 80 I=1,NI
80 PT(4+3*NI+I)=PS(4+2*NI+I)
PV(2)=PT(4+3*NI)
GO TO 388
384 PT(4+NI)=(PS(1)-PS(4+NI))-D1*((PS(4+NI)+ZM)*CE(ZW,0.0,G1)
1-ZM*CE(ZQ,0.0,G1))
DO 85 I=1,NI
85 TV(J)=TV(J)+PS(5+NI+I)
PT(5+NI)=(PS(2)-PS(5+NI))+B*D1*((PS(4+NI)+ZM)*CE(ZW,0.0,G1)
1-ZM*CE(ZQ,0.0,G1))-(BY(J)/SM)*(SM*PS(5+NI)-TV(J))
AX1=(Y3(J)+PY(4)-TVS(1,LQ,J)-PS(6+NI))
IF(MP.EQ.3.OR.MP.EQ.5) GO TO 386
C AX=(S4*(PS(2+NI)+PS(5+NI))+S5*TH*PS(6+2*NI)+S6*(PT(5+NI)/TH))
AX=(S4*PS(5+NI)+S5*TH*PS(6+2*NI)+S6*(PT(5+NI)/TH))
1*TQ*G1/FC(J)
GO TO 387
386 IF(MP.EQ.3.OR.MP.EQ.4) GO TO 388
C AX=(S4*(PS(1)+PS(4+NI))+S5*TH*PS(6+2*NI)+S6*(PT(4+NI)/TH))
AX=(S4*PS(4+NI)+S5*TH*PS(6+2*NI)+S6*(PT(4+NI)/TH))
1*CAO/FC(J)
387 PT(6+NI)=((BC(J)/SM)*(PS(5+NI)-PS(6+NI)))+(PY(4)
1-PS(6+NI))+(AX*AX1)*SM*(TH/(TK(1)))
DO 90 I=1,NI-1
AX1=(TVS(I,LQ,J)+PS(5+NI+I)-TVS(I+1,LQ,J)-PS(6+NI+I))
PT(6+NI+I)=((BC(J)/SM)*(PS(5+NI)-PS(6+NI+I)))+(PS(5+
1NI+I)-PS(6+NI+I))+(AX*AX1)*SM*(TH/(TK(J)))
90 CONTINUE
IF(MP.EQ.4) PT(6+2*NI)=PS(5+NI)
IF(MP.EQ.5) PT(6+2*NI)=PS(4+NI)
IF(MP.EQ.4) PV(2)=PT(5+NI)
IF(MP.EQ.5) PV(2)=PT(4+NI)
388 RETURN
END

```

```

SUBROUTINE NONINT(PT,PS,X,MP)
C Program describing dynamic state of
C Perturbed system near steady state value
C and controlled using cooling liquid flow.
C MP=6 Non-interacting control on reactor one & two.
REAL PT(105),PS(105),X
SPECIAL COMMON ZZ,XT,SV,XP,WX,VB,JP,BZ
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /JP/ J,IQ,LQ,LX,NS,NI,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
CALL BIXT(TV(1),TV(2),TV(3),TV(4))
SIS=SM*TH/TK(1)
S1S=SM*TH/TK(J)
FM=CIS(IQ,1)
ZM=CIS(LQ,J)
PT(1)=PY(1)-PS(1)-D1*((FM+PS(1))*CE(PS(2),TIS(IQ,1),G1)-FM*
1CE(TIS(IQ,1),0.0,G1))
PT(2)=PY(2)-S1*PS(2)
PT(3)=((BC(1)/SM)*(PS(2)-PS(3)))+(PY(3)-PS(3))*SIS

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```

DO 15 I=2,NI
15 PT(2+I)=((BC(1)/SM)*(PS(2)-PS(2+I))+((PS(1+I)-PS(2+I))))*SIS
TV(1)=PT(1)
TV(2)=PT(2)
PT(3+NI)=PS(1)-PS(3+NI)-D1*((ZM+PS(3+NI))*CE(PS(4+NI),
1TIS(LQ,J),G1)-ZM*CE(TIS(LQ,J),0.0,G1))
PT(4+NI)=PS(2)-S4*PS(4+NI)
PT(5+NI)=((BC(J)/SM)*(PS(4+NI)-PS(5+NI)))+(PY(4)-PS(5+NI))*SIS
DO 25 I=2,NI
25 PT(4+NI+I)=((BC(J)/SM)*(PS(4+NI)-PS(4+NI+I)))+(PS(3+NI+I)-
1PS(4+NI+I))*SIS
TV(3)=PT(3+NI)
TV(4)=PT(4+NI)
RETURN
END

```

```

SUBROUTINE INVART(PT,PS,X,MP)
C Program describing dynamic state of
C perturbed system near steady state value
C and controlled using cooling liquid flow.
C MP=7 Invariant control on reactor one & two.
REAL PT(3),PS(3),X
SPECIAL COMMON XT,SV,XP,JP
COMMON /JP/ J,IQ,LQ,LX,NS,NI,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
PT(1)=PY(1)-PS(1)-D1*PS(1)*CE(TIS(IQ,1),0.0,G1)
PT(2)=PS(1)-PS(2)-D1*PS(2)*CE(TIS(LQ,J),0.0,G1)
RETURN
END

```

```

SUBROUTINE NEFC(PA1,PA2,LM)
REAL A,D,FFC,PAF,X,X1,X2,X3I,Y,YS,Z,Z1
SPECIAL COMMON ZZ,XT,SV,XP,JP
COMMON /JP/ J,IQ,LQ,LX,NS,NI,NP,NB
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B,BC(4),TP,TK(4),TH,BY(4)
LH=0
PAF=PV(1)
IF(LM.EQ.10.OR.LM.EQ.1) PAF=FC(1)
TOL=.1E-10
5 CALL BIXT(X,Y,Z,Z1)
CALL BIXT(X3,X1,X2,YS)
A=(PAF/FC(1))+((BC(1)/SM)
D=PAF/FC(1)
X=D/A
DO 10 JE=1,NI
Z=Z+JE*(X**JE)
10 YS=YS+JE*(NI+1-JE)*(X**JE)
Z=Z*((A-D)/(A*D))*((Y3(1)+PY(3))/FC(1))
YS=(YS*BC(1)*TIS(IQ,1))/(D*A*SM*FC(1))
DO 15 JE=1,NI-1
15 Y=Y+JE*(NI-JE)*(X**JE)
Y=(Y*BC(1)*TIS(IQ,1))/(D*A*SM*FC(1))
Z1=(Z+Y-YS)*(BY(1)/SM)
DO 20 JE=1,NI
X1=X1+(X**JE)
20 X2=X2+(NI+1-JE)*(X**JE)
X3I=X1*(Y3(1)+PY(3))+((BC(1)/(SM*D))*X2*TIS(IQ,1))

```

```

FFC=Y2(1)+PY(2)-(1.+BY(1))*TIS(IQ,1)+B*D1*(CIS(IQ,1)+PA1)
1*CE(TIS(IQ,1),0.0,G1)+(BY(1)/SM)*X3I
PAF=PAF-FFC/Z1
LH=LH+1
IF(ABS(PAF-PV(1)).LT.TOL) GO TO 25
IF(LH.GT.101) GO TO 58
PV(1)=PAF
GO TO 5
25 PAF=PV(2)
IF(LM.EQ.10.OR.LM.EQ.1) PAF=FC(J)
LH=0
LM=5
30 CALL BIXT(X,Y,Z,Z1)
CALL BIXT(X3,X1,X2,YS)
A=(PAF/FC(J))+(BC(J)/SM)
D=PAF/FC(J)
X=D/A
DO 35 JE=1,NI
Z=Z+JE*(X**JE)
35 YS=YS+JE*(NI+1-JE)*(X**JE)
Z=Z*((A-D)/(A*D))*((Y3(J)+PY(4))/FC(J))
YS=(YS*BC(J)*TIS(LQ,J))/(D*A*SM*FC(J))
DO 40 JE=1,NI-1
40 Y=Y+JE*(NI-JE)*(X**JE)
Y=(Y*BC(J)*TIS(LQ,J))/(D*A*SM*FC(J))
Z1=(Z+Y-YS)*(BY(J)/SM)
DO 45 JE=1,NI
X1=X1+(X**JE)
45 X2=X2+(NI+1-JE)*(X**JE)
X3I=X1*(Y3(J)+PY(4))+((BC(J)/(SM*D))*X2*TIS(LQ,J))
FFC=Y2(J)-(1.+BY(J))*TIS(LQ,J)+B*D1*(CIS(LQ,J)+PA2)*
1CE(TIS(LQ,J),0.0,G1)+(BY(J)/SM)*X3I
PAF=PAF-FFC/Z1
LH=LH+1
IF(ABS(PAF-PV(2)).LT.TOL) GO TO 50
IF(LH.GT.101) GO TO 58
PV(2)=PAF
GO TO 30
50 RETURN
55 FORMAT(2X,I5,3E16.6)
56 FORMAT(5X,'WATCH-OUT!!! PROGRAM HEADING FOR A CRASH.!'*1**!')
58 WRITE(NS,56)
WRITE(NS,55) LH,PAF,PV(1),PV(2)
RETURN
END

```

```

SUBROUTINE D0INT(XO,XS,NI,HX,SZ,BIN,MP)
REAL XO,XS(105),SZ(105,4),XN(105),AS(105)
SPECIAL COMMON JP
COMMON /JP/ JQ,IQ,LQ,LX,NS,NC,NP,NB
INTEGER NI,I,MP
EXTERNAL BIN
XO=XO+HX
DO 412 I=1,NI
412 XN(I)=XS(I)
CALL BIN(AS,XN,XO,MP)
DO 414 I=1,NI
414 SZ(I,1)=HX*AS(I)
DO 420 J=1,2
DO 416 I=1,NI
416 XN(I)=(XN(I)+(SZ(I,J)/2.))
CALL BIN(AS,XN,XO,MP)

```



```

DO 418 I=1,NI
418 SZ(I,J+1)=HX*AS(I)
DO 420 I=1,NI
420 XN(I)=XS(I)
DO 422 I=1,NI
422 XN(I)=XN(I)+(SZ(I,3))
CALL BIN(AS,XN,XO,MP)
DO 424 I=1,NI
424 SZ(I,4)=HX*AS(I)
DO 426 I=1,NI
426 XS(I)=XS(I)+((SZ(I,1)+2.*SZ(I,2)+2.*SZ(I,3)+SZ(I,4))/6.)
RETURN
END

```

```

SUBROUTINE FIXT(XM,YM,X,Y,NM)
C This subroutine resets the axes ranges.
XM=10000.0
YM=10000.0
X=-10.0
Y=-10.0
RETURN
END

```

```

SUBROUTINE BIXT(XM,YM,X,Y)
C This subroutine resets variables to zero.
XM=0.0
YM=0.0
X=0.0
Y=0.0
RETURN
END

```

```

SUBROUTINE MOSES(SQ,SW,SE,SR,MI)
IF(MI.EQ.1) SQ=SQ-0.5
IF(MI.EQ.2.OR.MI.EQ.3) SQ=SQ-6.0
IF(MI.EQ.4) SQ=SQ-5.0E-06
IF(MI.EQ.4) SE=SE+5.0E-06
IF(MI.EQ.1) SE=SE+0.5
IF(MI.EQ.2.OR.MI.EQ.3) SE=SE+1.0
SW=SW-10.0
SR=SR+10.0
RETURN
END

```

```

SUBROUTINE SELECT(L,M,K,SI1,SI2,A1,A2,SZX,SY,P1,P2)
DIMENSION SI1(999),SI2(999),A1(999,2,8),A2(999,2,8)
SI1(L)=A1(L,M,K)
SI2(L)=A2(L,M,K)
IF(SI1(L).LE.SZX) SZX=SI1(L)
IF(SI1(L).GE.P1) P1=SI1(L)
IF(SI2(L).LE.SY) SY=SI2(L)
IF(SI2(L).GE.P2) P2=SI2(L)
RETURN
END

```

```

SUBROUTINE RELECT(L,M,K,SI1,SI2,A1,A2,SZX,SY,P1,P2)
DIMENSION SI1(451),SI2(451),A1(451,2,2),A2(451,2,2)
SI1(L)=A1(L,M,K)
SI2(L)=A2(L,M,K)
IF(SI1(L).LE.SZX) SZX=SI1(L)
IF(SI1(L).GE.P1) P1=SI1(L)
IF(SI2(L).LE.SY) SY=SI2(L)

```

```

IF(SI2(L).GE.P2) P2=SI2(L)
RETURN
END

```

```

SUBROUTINE EXPMNT
SPECIAL COMMON JP,SX,IBR
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
COMMON /JP/ JQ,IQ,LQ,LX,NS,NC,NP,NB
COMMON /SX/ AS1(451,2,2),AS2(451,2,2),
1AS3(451,2,2),AST(451,2,2),AS4(451,2,2)
INTEGER *6 BILN
15 FORMAT(I3)
17 FORMAT(5X,'READ GRAPHICAL OUTPUT FILE NAME[6CHAC]')
WRITE(NS,17)
READ(NS,21) BILN
CALL ASSIGN(16,BILN,LINM)
WRITE(NS,23) LINM,BILN
21 FORMAT(1X,A6)
23 FORMAT(5X,I3,5X,A6)
READ(16,-) NFX,NFY,CIS1,CIS2,FLC1,FLC2
WRITE(NS,35) NFX,NFY,CIS1,CIS2
N=0
L=0
DO 20 I=1,NFX
IF(N.EQ.0) L=L+1
N=N+1
READ(16,-) AST(N,1,L)
READ(16,-) AS2(N,1,L),AS3(N,1,L),AS3(N,2,L),AS2(N,2,L)
READ(16,-) AS1(N,1,L),AS1(N,2,L),AS4(N,1,L),AS4(N,2,L)
AST(N,2,L)=AST(N,1,L)
AS1(N,1,L)=AS1(N,1,L)*20.+CIS1
AS1(N,2,L)=AS1(N,2,L)*20.+CIS2
AS4(N,1,L)=AS4(N,1,L)-FLC1
AS4(N,2,L)=AS4(N,2,L)-FLC2
WRITE(NS,30) AS1(N,1,L),AS2(N,1,L),AS3(N,1,L),AS4(N,1,L)
1,AST(N,1,L)
WRITE(NS,30) AS1(N,2,L),AS2(N,2,L),AS3(N,2,L),AS4(N,2,L)
1,AST(N,2,L)
IF(N.EQ.NFY) MS(L,1)=NFY
IF(N.EQ.NFY) MS(L,2)=NFY
IF(I.EQ.NFX) MS(L,1)=N
IF(I.EQ.NFX) MS(L,2)=N
IF(I.EQ.NFX) NA(1)=L
IF(I.EQ.NFX) NA(2)=L
IF(N.EQ.NFY) N=0
20 CONTINUE
CLOSE 16
30 FORMAT(5F12.6)
35 FORMAT(2I6,2F12.6)
RETURN
END

```

```

SUBROUTINE CHAC(MIF,XMIF,YMIF,NMIF)
IF(NMIF.EQ.1) GO TO 10
CALL CHASWI(MIF)
CALL CHASIZ(XMIF,YMIF)
RETURN
10 CALL CHASWI(MIF)
RETURN
END

```

```

SUBROUTINE NKWOH

```

```

INTEGER *3 NIMX(10,4,2),NIMY(10,5,2),MX,MY
REAL BH(451),BA(451)
SPECIAL COMMON MXY,FX,SX,WP,JP,IBR
COMMON /MXY/ MX(10),MY(10)
COMMON /FX/ AX1(999,2,8),AX2(999,2,8),
1AX3(999,2,8),AXT(999,2,8),AX4(999,2,8)
COMMON /SX/ AS1(451,2,2),AS2(451,2,2),
1AS3(451,2,2),AST(451,2,2),AS4(451,2,2)
COMMON /WP/ BX(801),BM(801),YI(801)
COMMON /JP/ JQ,IQ,LQ,LX,NS,NC,NP,NB
COMMON /IBR/ MH(8,4),NZ(4),JS,IR,IH,MS(2,2),NA(2)
INTEGER *6 BILN
DATA NIMX/4*"[TIME          SECS]          ",
1      "[TEMP. *LOF *UREACTOR    oC] ",
1      3*"[TEMP. *LOF *UCOOLING COIL oC] "/
DATA NIMY/"[CONC. *LOF *UPRODUCT  Kg/m3] ",
1      "[TEMP. *LOF *UREACTOR    oC] ",
1      "[TEMP. *LOF *UCOOLING COIL oC] ",
1      "[CONC. *LOF *UREACTANT   Kg/m3] ",
1      "[COIL FLOW RATE          m3/SEC] ",
1      2*"[CONC. *LOF *UPRODUCT  Kg/m3] ",
1      2*"[TEMP. *LOF *UREACTOR    oC] ",
1      "[COIL FLOW RATE          m3/SEC] "/
XX=16.0
YY=XX*2.5
XN=0.0
WRITE(NS,448)
READ(NS,456) IQX
GO TO (438,440),IQX
438 CALL T4010
CALL UNITS(0.9)
PP=YY
GO TO 442
440 WRITE(NS,15)
READ(NS,21) BILN,NPAC
CALL ASSIGN(15,BILN,LINM)
WRITE(NS,23) LINM,BILN,NPAC
CALL OPEN
PP=YY*(7/4)
CALL UNITS(1.50)
CALL DEVPAP(1500.0,290.0,1)
DO 441 MAC=1,NPAC
IF(MAC.NE.1) XN=220.0
442 PA=1.2*PP
WRITE(NS,429)
READ(NS,456,ERR=494) JIM
WRITE(NS,452)
READ(NS,456,ERR=494) JS,IR
IF(JS.EQ.1) JX=1
IF(JS.GE.2) JX=2
IF(IR.GT.2) RETURN
429 FORMAT(5X,'SIMULATED(1) OR EXPERIMENTAL(2) OR BOTH(3)?',/)
WRITE(NS,454)
READ(NS,456,ERR=494) NIZ
IG=NZ(JS)
IS=NA(JX)
NOS=0
IF(JIM.EQ.2) GO TO 431
DO 430 IO=1,IG
430 WRITE(NS,460) IO,MH(IO,JS)
IF(JIM.EQ.1) GO TO 433
431 DO 14 IO=1,IS

```



```

14 WRITE(NS,461) IO,MS(IO,JS)
433 CONTINUE
    NV=0
    XX=XN+16.0
    IF(IQX.EQ.2.AND.MAC.NE.1) YY=0.0
    NIT=1
    CALL FIXT(XM,YM,X,Y,NIT)
    GO TO (432,480,506),IR
432 IF(JIM.EQ.2) GO TO 16
    DO 434 IX=1,IG
    IT=MH(IX,JS)
    DO 434 J=1,IT
    CALL SELECT(J,JX,IX,BX,BM,AXT,AX1,XM,YM,X,Y)
434 CONTINUE
15 FORMAT(5X,'READ GRAPHICAL OUTPUT FILE NAME[6CHAC] ',/,
1'    NUMBER OF GRAPHS TO BE PLOTTED?')
    IF(JIM.EQ.1) GO TO 20
16 DO 18 IX=1,IS
    IB=MS(IX,JX)
    DO 18 J=1,IB
    CALL RELECT(J,JX,IX,BH,BA,AST,AS1,XM,YM,X,Y)
18 CONTINUE
20 CONTINUE
    NV=NV+1
    CALL MOSES(YM,XM,Y,X,NV)
    ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
    ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
436 FORMAT(10A3)
    IF(NIZ.GE.2) XX=16.0+0.5*PA+XN
    CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
    CALL CHAC(1,0.5,0.5,2)
    IF(JIM.EQ.2) GO TO 22
    DO 446 IX=1,IG
    IT=MH(IX,JS)
    CALL ACALL(IT,JX,IX,BX,BM,AXT,AX1)
446 CALL GRACUR(BX,BM,IT)
21 FORMAT(1X,A6,I3)
    IF(JIM.EQ.1) GO TO 24
22 DO 25 IX=1,IS
    IB=MS(IX,JX)
    CALL GACALS(IB,JX,IX,BH,BA,AST,AS1)
25 CALL GRASYM(BH,BA,IB,5,0)
23 FORMAT(5X,I3,5X,A6,2X,I3)
    CALL CHAC(0,0.5,0.5,1)
448 FORMAT(10X,'INPUT GRAPH OUTPUT. SCREEN(1) OR PAPER(2)',/)
452 FORMAT(/,5X,'WHICH PHASE FOR DISPLAY(1,2,3 OR 4)?',/,
110X,'AND WHICH SET OF VARIABLES(1,2 or 3(return) ?',/)
454 FORMAT(10X,'FLOW RATE LABELING INVOLVED? YES(1) OR NO(2)',/)
456 FORMAT(2I3)
460 FORMAT(5X,'SIM LINE NUMBER ',I3,'SIM NUMBER OF POINTS ',I3,/)
461 FORMAT(5X,'EXPT LINE NUMBER=',I3,'EXPT NUMBER OF POINTS=',I3,/)
24 CALL FIXT(XM,YM,X,Y,NIT)
    IF(JIM.EQ.2) GO TO 26
    DO 462 IX=1,IG
    IT=MH(IX,JS)
    DO 462 J=1,IT
    CALL SELECT(J,JX,IX,BX,BM,AXT,AX2,XM,YM,X,Y)
462 CONTINUE
    IF(JIM.EQ.1) GO TO 30
26 DO 28 IX=1,IS
    IB=MS(IX,JX)
    DO 28 J=1,IB

```

```

CALL RELECT(J,JX,IX,BH,BA,AST,AS2,XM,YM,X,Y)
28 CONTINUE
30 CONTINUE
XX=0.0
IF(NIZ.GE.2) XX=-0.5*PA
YY=PA+10.0
NV=NV+1
CALL MOSES(YM,XM,Y,X,NV)
ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
CALL CHAC(1,0.5,0.5,2)
IF(JIM.EQ.2) GO TO 32
DO 466 IX=1,IG
IT=MH(IX,JS)
CALL ACALL(IT,JX,IX,BX,BM,AXT,AX2)
466 CALL GRACUR(BX,BM,IT)
IF(JIM.EQ.1) GO TO 36
32 DO 34 IX=1,IS
IB=MS(IX,JX)
CALL GACALS(IB,JX,IX,BH,BA,AST,AS2)
34 CALL GRASYM(BH,BA,IB,5,0)
CALL CHAC(0,0.5,0.5,1)
36 CALL FIXT(XM,YM,X,Y,NIT)
IF(JIM.EQ.2) GO TO 38
DO 468 IX=1,IG
IT=MH(IX,JS)
DO 468 J=1,IT
CALL SELECT(J,JX,IX,BX,BM,AXT,AX3,XM,YM,X,Y)
468 CONTINUE
IF(JIM.EQ.1) GO TO 42
38 DO 40 IX=1,IS
IB=MS(IX,JX)
DO 40 J=1,IB
CALL RELECT(J,JX,IX,BH,BA,AST,AS3,XM,YM,X,Y)
40 CONTINUE
42 CONTINUE
XX=PP+11.0
YY=0.0
NV=NV+1
CALL MOSES(YM,XM,Y,X,NV)
ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
CALL CHAC(1,0.5,0.5,2)
IF(JIM.EQ.2) GO TO 44
DO 472 IX=1,IG
IT=MH(IX,JS)
CALL ACALL(IT,JX,IX,BX,BM,AXT,AX3)
472 CALL GRACUR(BX,BM,IT)
IF(JIM.EQ.1) GO TO 48
44 DO 46 IX=1,IS
IB=MS(IX,JX)
CALL GACALS(IB,JX,IX,BH,BA,AST,AS3)
46 CALL GRASYM(BH,BA,IB,5,0)
CALL CHAC(0,0.5,0.5,1)
48 CALL FIXT(XM,YM,X,Y,NIT)
IF(JIM.EQ.2) GO TO 50
DO 474 IX=1,IG
IT=MH(IX,JS)
DO 474 J=1,IT
CALL SELECT(J,JX,IX,BX,BM,AXT,AX4,XM,YM,X,Y)

```

```

474 CONTINUE
    IF(JIM.EQ.1) GO TO 54
50 DO 52 IX=1,IS
    IB=MS(IX,JX)
    DO 52 J=1,IB
    CALL RELECT(J,JX,IX,BH,BA,AST,AS4,XM,YM,X,Y)
52 CONTINUE
54 CONTINUE
    NV=NV+1
    CALL MOSES(YM,XM,Y,X,NV)
    XX=0.0
    YY=(PA+10.0)
    ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
    IF(NIZ.GE.2) ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
    IF(NIZ.GE.2) GO TO 450
    ENCODE(30,436,MY) (NIMY(IZ,NV+1,IR),IZ=1,10)
    CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
    CALL CHAC(1,0.5,0.5,2)
    IF(JIM.EQ.2) GO TO 56
    DO 478 IX=1,IG
    IT=MH(IX,JS)
    CALL ACALL(IT,JX,IX,BX,BM,AXT,AX4)
478 CALL GRACUR(BX,BM,IT)
    IF(JIM.EQ.1) GO TO 60
56 DO 58 IX=1,IS
    IB=MS(IX,JX)
    CALL GACALS(IB,JX,IX,BH,BA,AST,AS4)
58 CALL GRASYM(BH,BA,IB,5,0)
    CALL CHAC(0,0.5,0.5,1)
60 CONTINUE
450 XX=(PP+11.0)
    IF(NIZ.EQ.1) YY=0.0
    NIT=2
    CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
    GO TO 441
480 IF(JIM.EQ.2) GO TO 62
    DO 482 IX=1,IG
    IT=MH(IX,JS)
    DO 482 J=1,IT
    CALL SELECT(J,JX,IX,BX,BM,AX2,AX1,XM,YM,X,Y)
482 CONTINUE
    IF(JIM.EQ.1) GO TO 66
62 DO 64 IX=1,IS
    IB=MS(IX,JX)
    DO 64 J=1,IB
    CALL RELECT(J,JX,IX,BH,BA,AS2,AS1,XM,YM,X,Y)
64 CONTINUE
66 CONTINUE
    NV=NV+1
    CALL MOSES(YM,XM,Y,X,NV)
    ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
    ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
    IF(NIZ.GE.2) XX=16.0+0.5*PA
    CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
    CALL CHAC(1,0.5,0.5,2)
    IF(JIM.EQ.2) GO TO 68
    DO 492 IX=1,IG
    IT=MH(IX,JS)
    CALL ACALL(IT,JX,IX,BX,BM,AX2,AX1)
492 CALL GRACUR(BX,BM,IT)
    IF(JIM.EQ.1) GO TO 72
68 DO 70 IX=1,IS

```



```

IB=MS(IX,JX)
CALL GACALS( IB,JX,IX,BH,BM,AS2,AS1)
70 CALL GRASYM(BH,BA,IB,5,0)
CALL CHAC(0,0.5,0.5,1)
72 CALL FIXT(XM,YM,X,Y,NIT)
IF(JIM.EQ.2) GO TO 74
DO 494 IX=1,IG
IT=MH(IX,JS)
DO 494 J=1,IT
CALL SELECT(J,JX,IX,BX,BM,AX3,AX1,XM,YM,X,Y)
494 CONTINUE
IF(JIM.EQ.1) GO TO 78
74 DO 76 IX=1,IS
IB=MS(IX,JX)
DO 76 J=1,IB
CALL RELECT(J,JX,IX,BH,BA,AS3,AS1,XM,YM,X,Y)
76 CONTINUE
78 CONTINUE
XX=0.0
IF(NIZ.GE.2) XX=-0.5*PA
YY=(PA+10.0)
NV=NV+1
CALL MOSES(YM,XM,Y,X,NV)
ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
CALL CHAC(1,0.5,0.5,2)
IF(JIM.EQ.2) GO TO 80
DO 498 IX=1,IG
IT=MH(IX,JS)
CALL ACALL(IT,JX,IX,BX,BM,AX3,AX1)
498 CALL GRACUR(BX,BM,IT)
IF(JIM.EQ.1) GO TO 84
80 DO 82 IX=1,IS
IB=MS(IX,JX)
CALL GACALS( IB,JX,IX,BH,BA,AS3,AS1)
82 CALL GRASYM(BH,BA,IB,5,0)
CALL CHAC(0,0.5,0.5,1)
84 CALL FIXT(XM,YM,X,Y,NIT)
IF(JIM.EQ.2) GO TO 83
DO 500 IX=1,IG
IT=MH(IX,JS)
DO 500 J=1,IT
CALL SELECT(J,JX,IX,BX,BM,AX3,AX2,XM,YM,X,Y)
500 CONTINUE
IF(JIM.EQ.1) GO TO 86
83 DO 85 IX=1,IS
IB=MS(IX,JX)
DO 85 J=1,IB
CALL RELECT(J,JX,IX,BH,BA,AS3,AS2,XM,YM,X,Y)
85 CONTINUE
86 CONTINUE
NV=NV+1
CALL MOSES(YM,XM,Y,X,NV)
XX=PP+11.0
YY=0.0
ENCODE(30,436,MX) (NIMX(IZ,NV,IR),IZ=1,10)
ENCODE(30,436,MY) (NIMY(IZ,NV,IR),IZ=1,10)
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
CALL CHAC(1,0.5,0.5,2)
IF(JIM.EQ.2) GO TO 88
DO 504 IX=1,IG

```

```

IT=MH(IX,JS)
CALL ACALL(IT,JX,IX,BX,BM,AX3,AX2)
504 CALL GRACUR(BX,BM,IT)
IF(JIM.EQ.1) GO TO 92
88 DO 90 IX=1,IS
IB=MS(IX,JX)
CALL GACALS(IB,JX,IX,BH,BA,AS3,AS2)
90 CALL GRASYM(BH,BA,IB,5,0)
CALL CHAC(0,0.5,0.5,1)
92 XX=(PP+11.0)
YY=(PA+10.0)
NIT=2
CALL XSCALE(IQX,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
441 CONTINUE
506 RETURN
END

```

```

SUBROUTINE ACALL(IK,IV,IM,D1,D2,S1,S2)
REAL D1(999),D2(999),S1(999,2,8),S2(999,2,8)
INTEGER J,IK,IV,IM
DO 94 J=1,IK
D1(J)=S1(J,IV,IM)
94 D2(J)=S2(J,IV,IM)
RETURN
END

```

```

SUBROUTINE GACALS(IK,IV,IM,D1,D2,S1,S2)
REAL D1(451),D2(451),S1(451,2,2),S2(451,2,2)
INTEGER J,IK,IV,IM
DO 94 J=1,IK
D1(J)=S1(J,IV,IM)
94 D2(J)=S2(J,IV,IM)
RETURN
END

```

```

SUBROUTINE XSCALE(IQ,XX,YY,PP,PA,XM,YM,X,Y,NIT,NOS)
C SUBROUTINE FOR SCALING DIAGRAM.
SPECIAL COMMON JP
COMMON /JP/ J,IQ,LQ,LX,NS,NC,NP,NB
IF(NIT.GE.2) GO TO 510
WRITE(NS,508) XM,YM
WRITE(NS,508) X,Y
508 FORMAT(2(F10.3,/))
C SHIFT ORIGIN
510 CALL SHIFT2(XX,YY)
CALL CHAC(1,1.2,1.6,2)
IF(NIT.GE.2) GO TO 512
C POSITION AXES
CALL AXIPOS(1,0.0,0.0,PP,1)
CALL AXIPOS(1,0.0,0.0,PA,2)
CALL AXISCA(3,2,XM,X,1)
CALL AXISCA(3,2,YM,Y,2)
C DRAW AXES
CALL AXIDRA(-1,1,1)
CALL AXIDRA(1,-1,2)
CALL MOVTO2(0.0,PA)
CALL LINTO2(PP,PA)
CALL LINTO2(PP,0.0)
CALL MOVTO2(2.0,PA-3.)
512 CALL AXLAB(NIT,PA)
CALL MOVTO2(0.0,0.0)
NOS=NOS+1

```

RETURN
END

```
C SUBROUTINE AXLAB(NIT,PP)
  Subroutine for labeling diagram.
  INTEGER*3 MI1(15),MI2(15),MI3(15)
  1,MI4(15),MX,MY
  SPECIAL COMMON MXY,JP
  COMMON /MXY/ MX(10),MY(10)
  COMMON /JP/ J,IQ,IQ,LX,NS,NC,NP,NB
  IF(NIT.GE.2) WRITE(NS,520)
  IF(NIT.LE.1) WRITE(NS,516)
  READ(NS,518) (MI1(I),I=1,15)
  READ(NS,518) (MI2(I),I=1,15)
  READ(NS,518) (MI3(I),I=1,15)
  READ(NS,518) (MI4(I),I=1,15)
  IF(NIT.LE.1) GO TO 522
516 FORMAT(5X,'INSERT TITLE ON DIAGRAM[4 LINES] *',/)
518 FORMAT(15A3)
520 FORMAT(5X,'OVERALL LABELS FOR DIAGRAM[4 LINES] *',/)
  IF(NIT.GE.2) GO TO 524
522 CONTINUE
  CALL CHAARR(MI1,10,3)
  CALL MOVTO2(15.0,PP-6.)
  CALL CHAARR(MI2,15,3)
  CALL MOVTO2(15.0,PP-9.0)
  CALL CHAARR(MI3,15,3)
  CALL MOVTO2(15.0,PP-12.0)
  CALL CHAARR(MI4,15,3)
  CALL MOVTO2(-6.0,6.0)
  CALL CHAANG(90.)
  CALL CHAARR(MY,10,3)
  CALL MOVTO2(-0.5,-6.0)
  CALL CHAANG(0.0)
  CALL CHAARR(MX,10,3)
  IF(NIT.EQ.1) GO TO 526
524 CALL MOVTO2(20.0,-18.0)
  CALL CHAARR(MI1,15,3)
  CALL MOVTO2(20.0,-22.0)
  CALL CHAARR(MI2,15,3)
  CALL MOVTO2(20.0,-26.0)
  CALL CHAARR(MI3,15,3)
  CALL MOVTO2(20.0,-29.0)
  CALL CHAARR(MI4,15,3)
  CALL MOVTO2(20.0,-33.0)
526 CALL CHAC(0,0.5,0.5,1)
  RETURN
  END
```

```
C SUBROUTINE LYAPON(LQV,JBX,JIB)
C CALCULATES THE LYAPONUV'S FUNCTION FOR
C SYSTEM.
C STEP ONE.CALCULATES INITIAL SYMMETRIC MATRIX.
  LOGICAL GROW,LBLOCK
  REAL CI(6,6),A(45),RHS(6),W(6)
  SPECIAL COMMON SK,SD,JP,BZ,ZZ,VB,XT,WX,XP,SV
  COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
  COMMON /SD/ SA(6,6),B(6,6),AO(3,3),BJ(3,3),RQ(3)
  COMMON /JP/ JS,IQ,IQ,LX,NS,NC,NT,N
  COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
  COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
  COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
```



```

COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B2,BC(4),TP,TK(4),TH,BY(4)
INTEGER I,IFAIL,LICN,LIRN,MTYPE,N,NS,NZ,NN,ISW,NT
INTEGER ICN(45),IDISP(10),IKEEP(30),IRN(25),IW(48)
LOGICAL ABORT(4)
C F01BRF, F04AXF
DATA CI,RHS,TENTH,TOL/42*0.0,1.0D-01,.1E-07/
CALL ZEROES(LS,FV(2),PM,QM,FV(1),SG,NN)
NZ=0
CI(1,1)=BJ(1,1)
CI(2,1)=BJ(1,2)
CI(3,1)=BJ(1,3)
RHS(1)=-0.5
CI(1,2)=BJ(2,1)
CI(2,2)=BJ(1,1)+BJ(2,2)
CI(3,2)=BJ(2,3)
CI(4,2)=BJ(1,2)
CI(5,2)=BJ(1,3)
CI(1,3)=BJ(3,1)
CI(2,3)=BJ(3,2)
CI(3,3)=BJ(1,1)+BJ(3,3)
CI(5,3)=BJ(1,2)
CI(6,3)=BJ(1,3)
CI(2,4)=BJ(2,1)
CI(4,4)=BJ(2,2)
CI(5,4)=BJ(2,3)
RHS(4)=-0.5
CI(2,5)=BJ(3,1)
CI(3,5)=BJ(2,1)
CI(4,5)=BJ(3,2)
CI(5,5)=BJ(2,2)+BJ(3,3)
CI(6,5)=BJ(2,3)
CI(3,6)=BJ(3,1)
CI(5,6)=BJ(3,2)
CI(6,6)=BJ(3,3)
RHS(6)=-0.5
DO 280 I=1,N
280 WRITE(NS,25) (CI(J,I),J=1,N)
WRITE(NS,25) (RHS(L),L=1,N)
DO 45 I=1,N
DO 45 J=1,N
IF(CI(I,J).EQ.0.0) GO TO 50
NZ=NZ+1
A(NZ)=CI(I,J)
IRN(NZ)=I
ICN(NZ)=J
50 CONTINUE
45 CONTINUE
C WRITE(NS,30) NZ
C DO 40 I=1,NZ
C WRITE(NS,35) A(I),IRN(I),ICN(I)
C 40 CONTINUE
C 35 FORMAT(2X,F10.4,2I4)
C 30 FORMAT(I4)
LICN = 45
LIRN = 25
ULA = TENTH
LBLOCK = .TRUE.
GROW = .TRUE.
ABORT(1) = .TRUE.

```

```

ABORT(2) = .TRUE.
ABORT(3) = .FALSE.
ABORT(4) = .TRUE.
IFAIL = 110
CALL F01BRF(N,NZ,A,LICN,IRN,LIRN,ICN,ULA,IKEEP,IW,W,
*LBLOCK,GROW,ABORT,IDISP,IFAIL)
IF (GROW) WRITE (NS,3) W(1)
MTYPE = 1
CALL F04AXF(N,A,LICN,ICN,IKEEP,RHS,W,MTYPE,IDISP,RESID)
C WRITE (NS,2) (RHS(I),I=1,N)
25 FORMAT(6F9.4)
15 FORMAT(3F17.9)
DO 10 ISW=1,NT
NN=NN+1
DO 10 J=NN,NT
LS=LS+1
10 AO(NN,J)=RHS(LS)
AO(2,1)=AO(1,2)
AO(3,1)=AO(1,3)
AO(3,2)=AO(2,3)
C DO 290 LI=1,NT
C290 WRITE(NS,15) (AO(LI,K),K=1,NT)
IKON=0
295 CALL MAXIZE(LQV,JBX,JIB)
IF(IKON.EQ.1) PV(1)=PV(2)
IKON=IKON+1
IF(IKON.NE.1.AND.ABS(PV(2)-PV(1)).LT.TOL) GO TO 298
IF(PV(1).GT.PV(2)) WRITE(NS,297)
IF(PV(1).GT.PV(2)) GO TO 298
IF(PV(2).GT.PV(1).AND.IKON.NE.1) PV(1)=PV(2)
DO 296 JHB=1,NT
DO 296 JHG=1,NT
296 CI(JHB,JHG)=AO(JHB,JHG)
297 FORMAT(5X,'MUST HAVE TAKEN A WRONG TURN!!!!')
WRITE(NS,4) IKON,PV(2),PV(1)
GO TO 295
298 DO 299 JHG=1,NT
WRITE(NS,15) (AO(JHG,JHB),JHB=1,NT)
C WRITE(NS,15) (CI(JHG,JHB),JHB=1,NT)
299 CONTINUE
WRITE(NS,4) IKON,PV(2),PV(1)
WRITE(NS,15) Z(1),Z(2),Z(3)
5 FORMAT (5(2X, F4.0, 2X, I1, 2X, I1))
4 FORMAT(5X,I3,2F15.10)
3 FORMAT (5X,'ON EXIT FROM F01BRFVALUE OF W(1) =', F10.4)
C 2 FORMAT (5X,'ON EXIT FROM F04AXF SOLUTION=', F10.4))
RETURN
END

```

```

SUBROUTINE ZEROES(LK,PL,PM,QM,PF,SG,IG)

```

```

SG=0.0
PF=0.0
LK=0
PL=0.0
PM=1.0
QM=1.0
IG=0
RETURN
END

```

```

SUBROUTINE ZEROED(NZEROS,CADS)
REAL CADS(50)

```

```

DO 10 JJ=1,NZEROS
10 CADS(JJ)=0.0
RETURN
END

C In search of Emax (X'AX=Emax)
SUBROUTINE TEST(V1,V2,PX,TS,AE,LN)
SPECIAL COMMON JP,SK,SD
COMMON /JP/ JS,IQ,LQ,LX,NS,NC,NT,NU
COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
COMMON /SD/ A(6,6),B(6,6),AO(3,3),AM(3,3),RQ(3)
DO 10 I=1,NT
DO 10 J=1,NT
10 AB(I,J)=AM(I,J)
V1=AO(1,1)*(X(1)**2)+AO(2,2)*(X(2)**2)+AO(3,3)*(X(3)**2)
+2*(AO(1,2)*X(1)*X(2)+AO(1,3)*X(1)*X(3)+AO(2,3)*X(2)*X(3))-AE
IF(ABS(V1-V2).LE.TS) GO TO 1
IF(V1.GT.V2) LN=1
IF(V1.LT.V2.AND.X(1).GT.PX) LN=2
IF(V1.LT.V2.AND.X(1).LE.PX) LN=3
IF(V1.GT.V2) V2=V1
C WRITE(NS,15) LN,V1
RETURN
1 LN=4
C WRITE(NS,15) LN,V1
15 FORMAT(I5,3X,4E15.9)
RETURN
END

SUBROUTINE MAXIZE(LCV,JCT,JET)
REAL UY(3)
SPECIAL COMMON SK,SD,JP,BZ,ZZ,VB,XT,WX,XP,SV
COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
COMMON /SD/ A(6,6),B(6,6),AO(3,3),AOE(3,3),RQ(3)
COMMON /JP/ JS,IQ,LQ,LX,NS,NC,NT,NP
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B2,BC(4),TP,TK(4),TH,BY(4)
DATA STEP,ALPA,BETA,TOL,EO/.1E-01,.9E-01,.8E-01,.1E-06,.1E-04/
DATA A,B/72*0.0/
LBON=10
CALL ZEROED(3,UY)
CALL ZEROES(L,PL,PM,QM,CHECK,PS,IQT)
DO 2 I=1,NT
C Starting co-ordinates for search.
S(1,I)=.1+FLOAT(I)*.1E-01
S(2,I)=S(1,I)+(2.65-FLOAT(I))*2
2 X(I)=S(2,I)
NY=1
3 L=L+1
C Calculates direction of step £
CALL FIRST(1,LBON)
II=1
10 I=0
GO TO 40
15 CONTINUE
I=I+1
C Search for Emax

```



```

CALL TEST(UY(3),UY(2),PS,TOL,EO,K)
CALL CONST(JET,UY(3),CHECK,1.0,1.0,LCV,JCT)
C Max$E subject to constraint f'(Yj/(Y'j(Ao/e)Yj)**.5)AoYj<0
IF(CHECK.GE.0.0) GO TO 85
GO TO (20,30,40,50),K
20 PM=PM+0.2
PS=X(1)
DO 25 JI=1,NT
25 X(JI)=X(JI)+ALPA*PM*STEP*E(II,JI)
CALL ZEROES(LP,QM,ZM,YA,VZ1,VZ2,IQT)
GO TO 55
30 QM=QM+0.2
DO 35 JI=1,NT
35 X(JI)=X(JI)-BETA*QM*STEP*E(II,JI)
CALL ZEROES(MAZ,PL,PM,YA,VZ1,VZ2,IQT)
GO TO 55
40 PL=PL+1.0
DO 45 JI=1,NT
45 X(JI)=X(JI)+ALPA*STEP*E(II,JI)/(PL+1.)
CALL ZEROES(MAZ,YA,PM,QM,VZ1,VZ2,IQT)
GO TO 55
50 WRITE(NS,80) X(1),X(2),X(3)
WRITE(NS,70) II
II=II+1
IF(II.GE.4) GO TO 60
GO TO 10
55 CONTINUE
C 55 WRITE(NS,80) X(1),X(2),X(3)
IF(I.GE.10) GO TO 60
GO TO 15
60 DO 65 JU=1,NT
65 S(2,JU)=X(JU)
C WRITE(NS,75) L
GO TO 3
70 FORMAT(5X,'COMPLETION OF PART',I3,' OF MAXIMIZATION.')
75 FORMAT(5X,'COMPLETION OF STAGE',I3,' OF MAXIMIZATION')
80 FORMAT(2X,6E11.4)
85 CONTINUE
DO 90 I=1,NT
DO 90 J=1,NT
90 AO(I,J)=AB(I,J)
C DO 95 I=1,NT
C 95 WRITE(NS,80) (AO(I,J),J=1,NT)
C Minimise maximum eigenvalue.
CALL MINIMI(LCV,JCT,JET)
RETURN
END

```

```

SUBROUTINE CONST(JAT,W1,CHECK,SKR,SKP,LF,LF1)
REAL Y(250,4),SI,SJ
SPECIAL COMMON SK,SD,JP,XT,WX,XP,SV,BZ,VB,ZZ
COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
COMMON /SD/ A(6,6),B(6,6),AO(3,3),AOE(3,3),RQ(3)
COMMON /JP/ JS,IQ,LQ,LX,NS,NC,NT,NP
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B2,BC(4),TP,TK(4),TH,BY(4)
DATA NN/240/

```

```

DO 95 J=1,NN
DO 95 I=1,NT
SI=FLOAT(NN)
SJ=FLOAT(J)
Y(J,I)=(SJ/SI)*(3.142/2.)
95 CONTINUE
IF(LF1.EQ.1) ZS1=S1
IF(LF1.GE.2) ZS1=S4
DO 100 I=1,NT
DO 100 J=1,NT
AOE(J,I)=AO(J,I)/W1
100 CONTINUE
105 FORMAT(2X,3F18.11)
X1S=CIS(LF,LF1)
X2S=TIS(LF,LF1)
YS=((Y(I,1)**2)*AOE(1,1)+(Y(I,2)**2)*AOE(2,2)+(Y(I,3)
1**2)*AOE(3,3)+2*(Y(I,1)*Y(I,2)*AOE(1,2)+Y(I,2)*Y(I,3)
2*AOE(2,3)+Y(I,1)*Y(I,3)*AOE(1,3))**0.5
YX1=((SKR/SKP)*Y(I,1))/YS
YX2=((SKR/SKP)*Y(I,2))/YS
YX3=((SKR/SKP)*Y(I,3))/YS
FY1=-YX1-D1*((X1S+YX1)*CE(X2S,YX2,G1)-X1S*CE(X2S,0.0,G1))
FY2=-YX2+B2*D1*((X1S+YX1)*CE(X2S,YX2,G1)-X1S*CE(X2S,0.0,G1))
1-BY(LF1)*YX2+(BY(LF1)/SM)*YX3
FY3=(BC(LF1)/SM)*(YX2-YX3)-YX3
GO TO (8,6,4,2,10),JAT
2 FY3=-ZS1*(TVS(24,LF,LF1)-TCS(LF,LF1))*(CAO/FC(LF1))
GO TO 8
4 FY3=((BC(LF1)/SM)+ZS1*(TVS(24,LF,LF1)-TCS(LF,LF1)
1)*(TQ*G1/FC(LF1)))
GO TO 8
6 FY3=-(1.+(BC(LF1)/SM)-ZS1*TQ*G1*(TVS(24,LF,
2LF1)-TCS(LF,LF1))/FC(LF1))
GO TO 8
10 FY3=-ZS1*YX2
8 CONTINUE
CHECK=(FY1*AO(1,1)+FY2*AO(1,2)+FY3*AO(1,3))*Y(I,1)+
1(FY1*AO(1,2)+FY2*AO(2,2)+FY3*AO(2,3))*Y(I,2)+(FY1*
2AO(1,3)+FY2*AO(2,3)+FY3*AO(3,3))*Y(I,3)
IF(CHECK.LT.0.0) CHECK1=CHECK
IF(CHECK.GE.0.0.AND.I.LT.2) WRITE(NS,105) CHECK,CHECK1,W1
110 CONTINUE
WRITE(NS,105) CHECK
RETURN
END

```

```

SUBROUTINE MINIMI(LEV,JOT,JAB)
REAL UY(3)
SPECIAL COMMON SK,SD,JP,BZ,ZZ,VB,XT,WX,XP,SV
COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
COMMON /SD/ A(6,6),B(6,6),AO(3,3),AOE(3,3),RQ(3)
COMMON /JP/ JS,IQ,LQ,LX,NS,NC,NT,NP
COMMON /ZZ/ TCI,TI,CA,VC(4),FC(4),V1,E1
COMMON /BZ/ TV(4),TVS(26,3,4),PVS(6)
COMMON /XT/ Y1(4),Y2(4),Y3(4),PV(2),PY(4),SM
COMMON /VB/ S1,S2,S3,S4,S5,S6,S7
COMMON /WX/ TQ,TCO,CAO,R1,CP,F,U(4),DEL,R
COMMON /XP/ TIS(3,4),CIS(3,4),TCS(3,4)
COMMON /SV/ D1,G1,B2,BC(4),TP,TK(4),TH,BY(4)
DATA STEP,ALPA,BETA,TOL/.1E-02,.9E-01,.8E-01,.1E-06/
DATA A,B/72*0.0/
LBON=10

```

```

CALL ZEROED(3,UY)
CALL ZEROES(L,PL,PM,QM,VZ1,PS,IQT)
S(1,1)=AO(1,1)
S(1,2)=AO(1,2)
S(1,3)=AO(1,3)
S(1,4)=AO(2,2)
S(1,5)=AO(2,3)
S(1,6)=AO(3,3)
DO 120 I=1,NP
S(2,I)=S(1,I)+(3.2-FLOAT(I))* .2E-04
120 X(I)=S(2,I)
125 L=L+1
CALL FIRST(2,LBON)
II=1
135 I=0
GO TO 165
140 CONTINUE
I=I+1
CALL BEST(UY(3),UY(2),PS,TOL,K)
CALL CONST(JAB,1.0,CHECK,1.0,1.0,LEV,JOT)
IF(CHECK.GE.0.0) GO TO 210
IF(UY(3).NE.UY(2)) GO TO 142
DO 183 JJ=1,NT
Z(JJ)=RQ(JJ)
DO 183 LJ=1,NT
AB(JJ,IJ)=AO(JJ,IJ)
183 CONTINUE
142 GO TO (145,155,165,175),K
145 PM=PM+0.5E-01
PS=X(1)
DO 150 JI=1,NP
150 X(JI)=X(JI)+ALPA*PM*STEP*E(II,JI)
CALL ZEROES(LP,QM,ZM,YA,VZ1,VZ2,IQT)
GO TO 180
155 QM=QM+0.5E-01
DO 160 JI=1,NP
160 X(JI)=X(JI)-BETA*QM*STEP*E(II,JI)
CALL ZEROES(MAZ,PL,PM,YA,VZ1,VZ2,IQT)
GO TO 180
165 PL=PL+1.0
DO 170 JI=1,NP
170 X(JI)=X(JI)+ALPA*STEP*E(II,JI)/(PL+1.)
CALL ZEROES(MAZ,YA,PM,QM,VZ1,VZ2,IQT)
GO TO 180
175 CONTINUE
C175 WRITE(NS,205) X(1),X(2),X(3),X(4),X(5),X(6)
C WRITE(NS,195) II
II=II+1
IF(II.GE.4) GO TO 185
GO TO 135
C180 WRITE(NS,205) X(1),X(2),X(3),X(4),X(5),X(6)
180 CONTINUE
C DO 184 JJ=1,NT
C184 WRITE(NS,205) (AO(JJ,IJ),IJ=1,NT)
IF(I.GE.10) GO TO 185
GO TO 140
185 DO 190 JU=1,NP
190 S(2,JU)=X(JU)
C WRITE(NS,200) L
GO TO 125
195 FORMAT(5X,'COMPLETION OF PART',I3,' OF MINIMIZATION.')
200 FORMAT(5X,'COMPLETION OF STAGE',I3,' OF MINIMIZATION')

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205 FORMAT(2X,6F12.8)
210 DO 213 I=1,NT
    DO 213 J=1,NT
213 AO(I,J)=AB(I,J)
C   DO 214 I=1,NT
C214 WRITE(NS,205) (AO(I,J),J=1,NT)
    PV(2)=Z(1)*Z(2)*Z(3)
    RETURN
    END

C   Calculates best direction of advance
C   An are the unit vectors joining the initial and final points.
SUBROUTINE FIRST(ML,LBOM)
SPECIAL COMMON SK,SD,JP
COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
COMMON /SD/ A(6,6),B(6,6),AO(3,3),AM(3,3),RQ(3)
COMMON /JP/ JS,IQ,LQ,LX,NS,NC,NT,NP
IF(LBOM.EQ.10) CALL BIXT(EI,SI,TI,WI)
IF(LBOM.EQ.10) CALL BIXT(EI,SI,QI,AI)
LBOM=10
IF(ML.EQ.2) GO TO 273
DO 215 I=1,NT
215 A(1,I)=S(2,I)-S(1,I)
    A(2,1)=0.0
    DO 220 I=2,NT
220 A(2,I)=S(2,I)-S(1,I)
    DO 225 I=1,2
225 A(3,I)=0.0
    A(3,I)=S(2,3)-S(1,3)
    DO 230 I=1,NT
230 EI=EI+A(1,I)**2
    EI=EI**0.5
    DO 235 I=1,NT
235 E(1,I)=A(1,I)/EI
    DO 240 I=1,NT
240 B(2,I)=A(2,I)-E(1,I)*(A(2,1)*E(1,1)+A(2,2)*E(1,2)+A(2,3)*E(1,3))
    DO 245 I=1,NT
245 SI=SI+B(2,I)**2
    SI=SI**0.5
    DO 250 I=1,NT
250 E(2,I)=B(2,I)/SI
    DO 255 I=1,NT
255 B(3,I)=A(3,I)-E(2,I)*(A(3,1)*E(2,1)+A(3,2)*E(2,2)+A(3,3)*E(2,3))
    TI=(B(3,1)**2+B(3,2)**2+B(3,3)**2)**0.5
    DO 265 I=1,NT
265 E(3,I)=B(3,I)/TI
    DO 270 I=1,NT
270 B(1,I)=B(2,I)
    RETURN
273 CONTINUE
    DO 290 I=1,NP
    IF(I.EQ.1) GO TO 285
    DO 275 J=1,I-1
275 A(I,J)=0.0
    DO 280 JI=I,NP
280 A(I,JI)=S(2,JI)-S(1,JI)
285 CONTINUE
290 A(1,I)=S(2,I)-S(1,I)
    EI=(A(1,1)**2+A(1,2)**2+A(1,3)**2+A(1,4)**2+A(1,5)**2
    1+A(1,6)**2)**0.5
    DO 295 I=1,NP
295 E(1,I)=A(1,I)/EI

```

```

DO 300 I=1,NP
300 B(2,I)=A(2,I)-E(1,I)*(A(2,1)*E(1,1)+A(2,2)*E(1,2)+A(2,3)
1+E(1,3)+A(2,4)*E(1,4)+A(2,5)*E(1,5)+A(2,6)*E(1,6))
SI=(B(2,1)**2+B(2,2)**2+B(2,3)**2+B(2,4)**2+B(2,5)**2
1+B(2,6)**2)**0.5
DO 305 I=1,NP
305 E(2,I)=B(2,I)/SI
DO 310 I=1,NP
310 B(3,I)=A(2,I)-E(2,I)*(A(3,1)*E(2,1)+A(3,2)*E(2,2)+A(3,3)
1+E(2,3)+A(3,4)*E(2,4)+A(3,5)*E(2,5)+A(3,6)*E(2,6))
TI=(B(3,1)**2+B(3,2)**2+B(3,3)**2+B(3,4)**2+B(3,5)**2
1+B(3,6)**2)**0.5
DO 315 I=1,NP
315 E(3,I)=B(3,I)/TI
DO 320 I=1,NP
320 B(4,I)=A(4,I)-E(3,I)*(A(4,1)*E(3,1)+A(4,2)*E(3,2)+A(4,3)
1+E(3,3)+A(4,4)*E(3,4)+A(4,5)*E(3,5)+A(4,6)*E(3,6))
QI=(B(4,1)**2+B(4,2)**2+B(4,3)**2+B(4,4)**2+B(4,5)**2
1+B(4,6)**2)**0.5
DO 325 I=1,NP
325 E(4,I)=B(4,I)/QI
DO 330 I=1,NP
330 B(5,I)=A(5,I)-E(4,I)*(A(5,1)*E(4,1)+A(5,2)*E(4,2)+A(5,3)
1+E(4,3)+A(5,4)*E(4,4)+A(5,5)*E(4,5)+A(5,6)*E(4,6))
WI=(B(5,1)**2+B(5,2)**2+B(5,3)**2+B(5,4)**2+B(5,5)**2
1+B(5,6)**2)**0.5
DO 335 I=1,NP
335 E(5,I)=B(5,I)/WI
DO 340 I=1,NP
340 B(6,I)=A(6,I)-E(5,I)*(A(6,1)*E(5,1)+A(6,2)*E(5,2)+A(6,3)
1+E(5,3)+A(6,4)*E(5,4)+A(6,5)*E(5,5)+A(6,6)*E(5,6))
AI=(B(6,1)**2+B(6,2)**2+B(6,3)**2+B(6,4)**2+B(6,5)**2
1+B(6,6)**2)**0.5
DO 345 I=1,NP
345 E(6,I)=B(6,I)/AI
DO 347 I=1,NP
347 B(1,I)=B(2,I)
RETURN
END

```

```

SUBROUTINE BEST(V1,V2,PX,TS,N)
REAL RI(3)
SPECIAL COMMON SK,SD,JP
COMMON /SK/ X(6),E(6,6),S(2,6),Z(6),AB(3,3)
COMMON /SD/ A(6,6),B(6,6),AO(3,3),AM(3,3),RR(3)
COMMON /JP/ JS,IQ,LQ,LX,NS,NC,NT,NP
INTEGER INTEG(3),IA,IN,IFAIL
DATA IA,IN/2*3/
IFAIL=1
VMAX=0.0
DO 350 I=1,3
AO(1,I)=X(I)
IF(I.EQ.1) GO TO 348
AO(2,I)=X(2+I)
AO(I,1)=AO(1,I)
348 CONTINUE
350 CONTINUE
AO(3,2)=AO(2,3)
AO(3,3)=X(6)
DO 352 JZT=1,NT
DO 351 IZT=1,NT
351 AM(JZT,IZT)=AO(JZT,IZT)

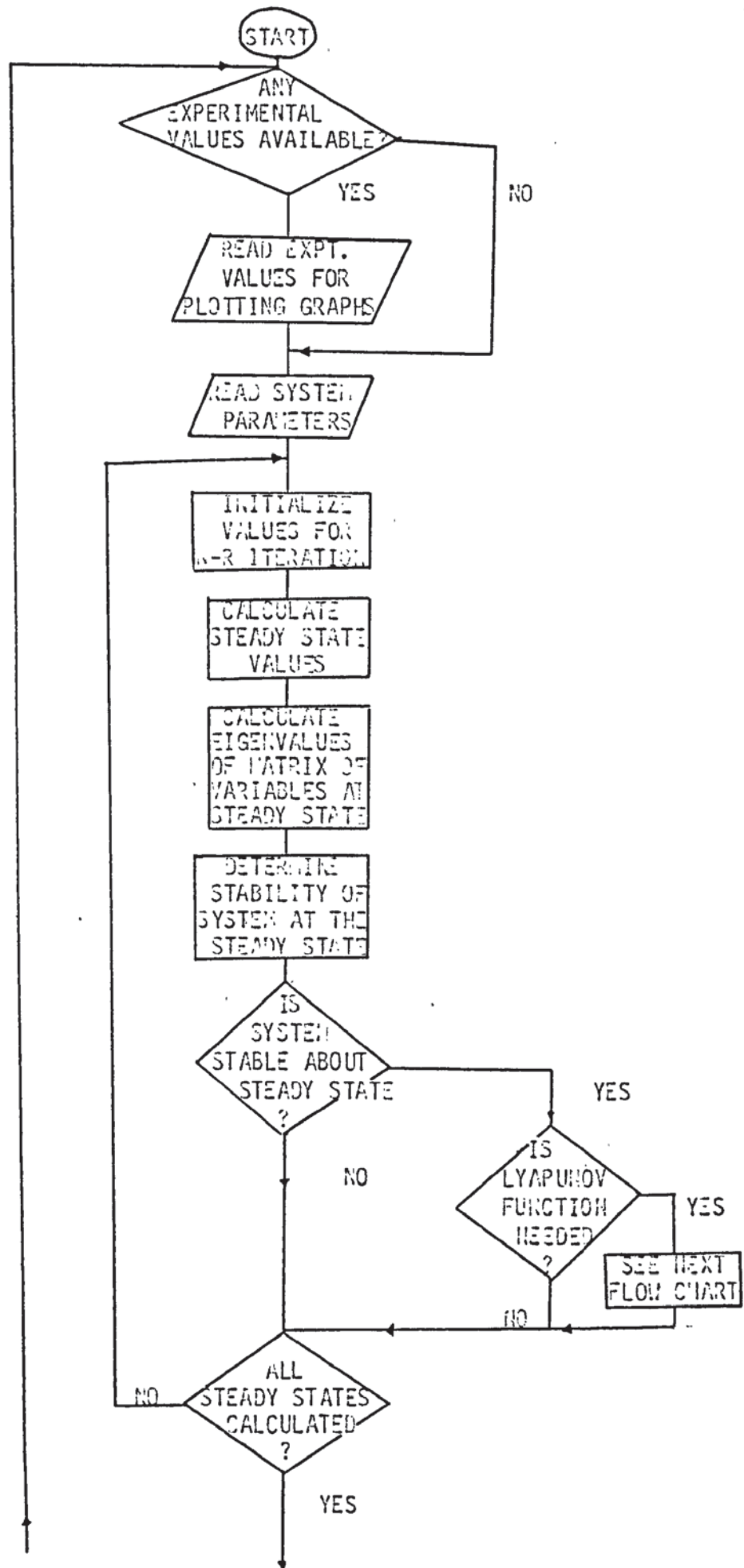
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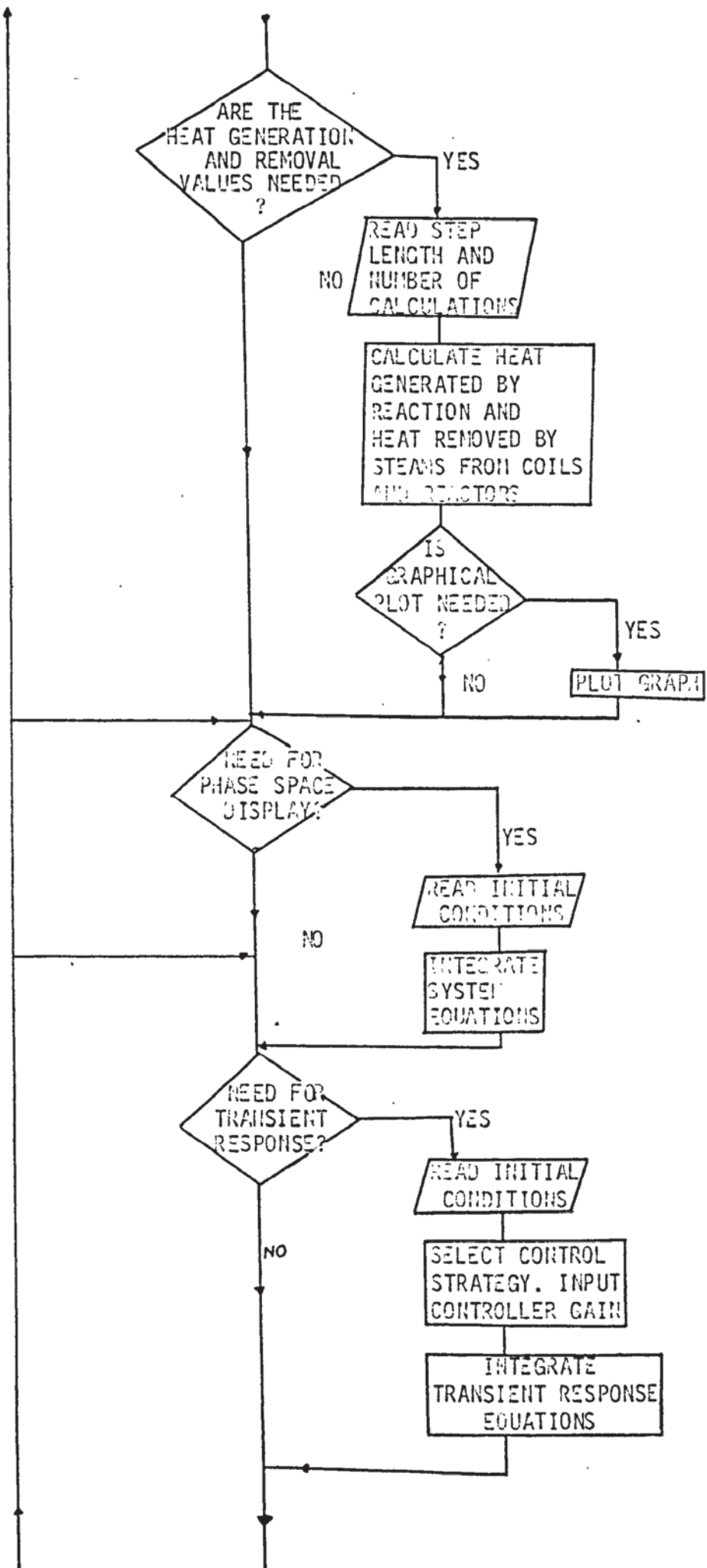
```

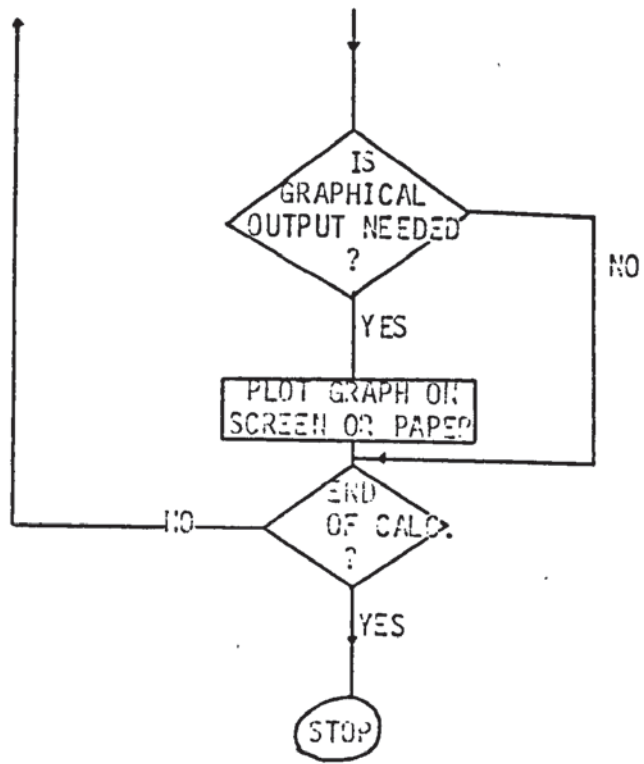
352 CONTINUE
CALL F02AFF(AO, IA, IN, RR, RI, INTEG, IFAIL)
DO 354 JZT=1,NT
DO 354 IZT=1,NT
354 AO(JZT, IZT)=AM(JZT, IZT)
C353 WRITE(NS, 356) (AO(JZT, ILL), ILL=1, NT)
C356 FORMAT(3F20.10)
IF(IFAIL.EQ.0) GO TO 360
WRITE(NS, 355) IFAIL
355 FORMAT(5X, 'ERROR IN IFAIL=', I3)
RETURN
360 CONTINUE
C360 WRITE(NS, 365) (RR(I), RI(I), I=1, IN)
365 FORMAT(2(7X, E12.5, 7X))
VMIN=RR(1)
DO 370 I=1, IN
IF(RR(I).GE.VMAX) VMAX=RR(I)
IF(RR(I).LE.VMIN) VMIN=RR(I)
370 IF(RR(I).LE.0.0) WRITE(NS, 375) RR(I)
375 FORMAT(5X, 'ERROR IN EIGEN VALUE', E10.3)
V1=(ABS(VMAX)-ABS(VMIN))
IF(ABS(V1-V2).LE.TS) GO TO 380
IF(V1.LT.V2) N=1
IF(V1.GT.V2.AND.X(1).GT.PX) N=2
IF(V1.GT.V2.AND.X(1).LE.PX) N=3
C WRITE(NS, 385) N, V1, V2
IF(V1.LT.V2.OR.V2.EQ.0.0) V2=V1
RETURN
380 N=4
C WRITE(NS, 385) N, V1, V2
385 FORMAT(5X, I3, 2F17.9)
RETURN
END

```

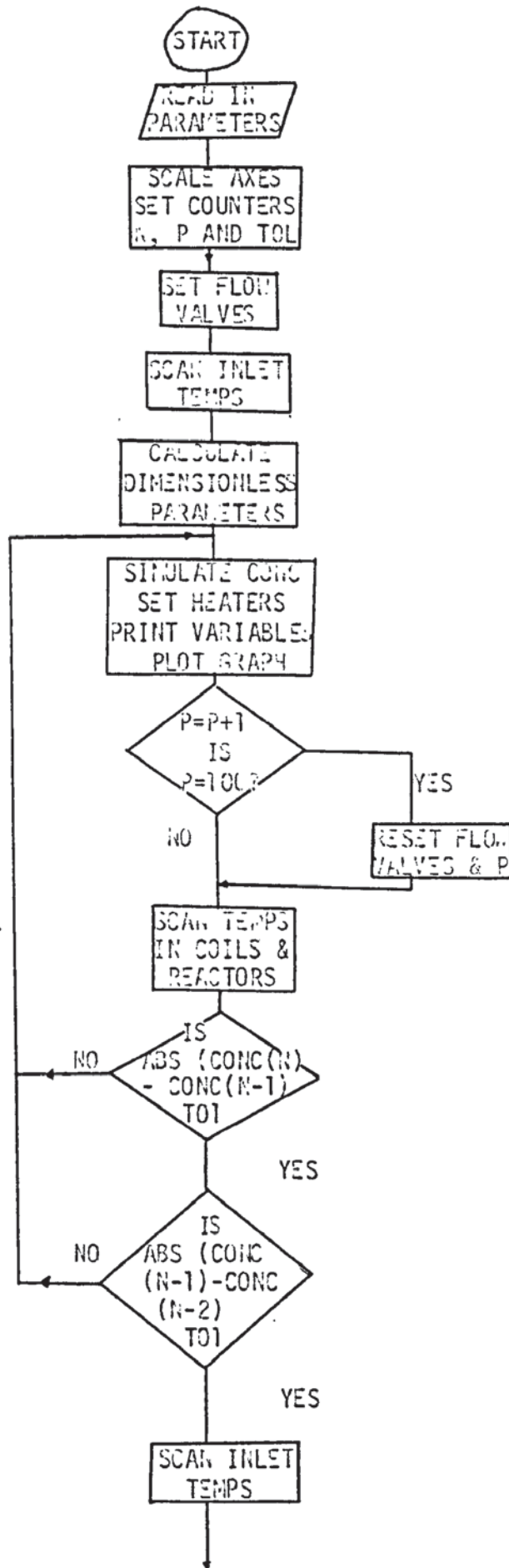

A.4.7.1 FLOW CHART FOR TOTAL SIMULATION PROGRAMME

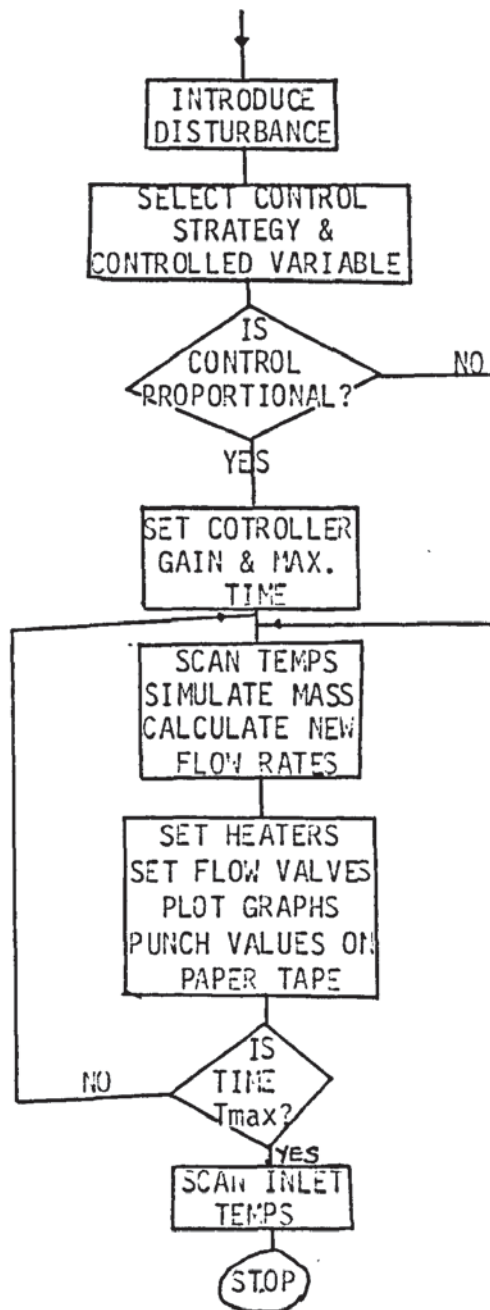




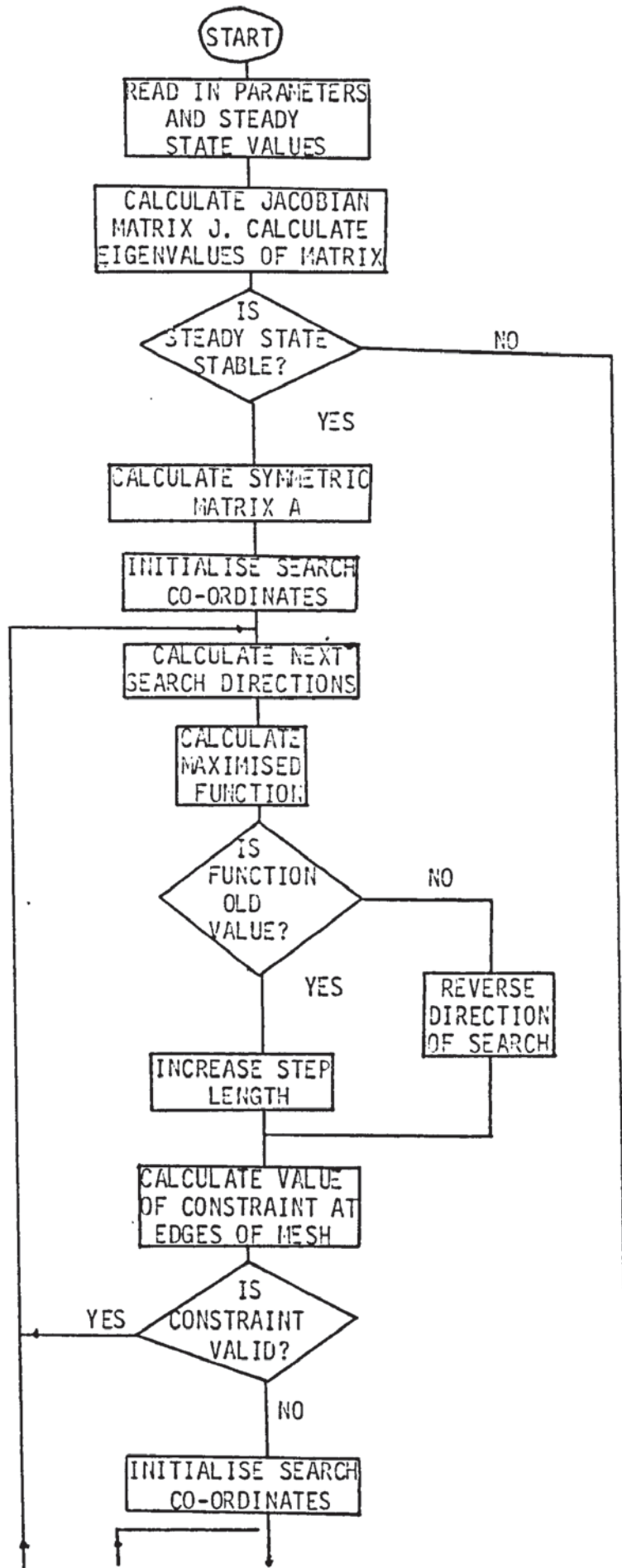


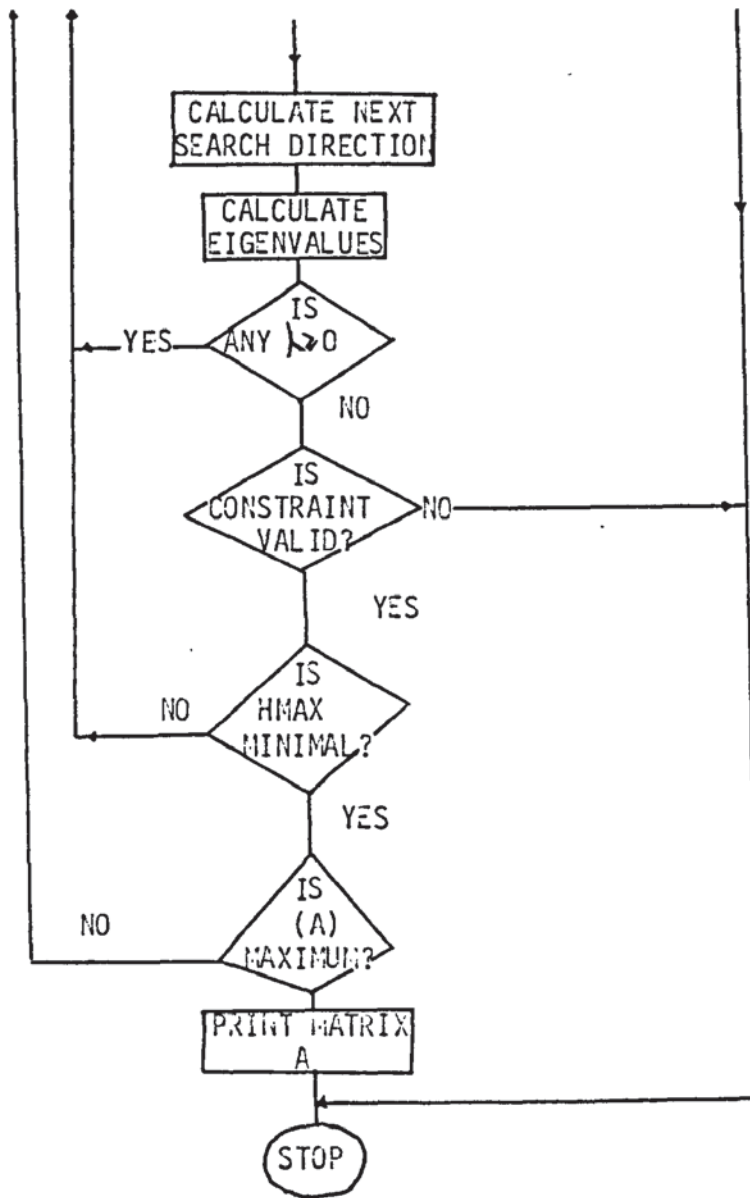
A.4.7.2 FLOW CHART OF ON-LINE SIMULATION PROGRAMME

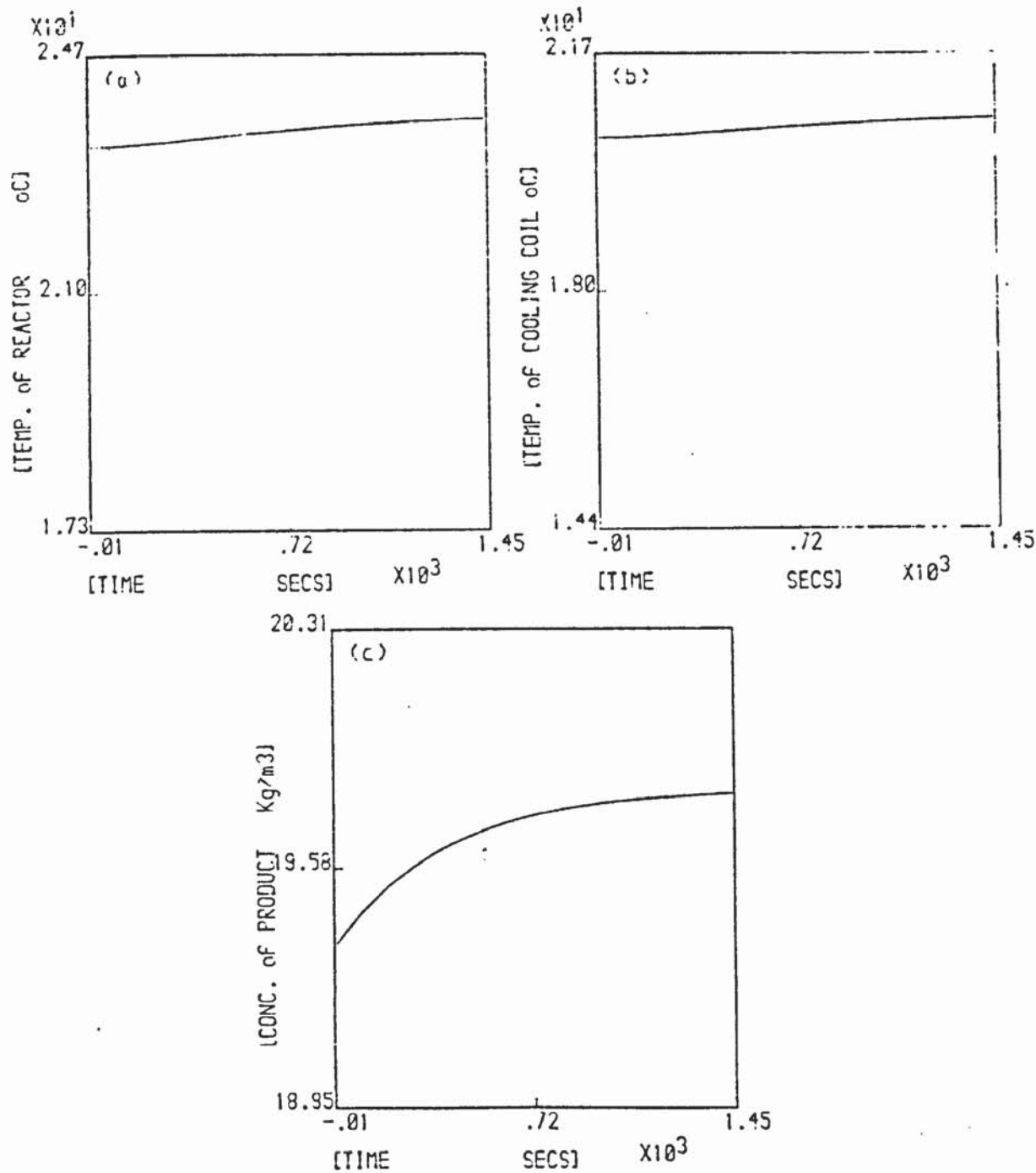




A.4.7.3 FLOW CHART OF LYAPUNOV FUNCTION PROGRAMME

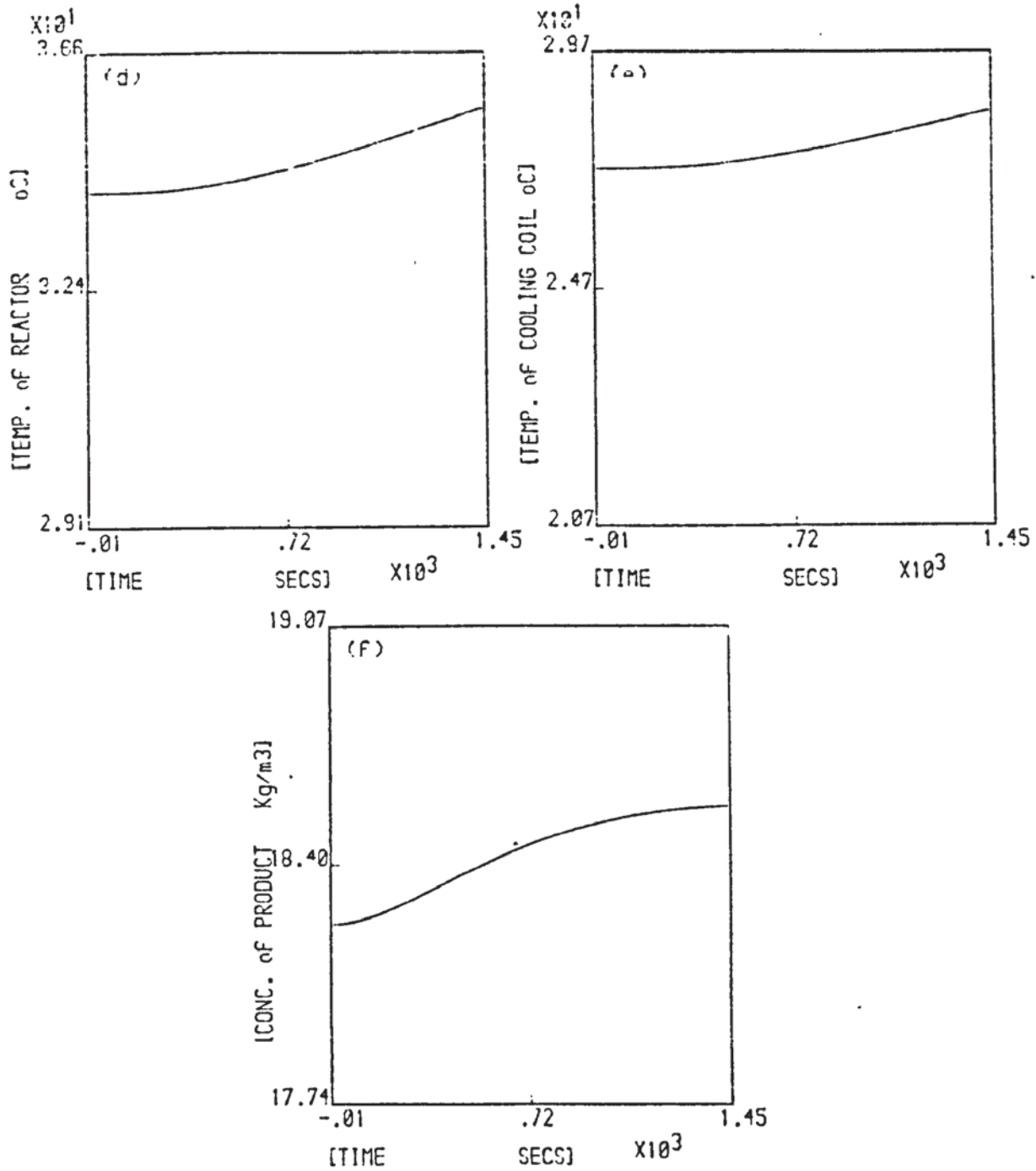






Step in Feed concentration (0.5 kg/m^3),
 Open loop stable steady state.

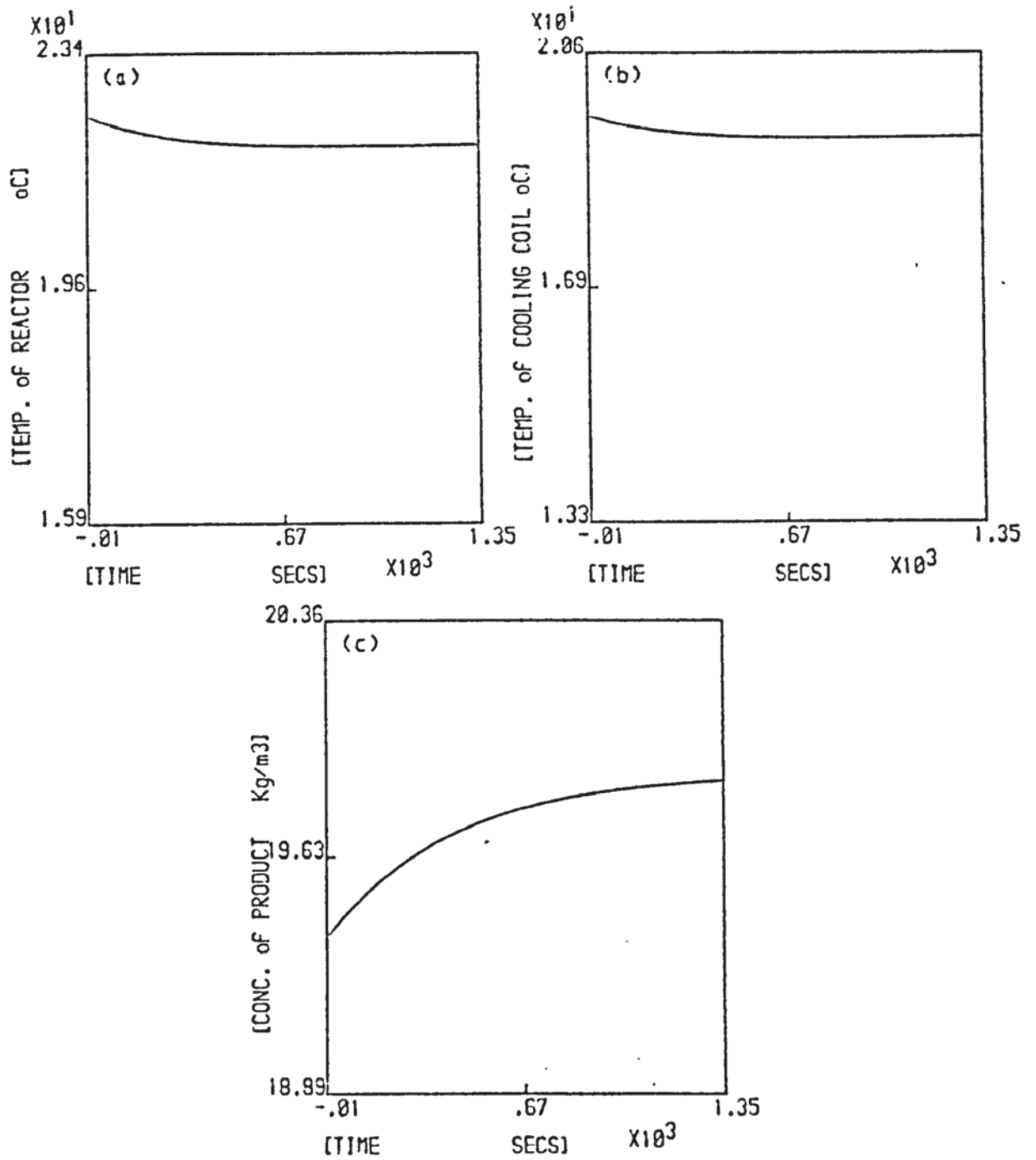
Fig A.6.1.1 Reactor One. Experiment no: i



Step in Feed concentration (0.5 kg/m^3).

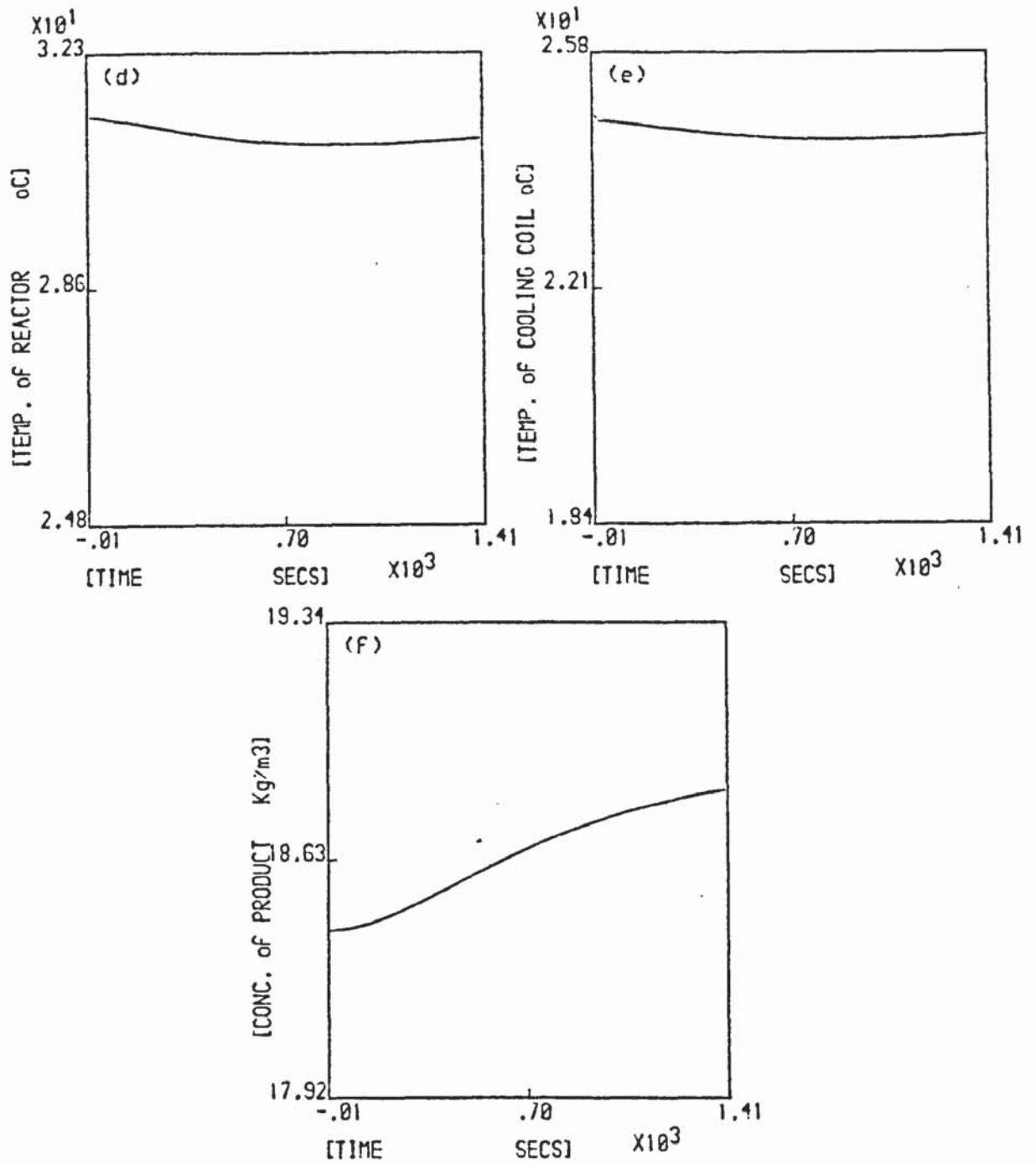
No control.

Fig A.6.1.1 Reactor Two. Experiment no: 1



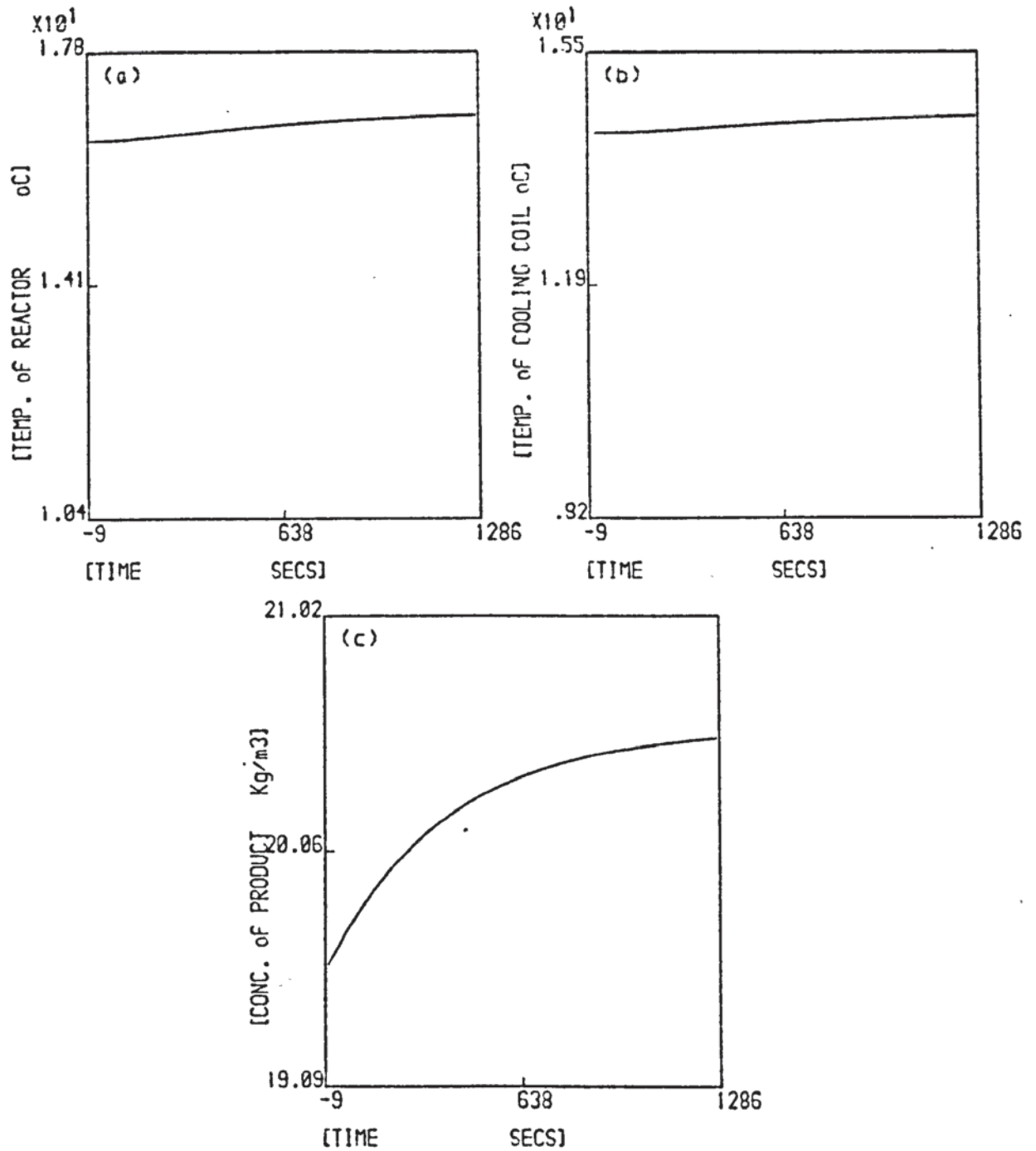
Step in feed concentration (0.5 kg/m^3) & inlet reactor temperature (-0.9 K). No control.

Fig A.6.1.2 Reactor One. Experiment no: 2



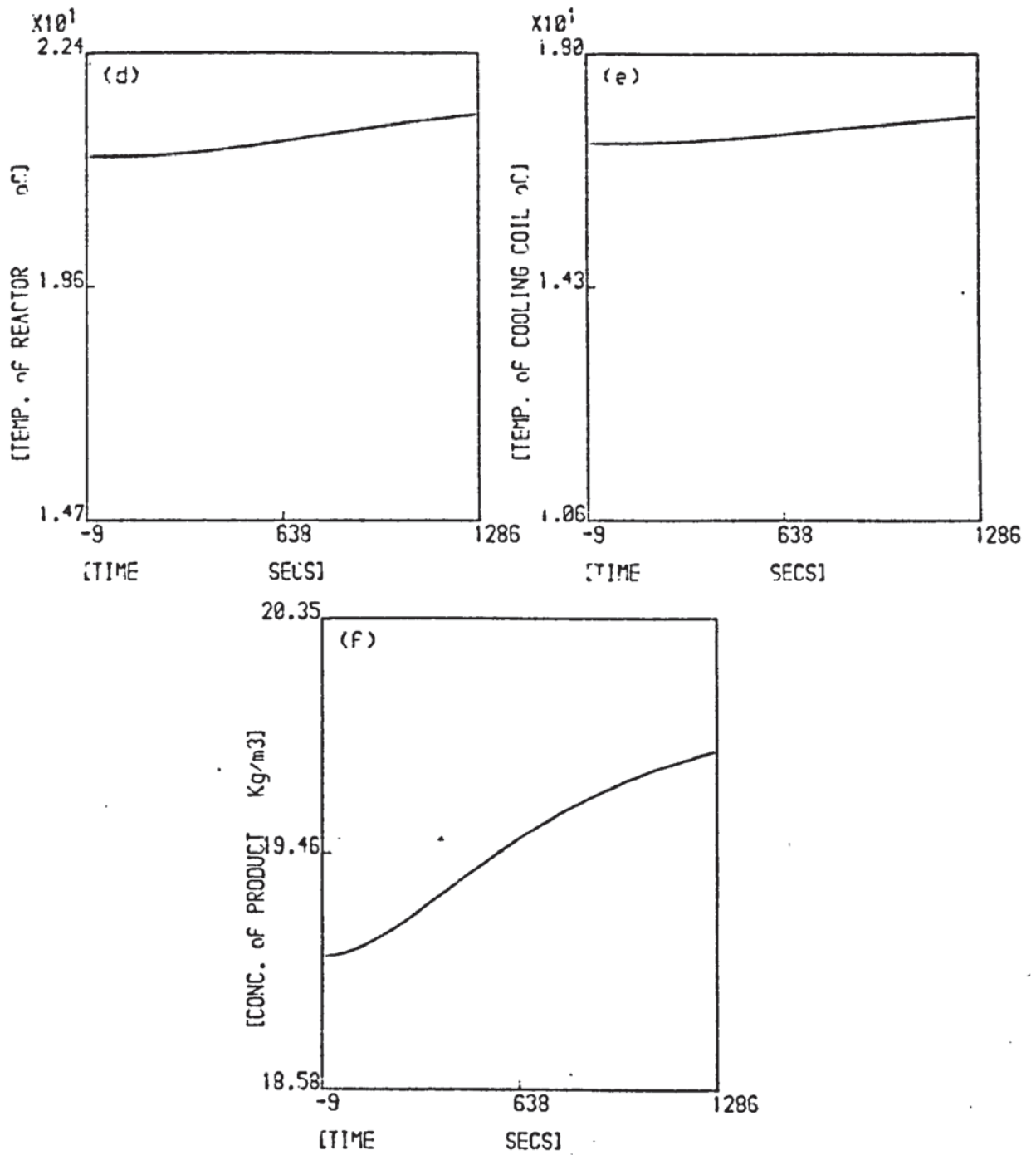
Step in feed concentration (0.5 kg/m^3) & inlet cooling coil temperature (-0.2°K). No control.

Fig.A.6.i.2 Reactor Two. Experiment no: 2



Step in feed concentration(1.0kg/m³),
 No control.

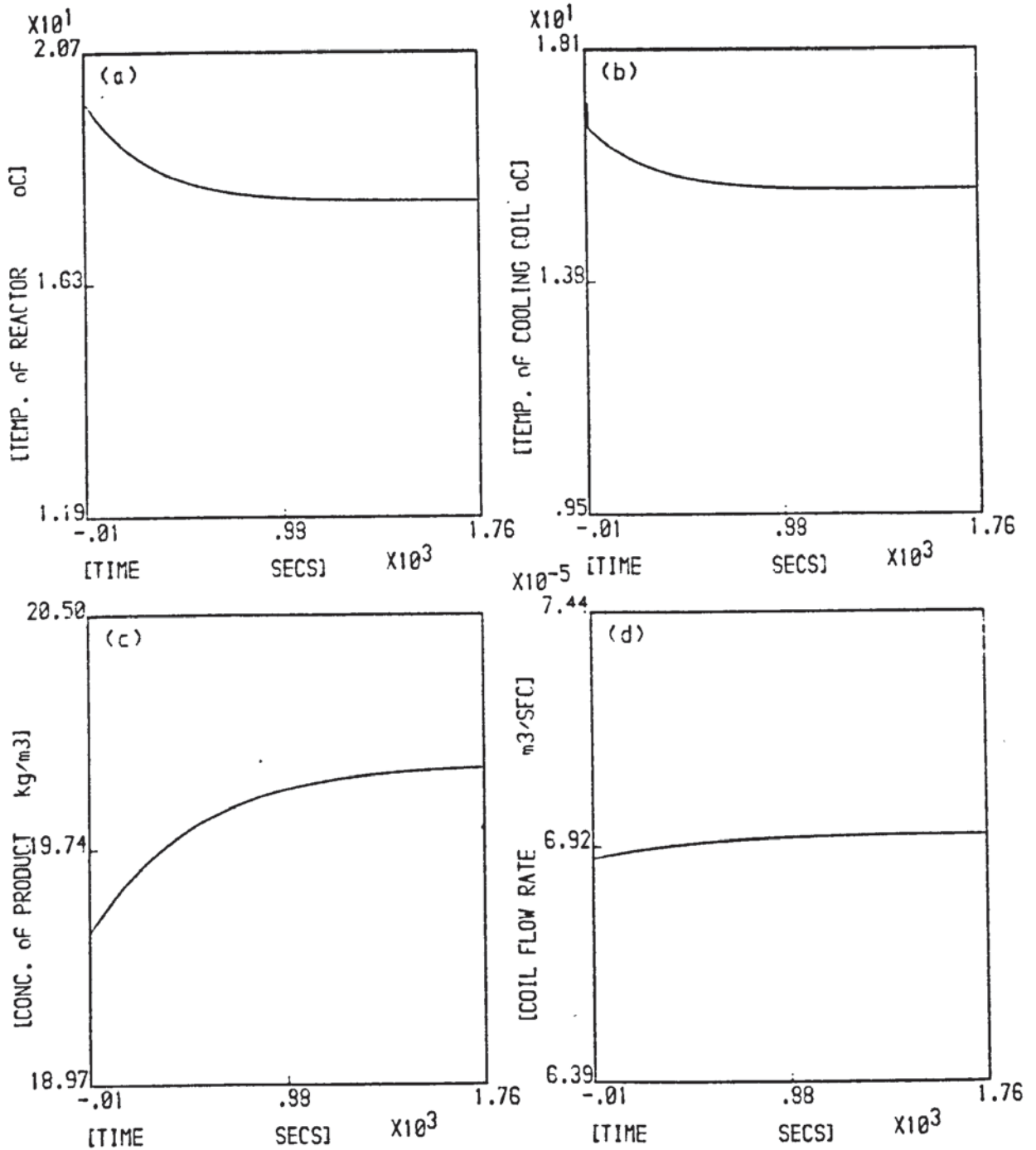
Fig A.6.i.3 Reactor One. Experiment no: 3



Step in feed concentration (1.0 kg/m^3).

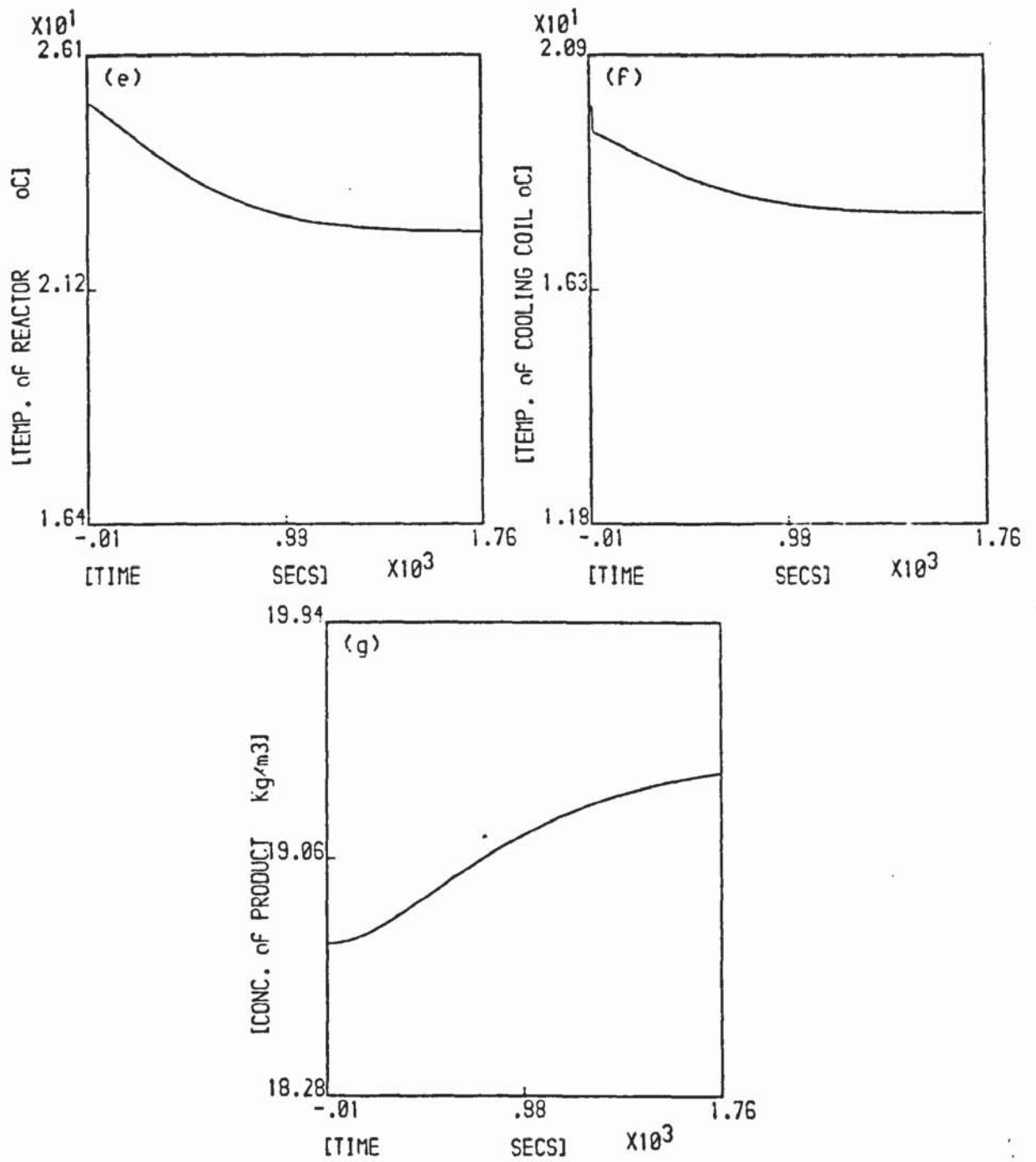
No control.

Fig A.C.1.3 Reactor Two. Experiment no: 3



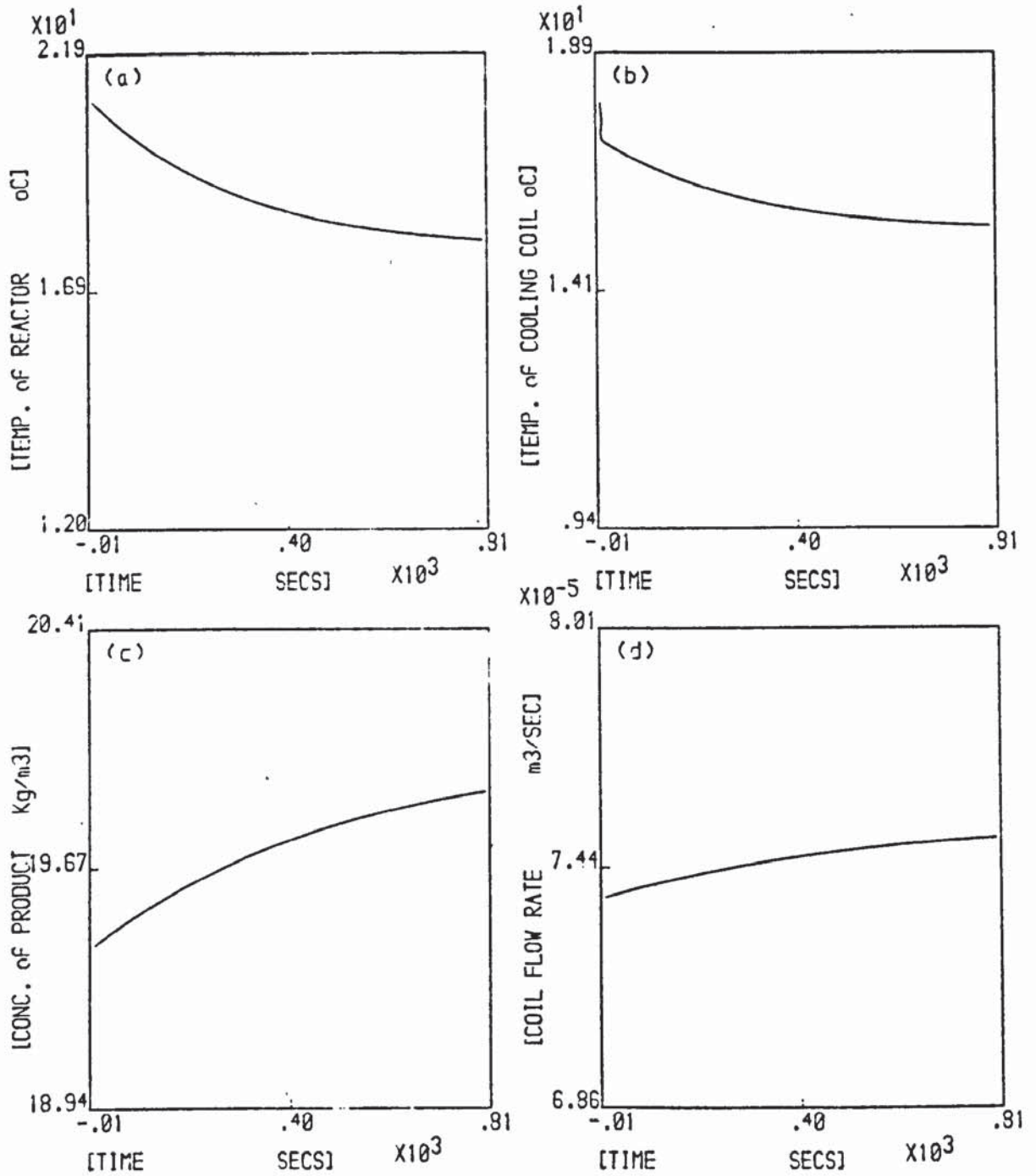
183

Step in feed conc. (0.5 kg/m^3) & inlet reactor (-1.3 K) & coil (-1.26 K) temperatures. Prop. Feedback control of reactant conc. $K_c = 1 \text{ E} - 06$
 Fig. A.6.1.4 Reactor One. Experiment no: 4

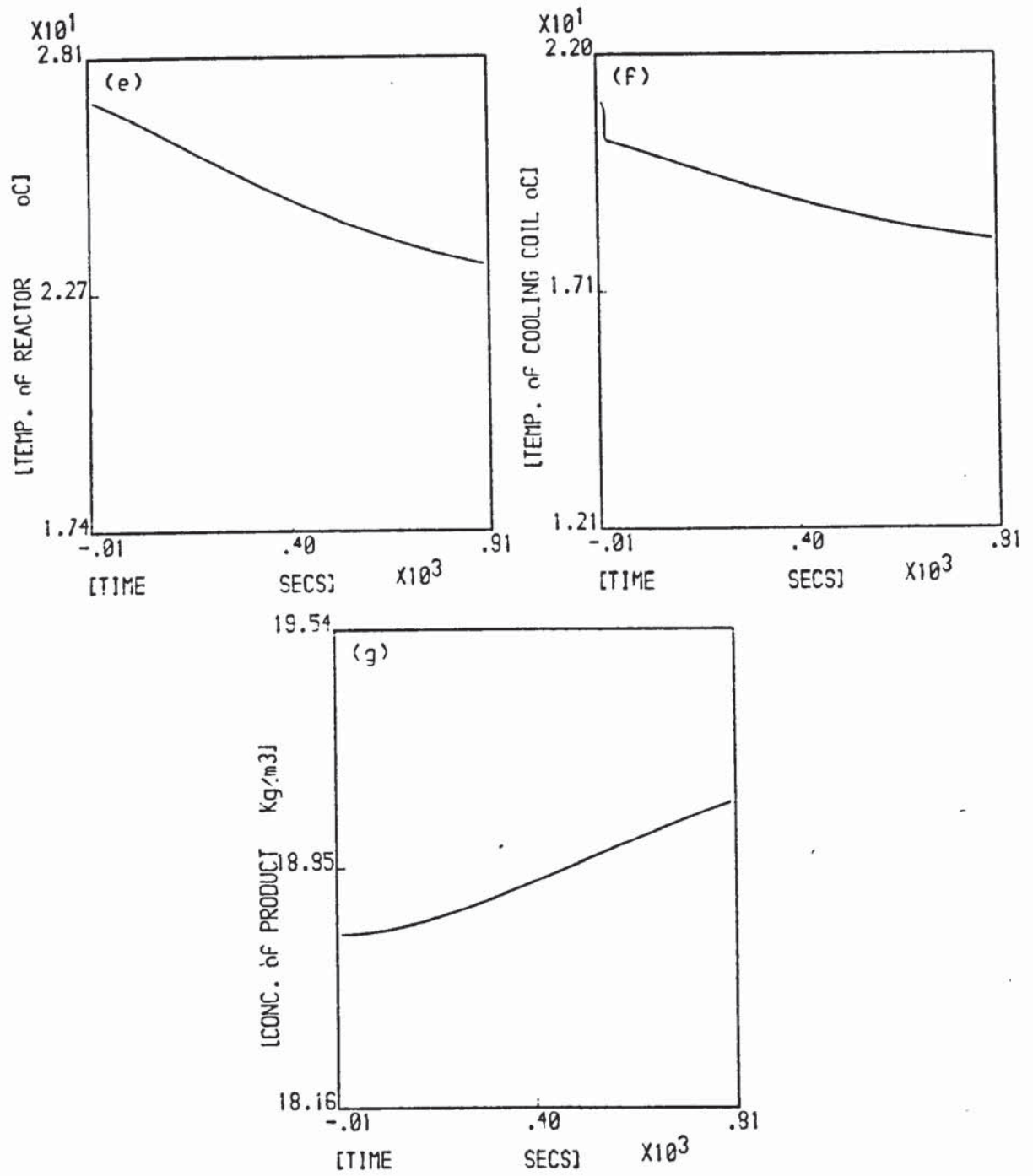


Step in inlet temperature of cooling coil (-1.23°K). No control of state variables.

Fig. A.6.1.4 Reactor Two. Experiment no: 4

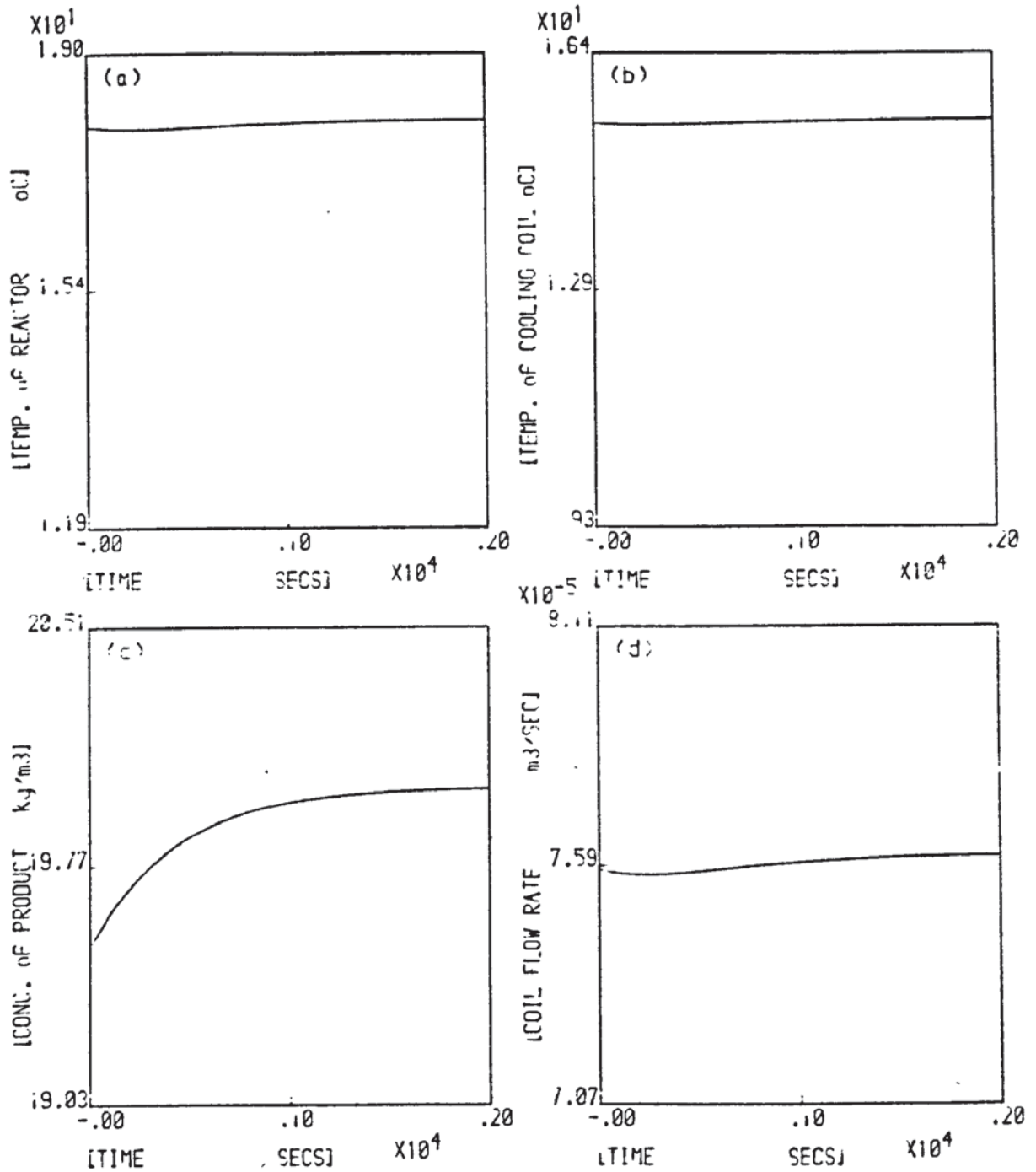


Step in feed conc.(0.5kg/m³) & inlet reactor (-2.1 K) & coil(-1.93 K) temperatures. Prop. Feedback control of reactant conc. Kc=3E-06
 Fig. A.6.i.5 Reactor One. Experiment no: 5

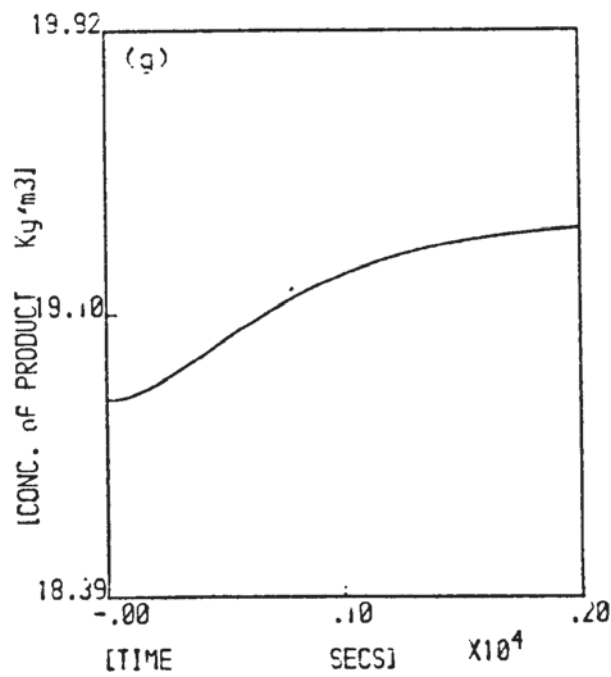
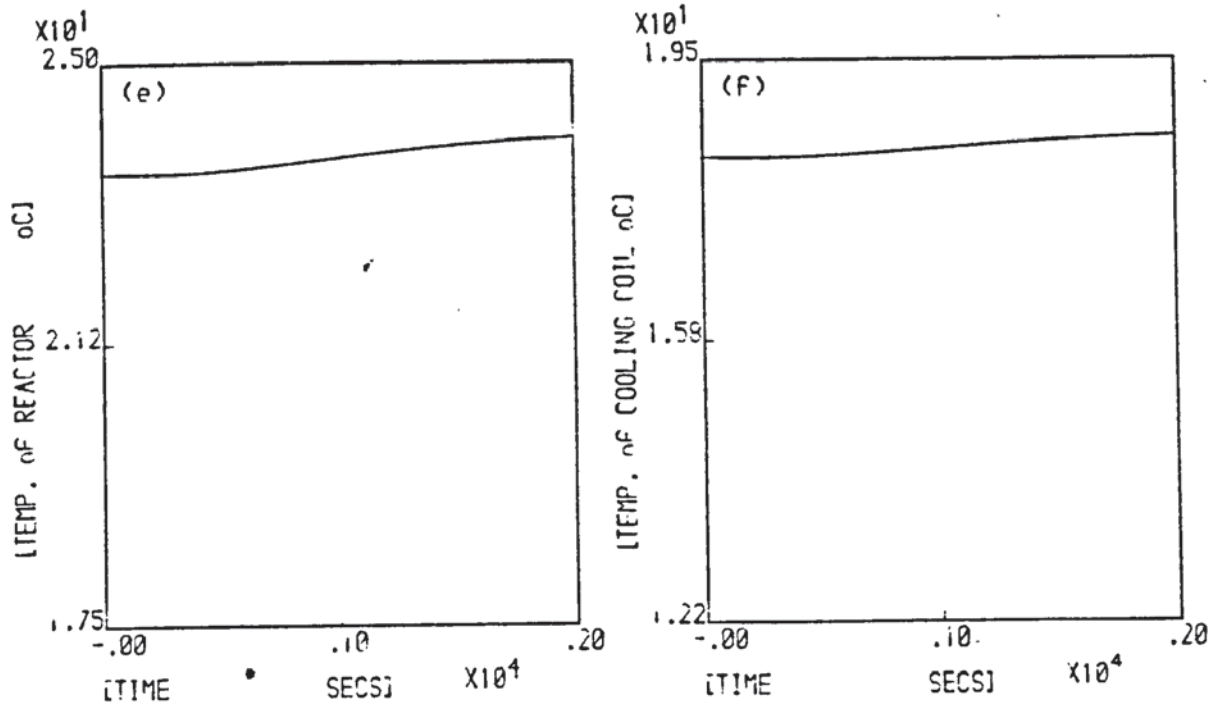


Step in cooling coil inlet temperature
 (-1.94 K). No control of state variables.

Fig. A.6.1.5 Reactor Two. Experiment no: 5

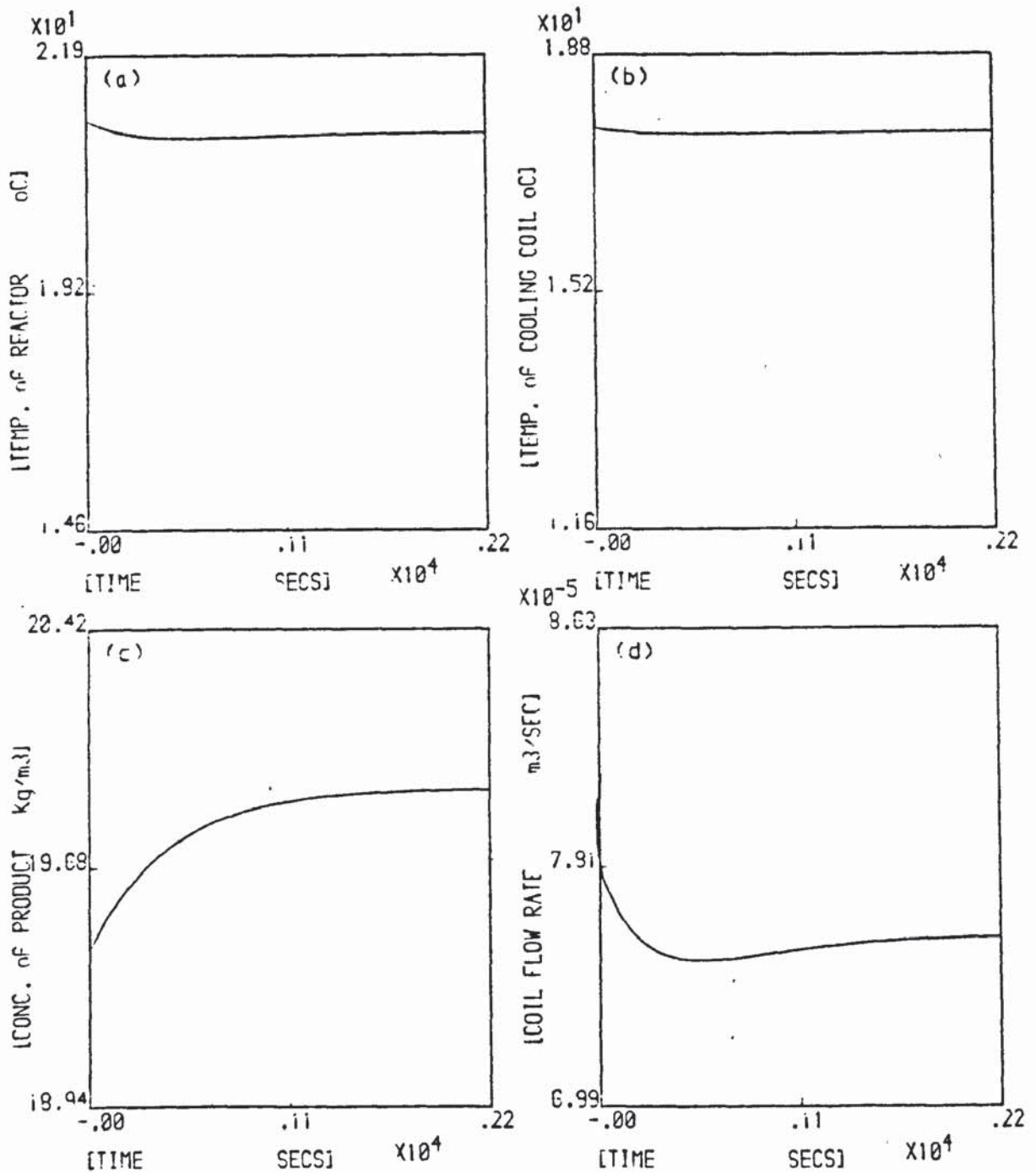


Step in Feed concentration ($.5\text{kg/m}^3$) and temperature (-0.2K). Proportional Feedback control of reactor temperature. $K_c=0.3\text{E}-05$
 Fig. A.G.1.6 Reactor One. Experiment no: 6

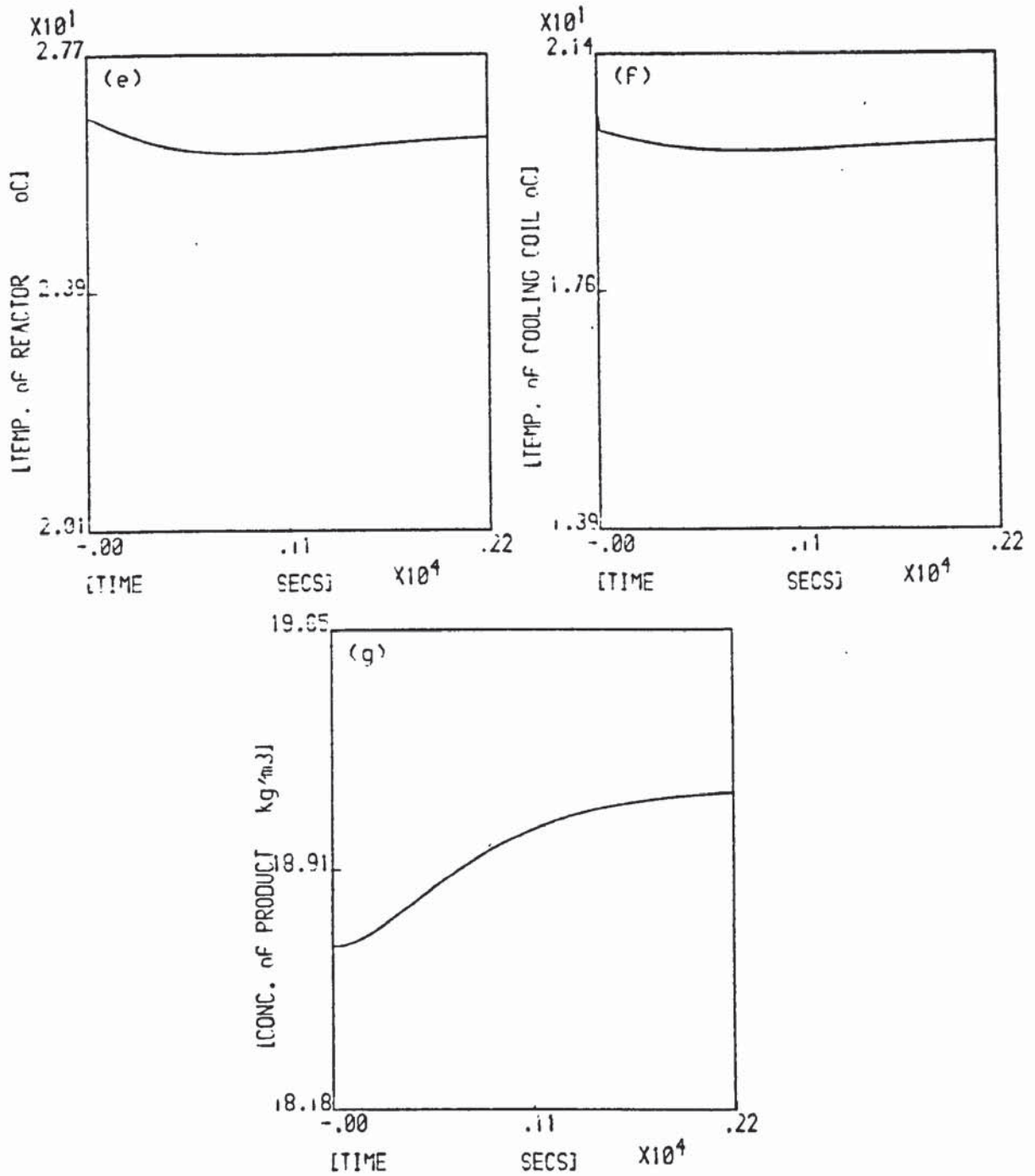


Disturbances are carry-overs From Reactor One. No control of state variables.

Fig. A.G.i.6 Reactor Two. Experiment no: 6

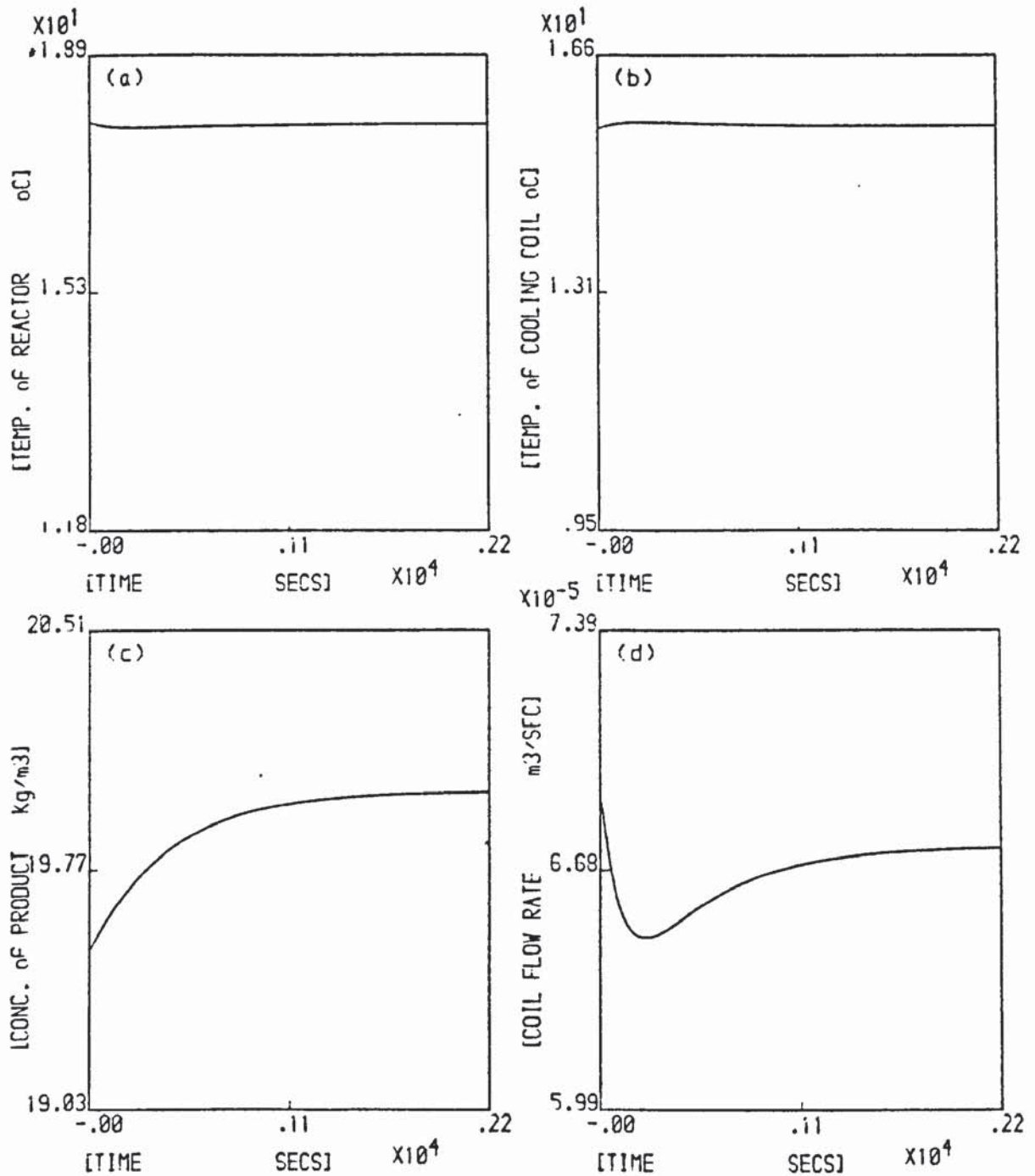


Step in Feed conc. (0.5 kg/m^3) and inlet coil (-1.5°K) temperature. Proportional feedback control of coil temperature. $K_c = 0.3E-04$
 Fig. 1.6.1.7 Reactor One. Experiment no: 7

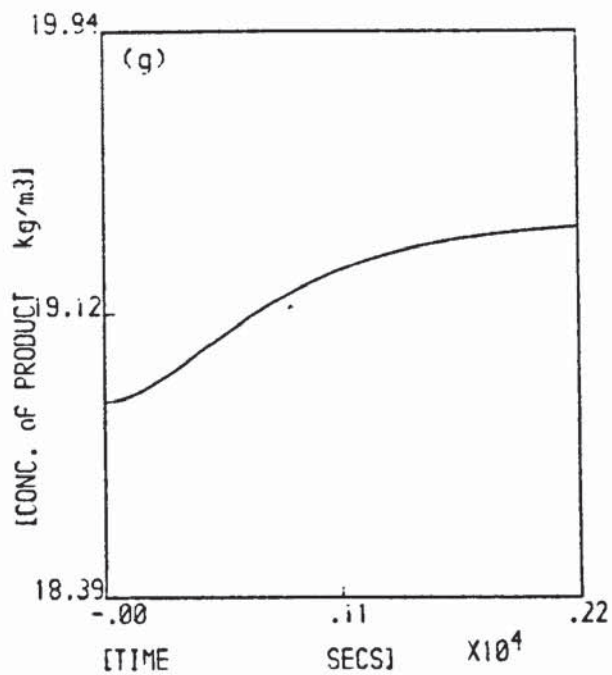
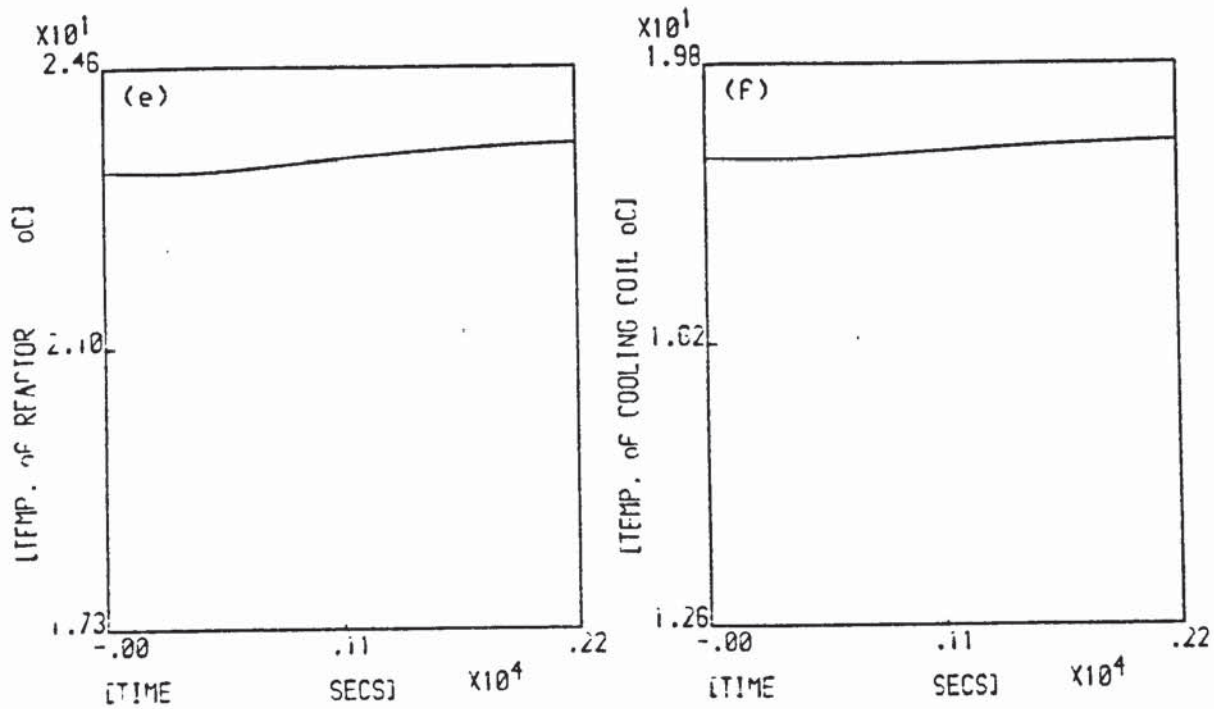


Step in inlet temperature to cooling coil
 (-0.5 K). No control of state variables.

Fig. A.6.1.7 Reactor Two. Experiment no: 7

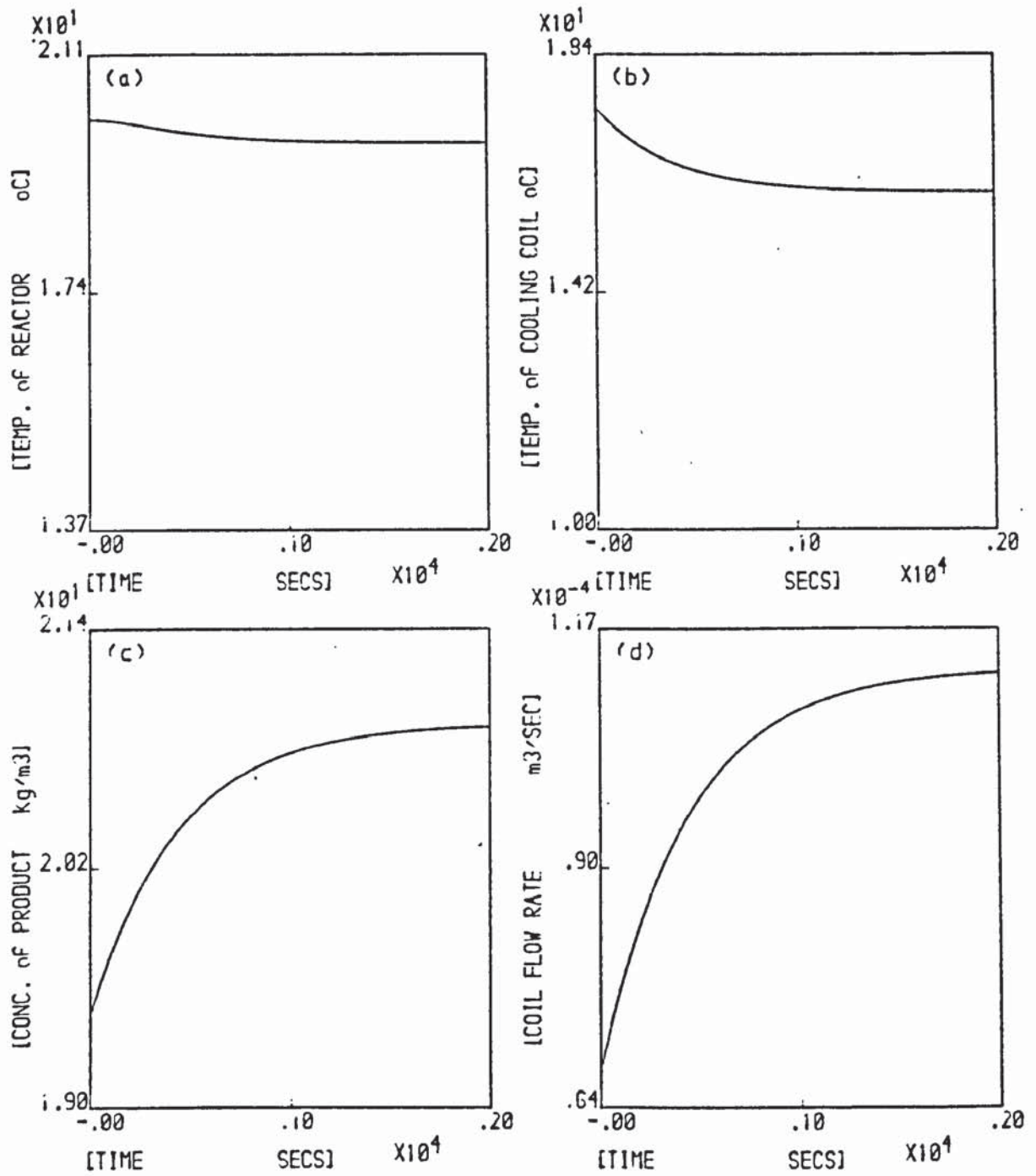


Step in feed conc. (0.5 kg/m^3) and temperature (-0.4632 K). Proportional feedback control of reactor temperature. $K_c = 0.5E-04$
 Fig. 1.6.1.9 Reactor One. Experiment no: 8A



Disturbances From Reactor One only.
 No control of state variables.

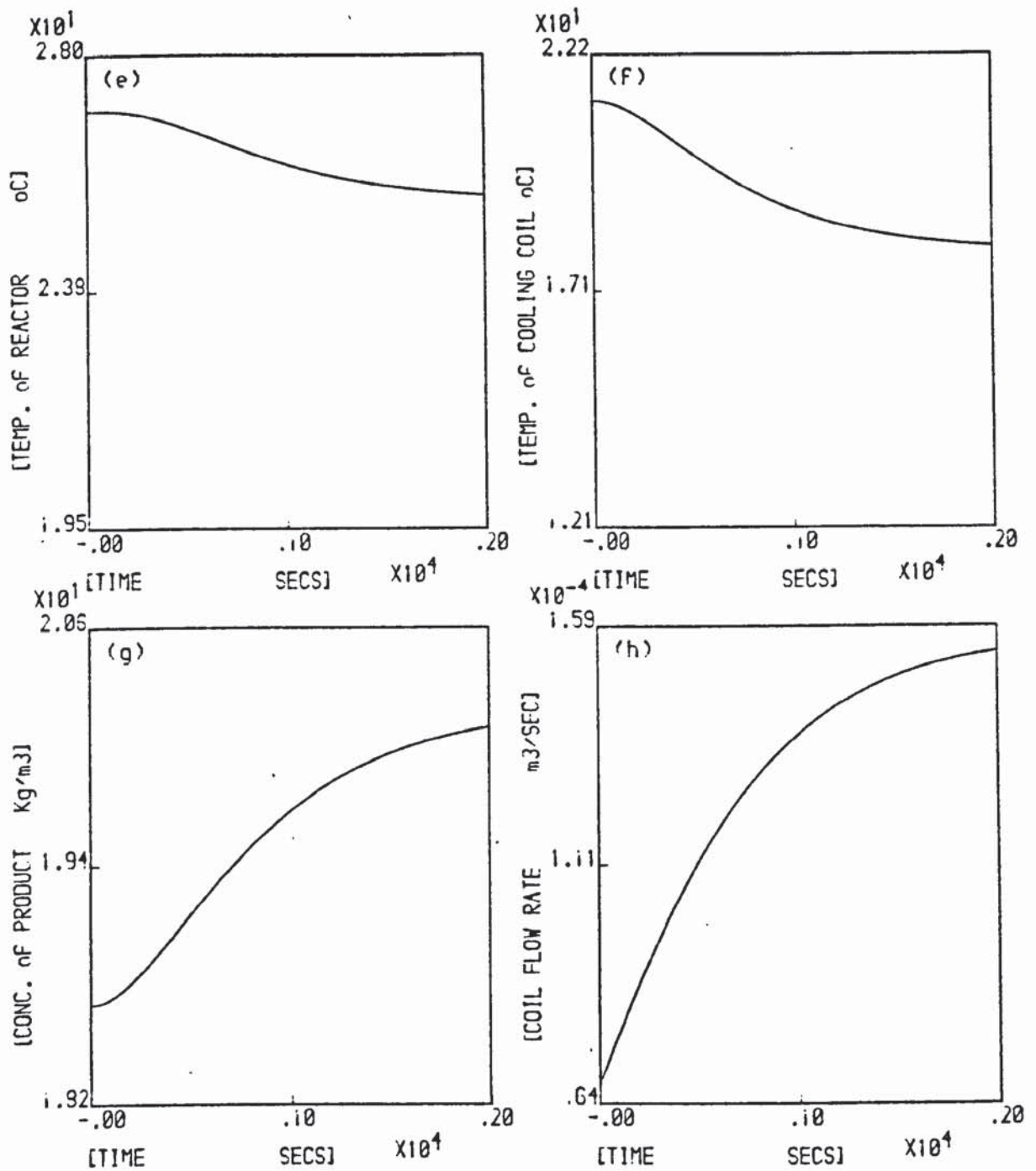
Fig. A.6.1.8 Reactor Two. Experiment no: 9A



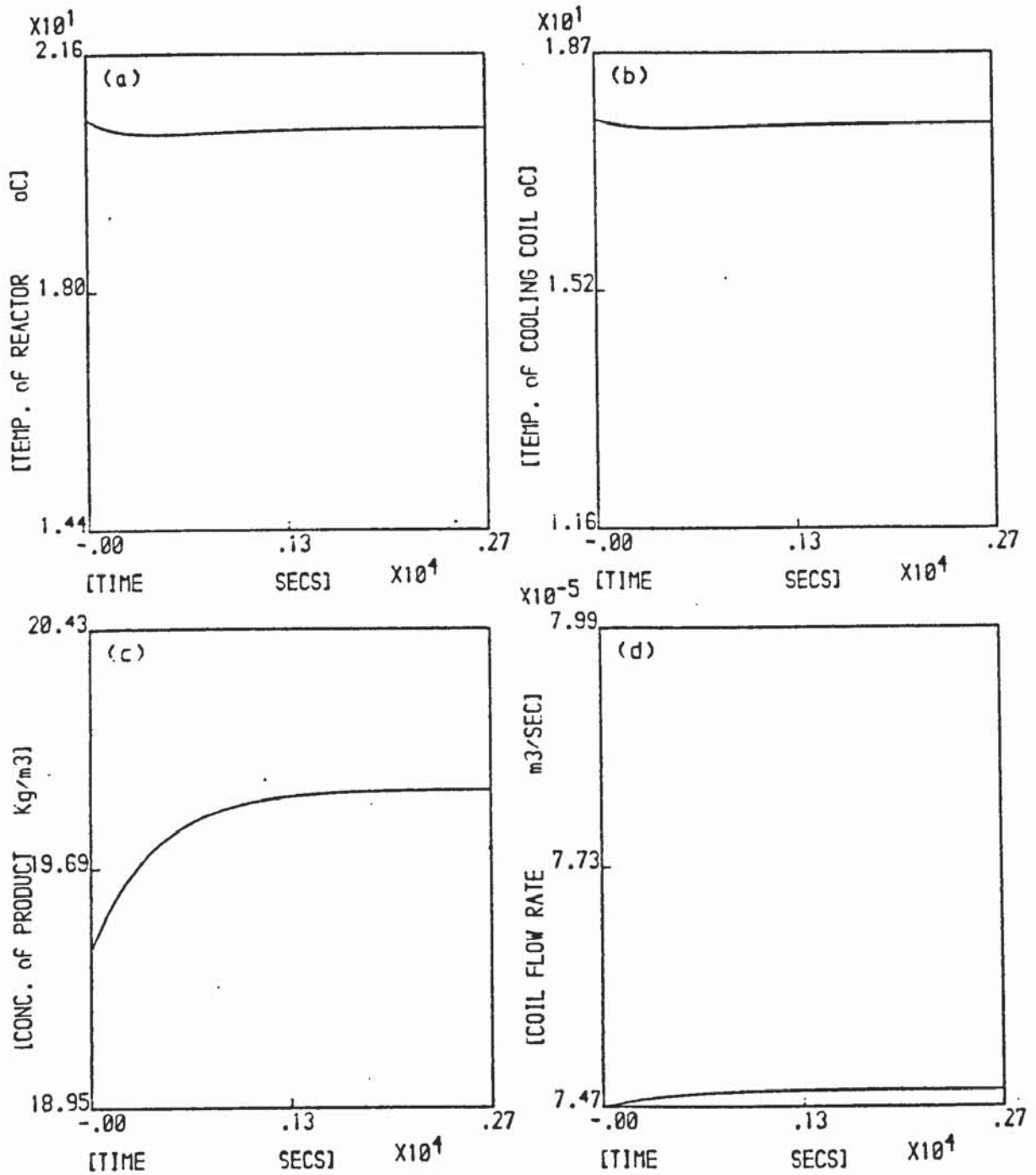
Step in feed concentration (1.5 kg/m^3).

Proportional feedback control of reactant concentration. $K_c = 0.3E-04$

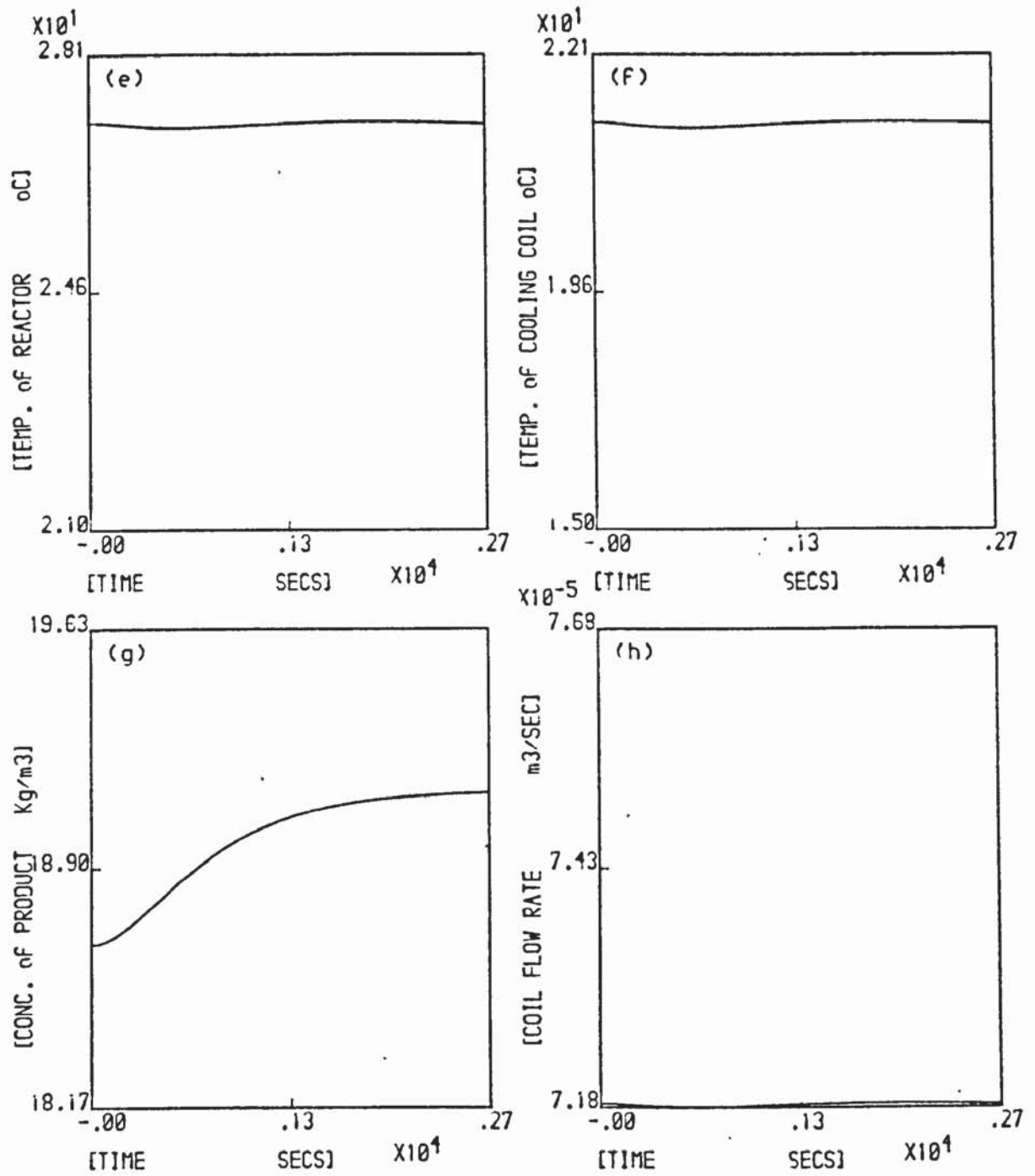
Fig. 4.6.1.9 Reactor One. Experiment no: 9



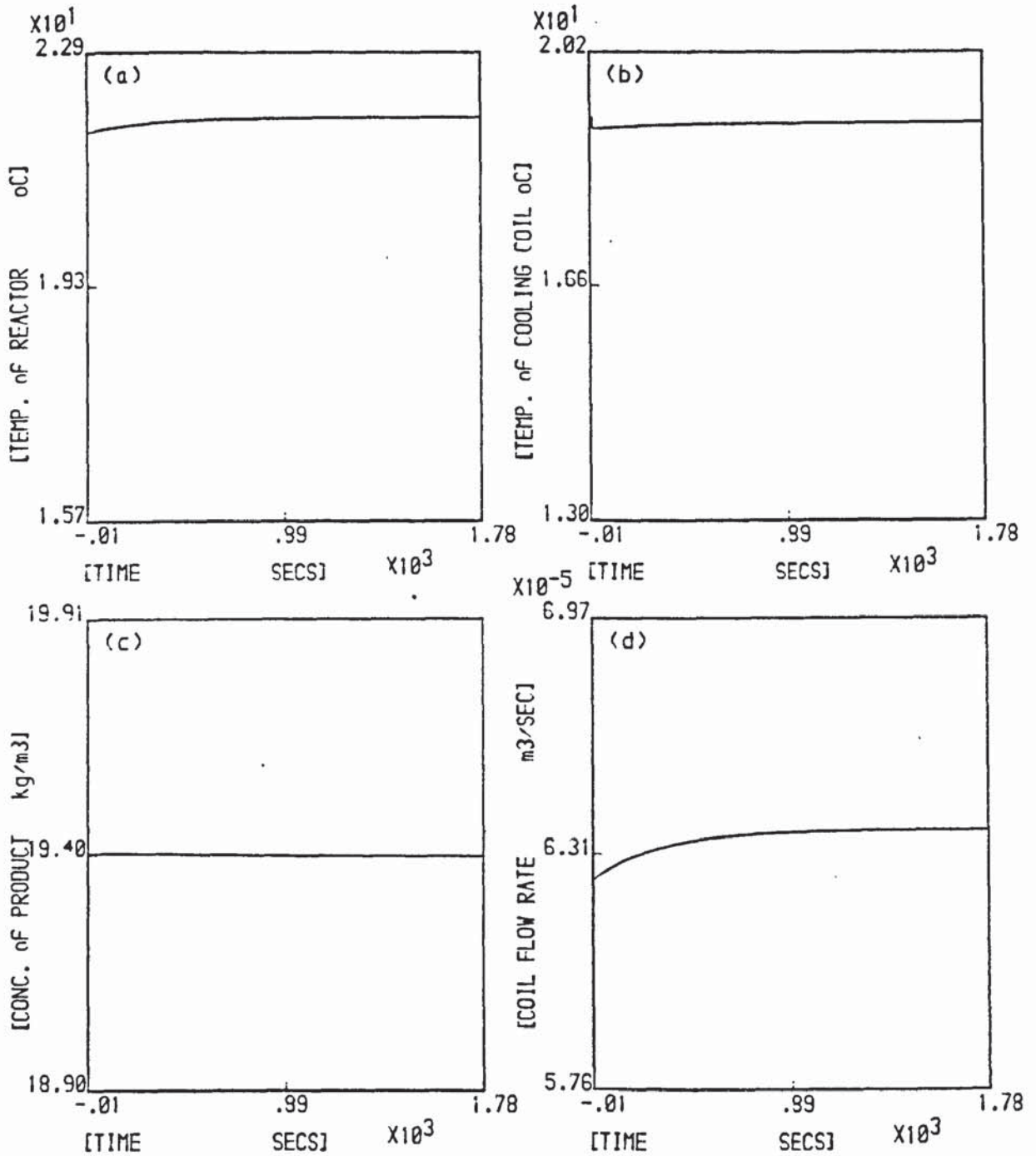
Disturbances from First reactor only.
 Proportional feedback control of reactant
 concentration.
 Fig. A.6.i.9 Reactor Two. Experiment no: 9



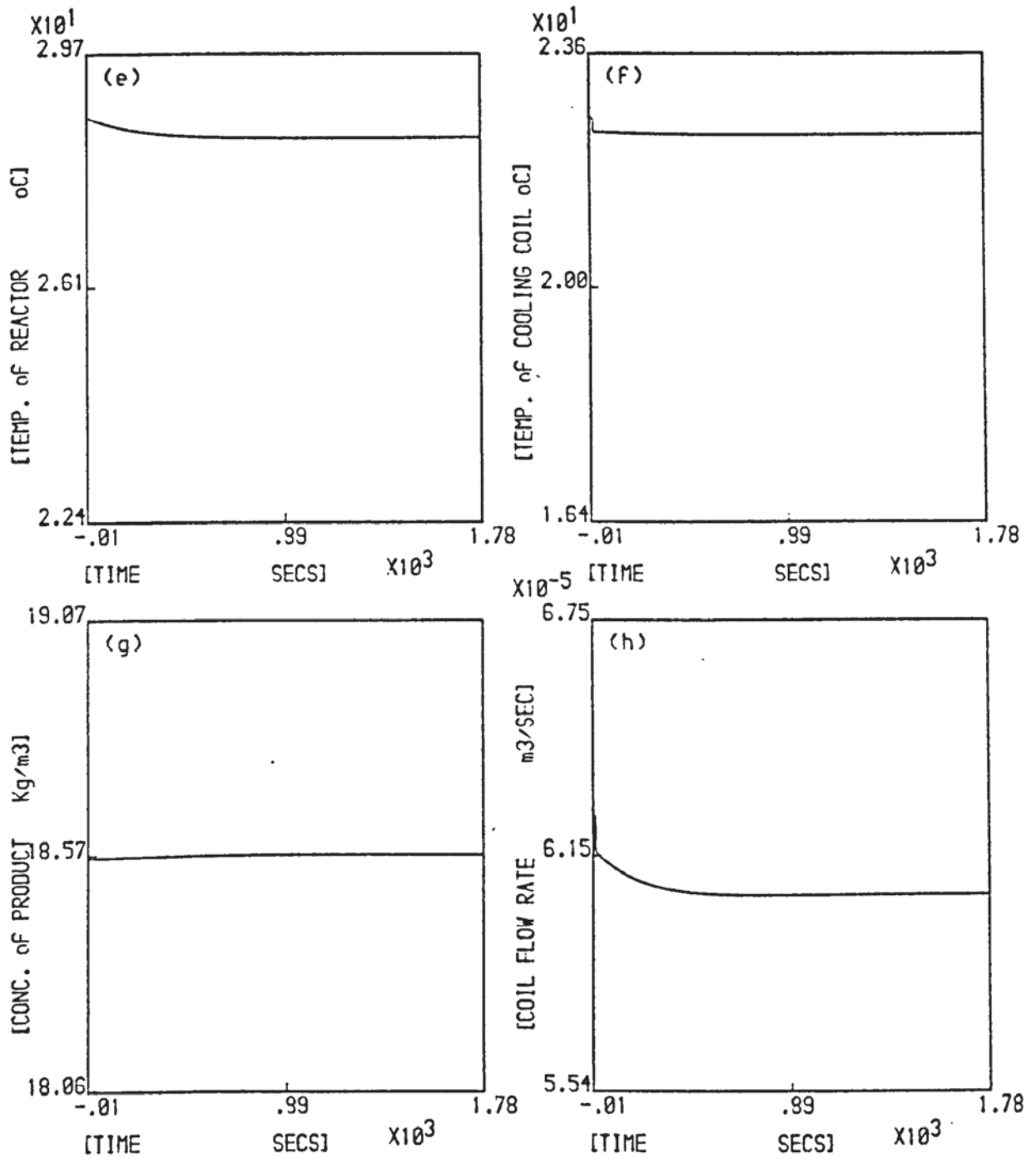
Step in feed concentration(0.5kg/m³) and reactor(-0.58 K) temperature. Proportional control of reactor concentration. Kc=5E-07
 Fig. A.6.1.10 Reactor One. Experiment no: 10



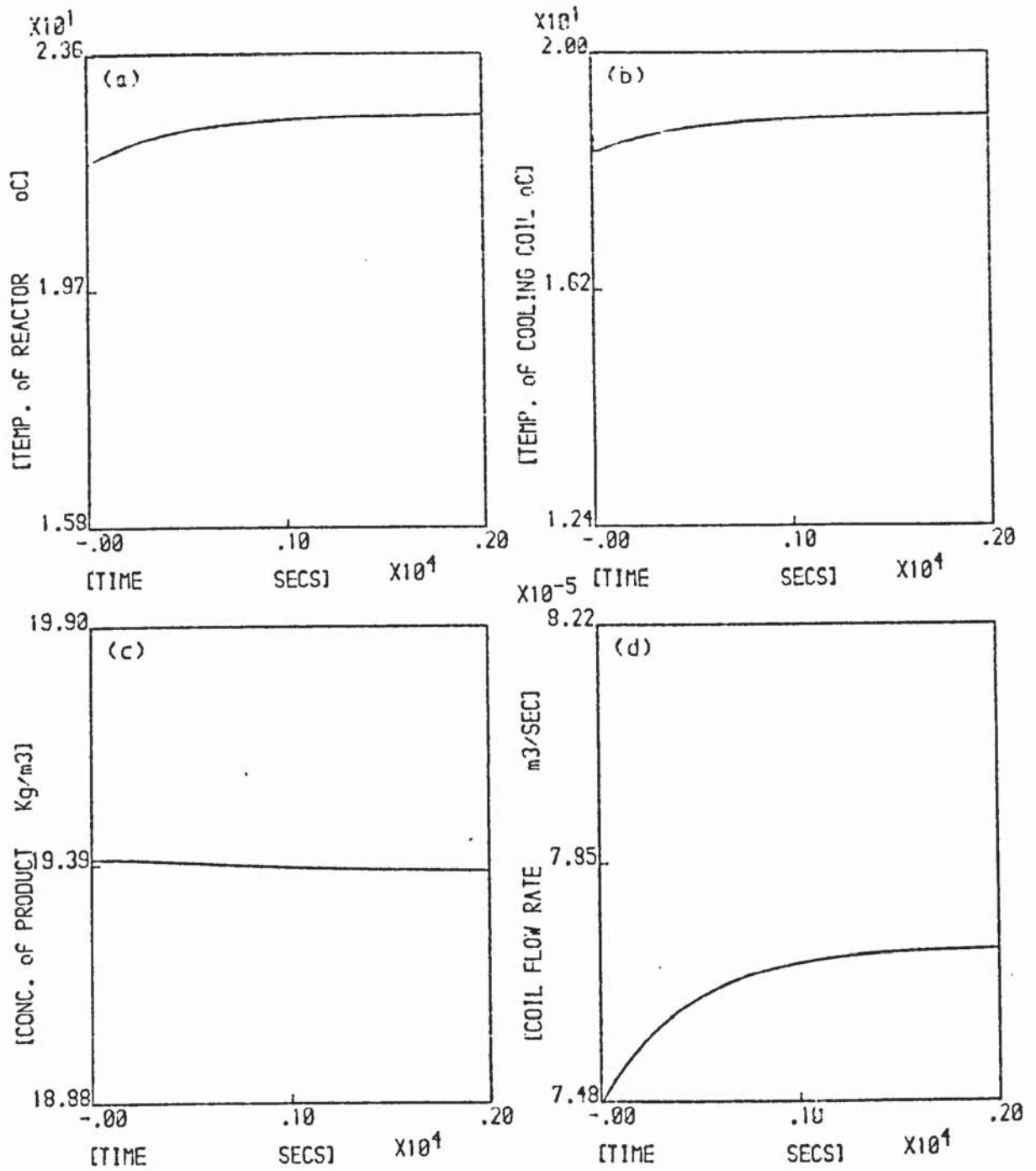
Disturbances introduced from first reactor only. Proportional control of reactor temperature. $K_c=5E-07$
 Fig. A.6.1.10 Reactor Two. Experiment no: 10



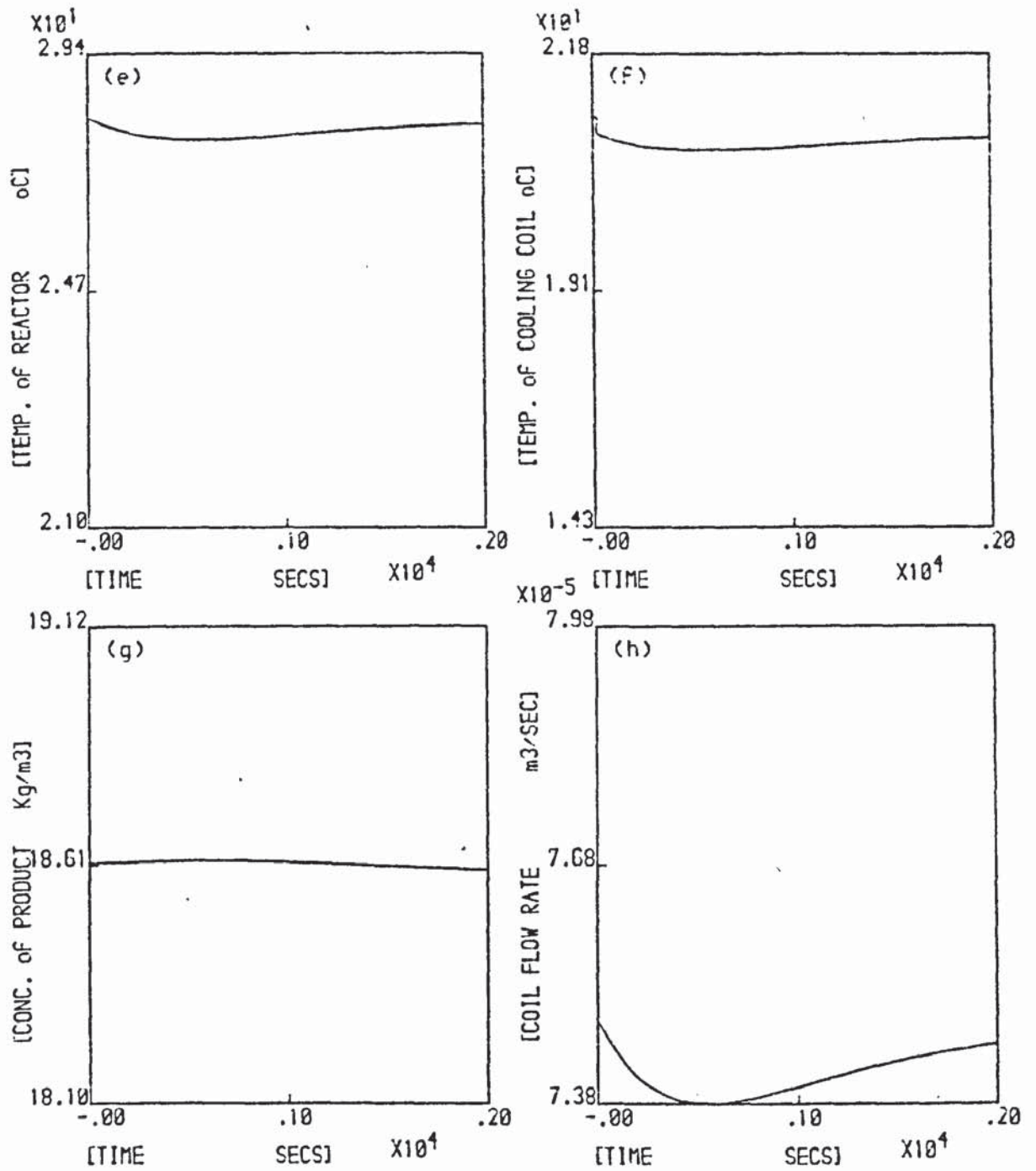
Step in inlet reactor(1.014 K) & cooling coil (-.58 K) temperatures. Proportional Feedback control of reactor temperature. $K_c=5E-06$
 Fig. 1.6.1.11 Reactor One. Experiment no: 11



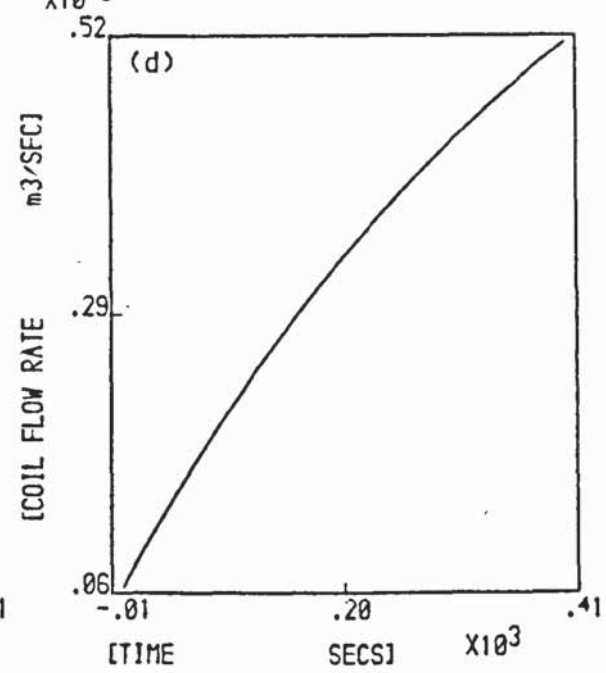
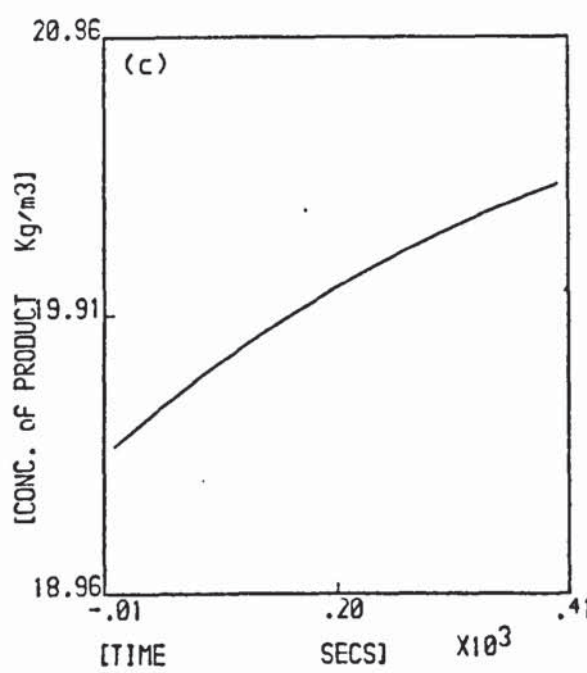
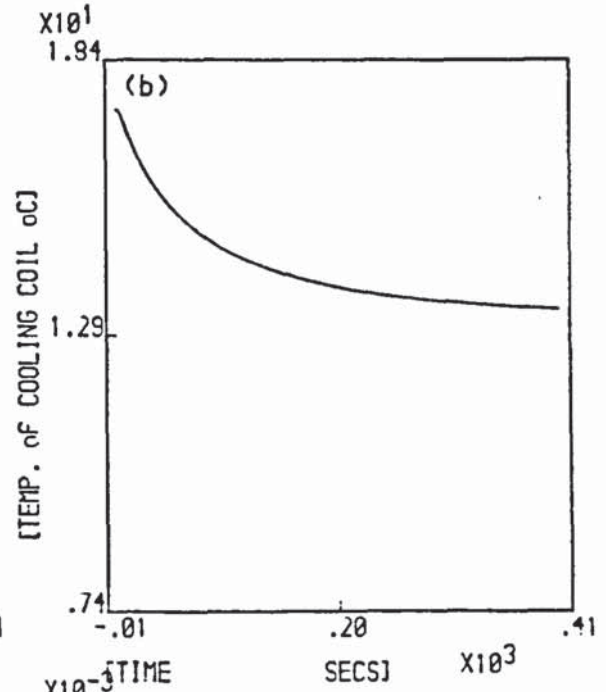
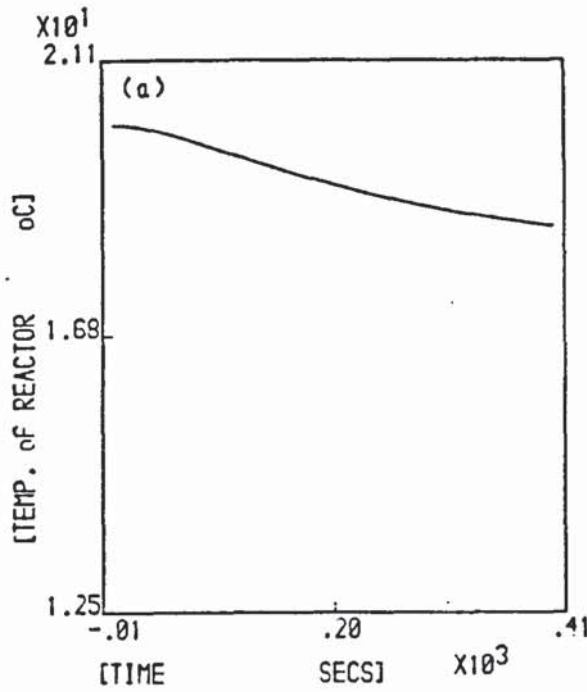
Step in inlet cooling coil(-.61 K) temperature
 Proportional Feedback control of reactor
 temperature. $K_c=5E-06$
 Fig. A.G.1.11 Reactor Two. Experiment no: 11



Step in inlet reactor(1.614 K) & cooling coil (-0.65 K) temperatures. Proportional control of reactor temperature. $K_c=0.3E-05$
 Fig A.G.1.12 Reactor One. Experiment no: 12



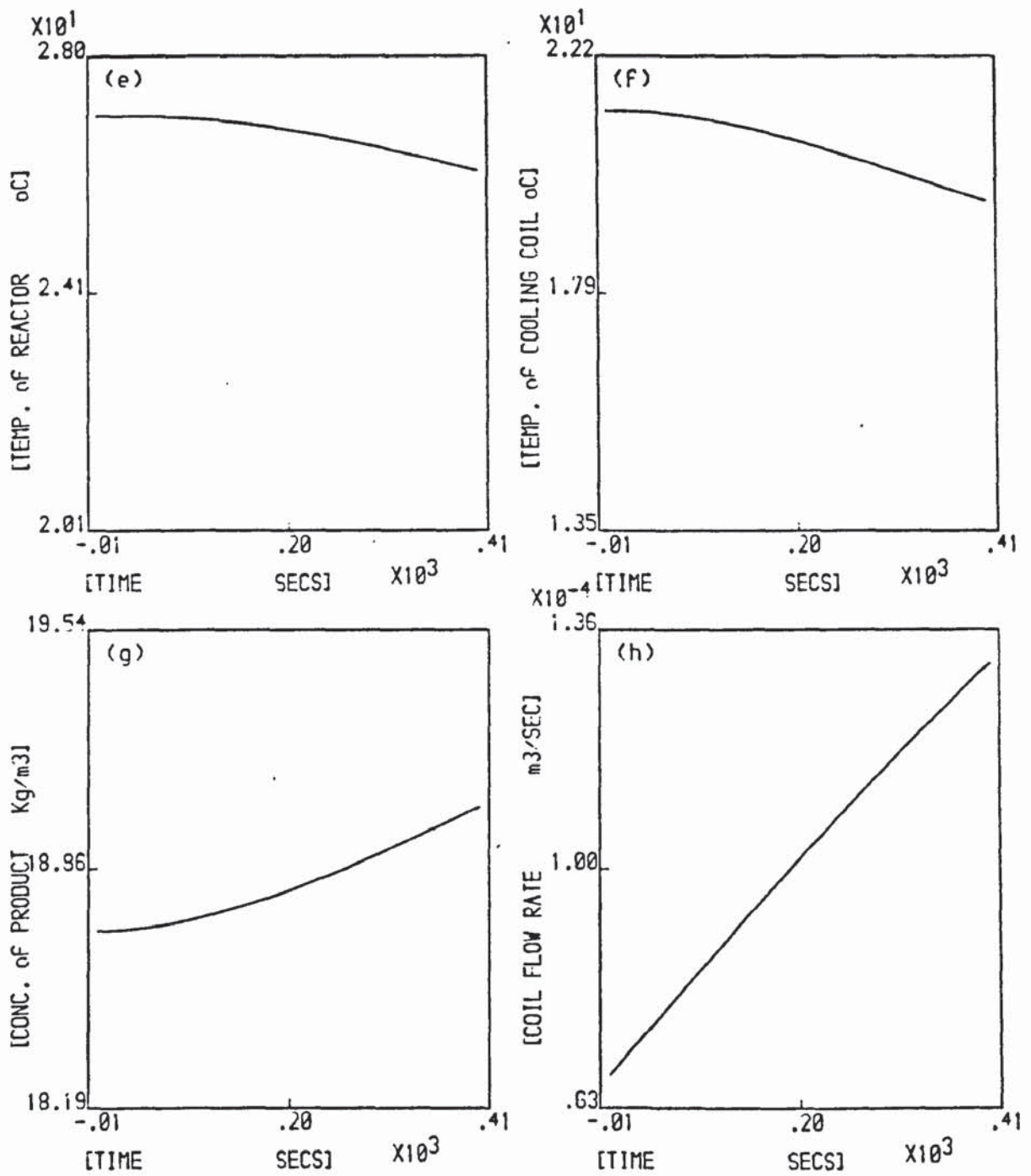
Step in cooling coil temperature(-0.652 K).
 Proportional control of reactor temperature.
 $K_c=0.3E-05$
 Fig A.6.1.12 Reactor Two. Experiment no: 12



Step in feed concentration (1.5 kg/m^3).

Proportional feedback control of reactant concentration. $K_c = 0.5E-03$

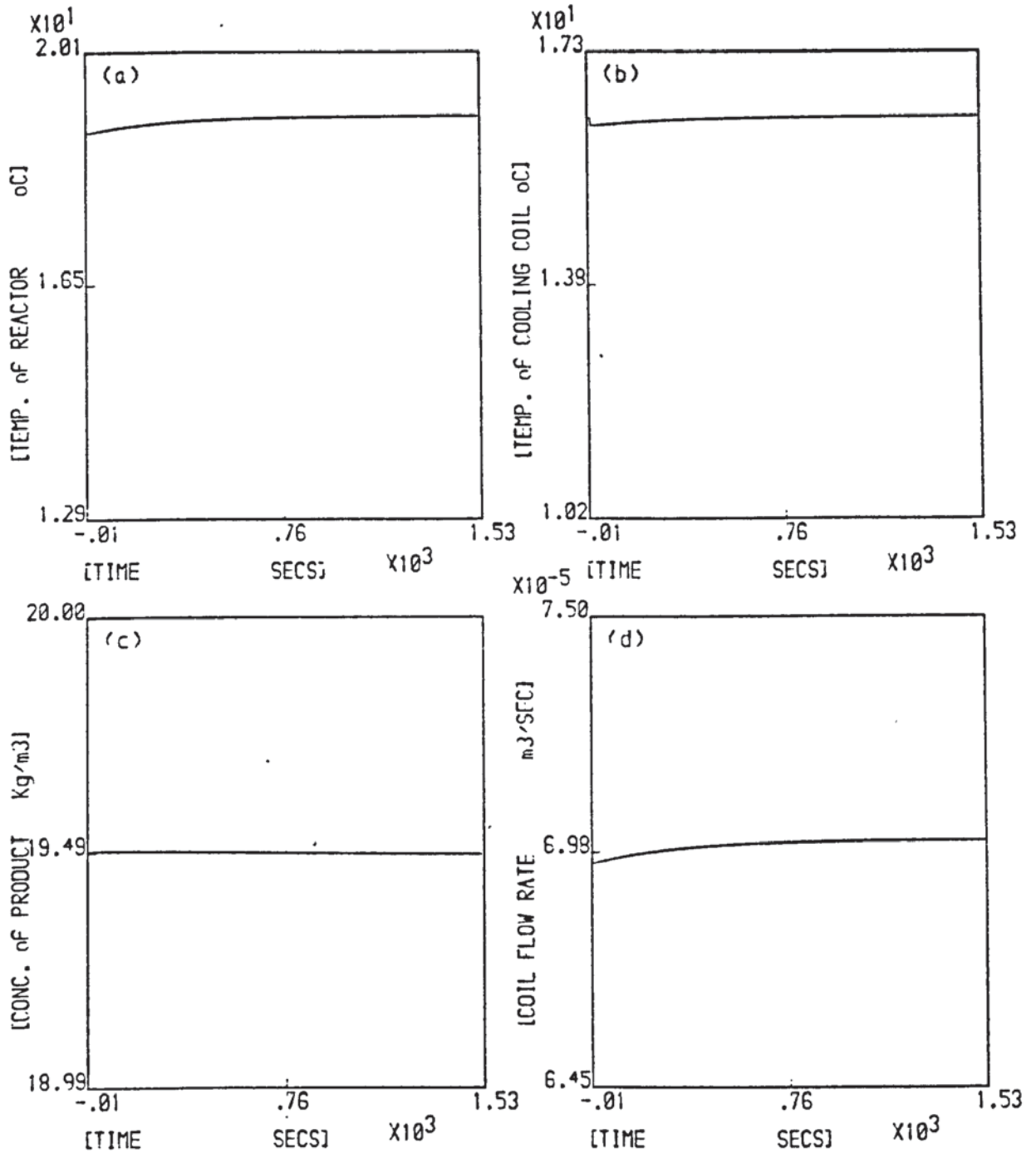
Fig. A.6.1.13 Reactor One. Experiment no: 9



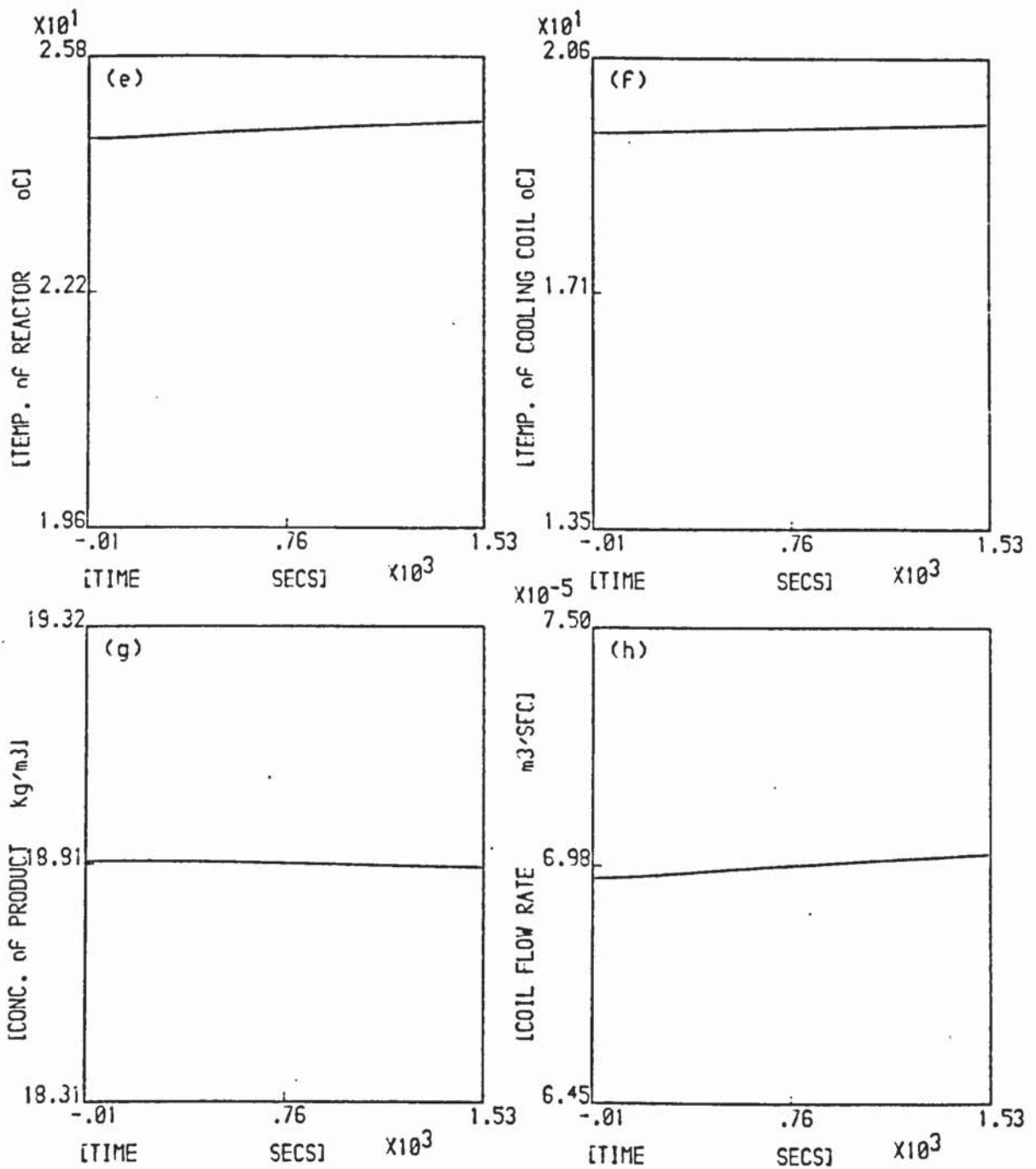
Disturbances From First reactor.

Proportional feedback control of reactant concentration. $K_c=0.5E-04$

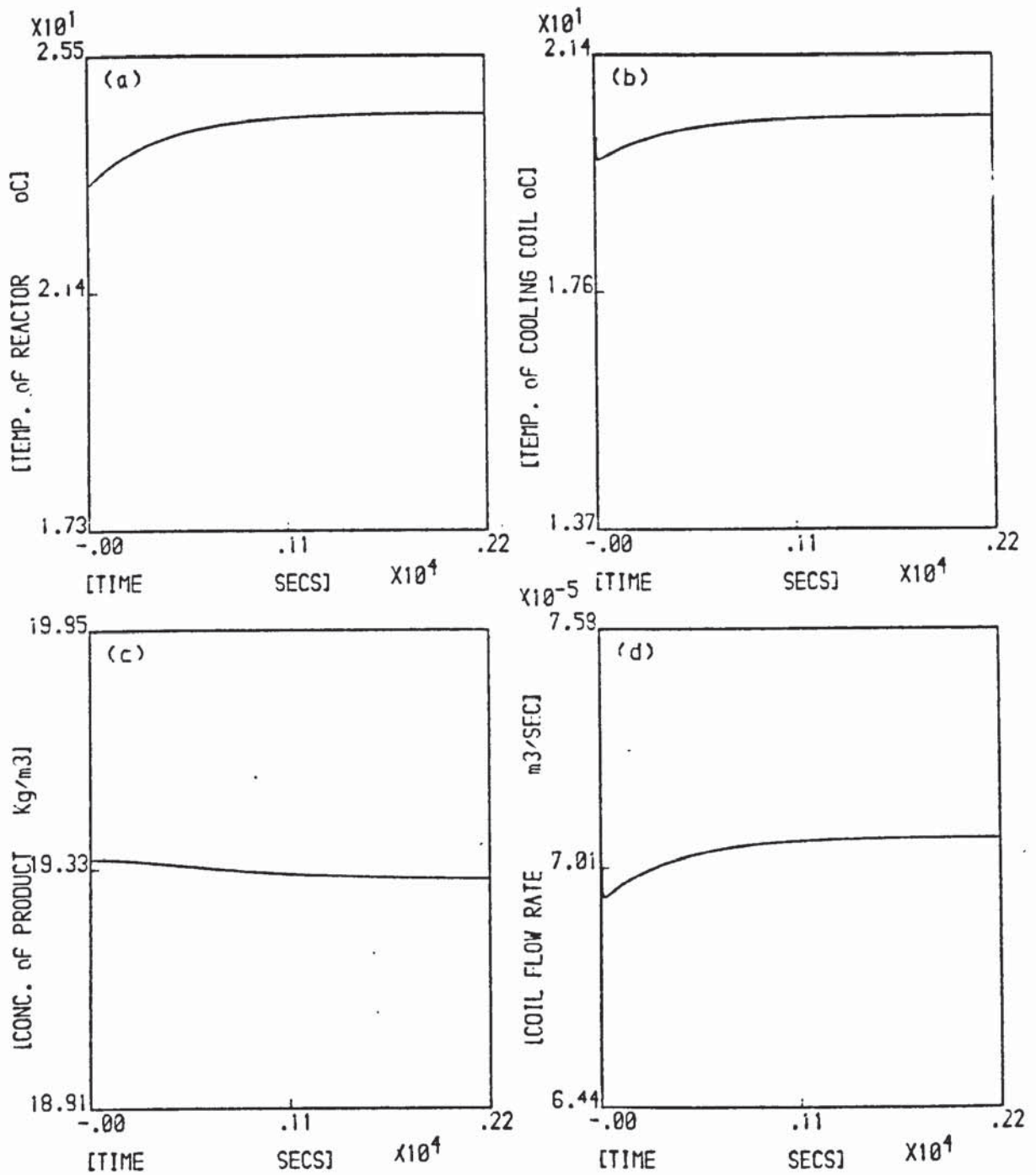
Fig. A.6.1.13 Reactor Two. Experiment no: 9



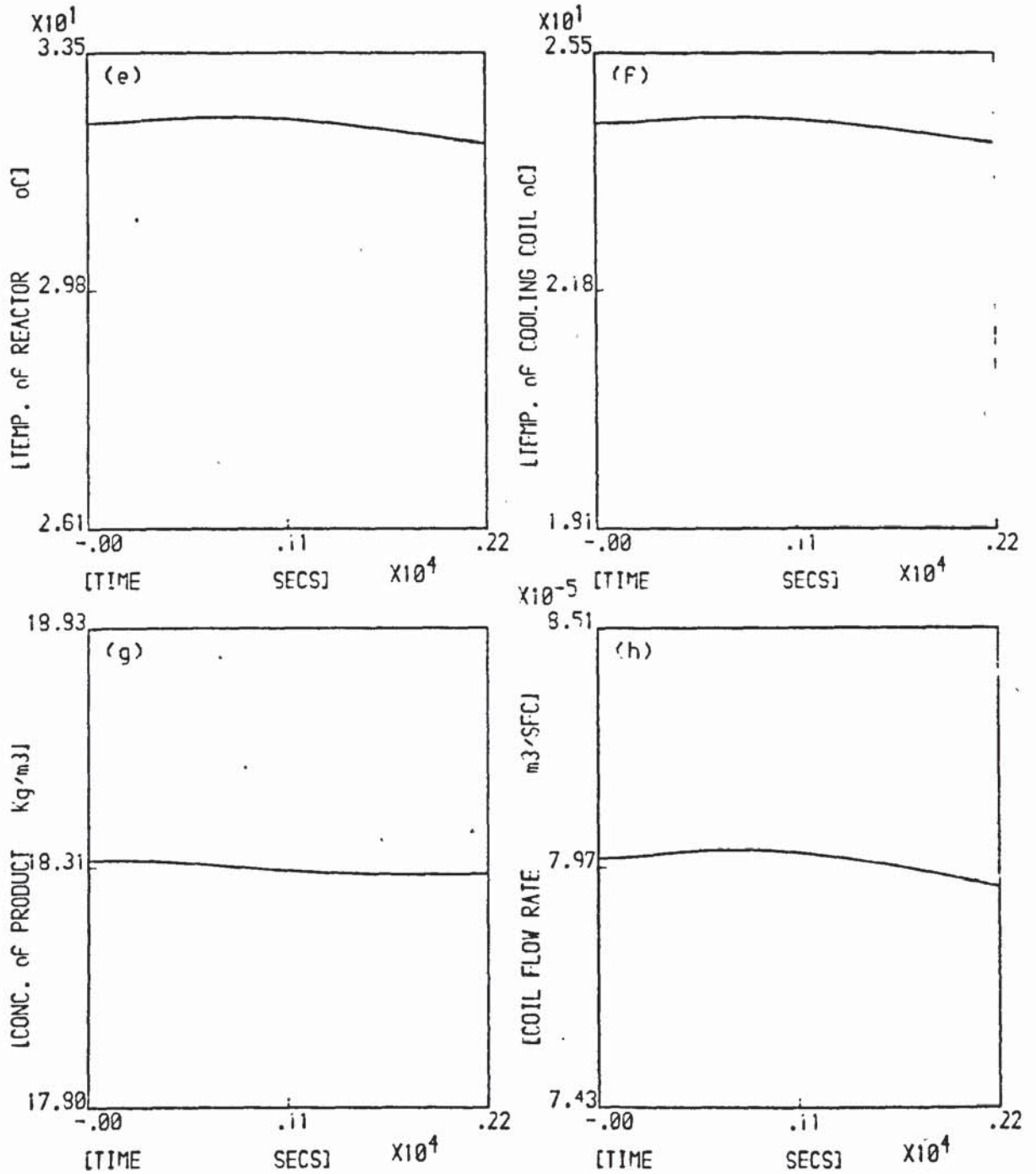
Step in Feed temperature(0.79 K) & inlet coil (-0.35)temperature. Proportional Feedback control of reactor temperature. $K_c=2E-06$
 Fig. A.6.1.14 Reactor One. Experiment no:14



Disturbances from first reactor only.
 Proportional feedback control of cooling
 coil temperature. $K_c=2E-06$
 Fig. 1.6.1.14 Reactor Two. Experiment no: 14



Step in Feed temperature to reactor(2.76°K) & cooling coil(-1.23°K). Proportional feedback control of coil temperature. $K_c=2E-06$
 Fig. A.6.1.15 Reactor One. Experiment no: 15

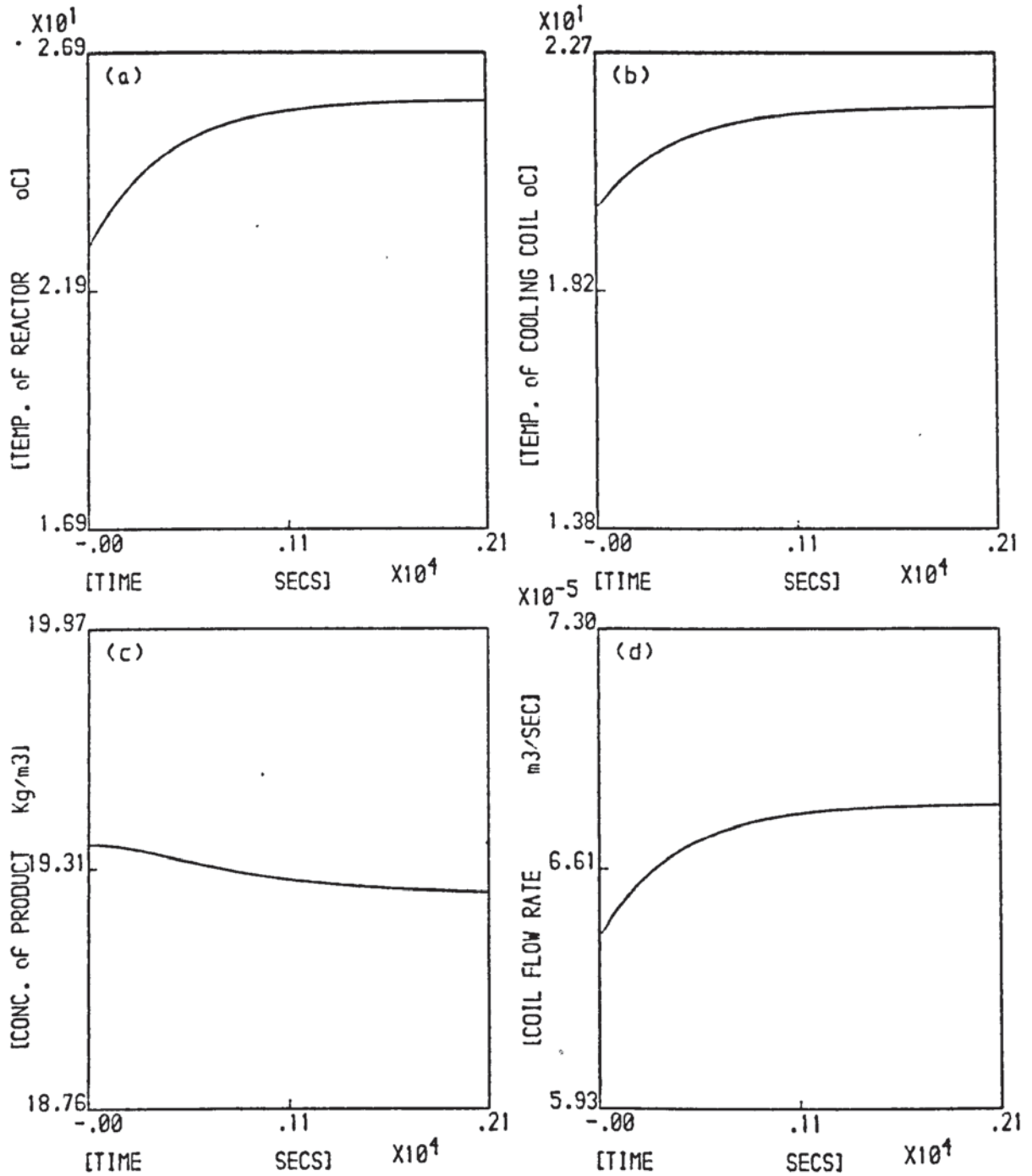


Step in temperature into cooling coil (-.58 K)

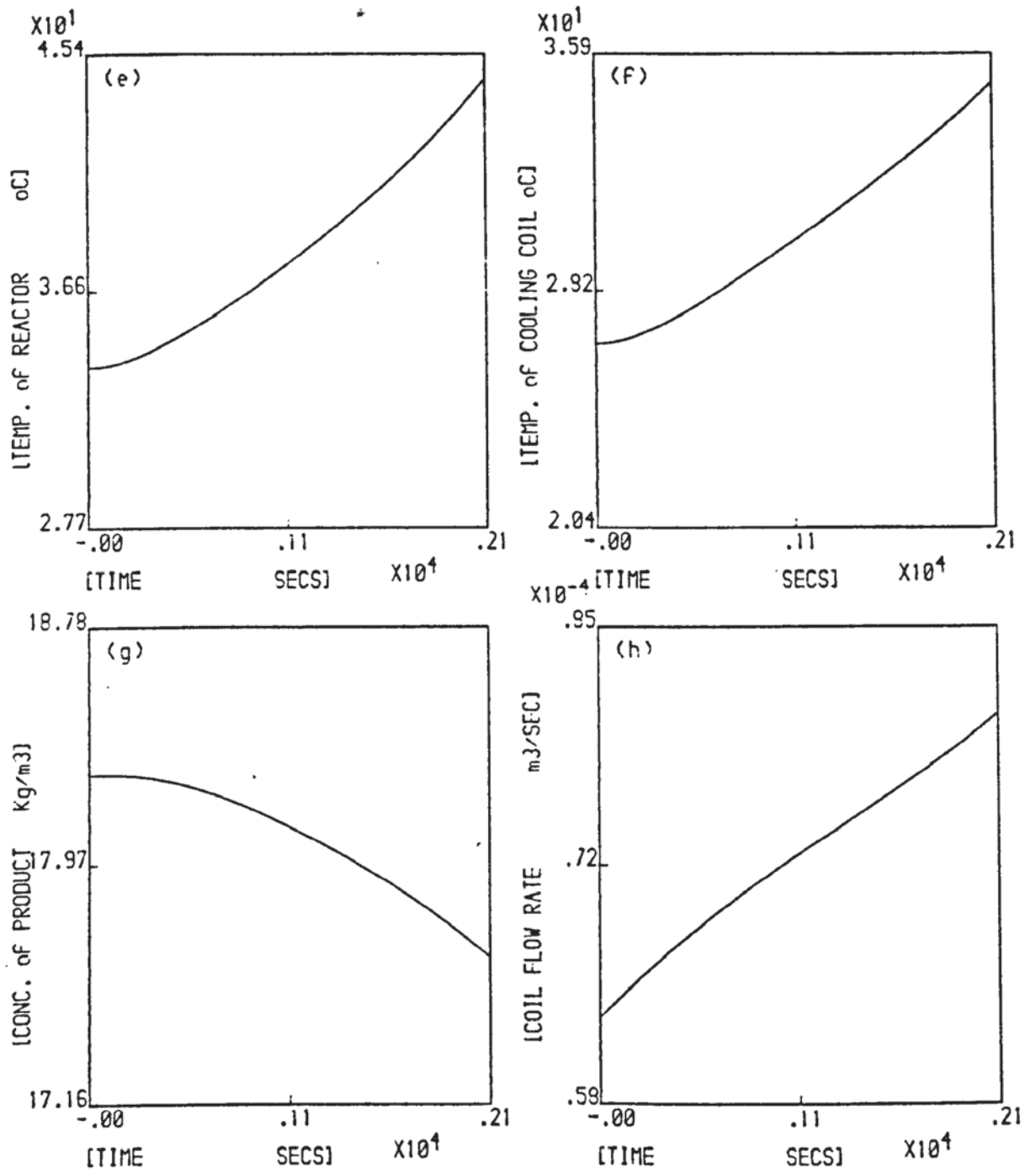
Proportional feedback control of reactor

temperature. $K_c = 2E-06$

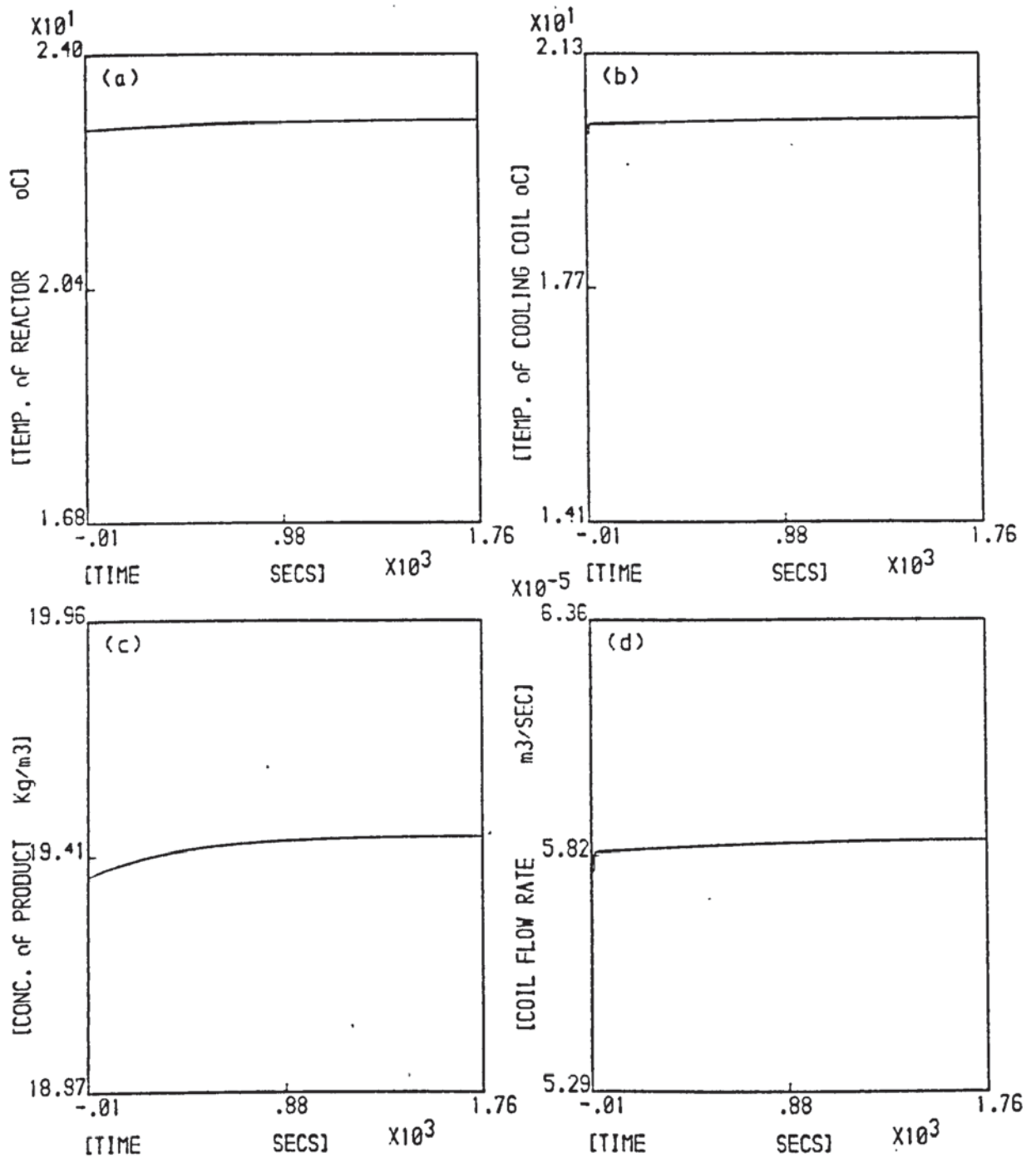
Fig. A.6.1.15 Reactor Two. Experiment no: 15



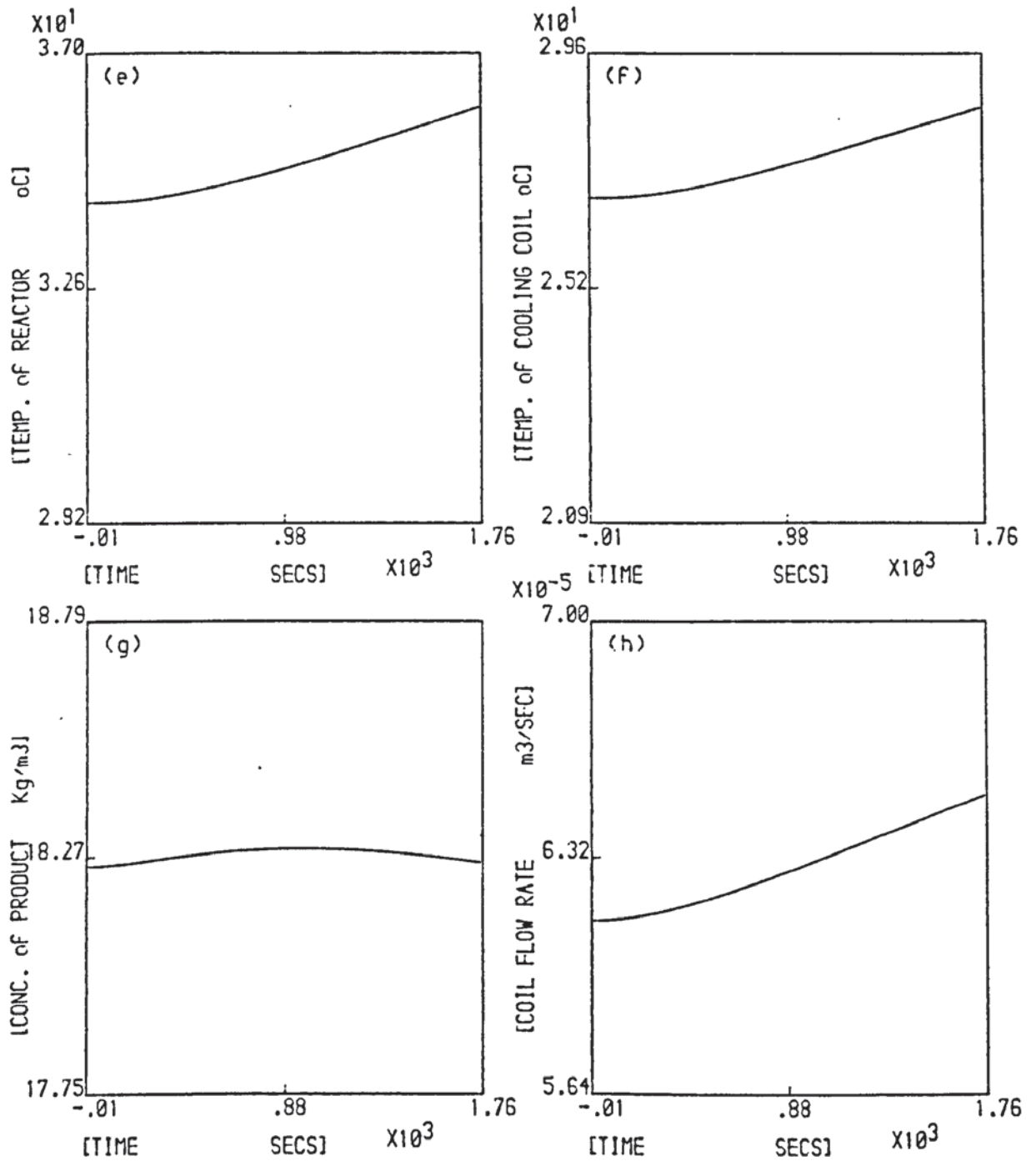
Step in feed reactor(3.38 K) & coil(-0.1 K) temperatures. Feedback proportional control of coil temperature. $K_c=2E-06$
 Fig. A.6.1.16 Reactor One. Experiment no:i6



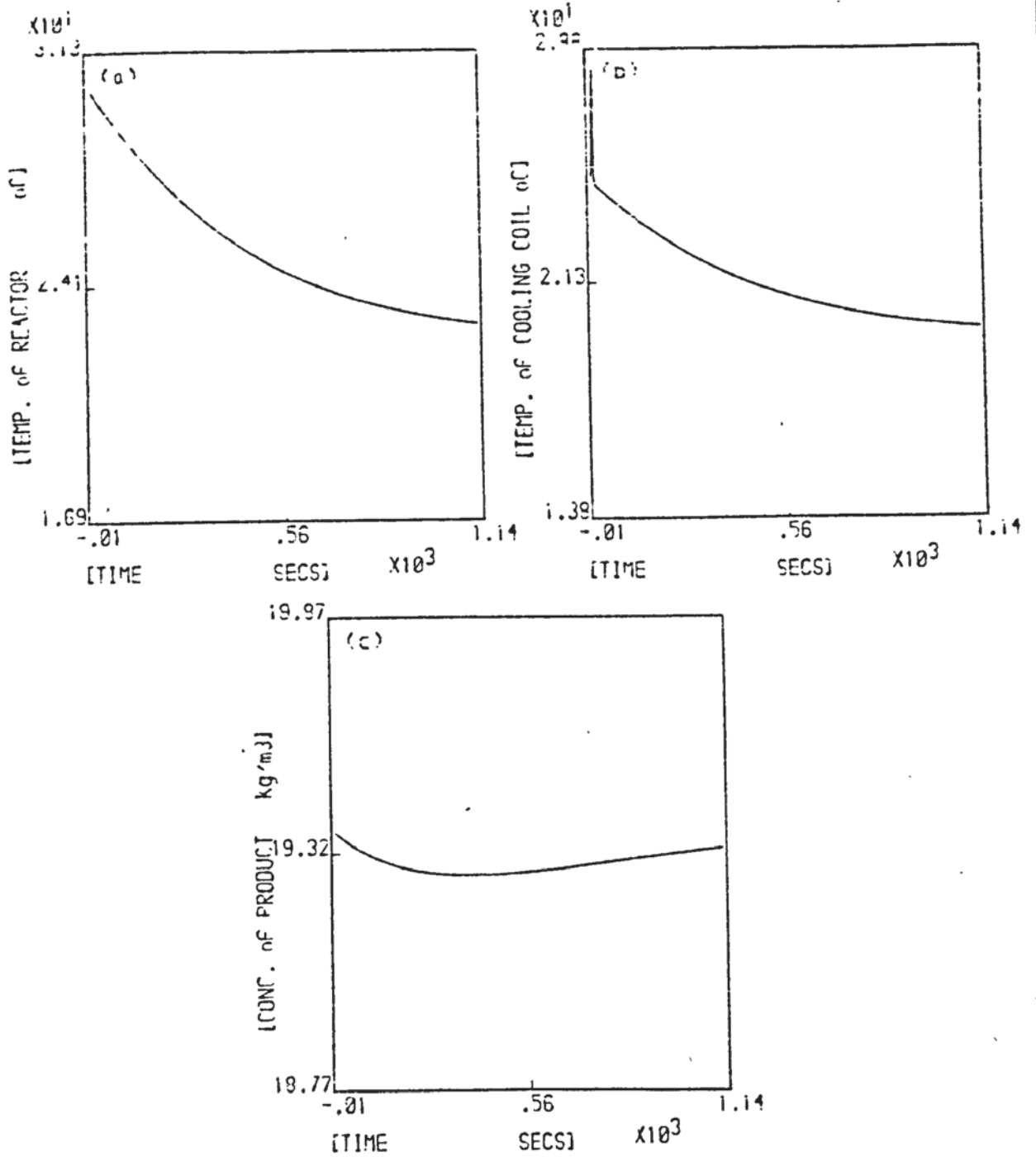
Step in inlet coil (-0.66 K) temperature.
 Feedforward & feedback proportional control
 of reactor temperature. $K_c=1.5\text{E}-06$
 Fig. 1.6.1.16 Reactor Two. Experiment no:16



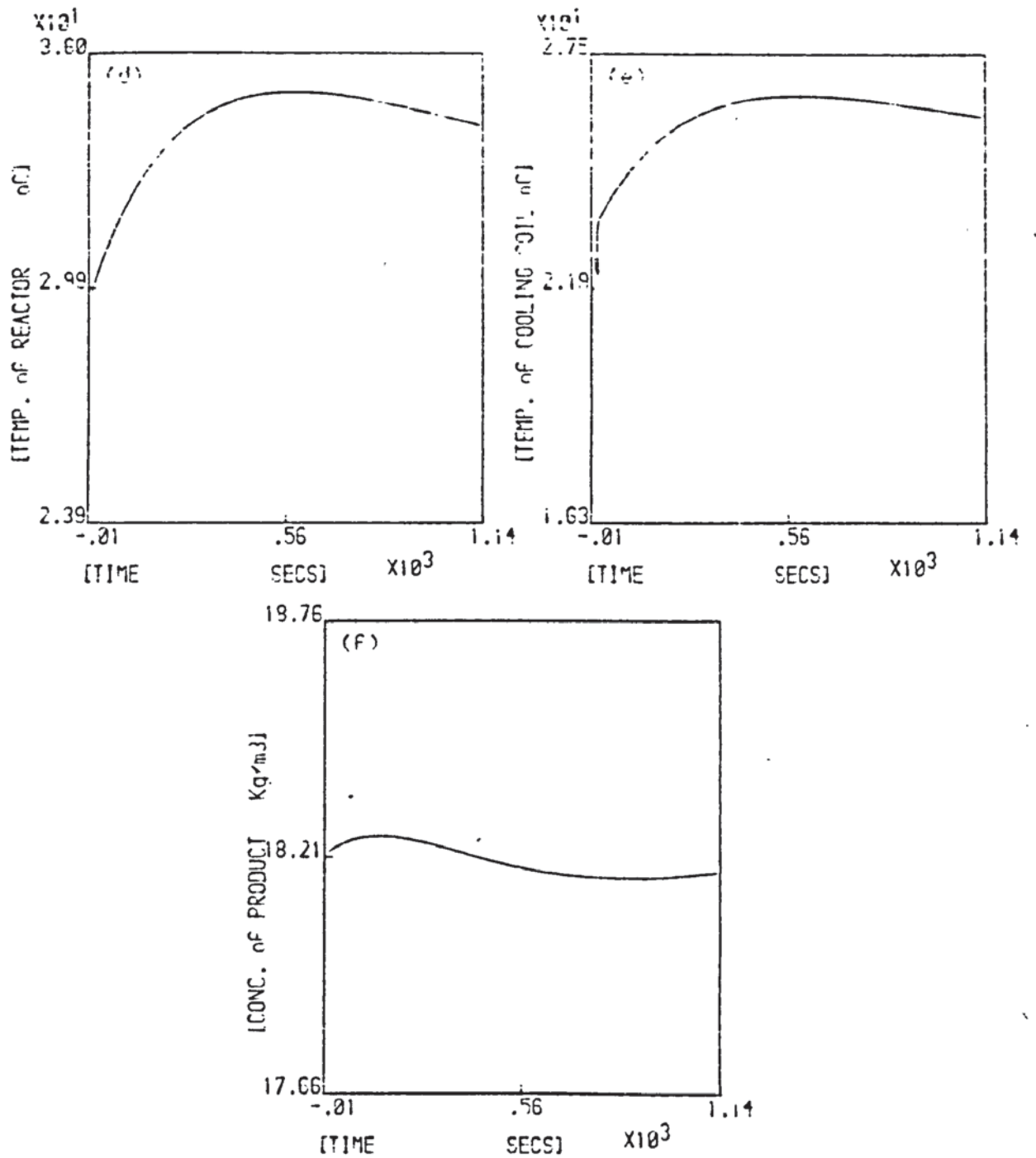
Step in Feed conc. (0.1 kg/m^3) & temp. (-0.56 K)
 & inlet coil (0.65 K) temperature. Feedback
 proportional control of coil temp. $K_c = 3\text{E}-06$
 Fig. A.6.1.17 Reactor One. Experiment no: 17



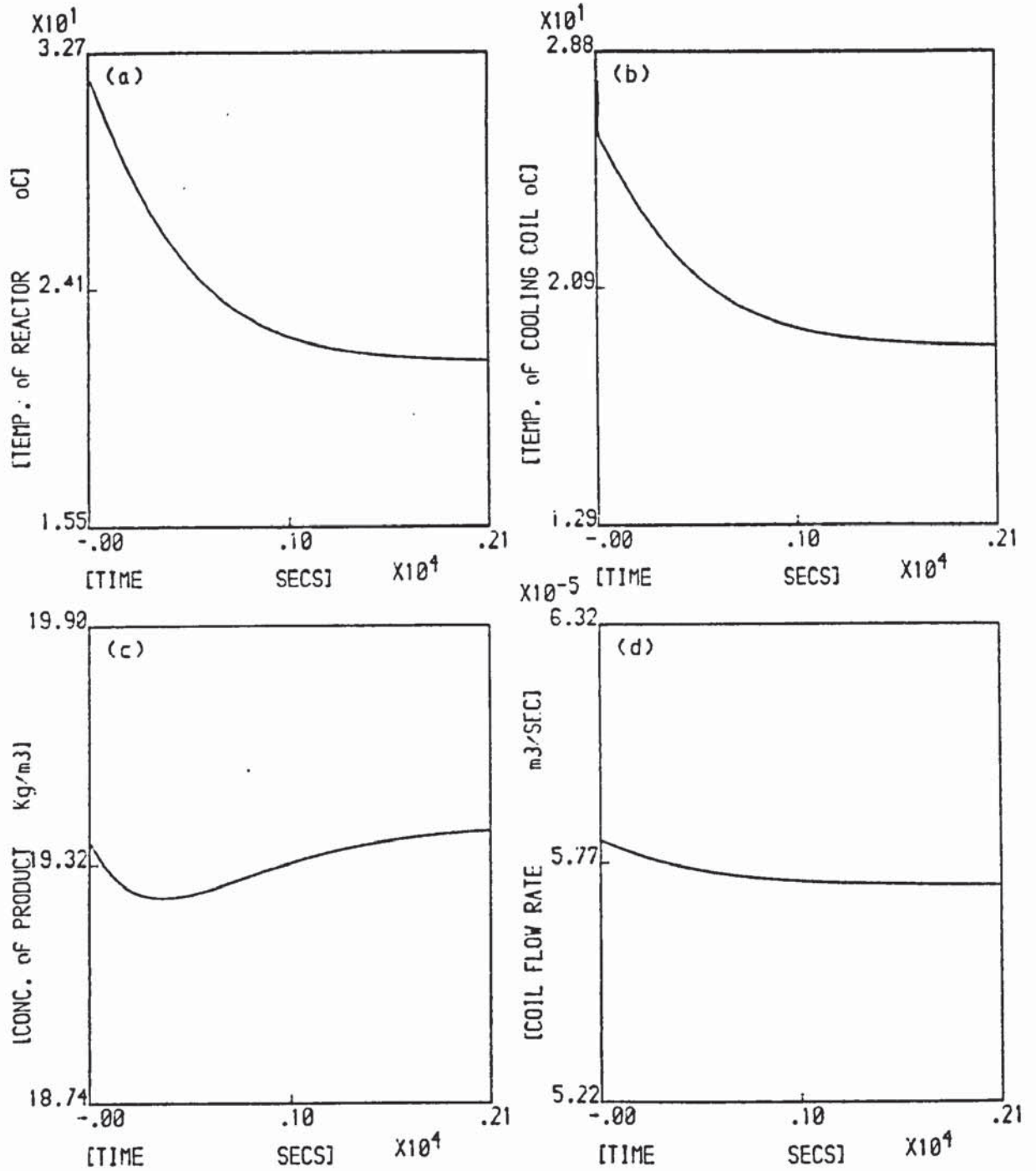
Step in inlet coil(-0.56 k) temperature.
 Feedforward & feedback proportional control
 of reactor temperature. $K_c=2E-06$
 Fig. A.6.1.17 Reactor Two. Experiment no: 17



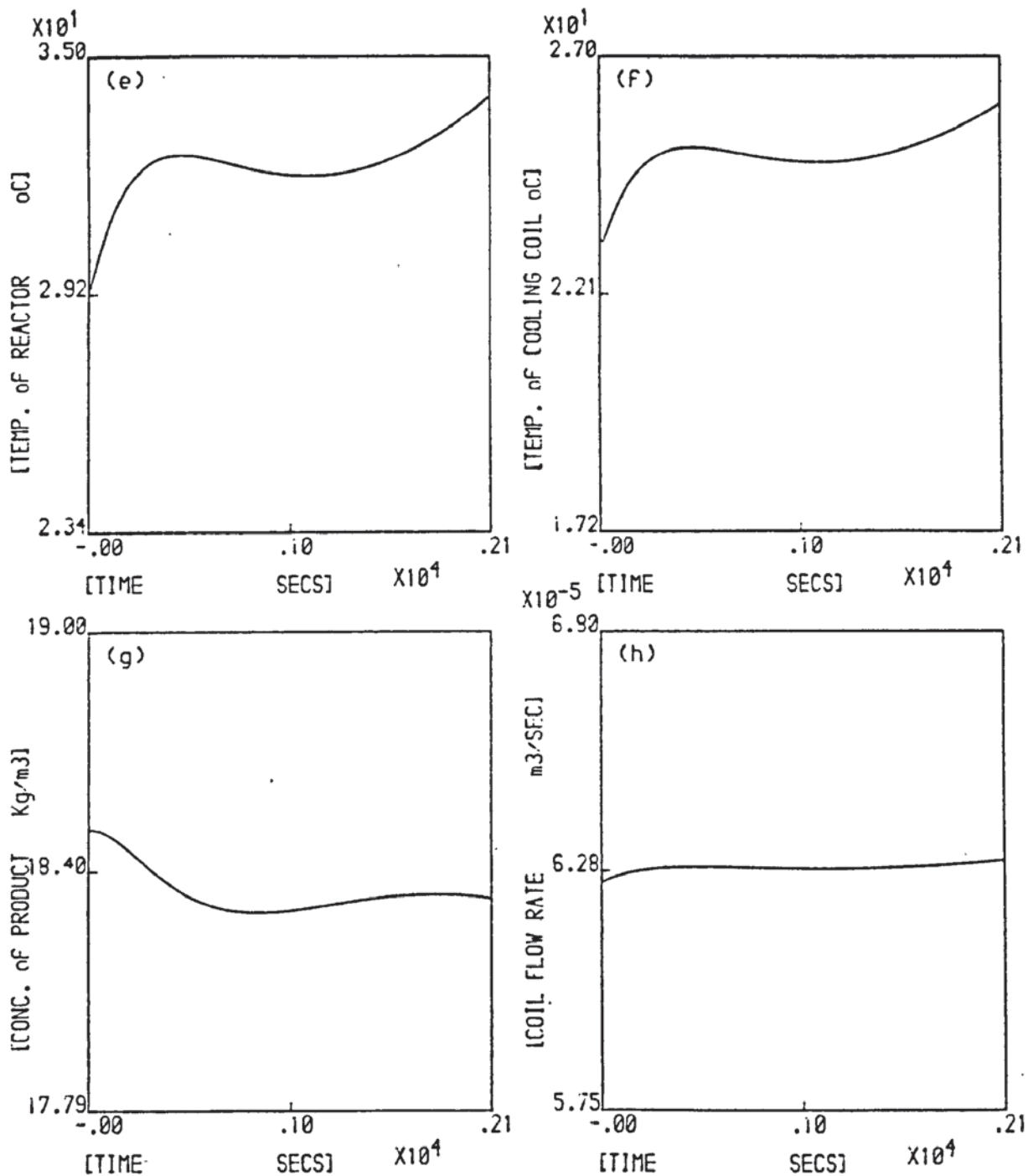
Initial perturbation of state variables & step in reactor (-0.06 K) & cooling coil (-0.41 K) temperatures. No state variable control.. Fig A.C.1.18 Reactor One. Experiment no: 18



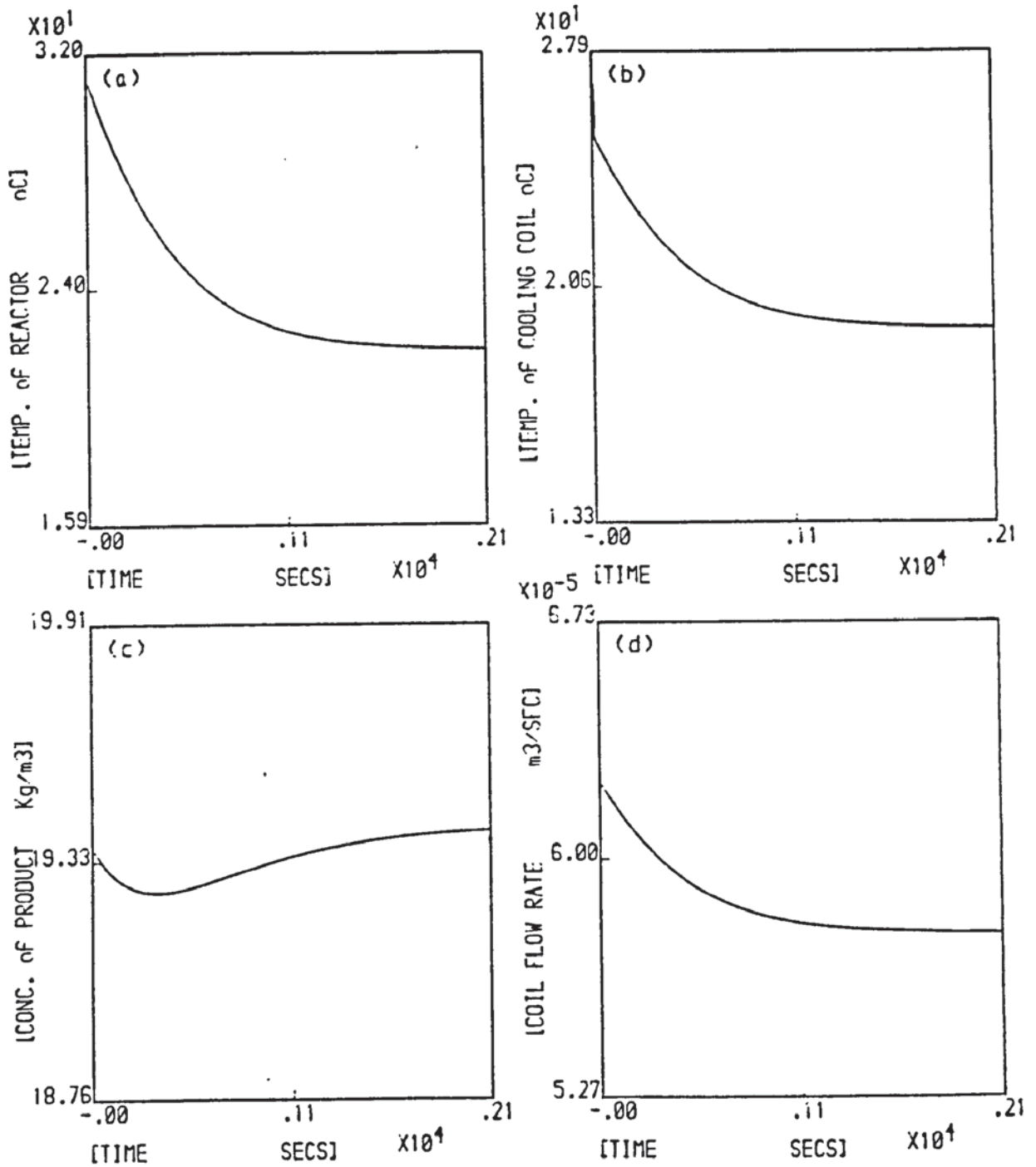
Initial perturbation in state variables &
 Step in cooling coil (-0.188 K) inlet tempera-
 ture. No control on state variables.
 Fig A.6.1.18 Reactor Two. Experiment no. 18



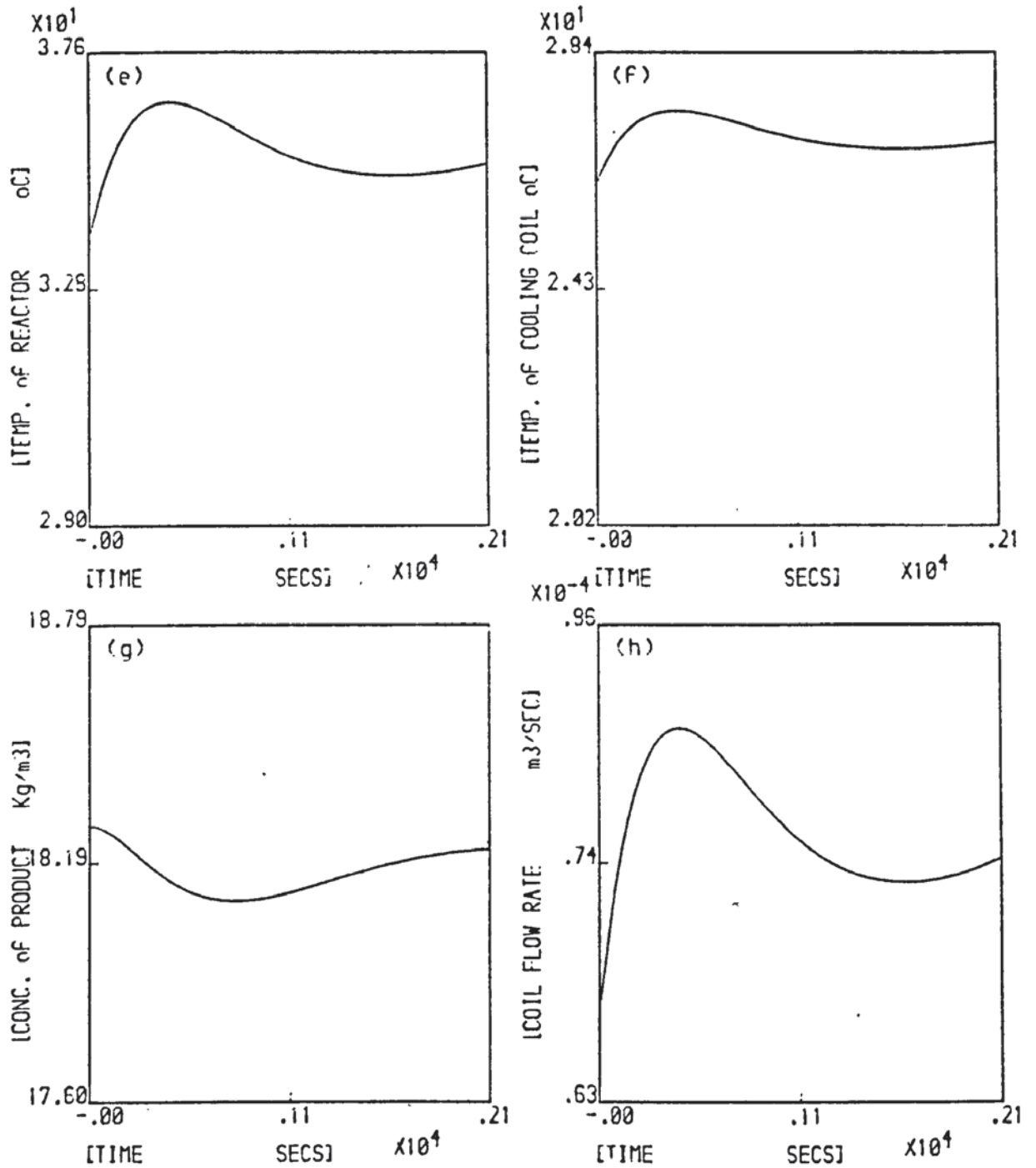
Initial perturbation of state variables and step in reactor(-.37°K) & coil(-.9°K) temps.
 Prop. feedback control of reactor temp. $K_c=1E-07$
 Fig. A.6.1.19 Reactor One. Experiment no: 19



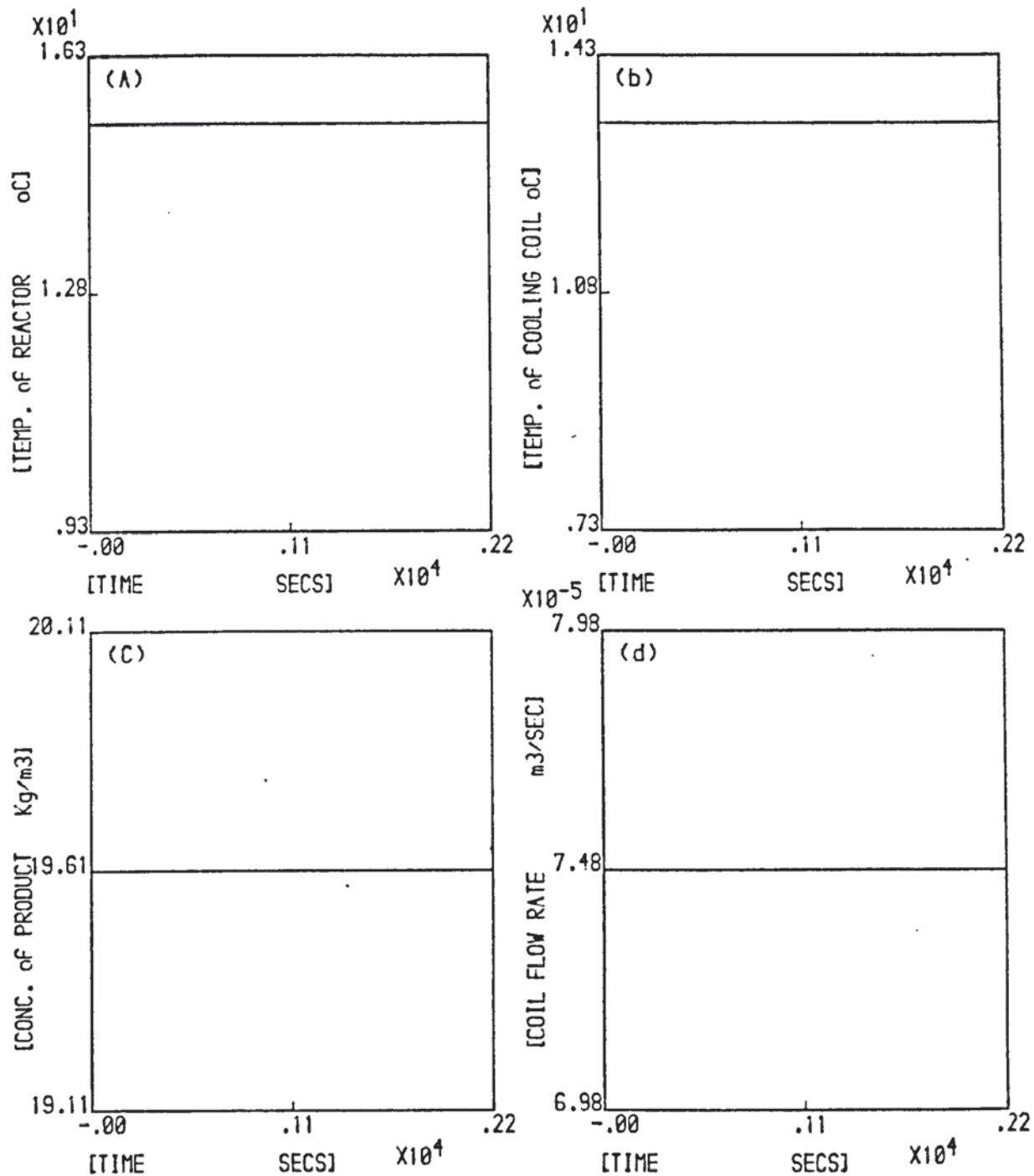
Initial perturbation of state variables & ste
 in inlet coil(-.113 K) temperature. Feedback
 Proportional control of coil temp. $K_c=1E-07$
 Fig. A.6.1.19 Reactor Two. Experiment no: 19



Initial perturbation of state variables & step in feed reactor (-0.68°K) & coil (-0.98°K) temps.
 Prop. feedback control of reactor temp. $K_c=5E$
 Fig. A.6.1.20 Reactor One. Experiment no: 20



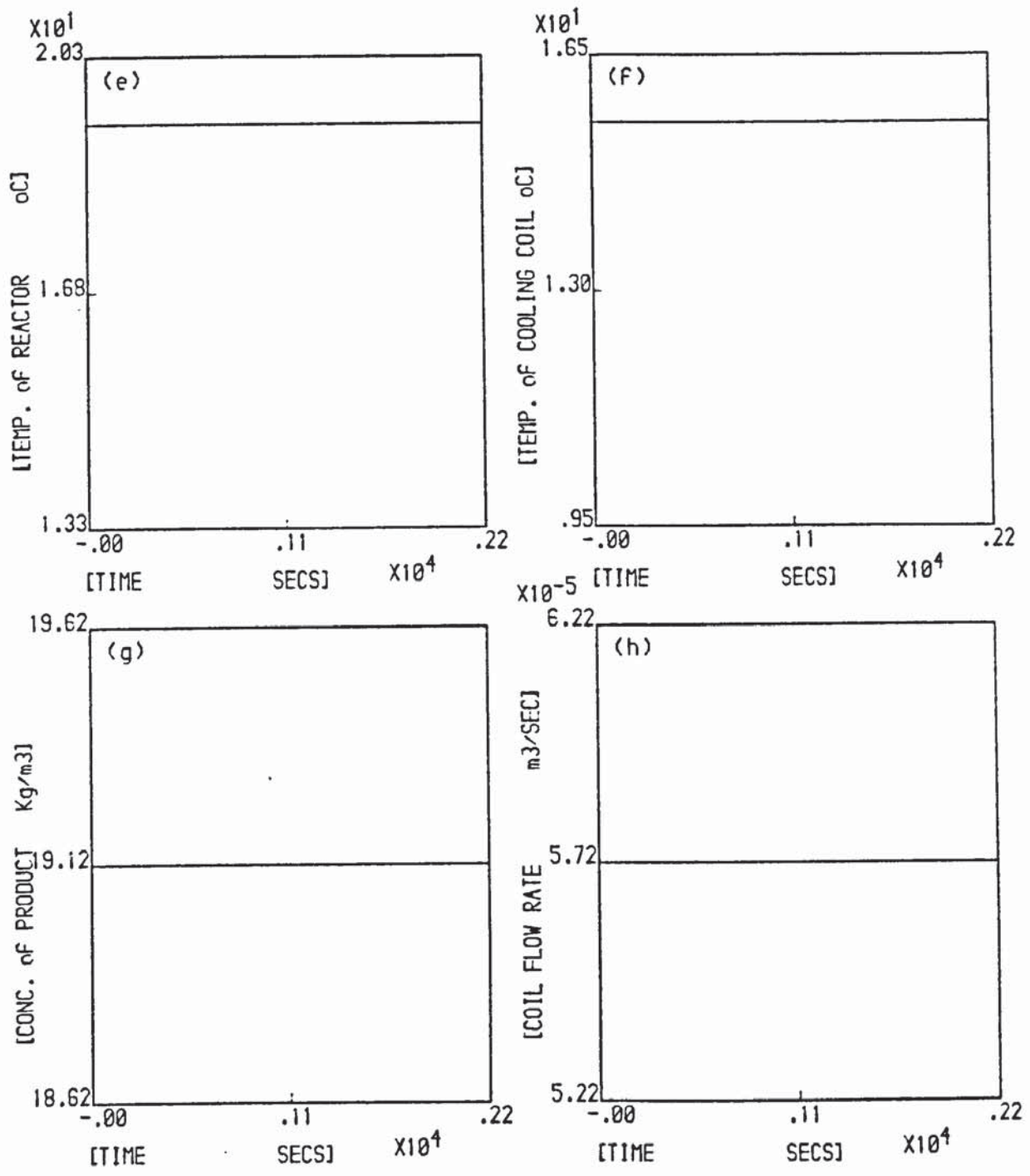
Initial perturbation of state variables & step in feed coil (-0.23 K) temperature. Proportional feedback control of coil temperature. $K_c = 5E-6$
 Fig. A.6.1.20 Reactor Two. Experiment no: 20



Step in reactor and cooling coil inlet
temperatures (0.772 K, -0.41 K).

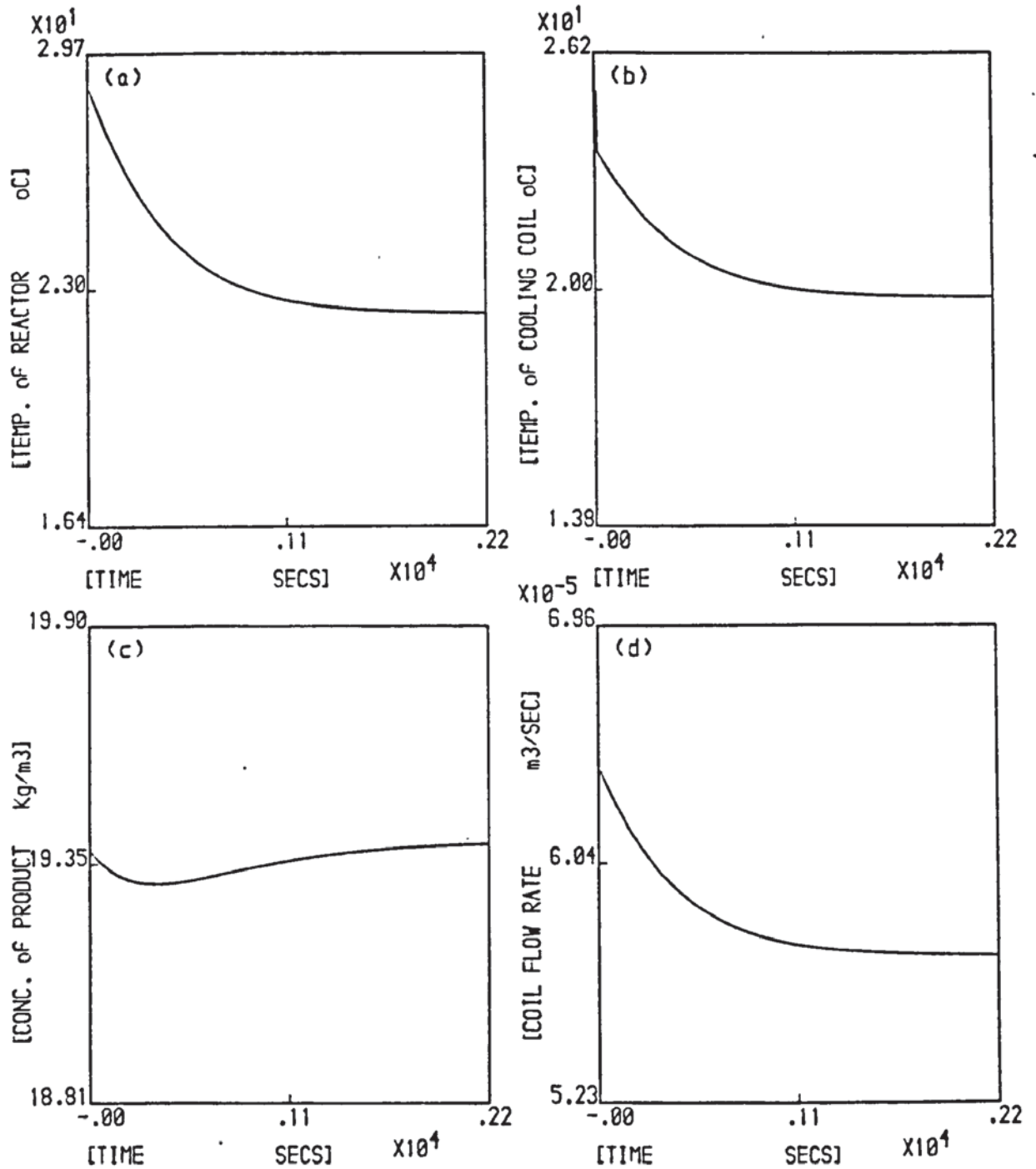
Invariance control.

Fig. A.6.1.21 Reactor-One. Experiment no:28

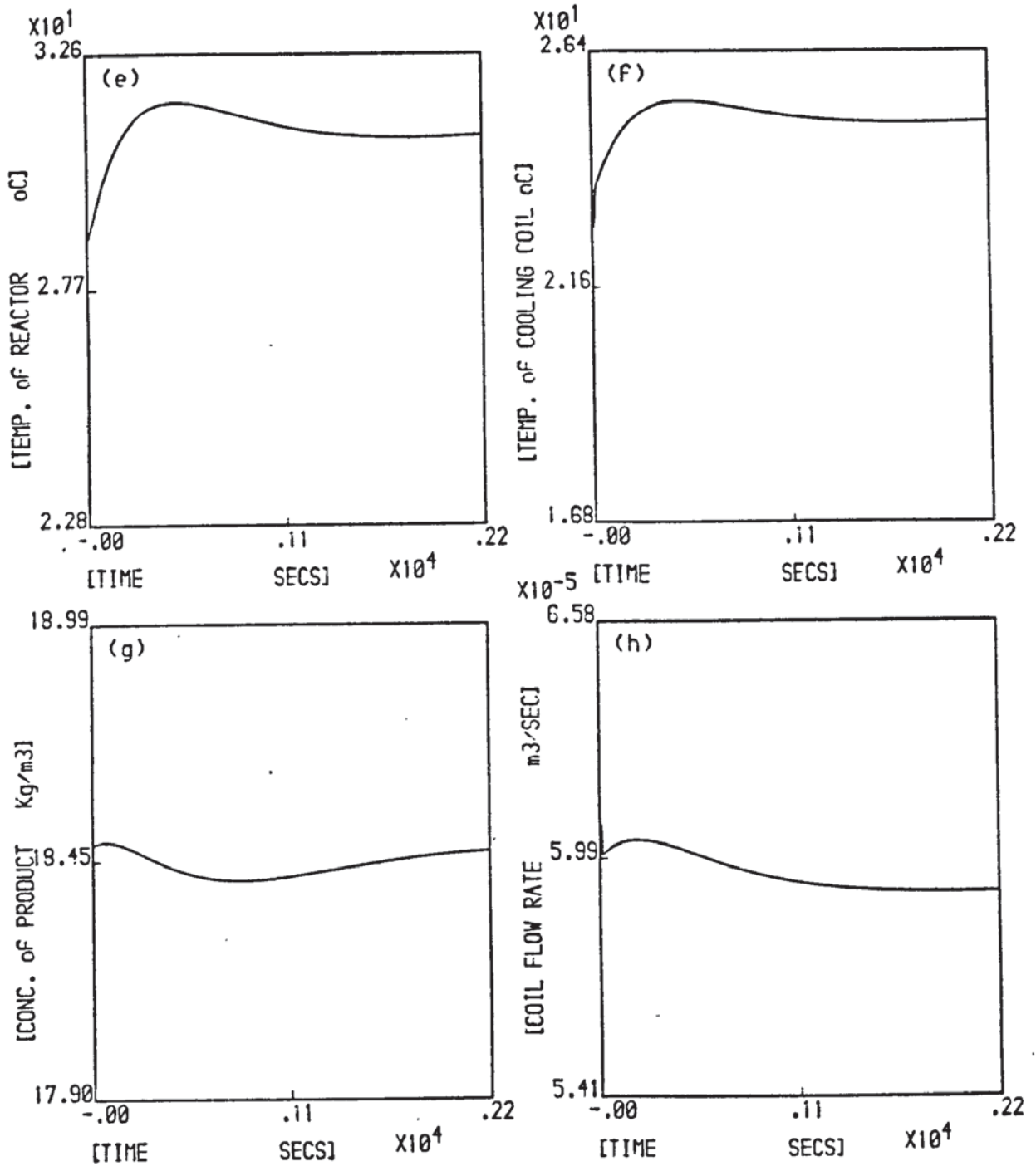


Step in temperature into cooling coil (-0.75 K)
 Invariance control.

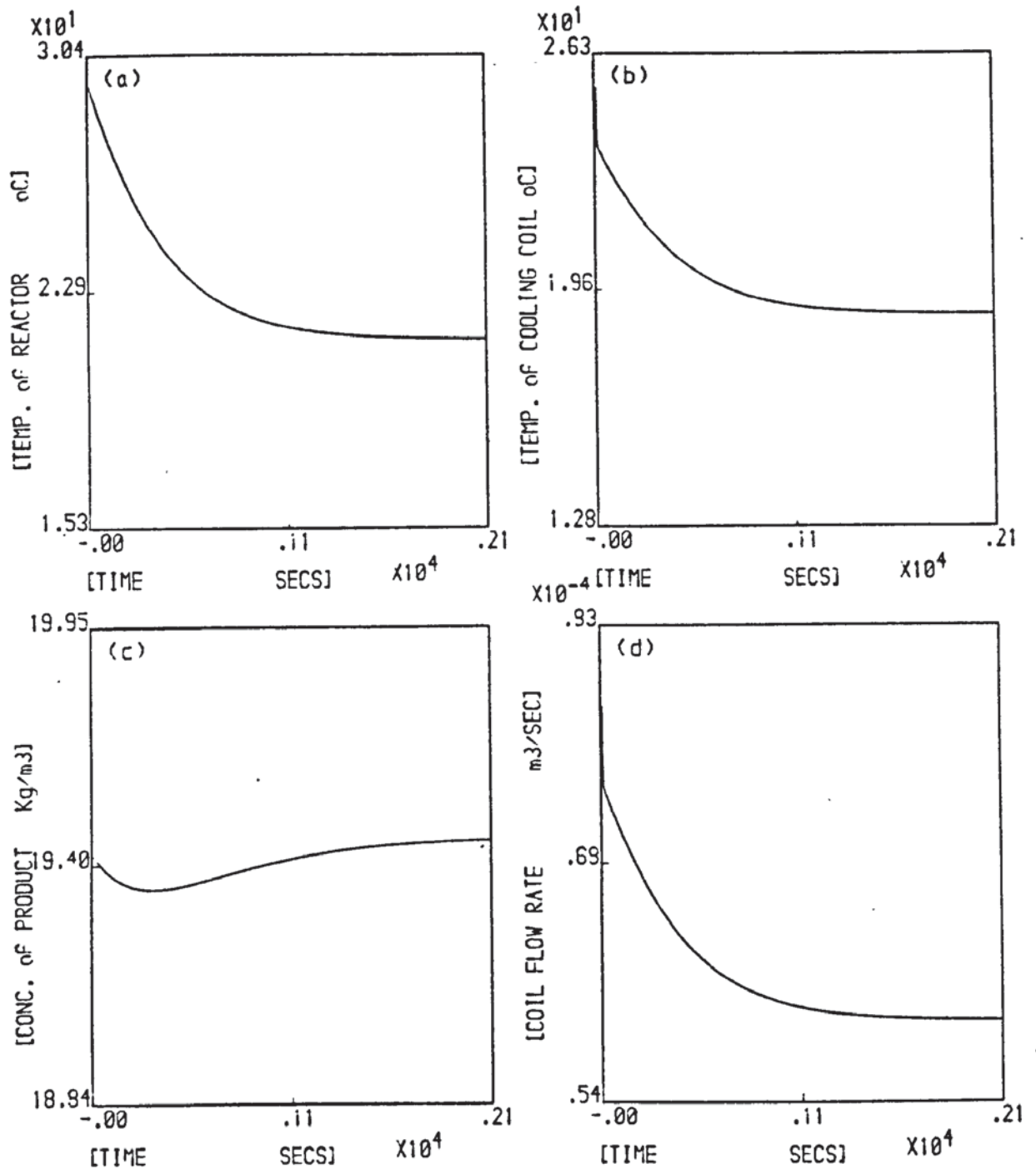
Fig. 1.6.1.21 Reactor Two. Experiment no:28



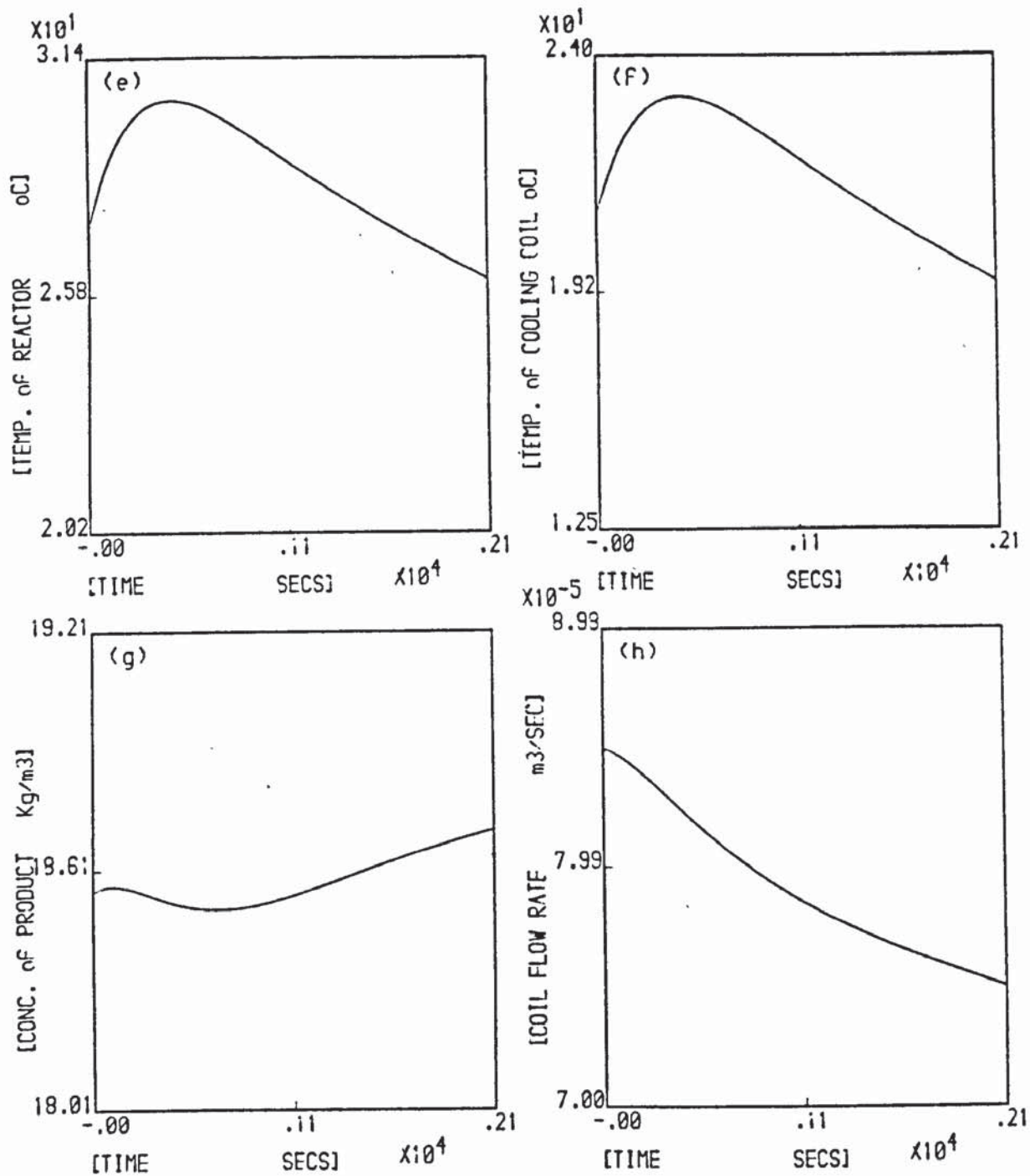
Initial perturbation of state variables and step in inlet temps. to reactor (-.44 K) & coil (-.26 K). Prop. feedback control of reactor temp. $K_c=1E-06$. Fig. 1.6.1.22 Reactor One.



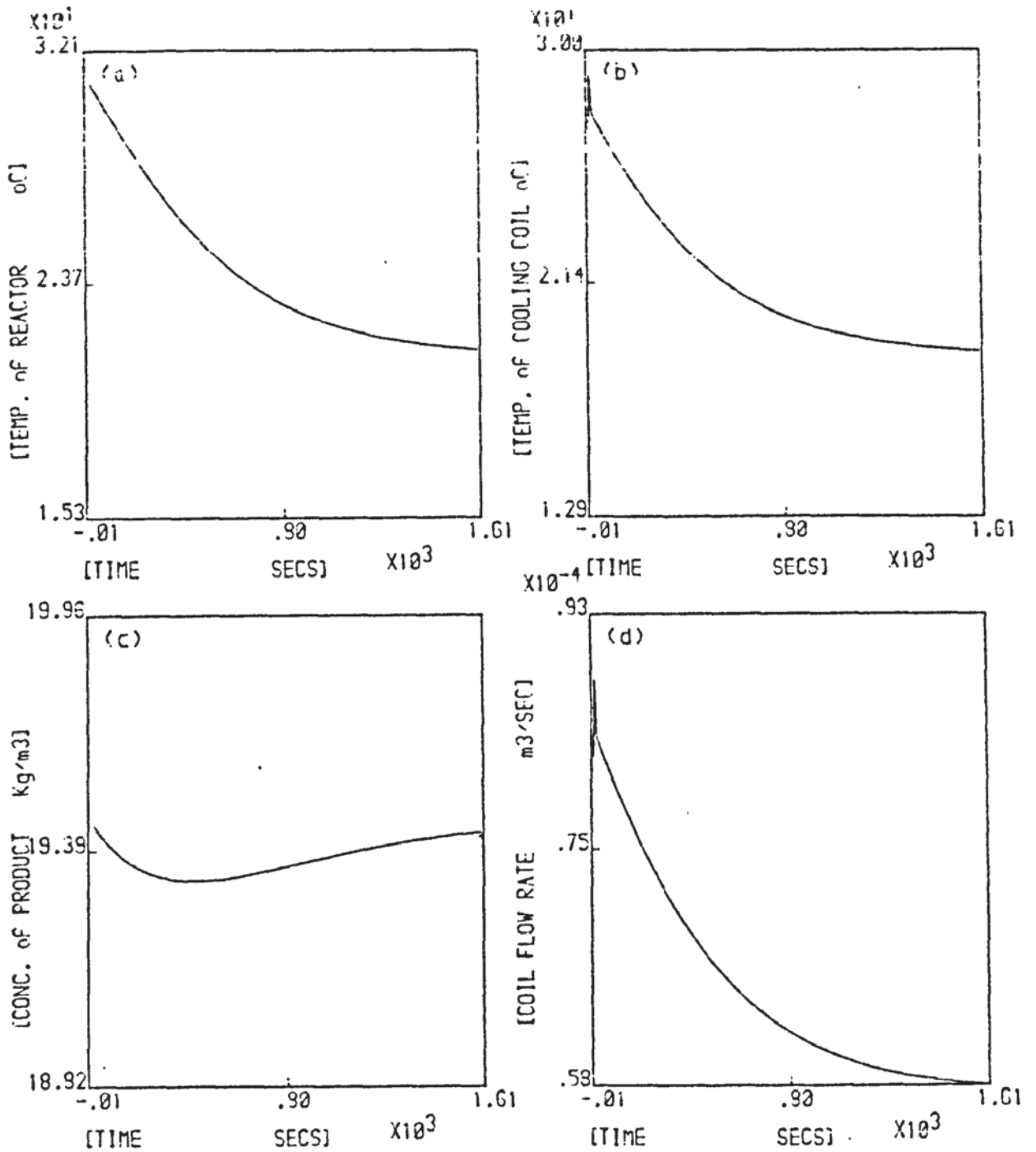
Initial perturbation of state variables and step in inlet temperature to coil (-.11 K). Proportional feedback control of coil temp. $K_c=5E-07$. Fig. A.6.1.22 Reactor Two. Expt.21



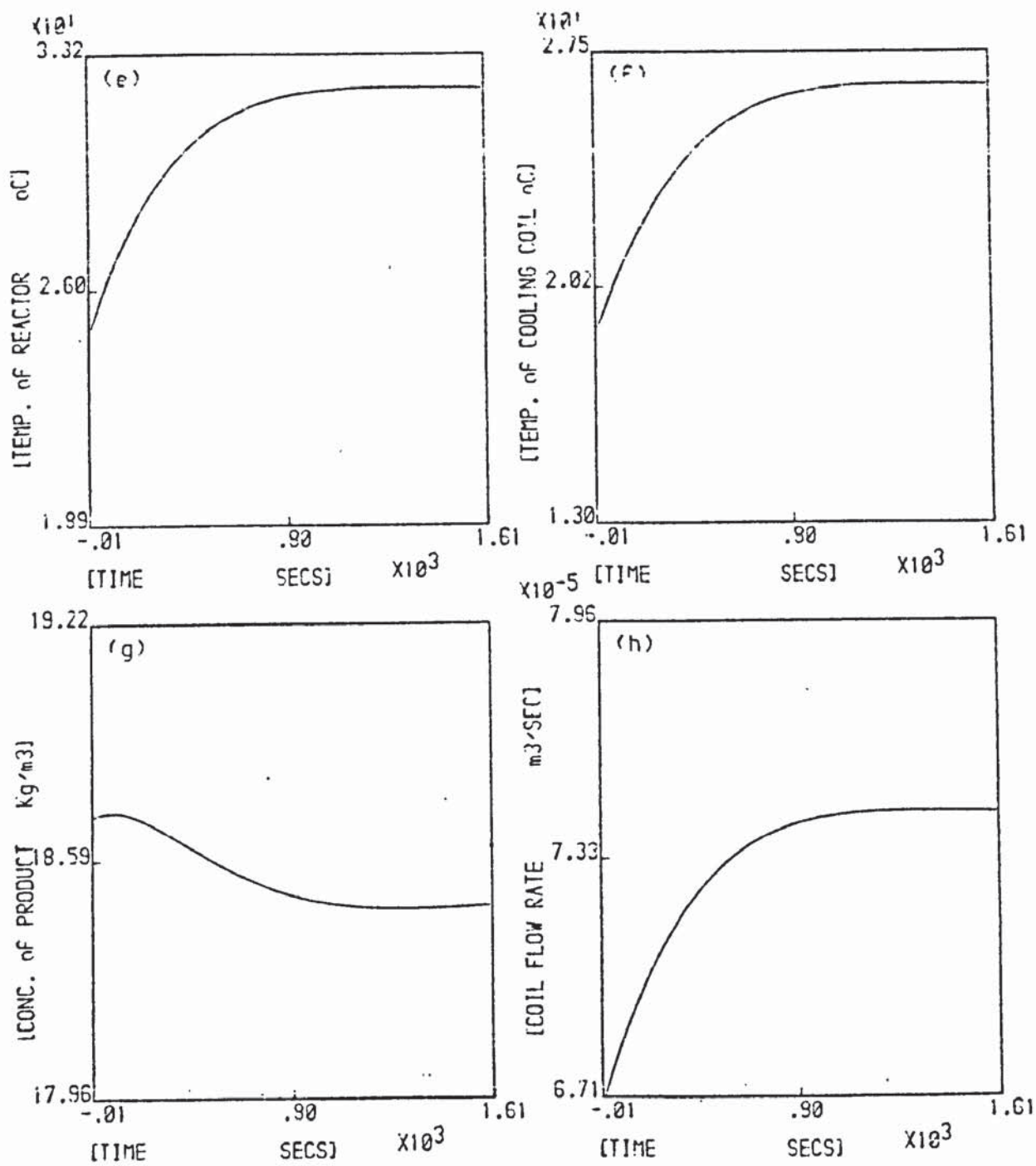
Initial perturbation of state variables and step in reactor ($-0.68^{\circ}K$) & coil ($-0.82 K$) inlet temps. Prop. Feedback control of coil temp. $K_c=3E-06$. Fig. 1.6.1.23 Reactor One. Expt. 22



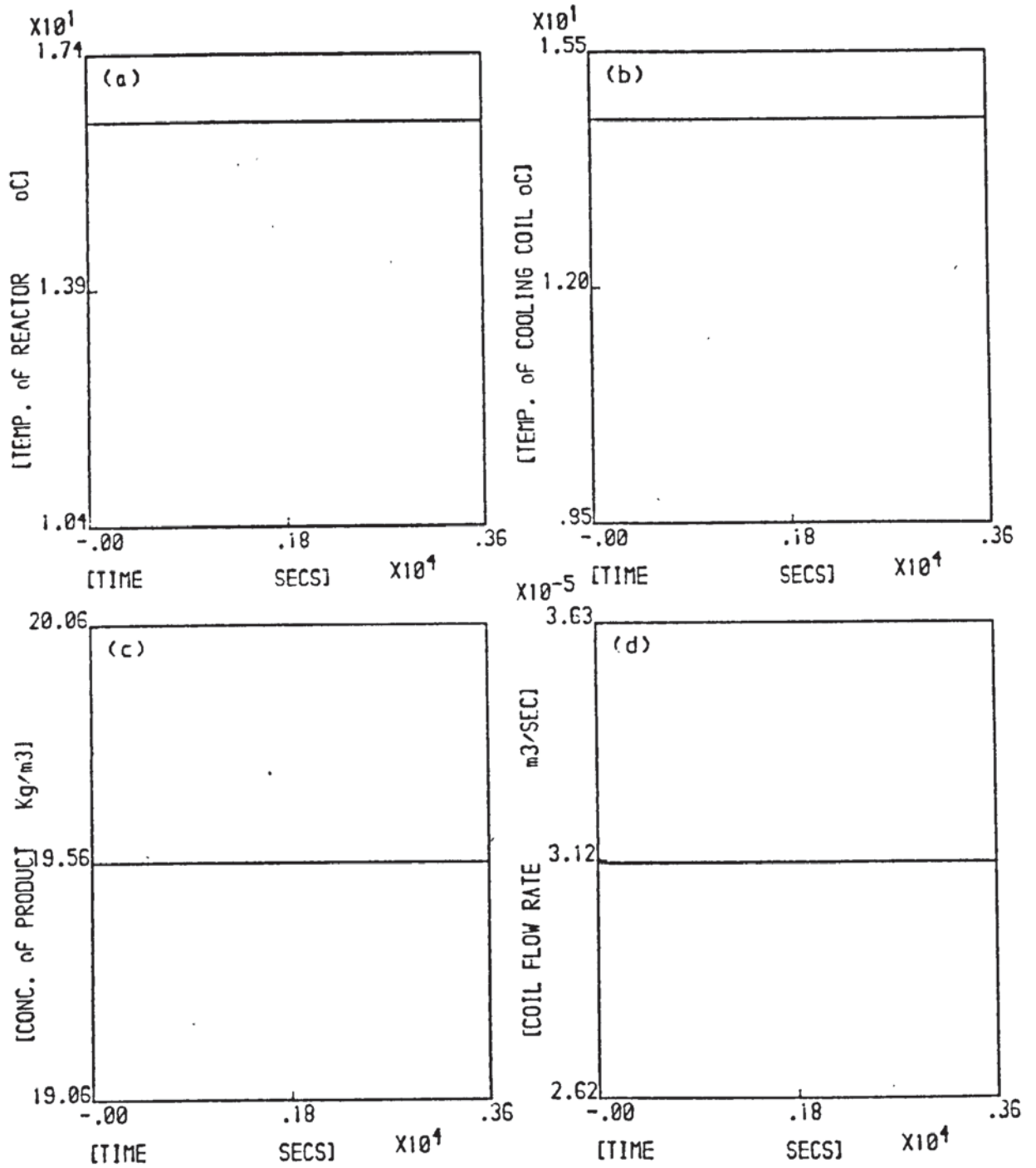
Initial perturbation of state variables and step in coil(-0.07 K) inlet temp. Proportional FeedForward & feedback control of reactor tem $K_c=1\text{E}-06$. Fig. A.6.i.23 Reactor Two. Expt. 22



Perturbation in state variables and step in Feed reactor(0.1 K) temperature. Proportional feedback control of coil temperature. $k_c=3E-6$ Fig. 1.6.1.24 Reactor One. Experiment no:24

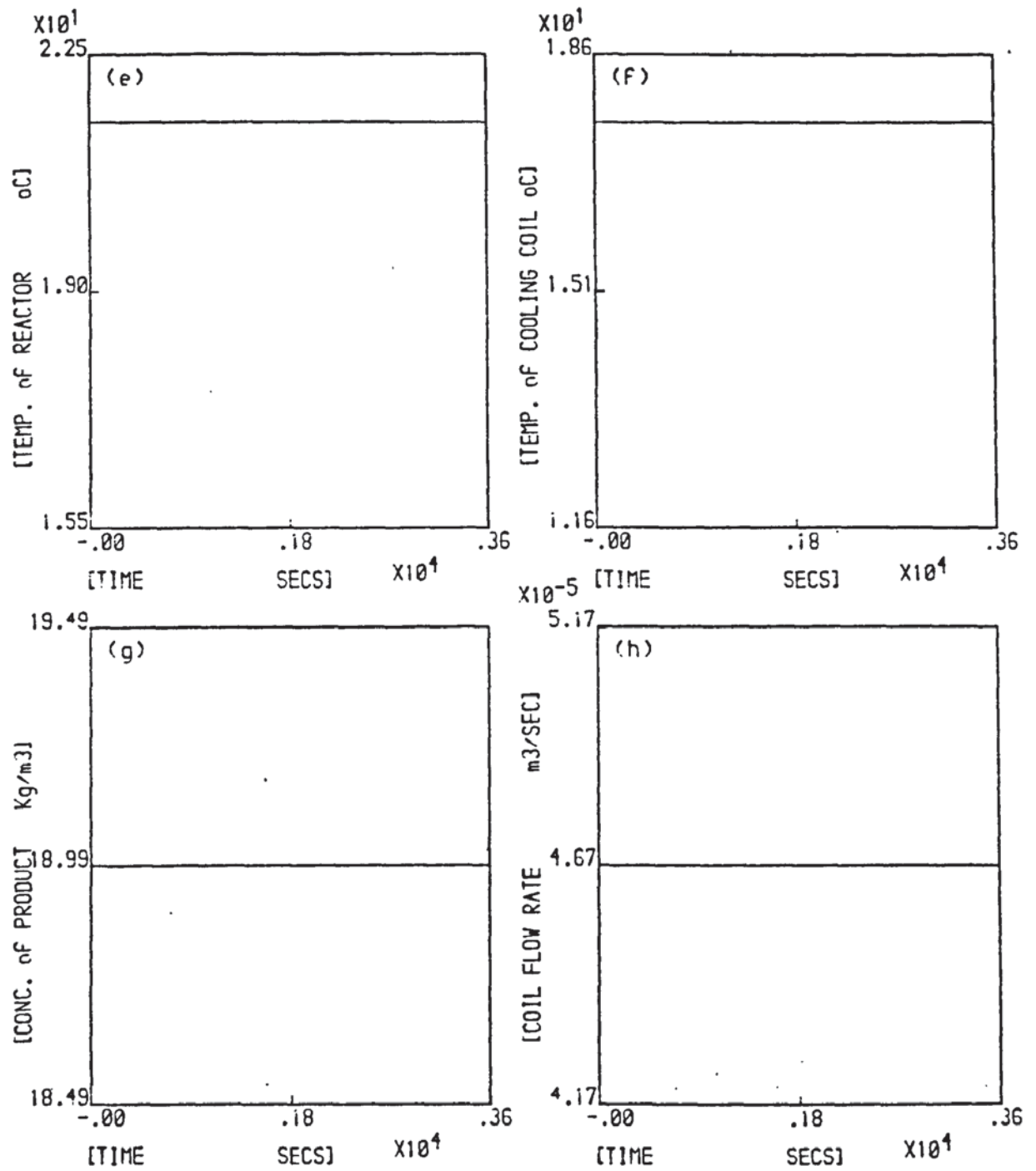


Perturbation of state variables and step in cooling coil (0.49 K) temperature. Proportional control of reactor temperature. $k_c = 1E-06$
 Fig. A.G.1.24 Reactor Two. Experiment no:24

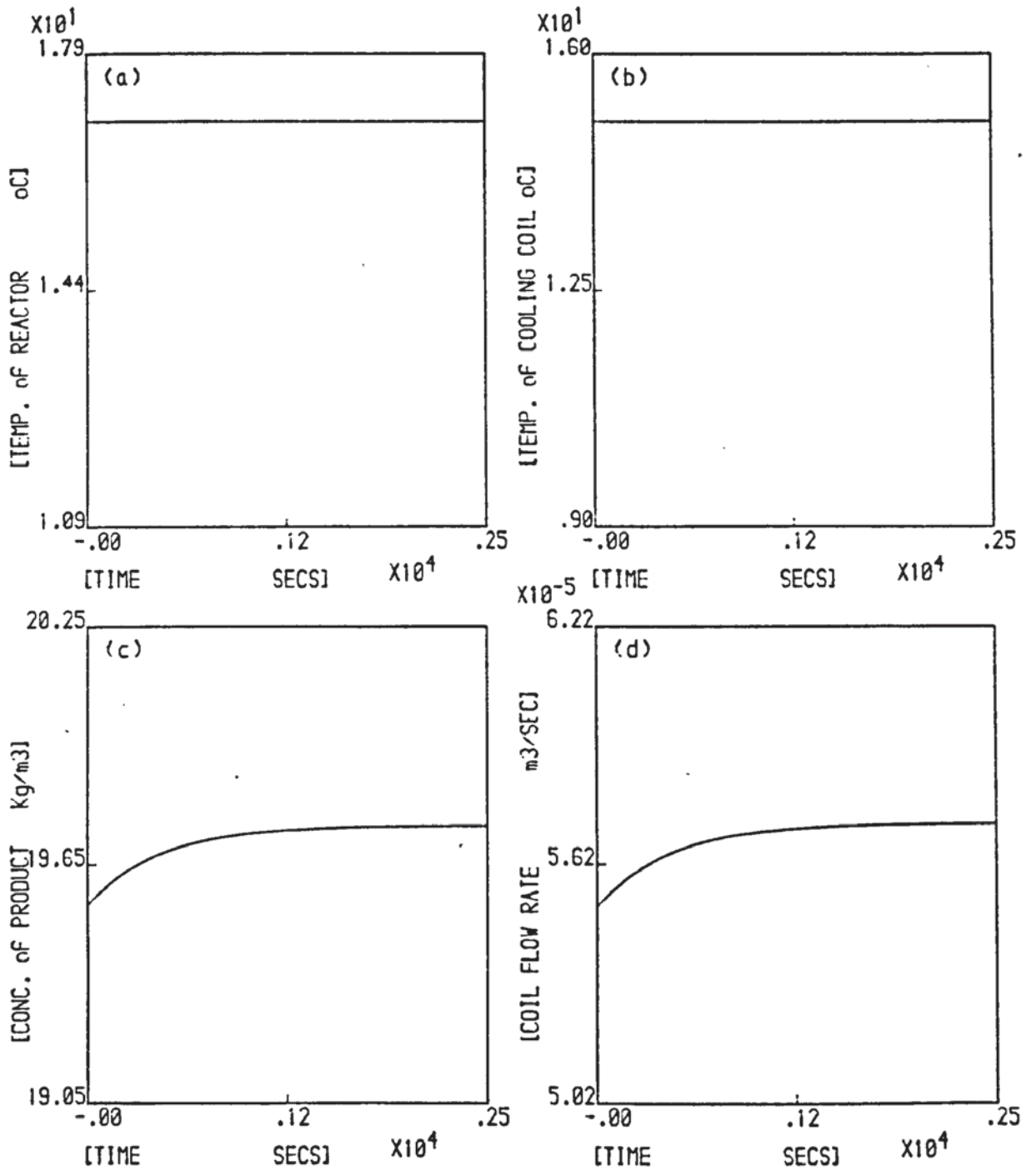


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Step in feed temperature of reactor(-1.062 K) and cooling coil(-1.64K). Invariance control of reactor and cooling coil temperature. Fig. 1.6.1.25 Reactor One. Experiment no:25



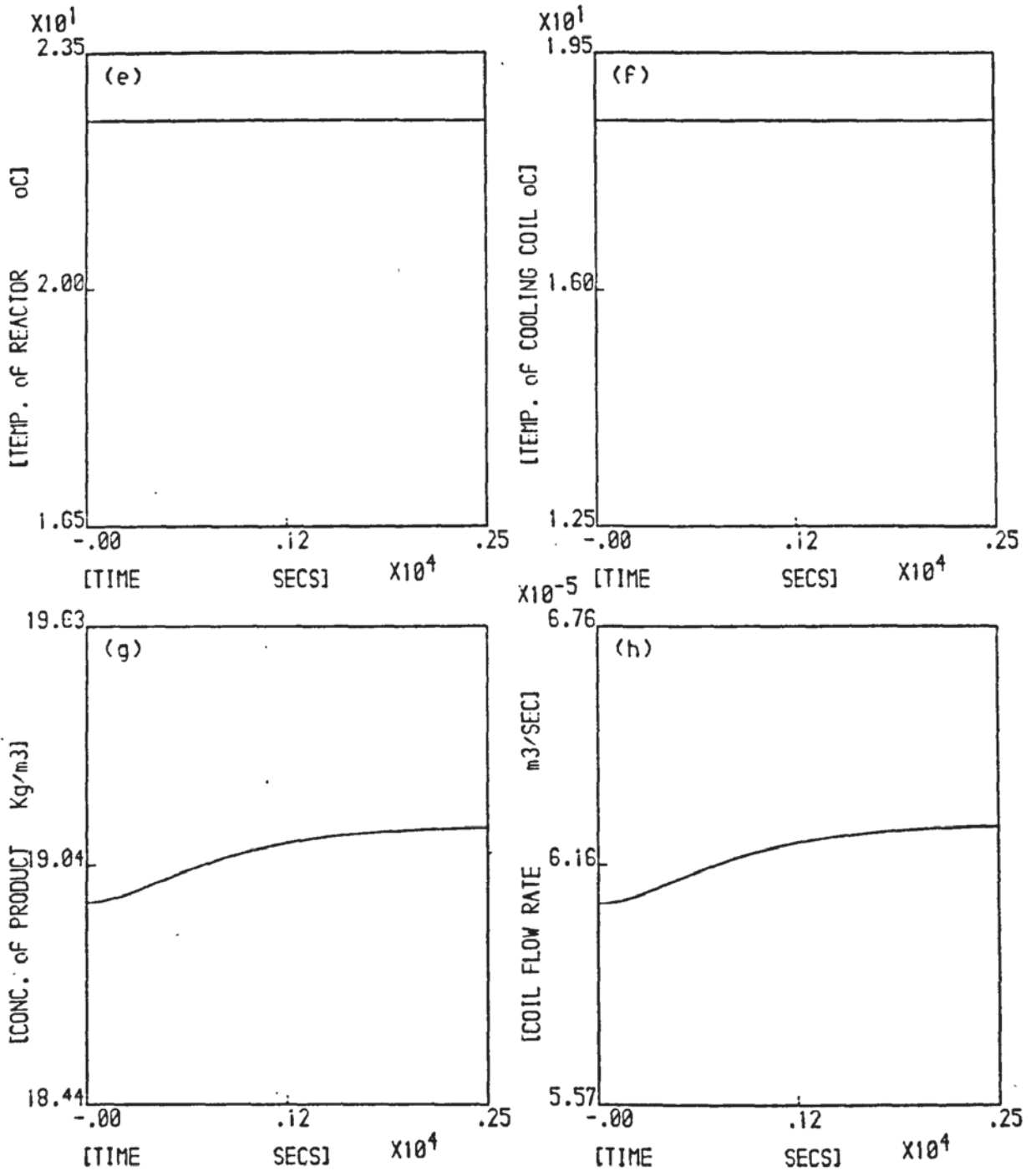
Step in feed temperature of cooling coil
 (-1.5 K). Invariance control of reactor &
 cooling coil temperature.
 Fig. A.6.1.25 Reactor Two. Experiment no: 25



Step in feed concentration (0.2 kg/m^3) and coil inlet temperature (-0.92 K).

Invariance control.

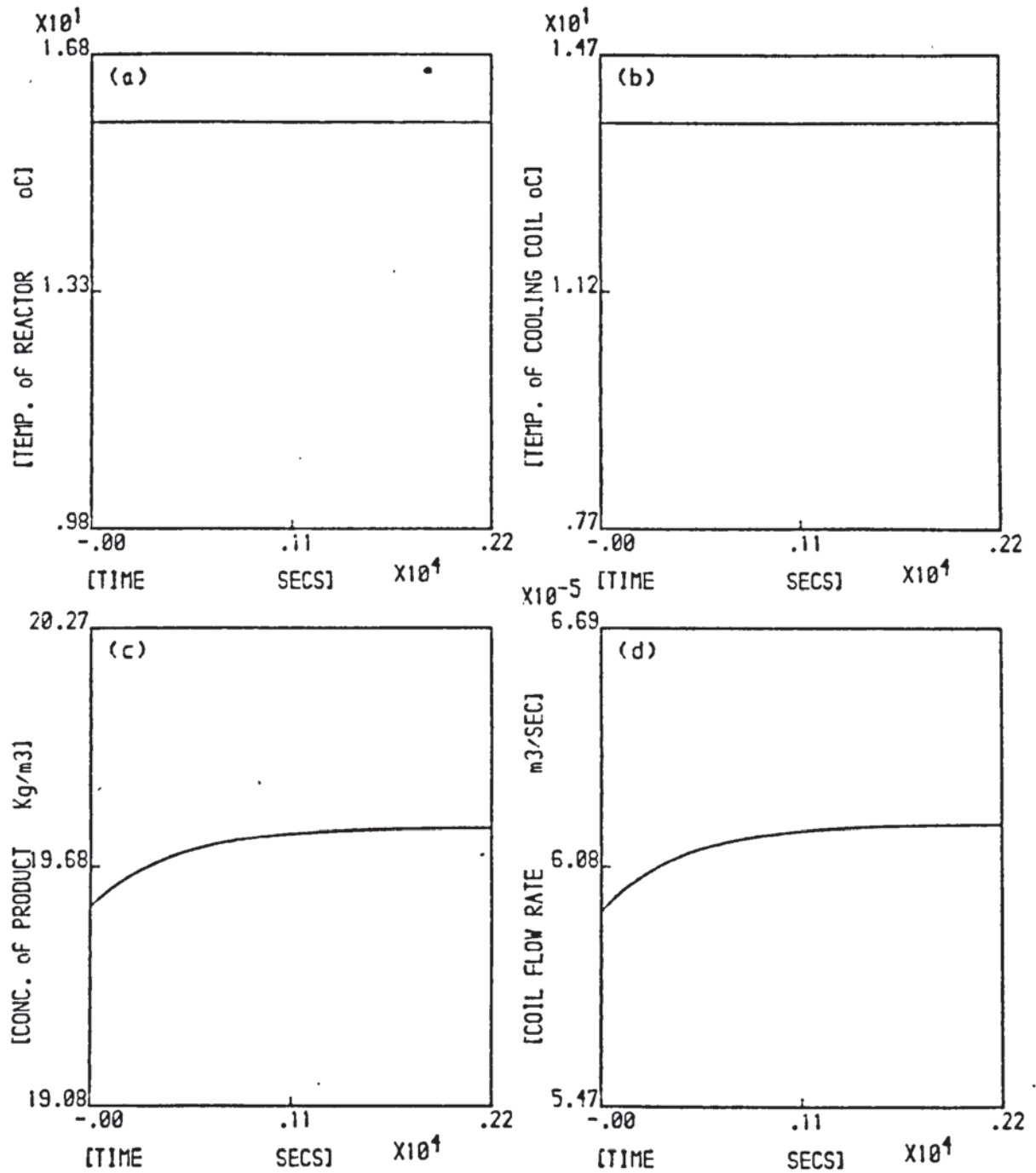
Fig. A.6.1.26 Reactor One. Experiment no:26



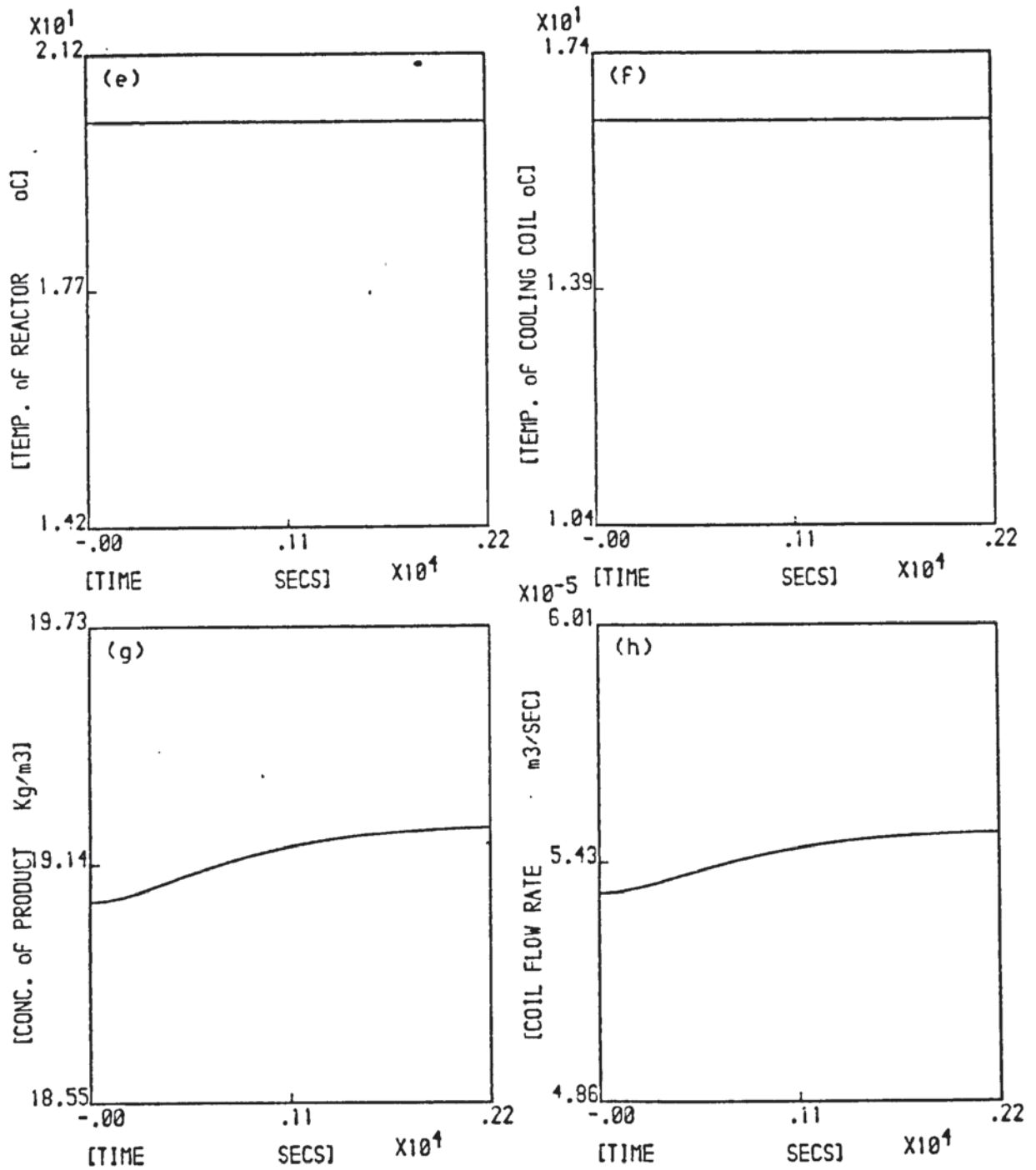
Step in temperature of coolant into coil
 (-0.75 K).

Invariance control.

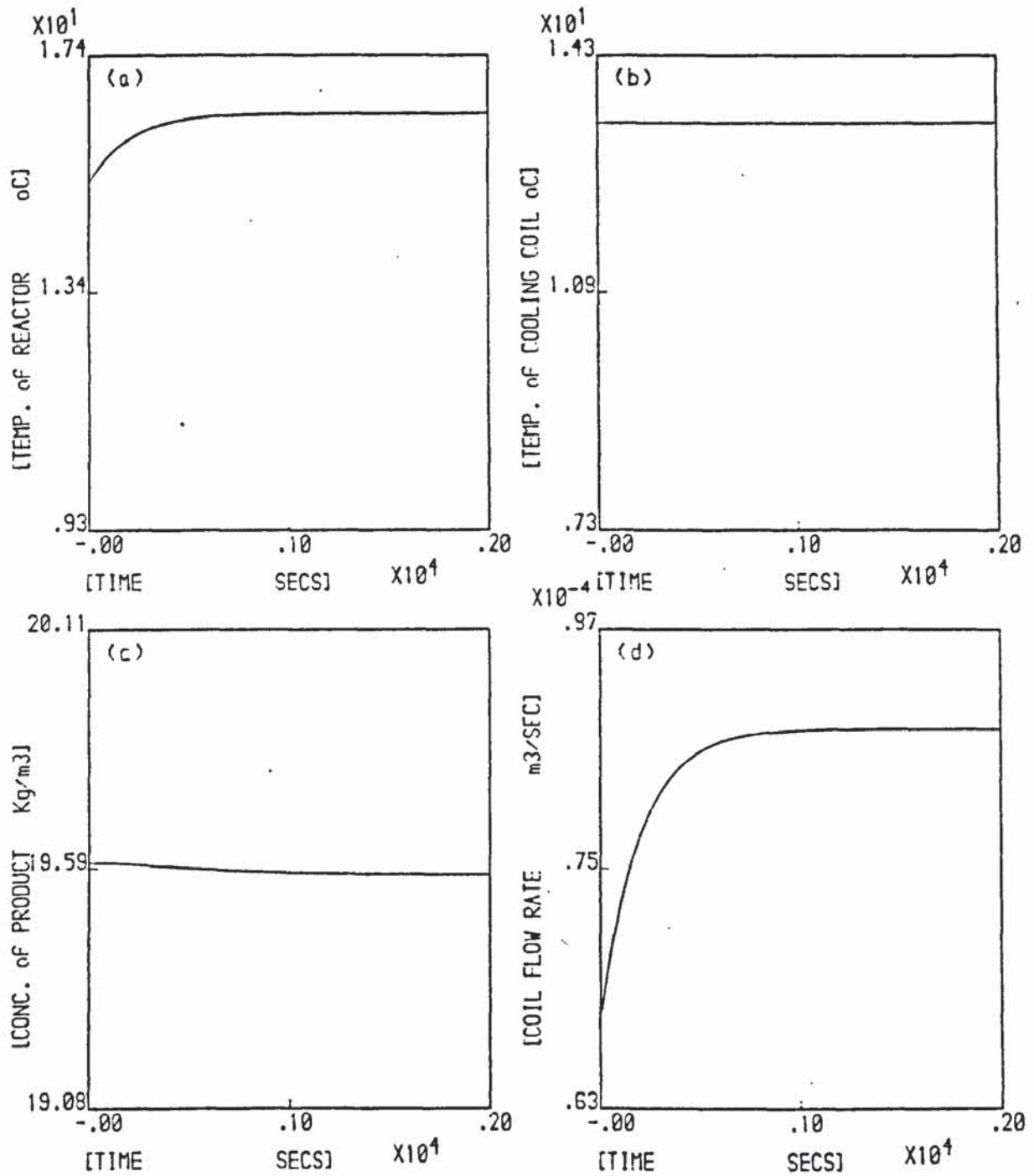
Fig. A.6.1.26 Reactor Two. Experiment no:26



Step in Feed concentration(0.2kg/m³) and reactor(-0.193 K) temperature. Invariance control of reactor & cooling coil temperature Fig. A.6.1.27 Reactor one. Experiment no:27



Step in feed temperature into cooling coil
 (-0.752 K). Invariance control of reactor
 and cooling coil temperatures.
 Fig. 1.6.1.27 Reactor Two. Experiment no:27

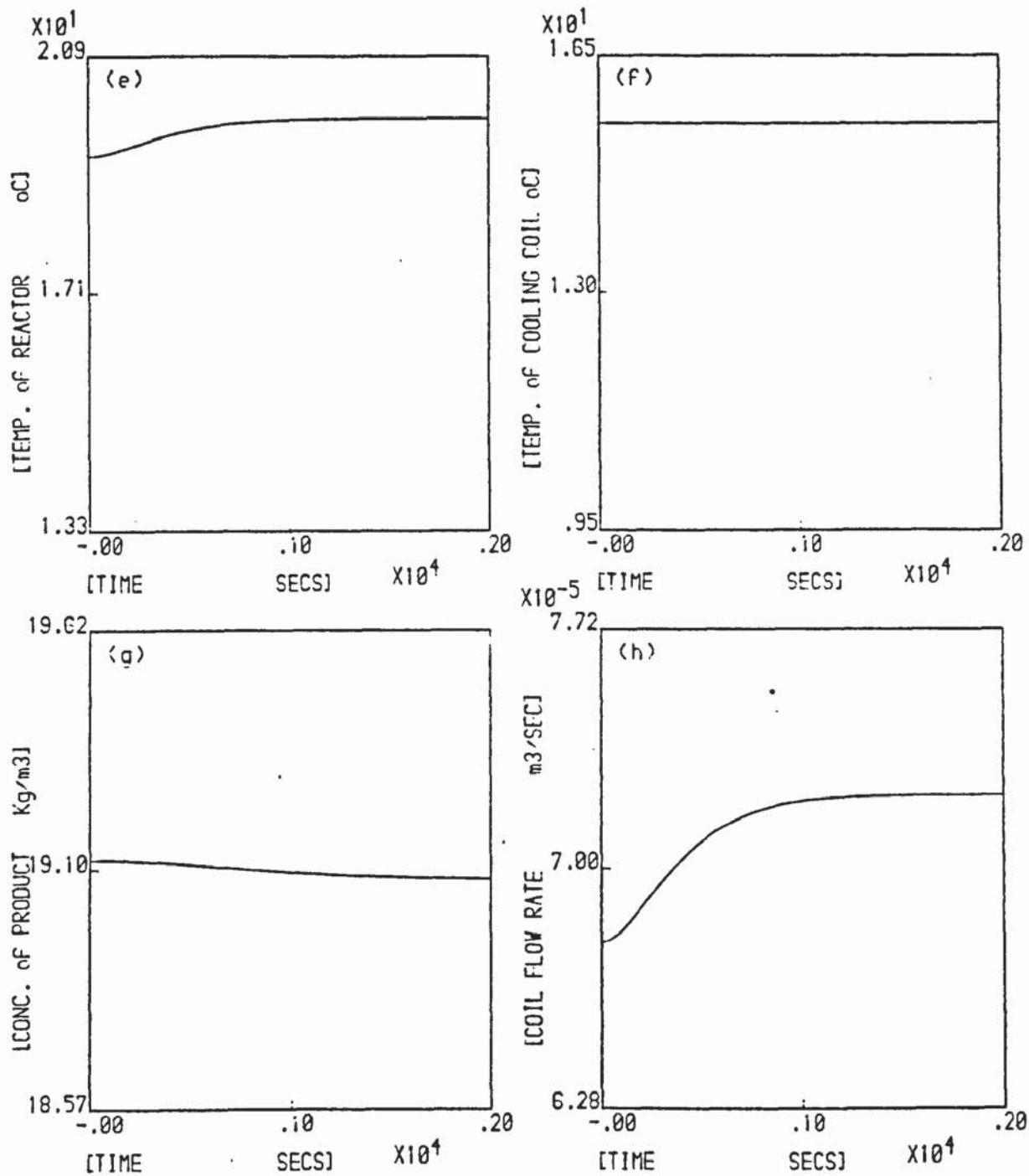


Step in feed temperature(2.5 K).

Non-interacting control of coil

temperature.

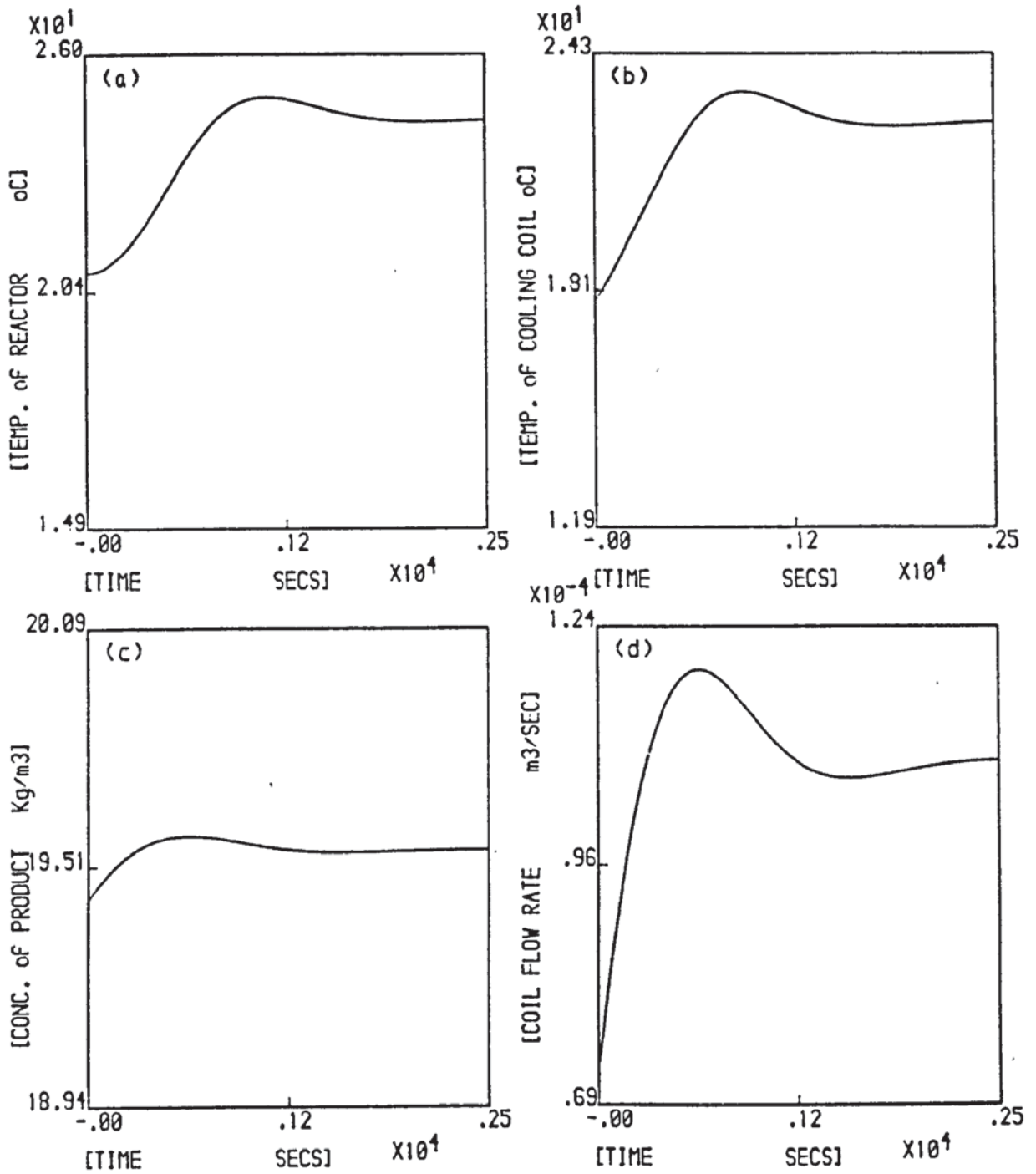
Fig. A.6.1.28 Reactor One. Experiment no:28



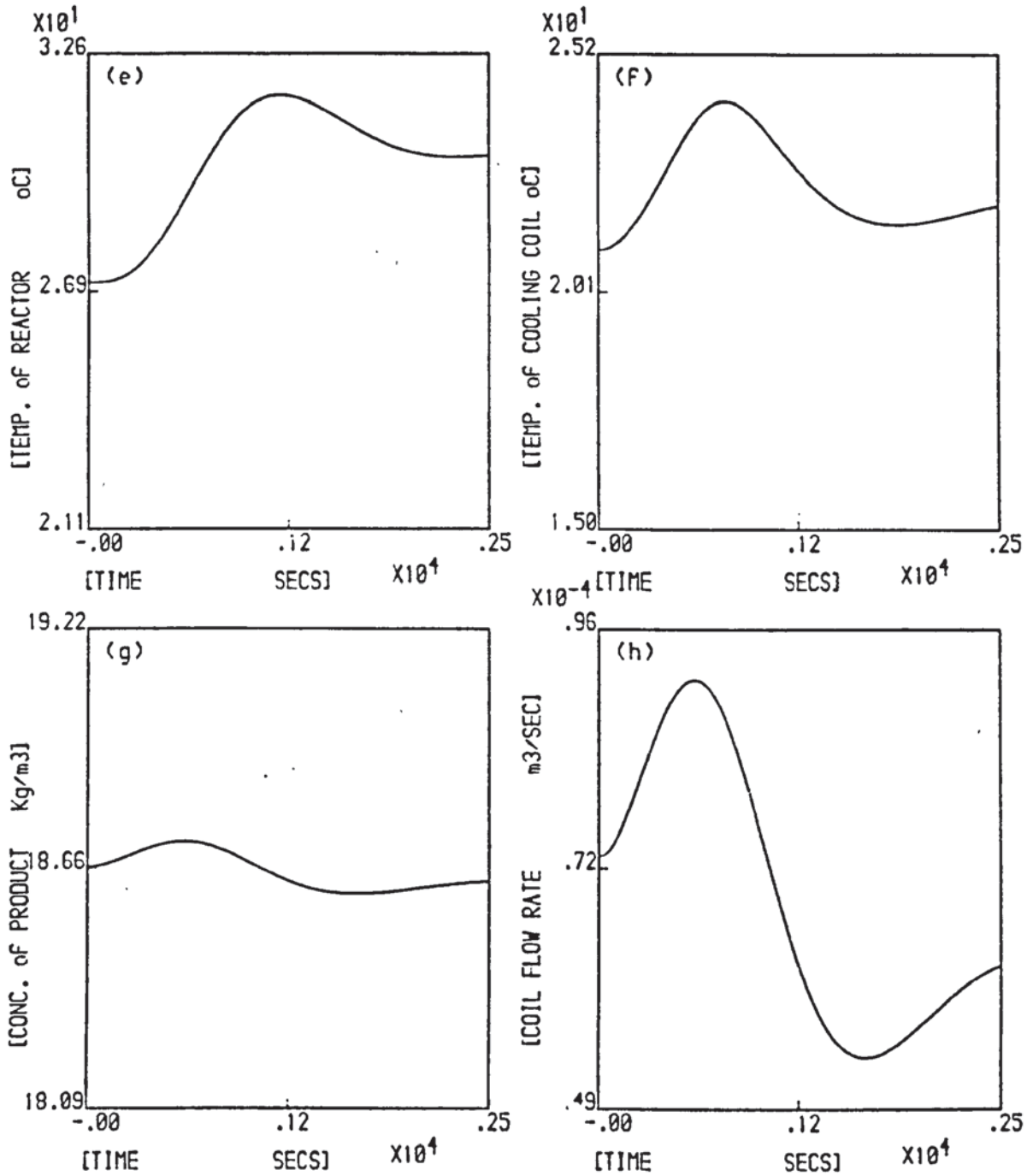
Disturbances From first reactor only.

Non-interacting control of cooling coil
temperature.

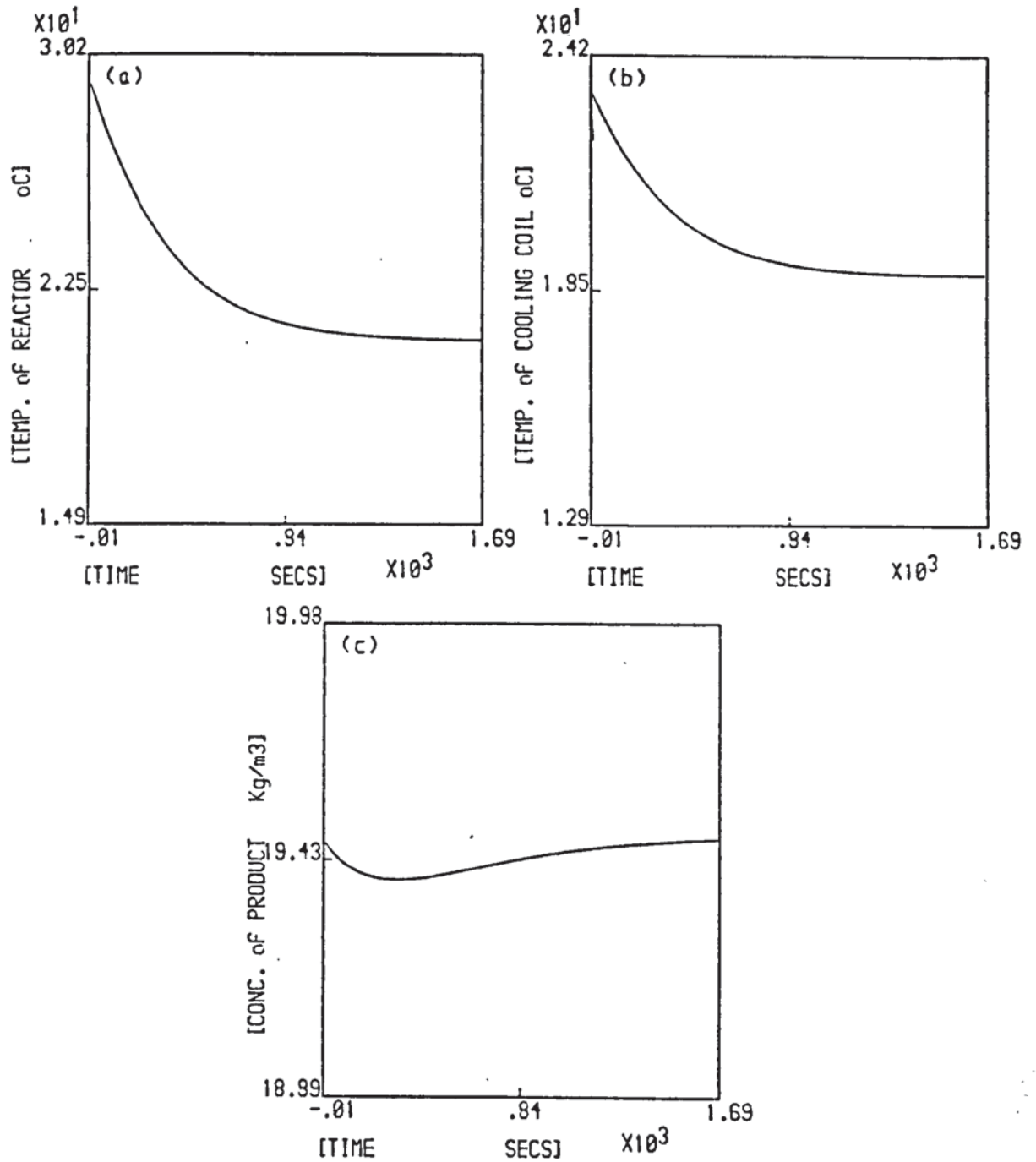
Fig. A.6.1.28 Reactor Two. Experiment no:28



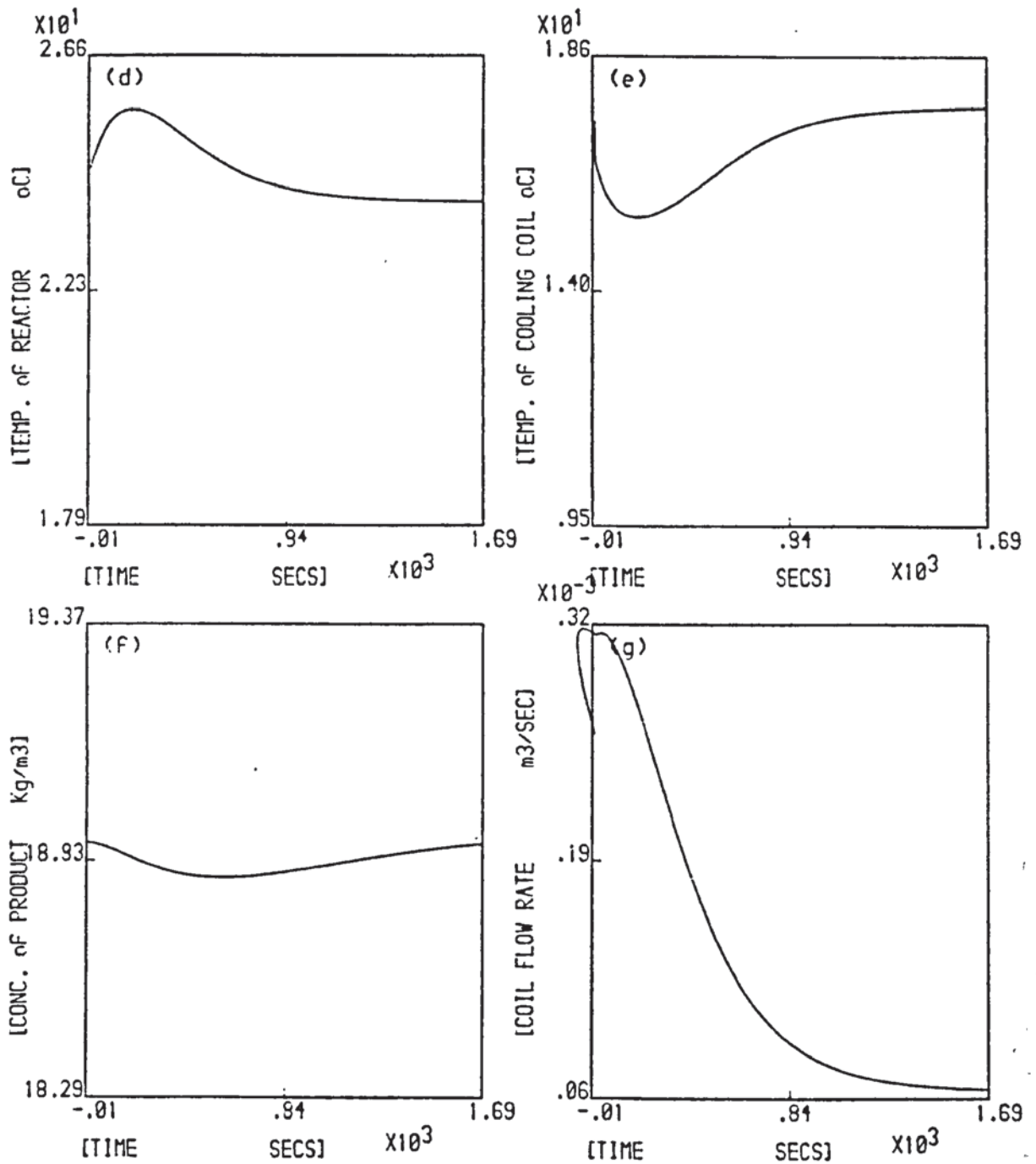
Step in Feed concentration(0.25kg/m³).
 Proportional feedback control of
 reactant concentration. $K_c=3E-04$
 Fig. 1.6.1.29 Reactor One. Experiment no: 5



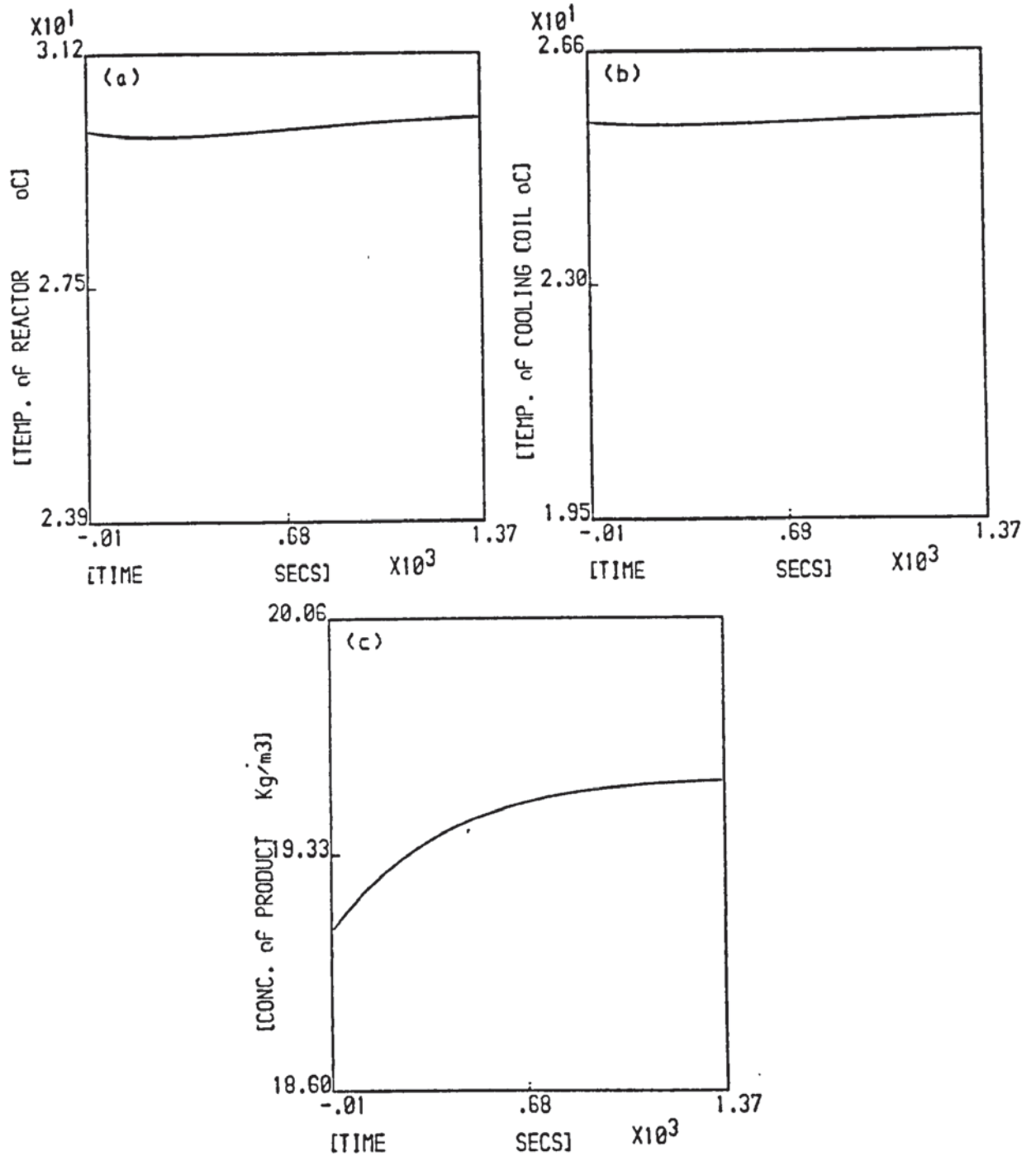
Disturbances from First reactor only.
 Proportional feedback control of
 reactant concentration. $K_c=3E-04$
 Fig. 1.6.1.29 Reactor Two. Experiment no: 5



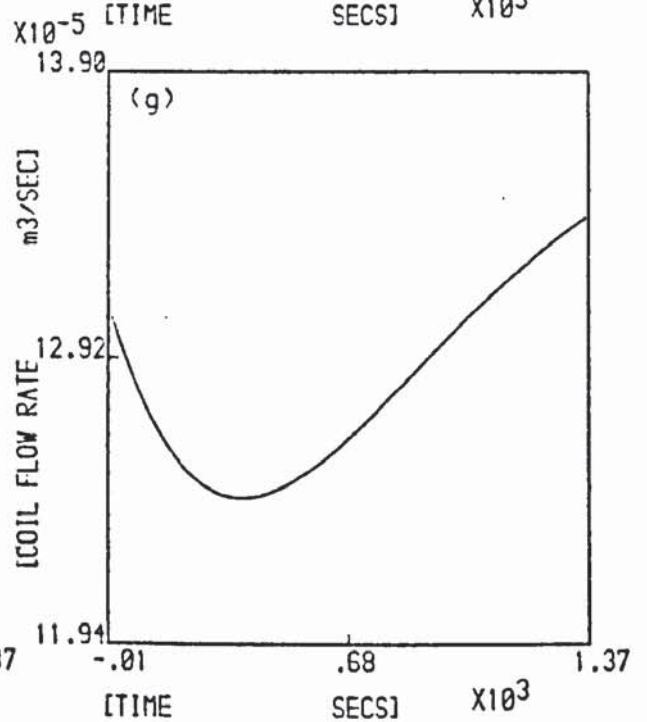
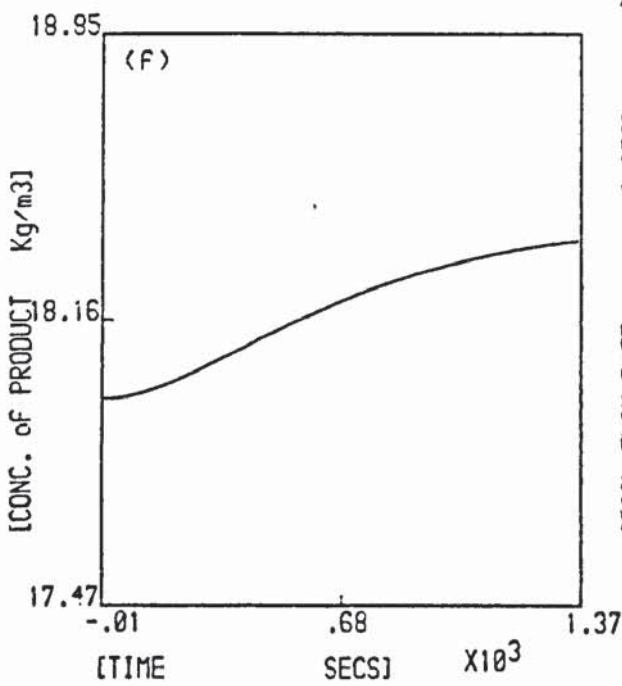
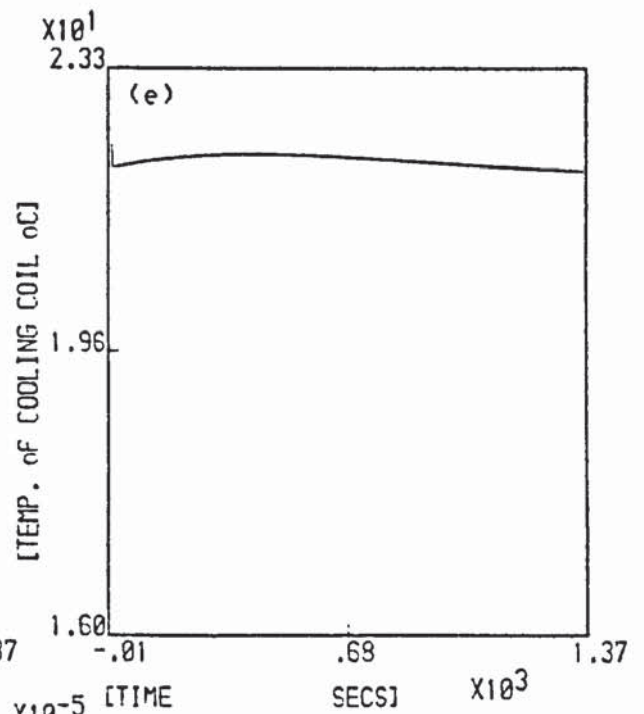
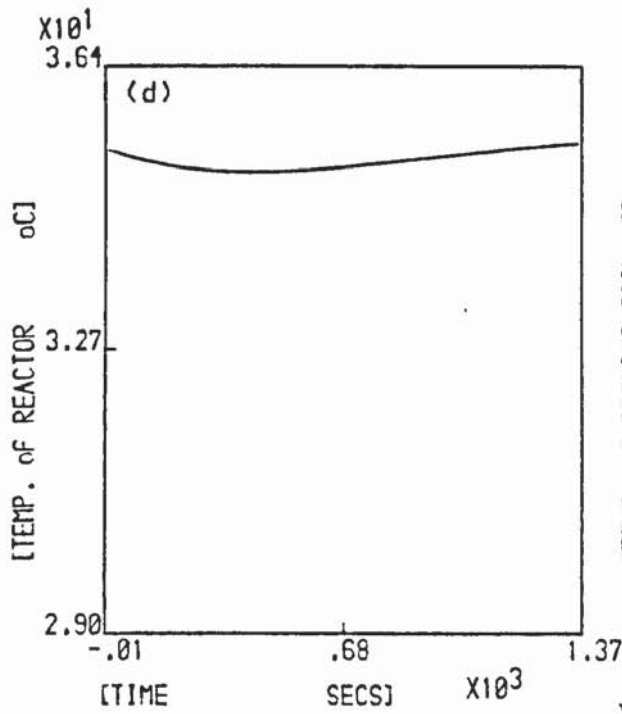
Initial perturbation in state variables & step in feed temperature(-0.212 K). Single cooling stream for both reactors.
 Fig. A.6.1.30 Reactor One. Experiment no:32



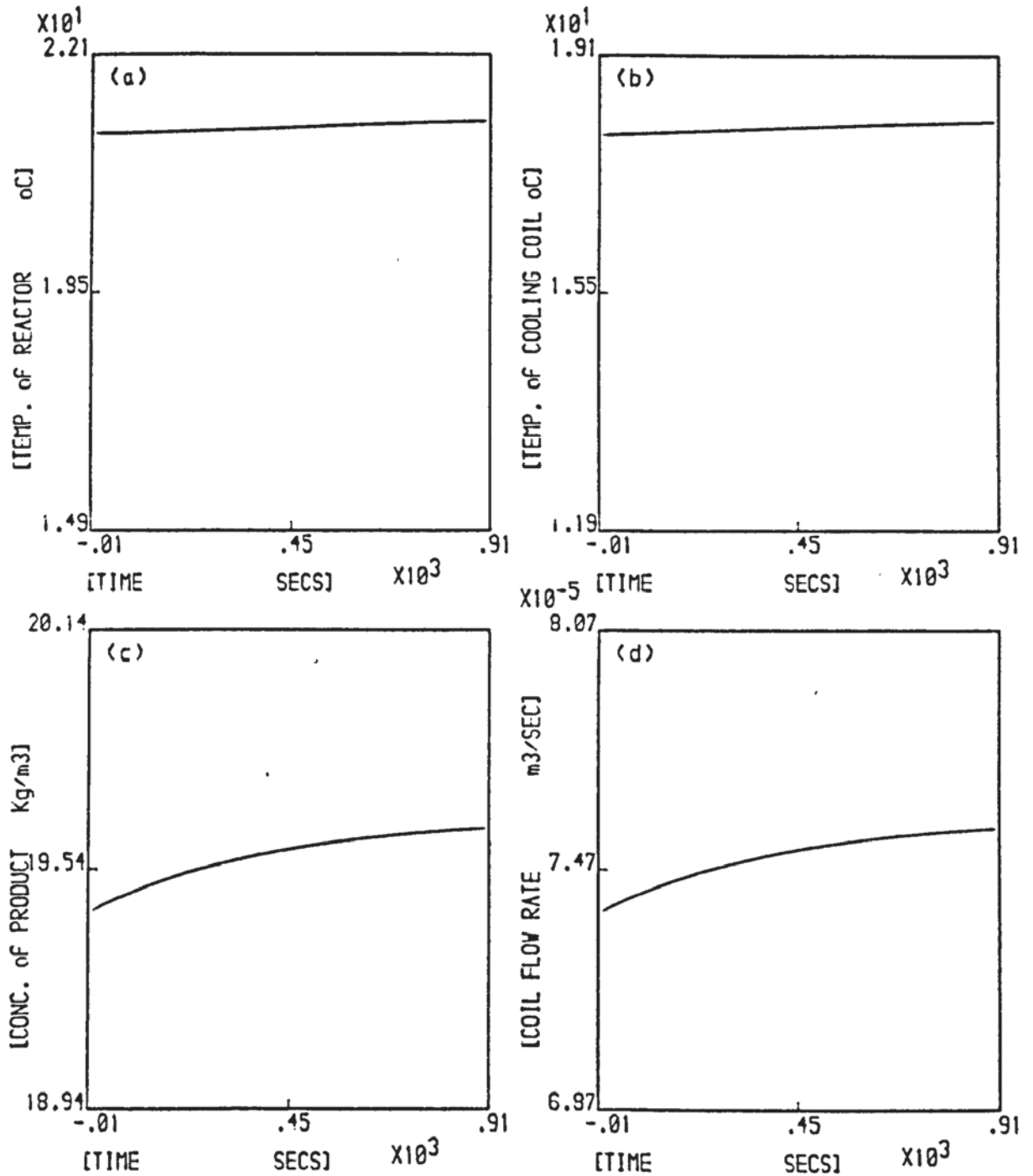
Initial perturbation in state variables and step in coolant temperature (-0.53 K). Prop. Feedback control of reactor temp. $K_c = 5E-05$
 Fig. A.6.1.30 Reactor Two. Experiment no:32



Step in Feed concentration (0.5 kg/m^3) and temperature (-0.39 K). Cooling stream from coil in second reactor.
 Fig. A.6.1.31 Reactor One. Experiment no:29



Step in coolant temperature (-0.47 K). Counter-current contacting of feed and coolant streams. Prop. feedback control of reactor temp. $K_c = 2 \times 10^{-5}$. Fig. A.6.1.31 Expt. no:29

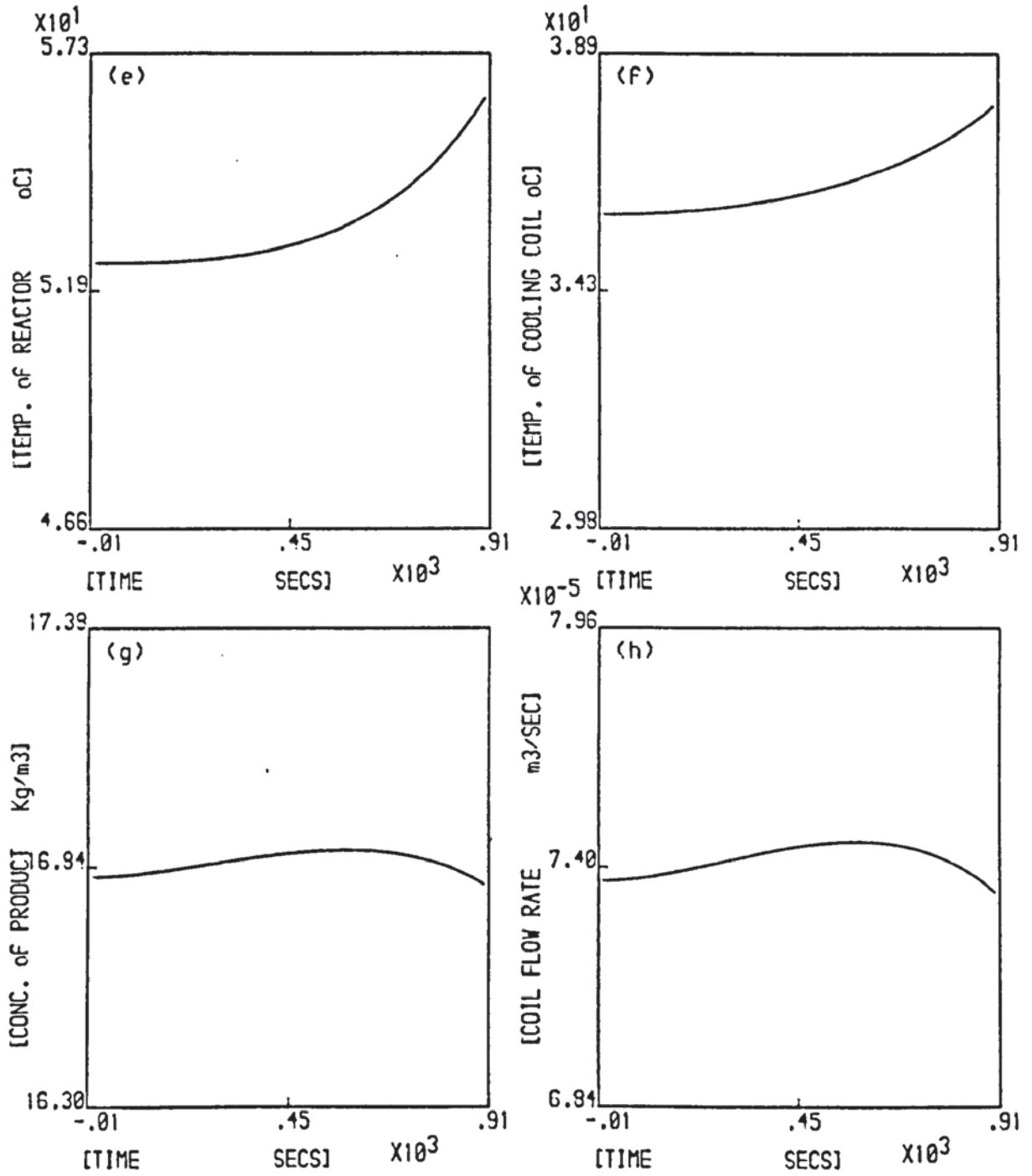


Step in feed concentration(0.25kg/m^3).

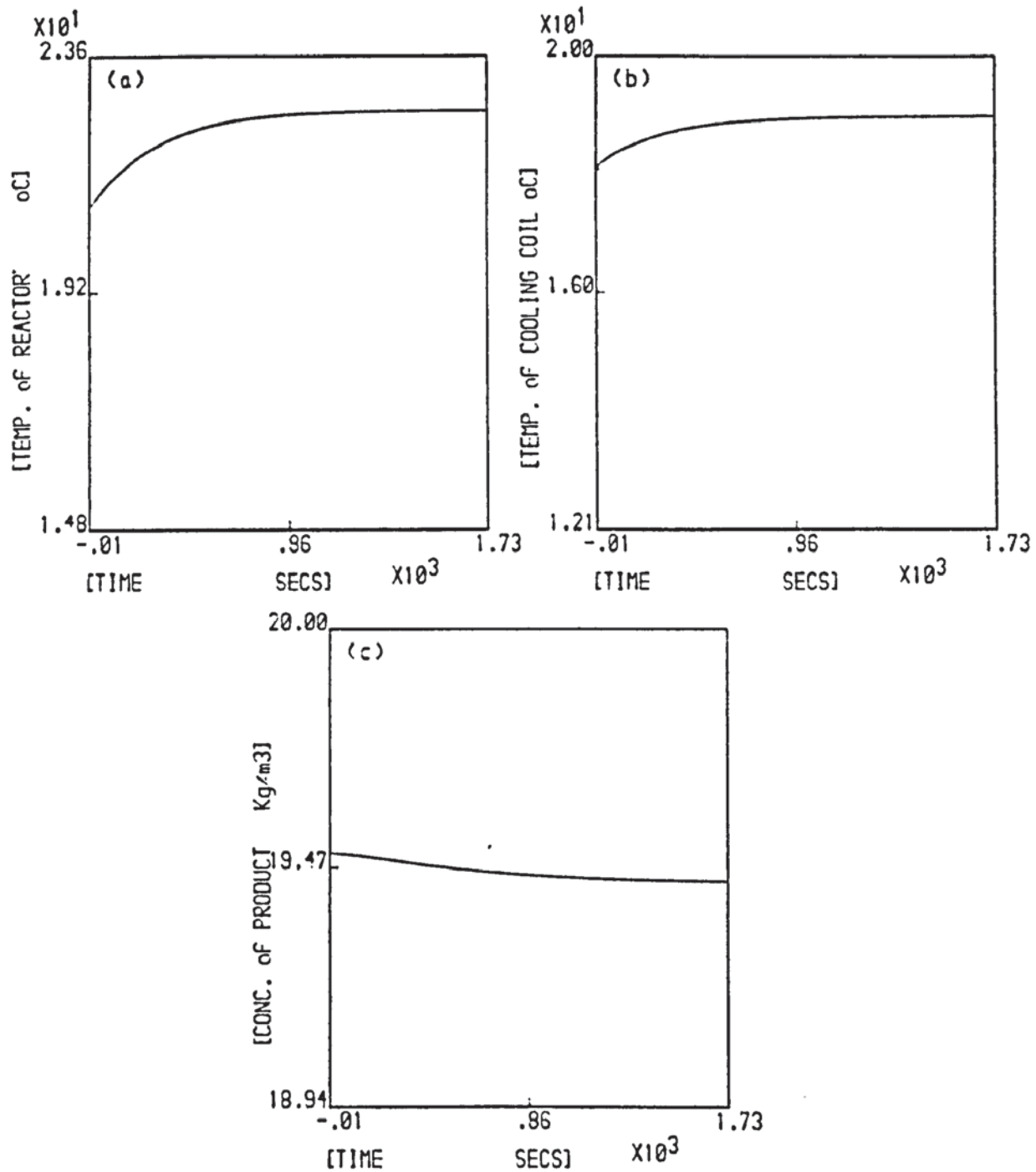
Proportional Feedback control of

reactant concentration. $K_c=1E-05$

Fig. A.6.1.32 Reactor One. Experiment no: 5

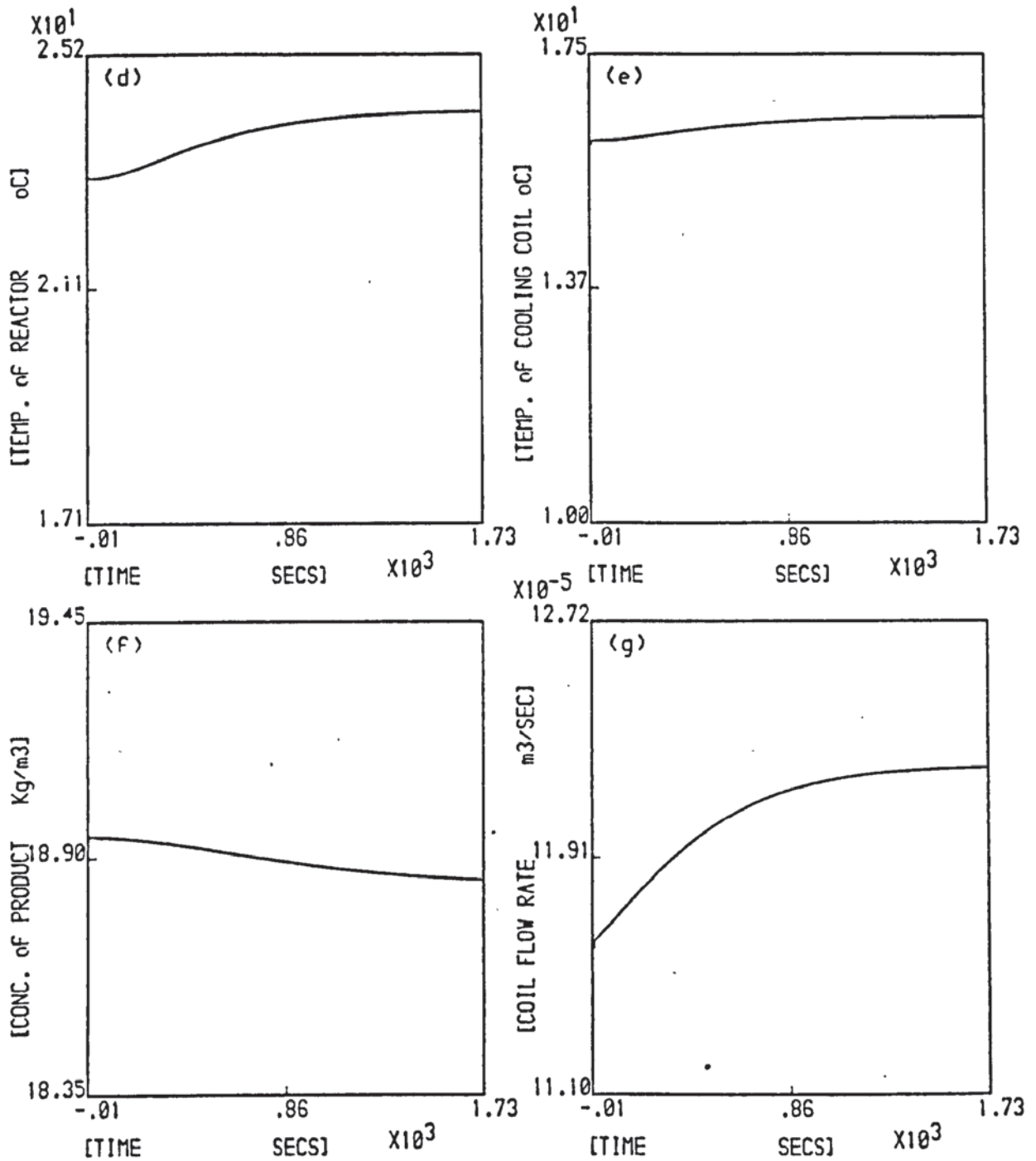


Disturbances From first reactor only.
 Proportional feedback control of reactant
 concentration at unstable state. $K_c=1.5E-05$
 Fig. A.6.1.32 Reactor Two. Experiment no: 5

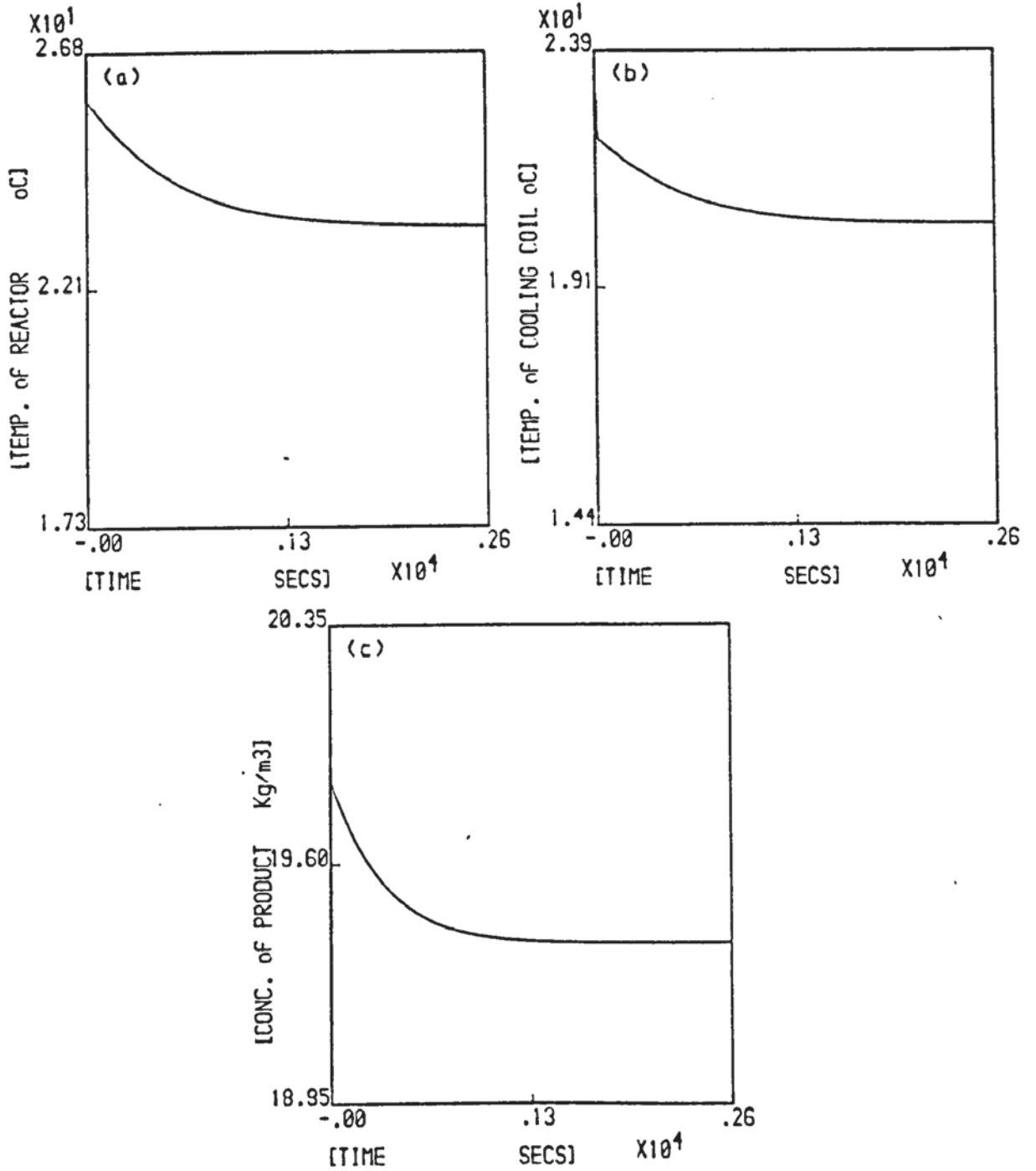


Step in Feed temperature(3.09 K). Cooling stream from coil in second reactor.

Fig. A.G.1.33 Reactor One. Experiment no:33

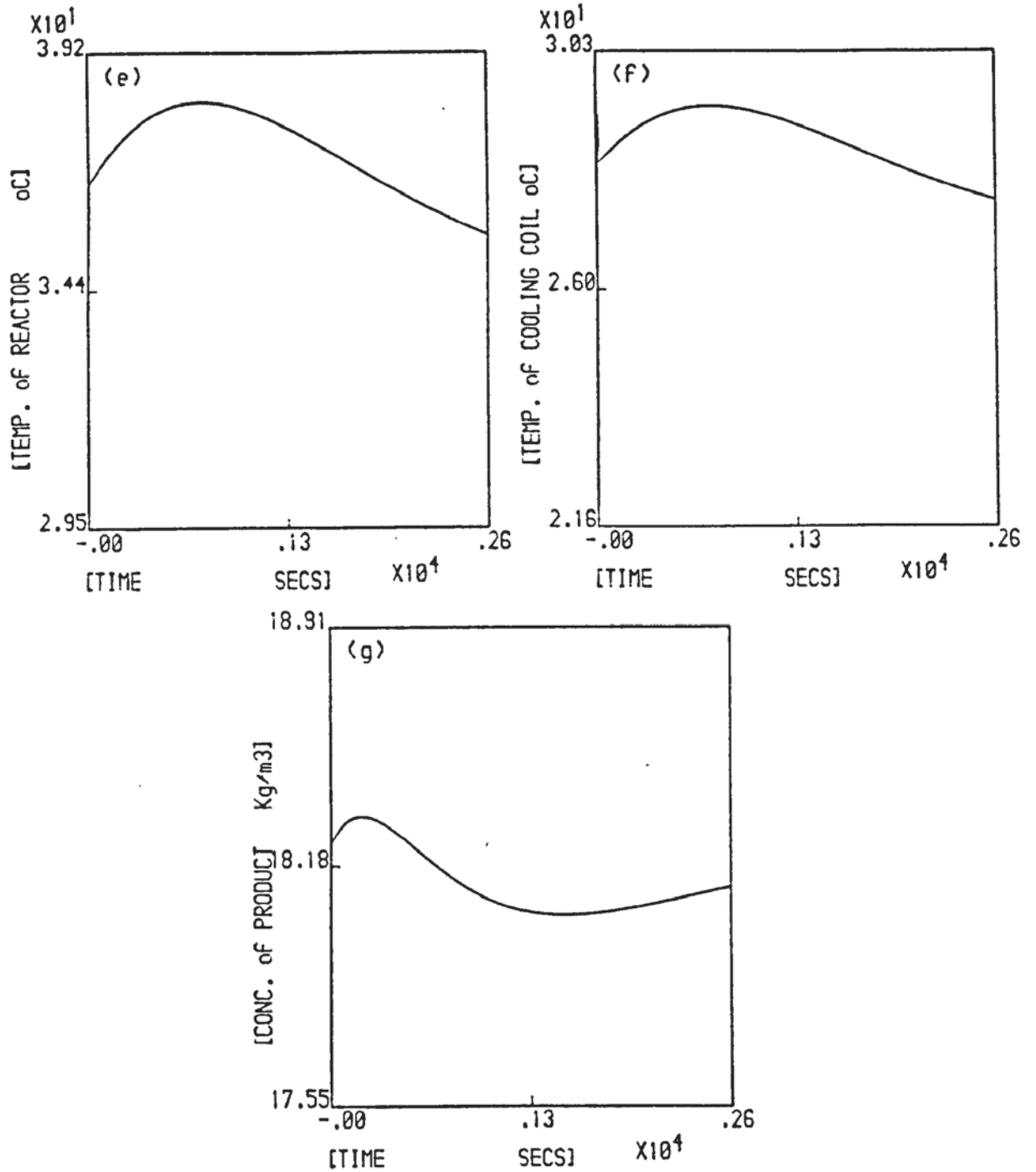


Disturbances from First reactor. Counter-current contacting of feed & coolant streams.
 Prop. Feedback control of reactor temperature
 Fig. A.6.1.33 Reactor Two. $K_c=3E-06$. Expt. no:33



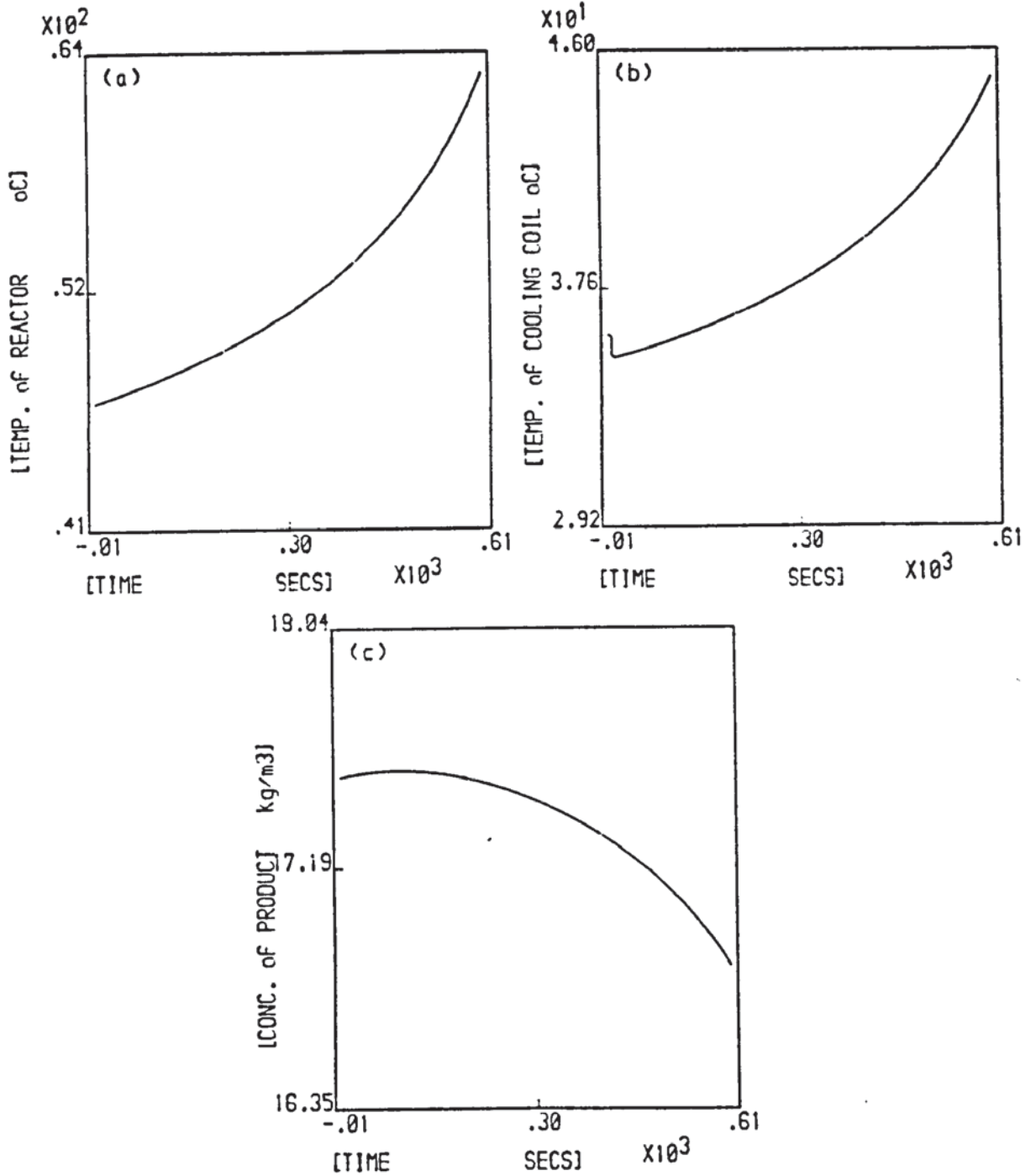
Initial perturbation in state variables.
 Open loop stable steady state.

Fig. A.6.1.34 Reactor One. Experiment no: 1



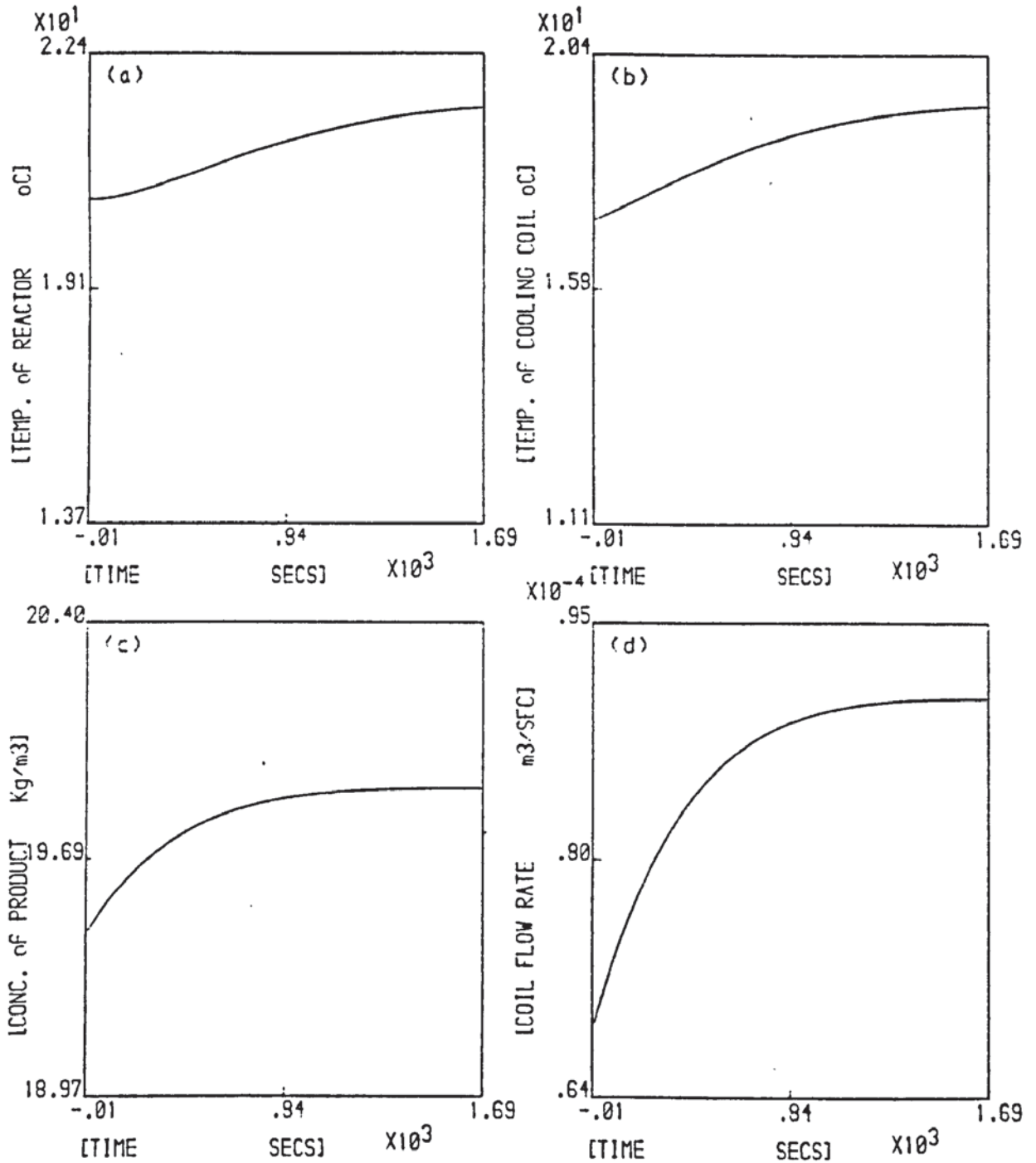
Initial perturbation in state variables.
 No control of stable steady state.

Fig. A.6.1.34 Reactor Two. Experiment no: 1

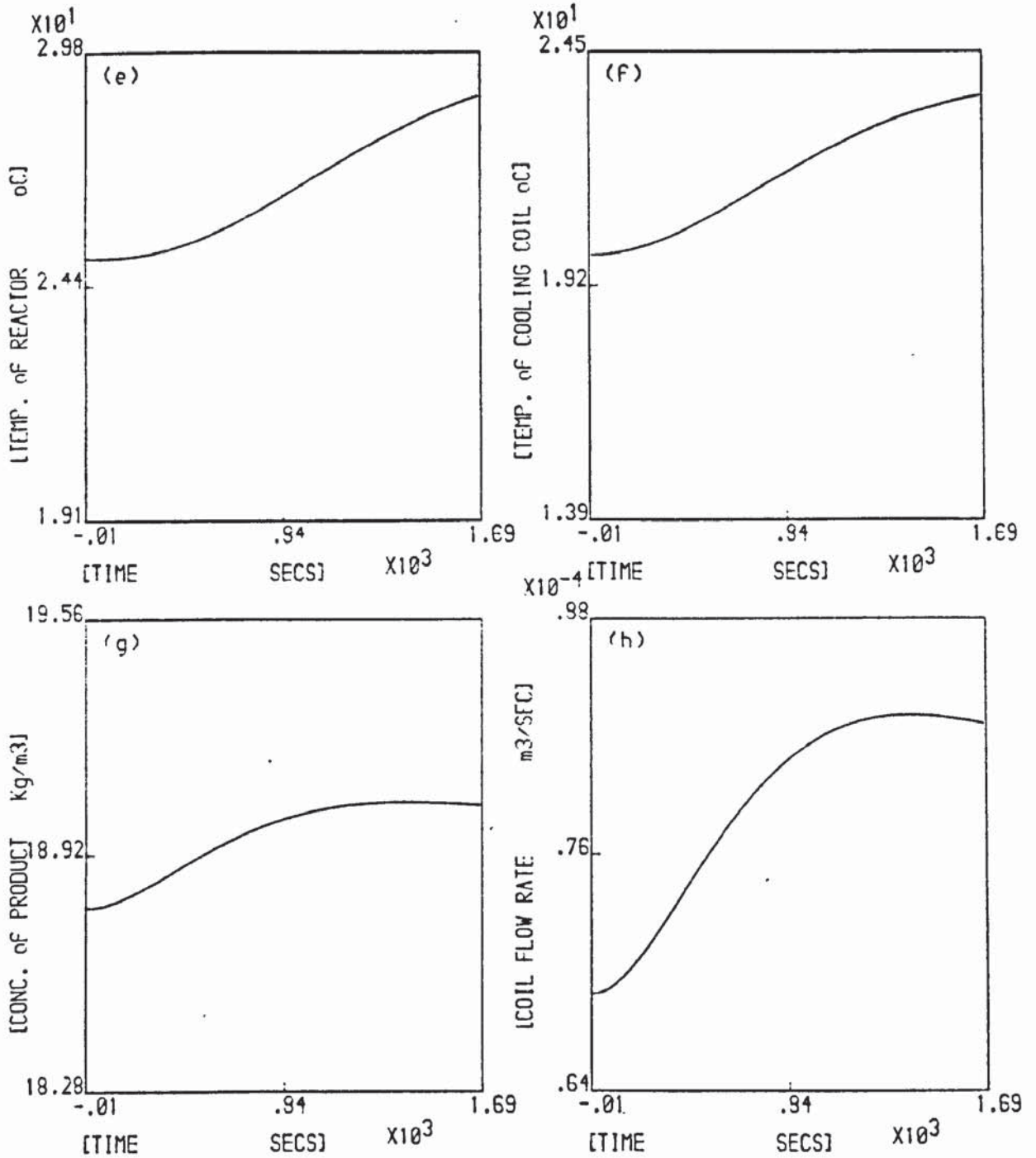


Initial perturbation in state variables.
 Open loop unstable steady state.

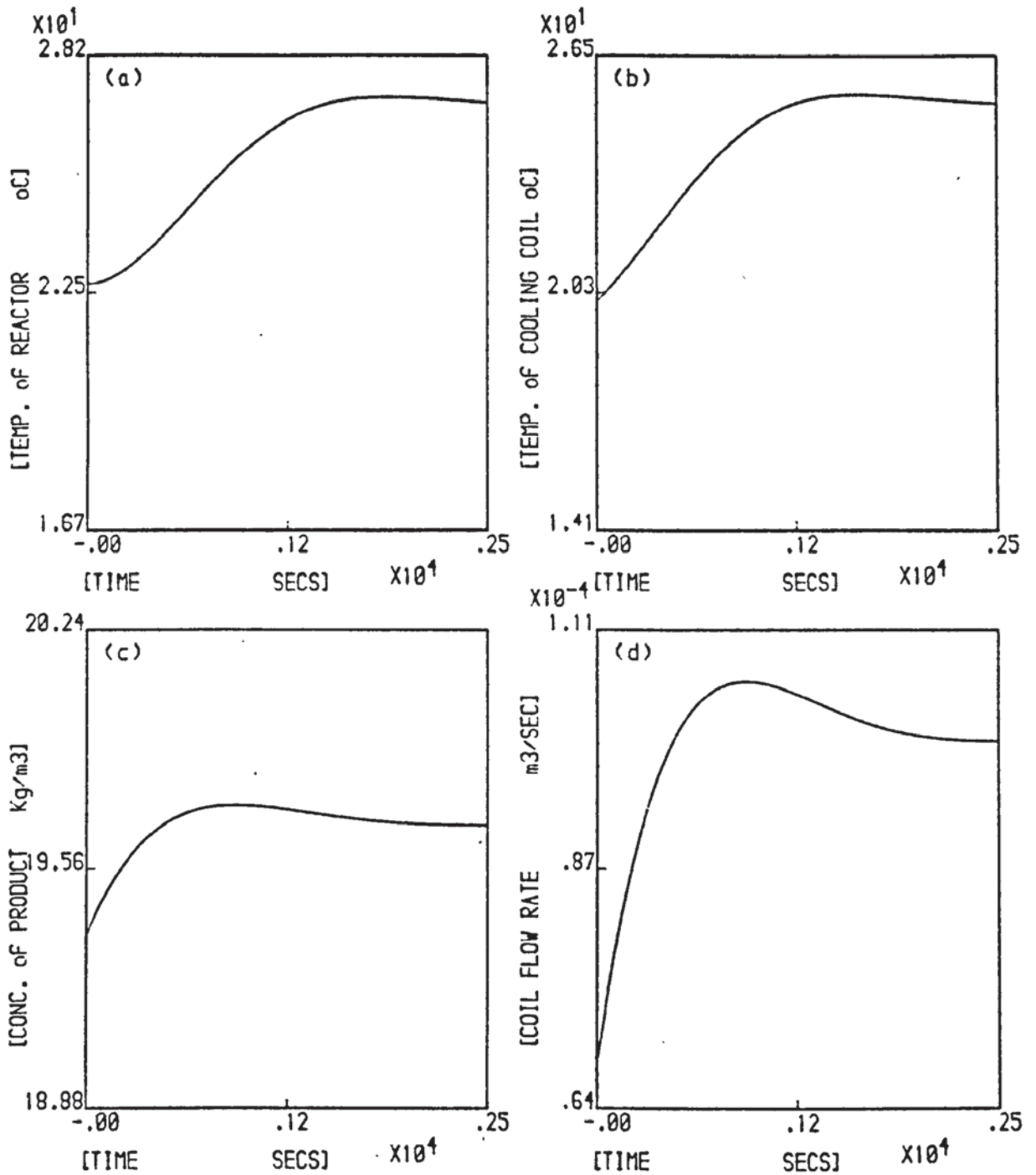
Fig. A.6.1.35 Reactor Two. Experiment no: 1



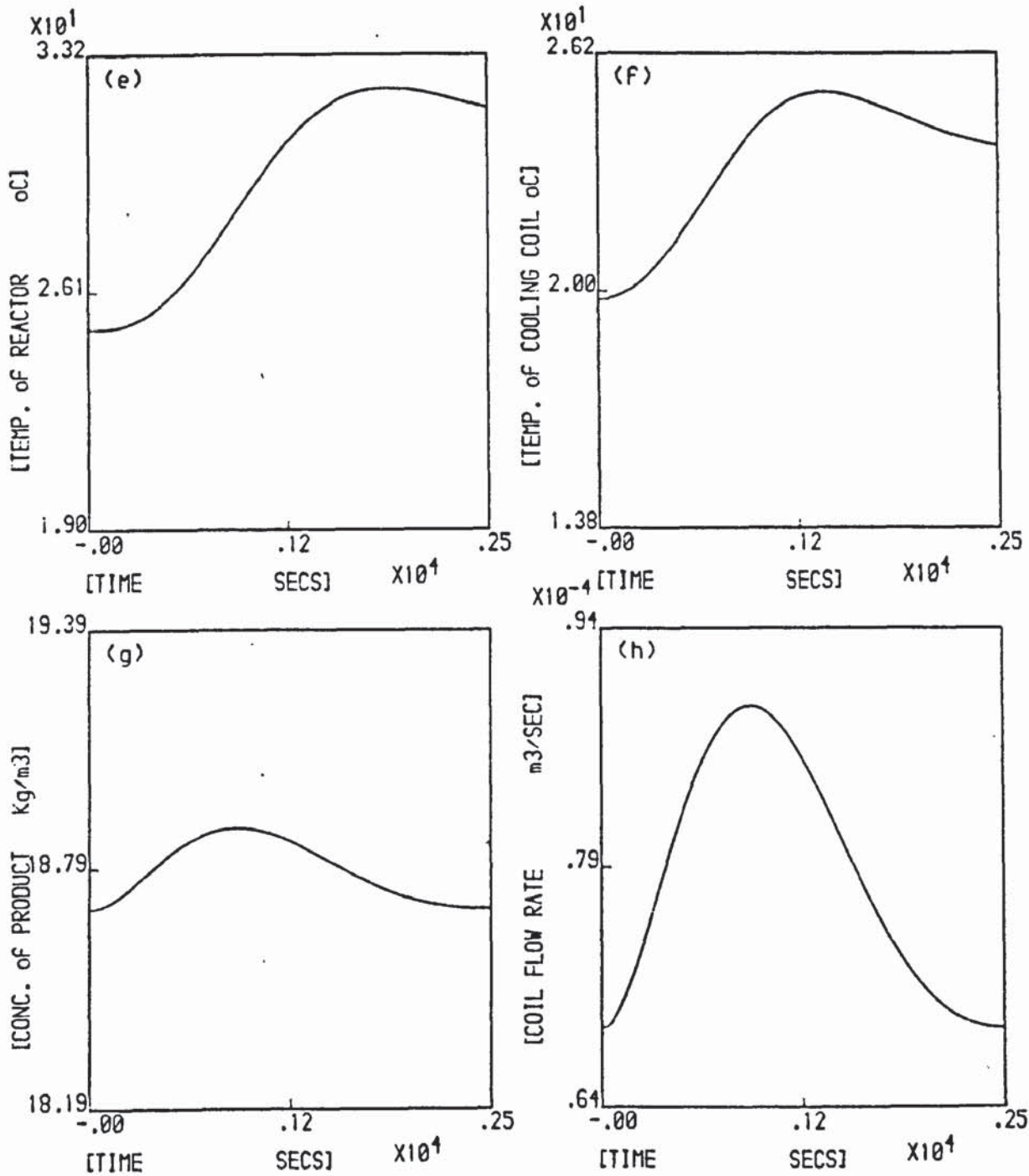
Step in feed concentration (0.5 kg/m^3),
 Proportional feedback control of
 reactant concentration. $K_c = 5E-05$
 Fig. A.6.1.36 Reactor One. Experiment no: 4



Disturbances from First reactor only.
 Proportional feedback control of
 reactant concentration. $K_c=5E-05$
 Fig. A.6.1.36 Reactor Two. Experiment no: 4



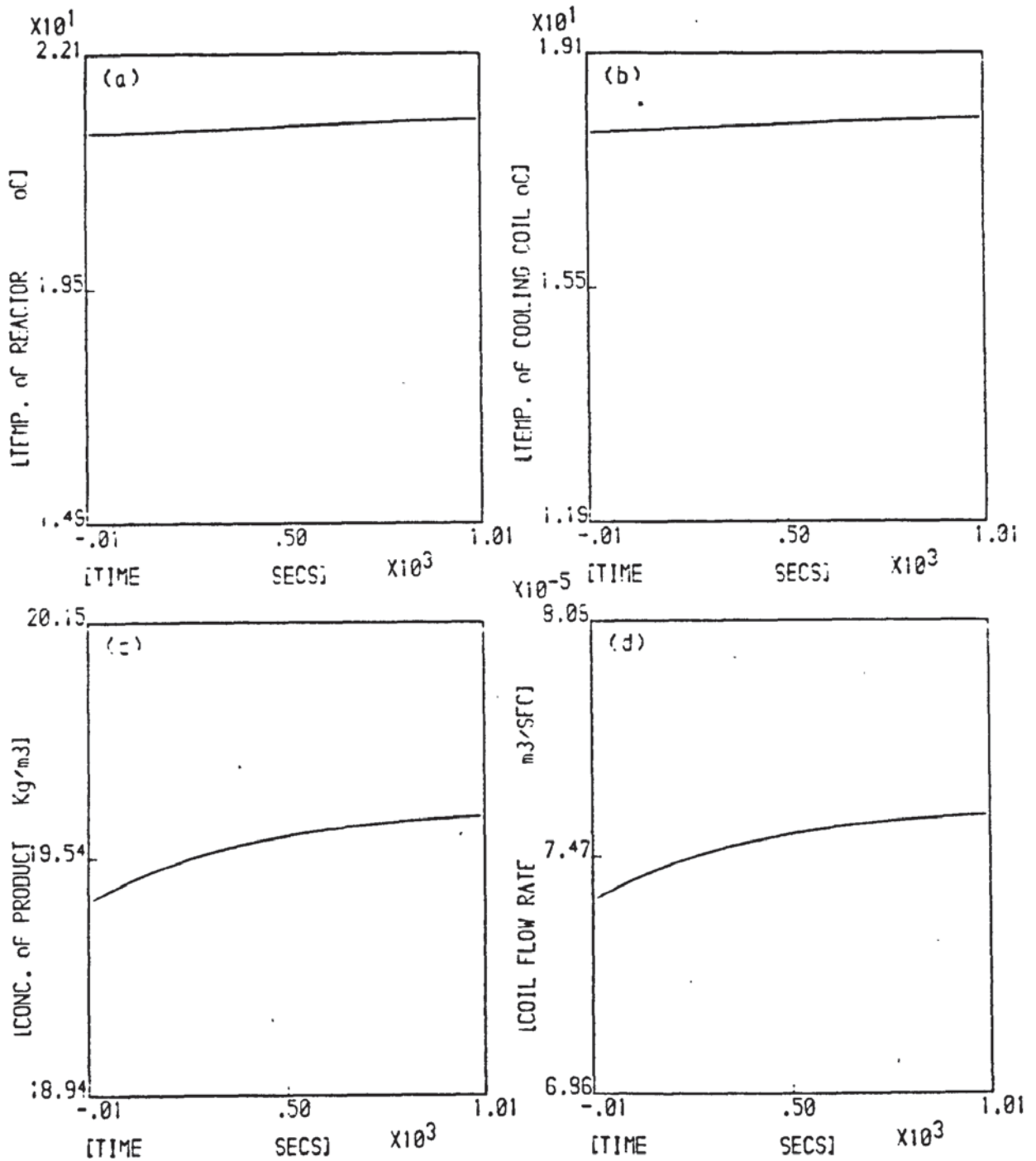
Step in Feed concentration (0.5 kg/m^3).
 Proportional feedback control of
 reactant concentration. $K_c = 1E-04$
 Fig. A.6.1.37 Reactor One. Experiment no: 4



Disturbances from first reactor only.

Proportional feedback control of
reactant concentration. $K_c=1E-04$

Fig. 1.6.1.37 Reactor Two. Experiment no: 4

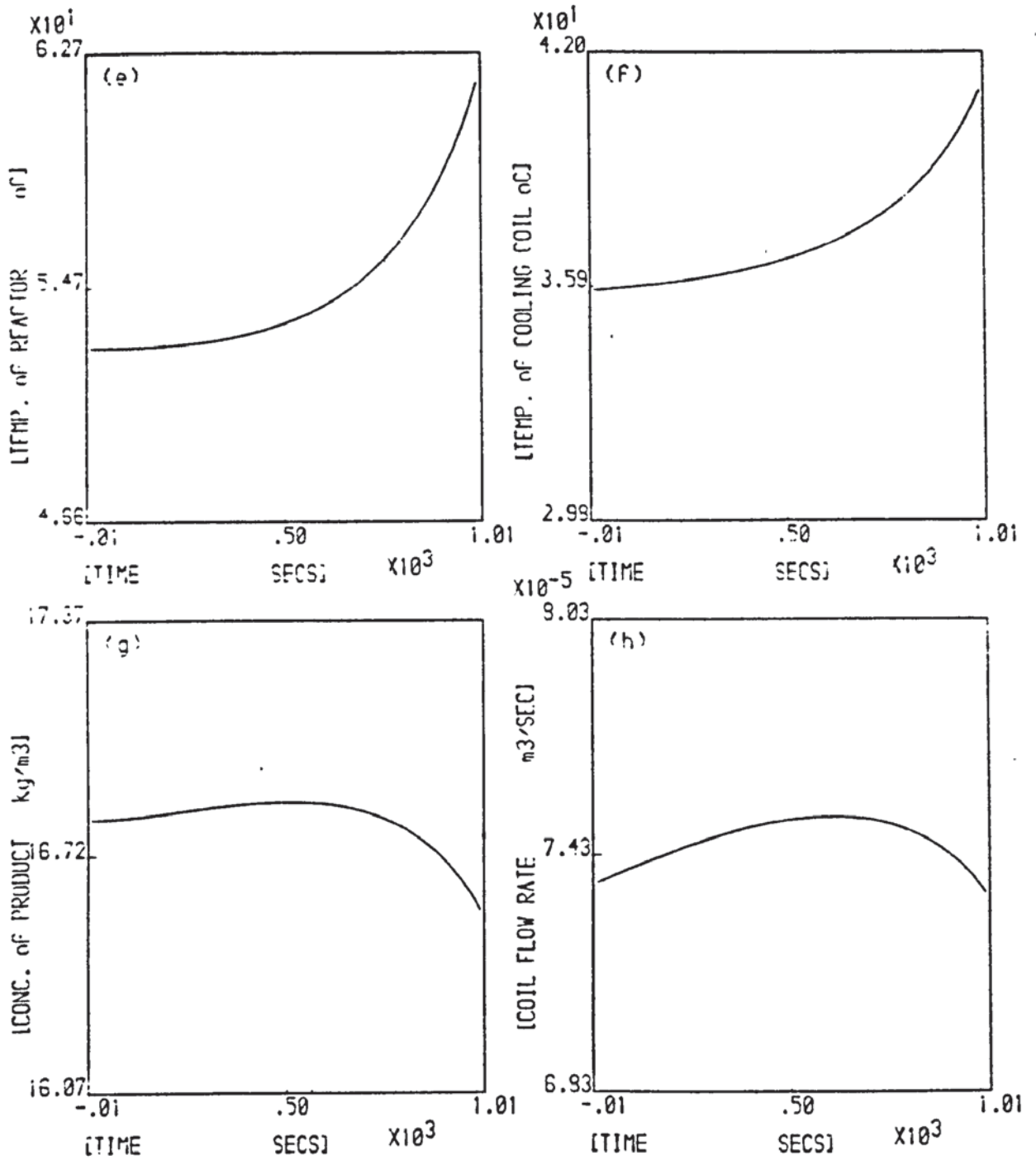


Step in feed concentration (0.25 kg/m^3).

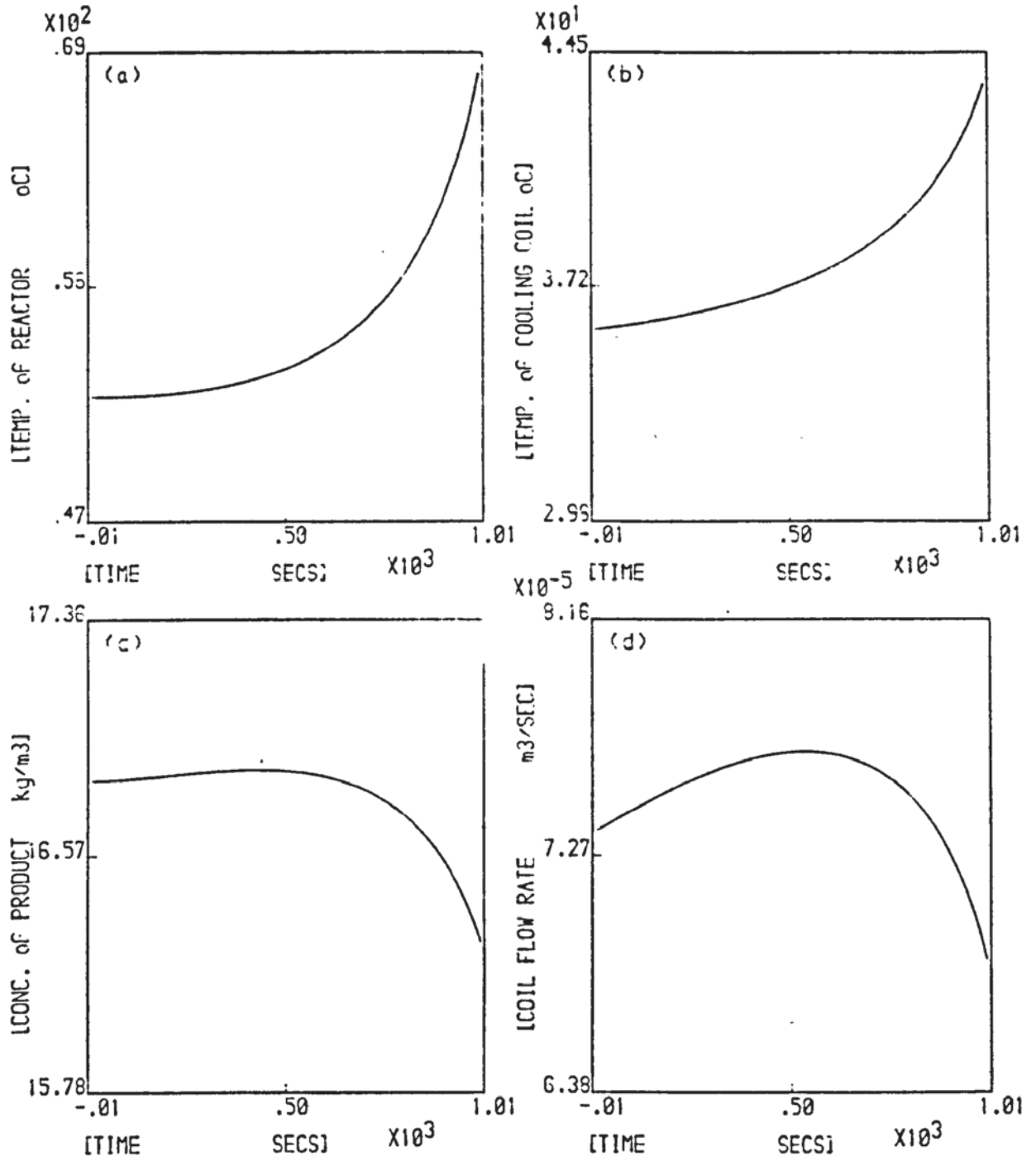
Proportional Feedback control of

reactant concentration. $K_c = 1E-05$

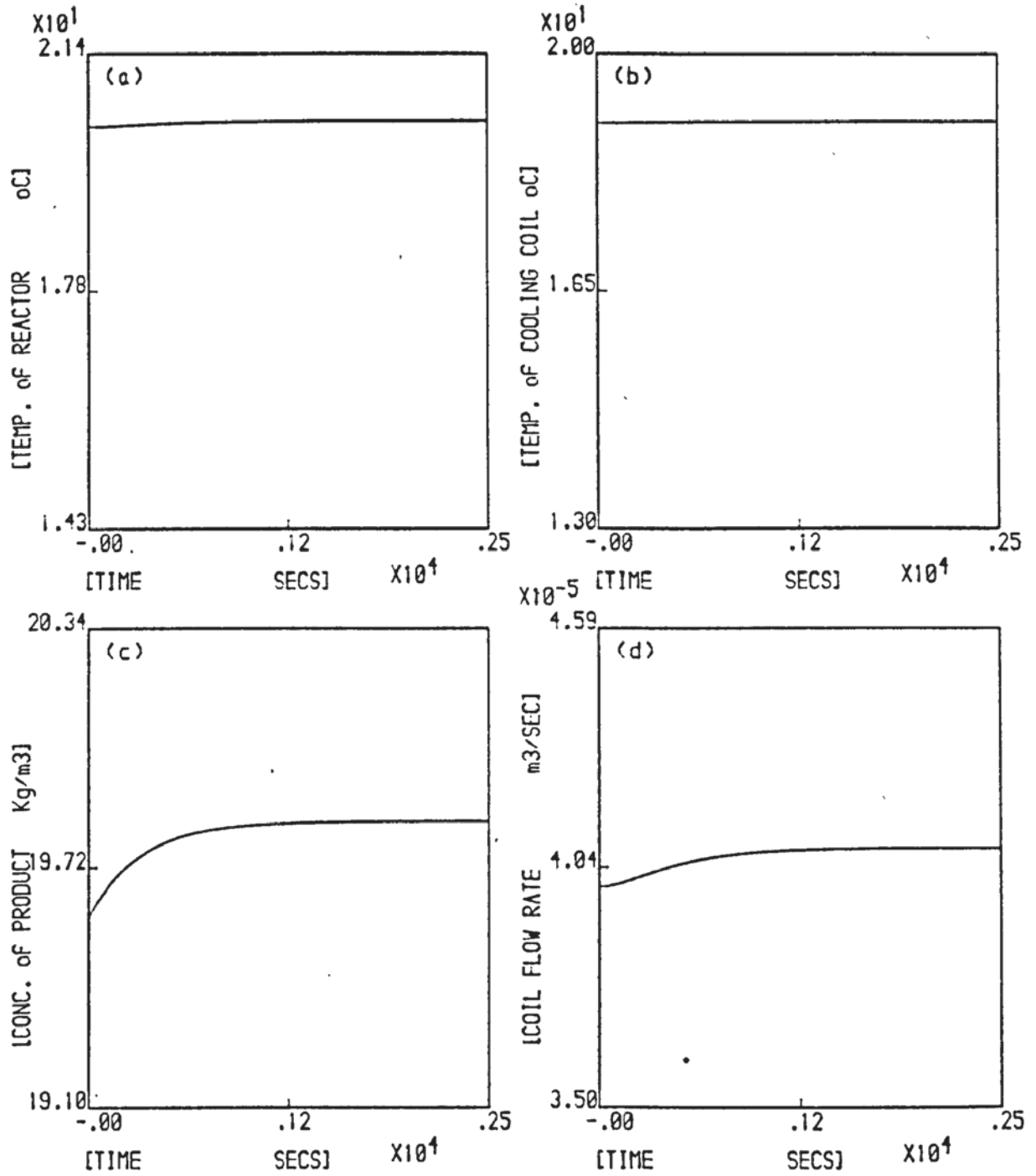
Fig. A.6.1.38 Reactor One. Experiment no: 5



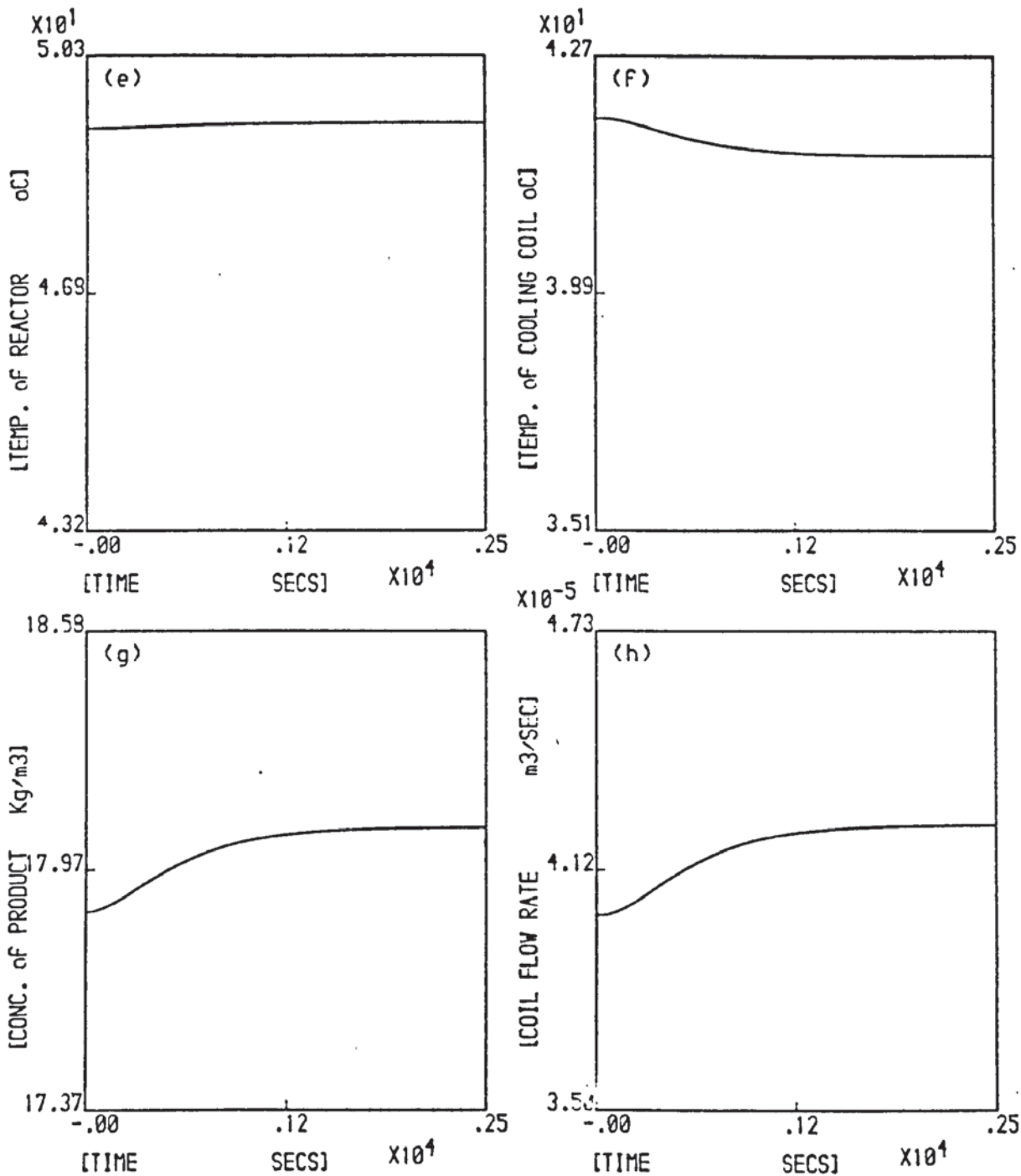
Proportional Feedforward & Feedback control
of reactant concentration at unstable steady
state. $K_c=7.5E-06$
Fig. A.6.i.39 Reactor Two. Experiment no: 5



Proportional Feedforward & Feedback control
of reactant concentration at unstable steady
state. Disturbances from reactor one. $K_c=1.5E$
Fig. 4.6.1.39 Reactor Two. Experiment no: 5

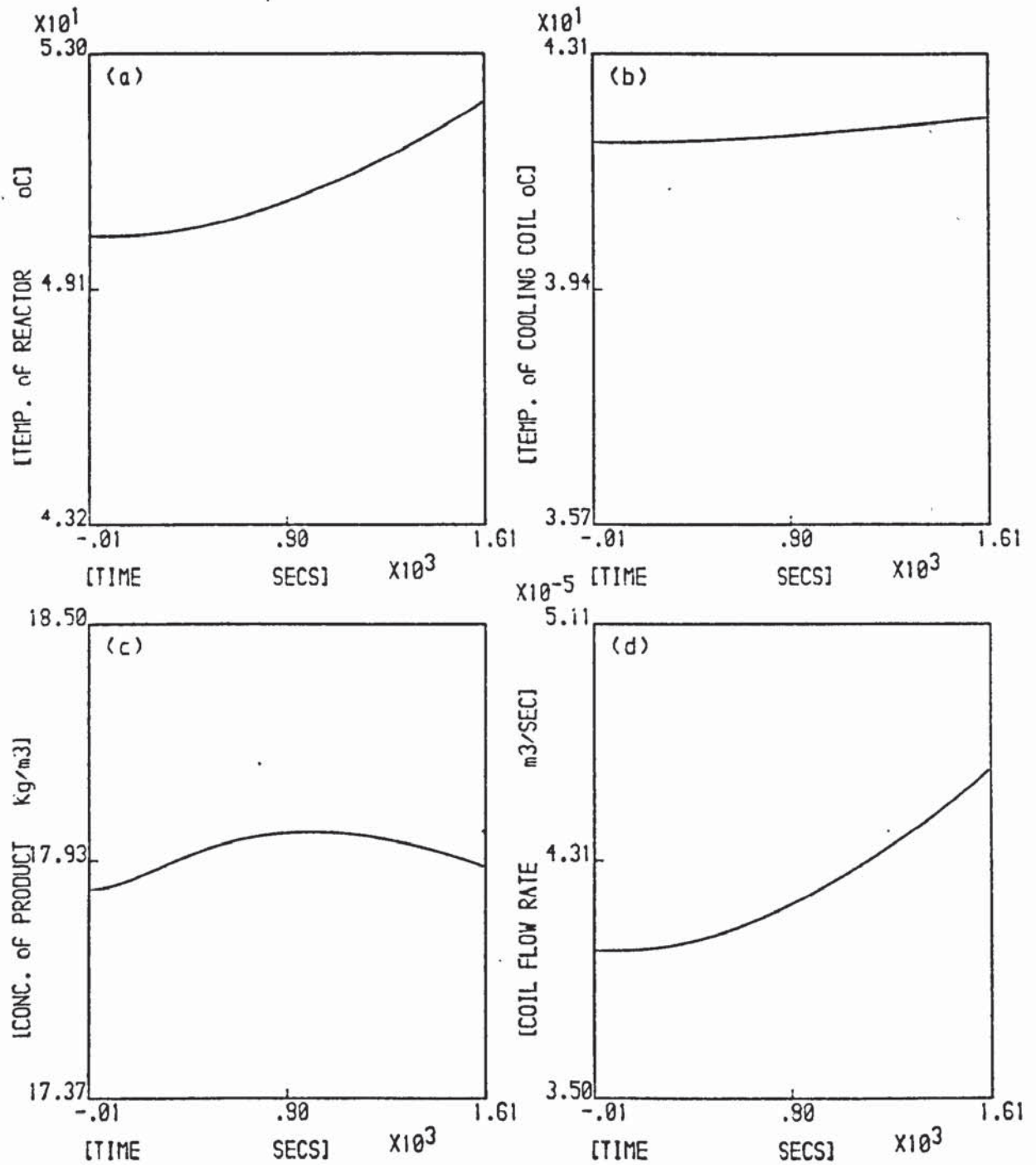


Step in feed concentration (0.25 kg/m^3).
 Proportional feedback control of
 reactor temperature. $K_c = 1 \text{E-}05$
 Fig. A.6.1.40 Reactor One. Experiment no:31

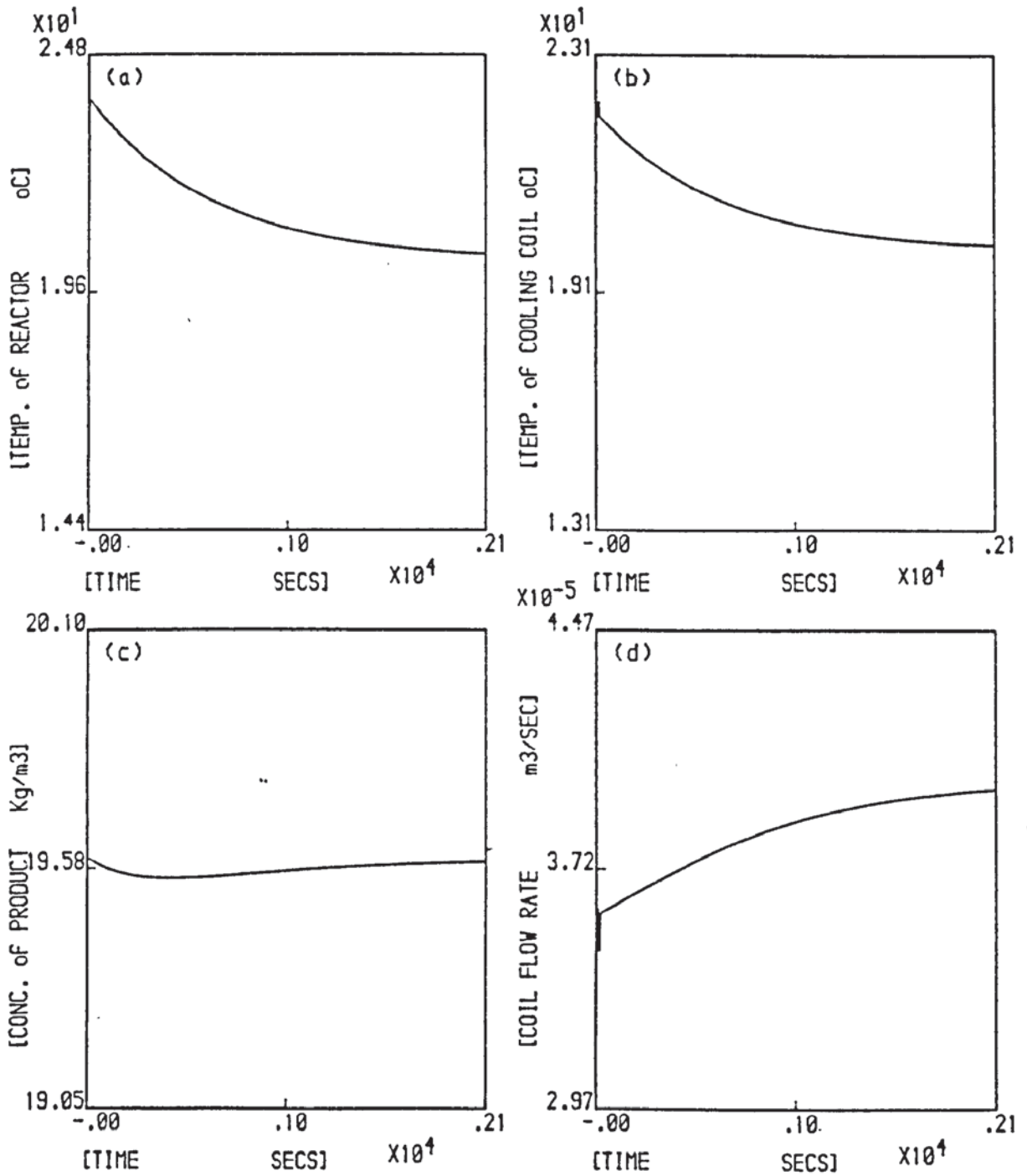


Proportional feedback control of reactor temperature at unstable steady state.

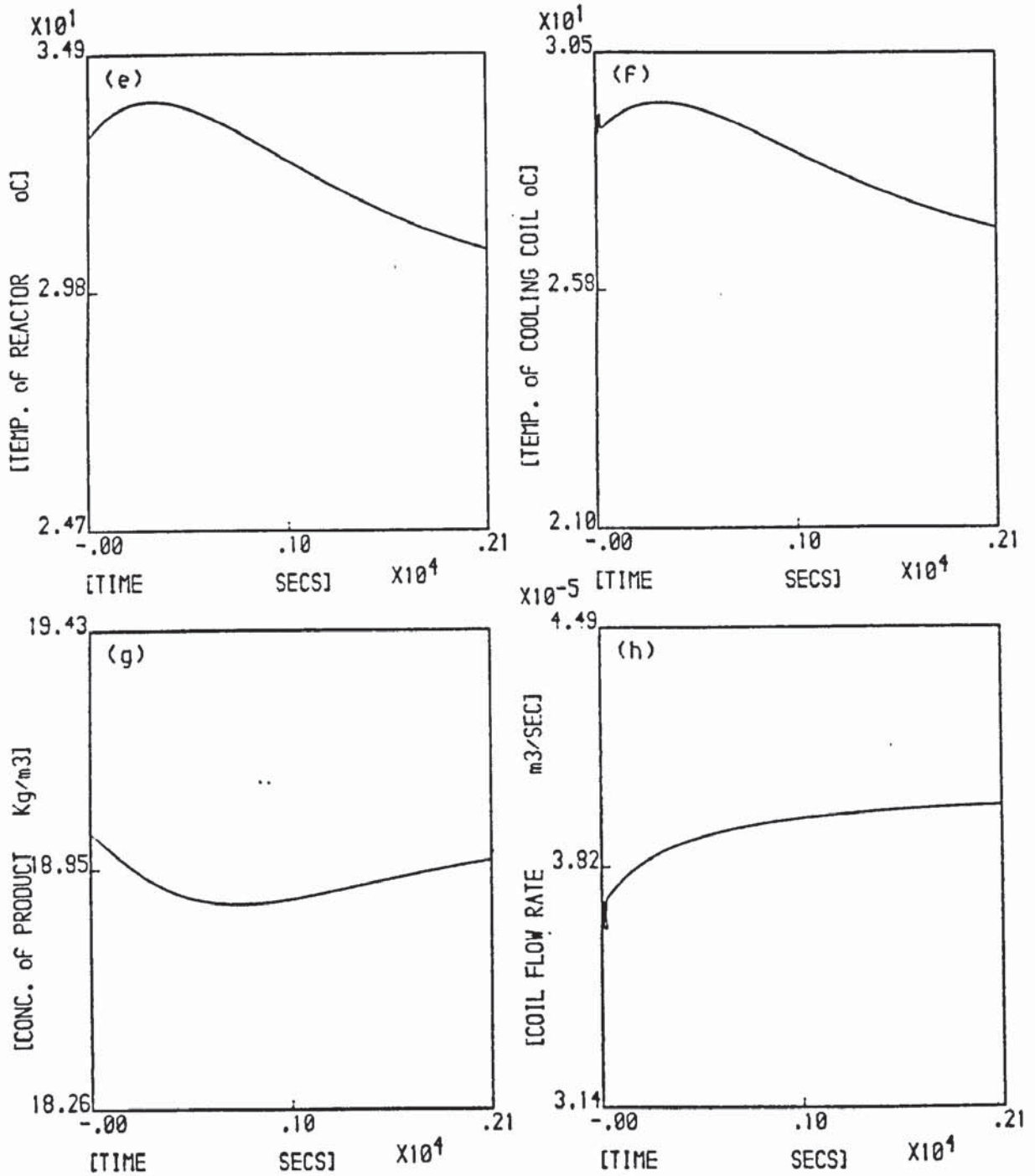
Disturbances from first reactor. $K_c=3E-05$
 Fig. A.6.1.40 Reactor Two. Experiment no:31



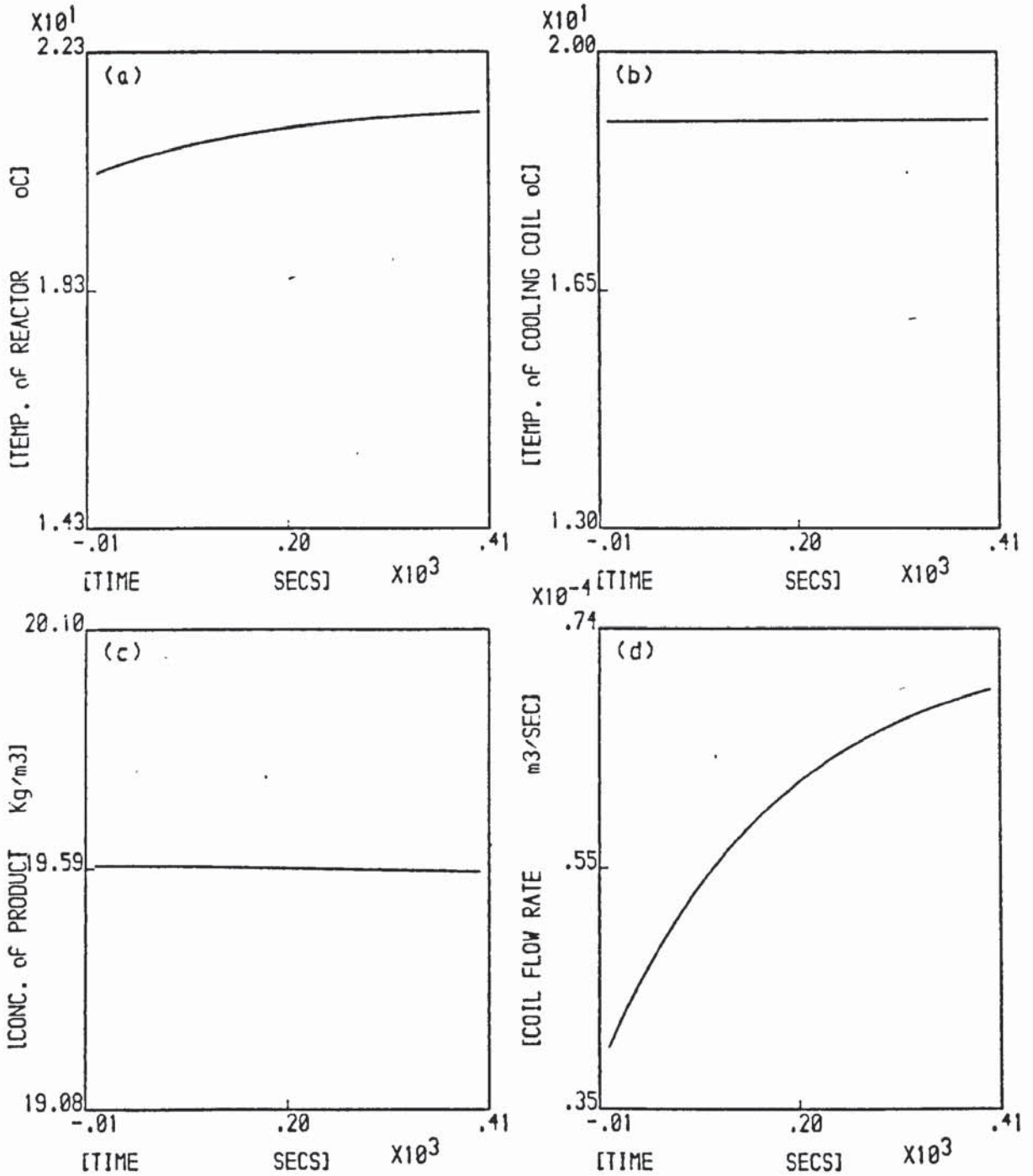
Proportional control of reactor temperature
 at unstable steady state. $K_c=2.2E-06$
 Disturbances from first reactor only.
 Fig. A.6.1.41 Reactor Two. Experiment no:31



Initial perturbation in state variables.
 Noninteracting control of reactor
 temperature. $a_2 = 0.5$
 Fig. A.6.1.42 Reactor One. Experiment no:31



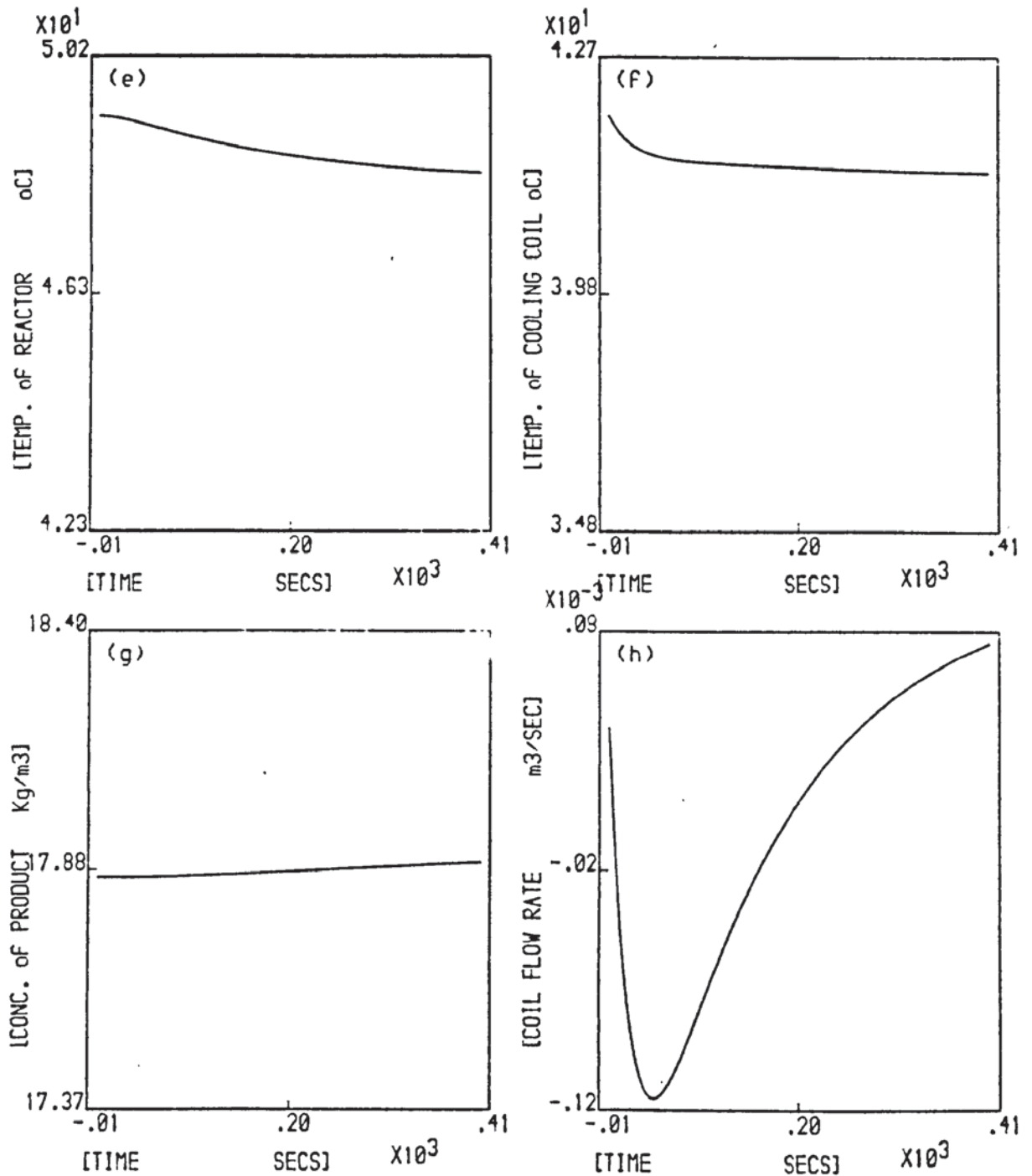
Initial perturbation in state variables.
 Noninteracting control of reactor
 temperature. $a_2=0.5$
 Fig. A.6.1.42 Reactor Two. Experiment no:31



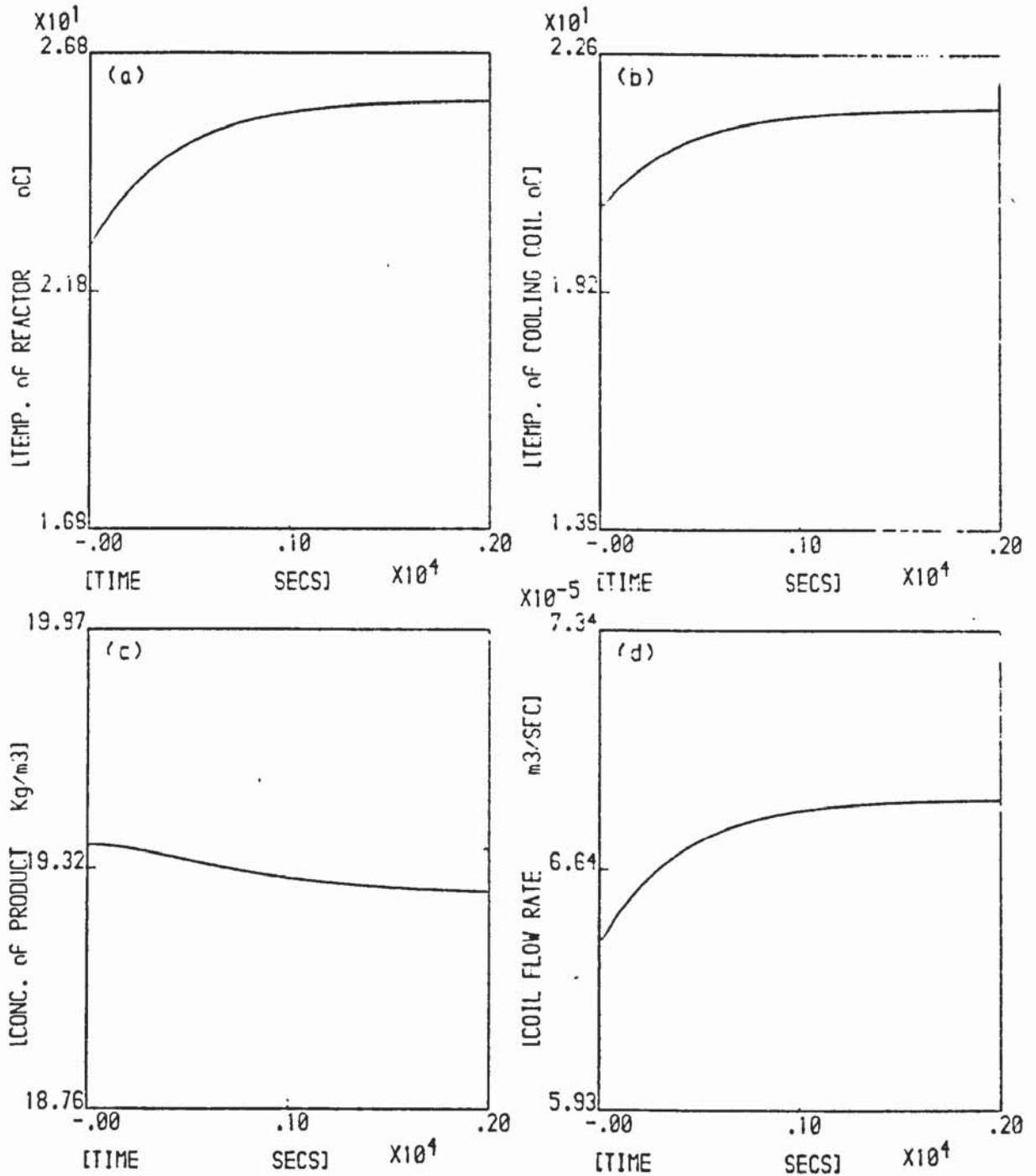
Step in Feed temperature(2.0 K). Proportional Feedback control of cooling coil temperature.

$$K_c = 8E-04$$

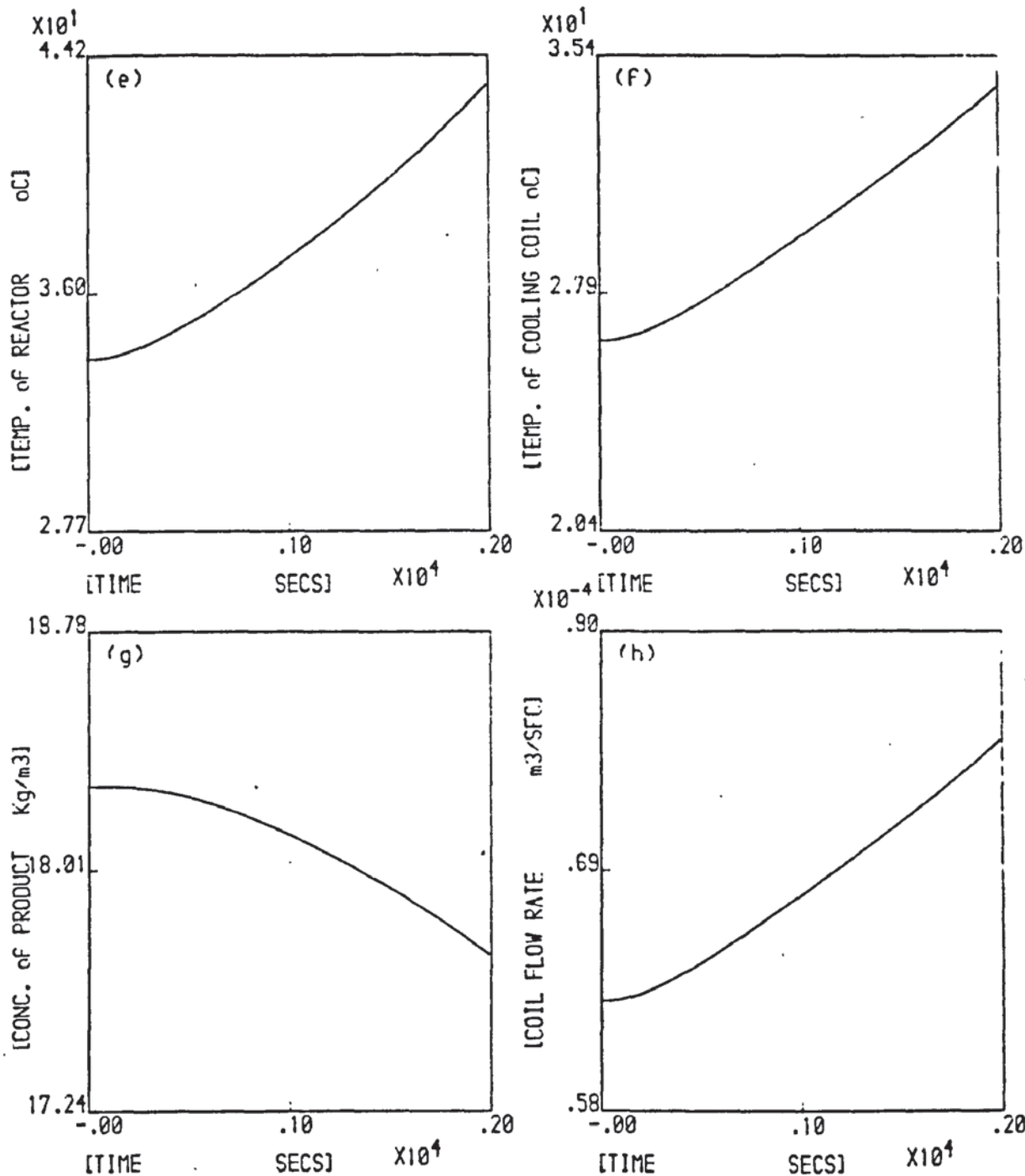
Fig. A.6.1.43 Reactor One. Experiment no:31



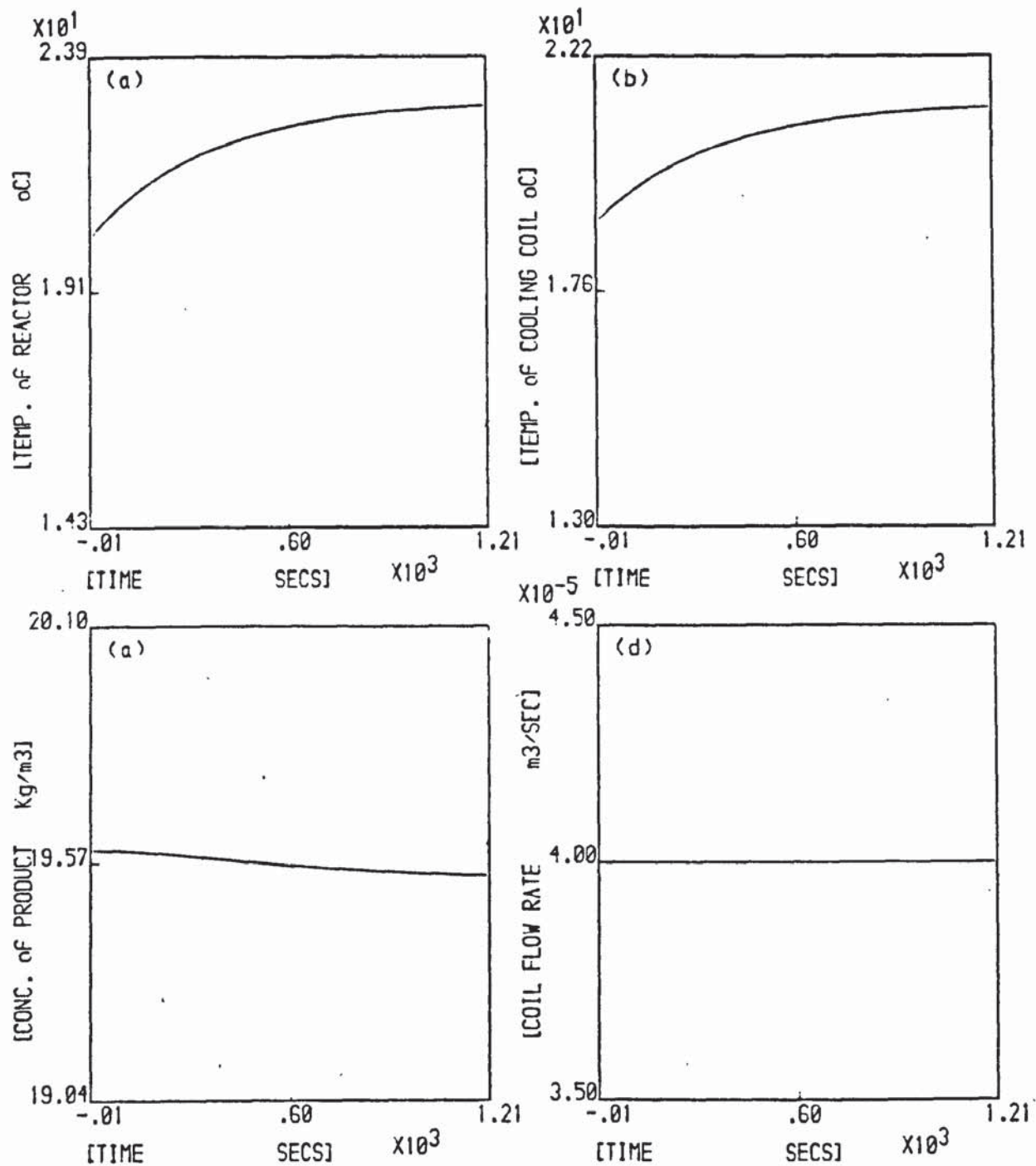
Disturbances from reactor one. FeedForward & feedback proportional control of reactor temperature. $K_c=4E-04$
 Fig. A.6.1.43 Reactor Two. Experiment no:31



Step in Feed temperature(3.4 K) and temperature of liquid into cooling coil(-0.1 K).
 Prop. feedback control of coil temp. $K_c = .23E-06$
 Fig. A.6.1.44 Reactor One. Experiment no: 16

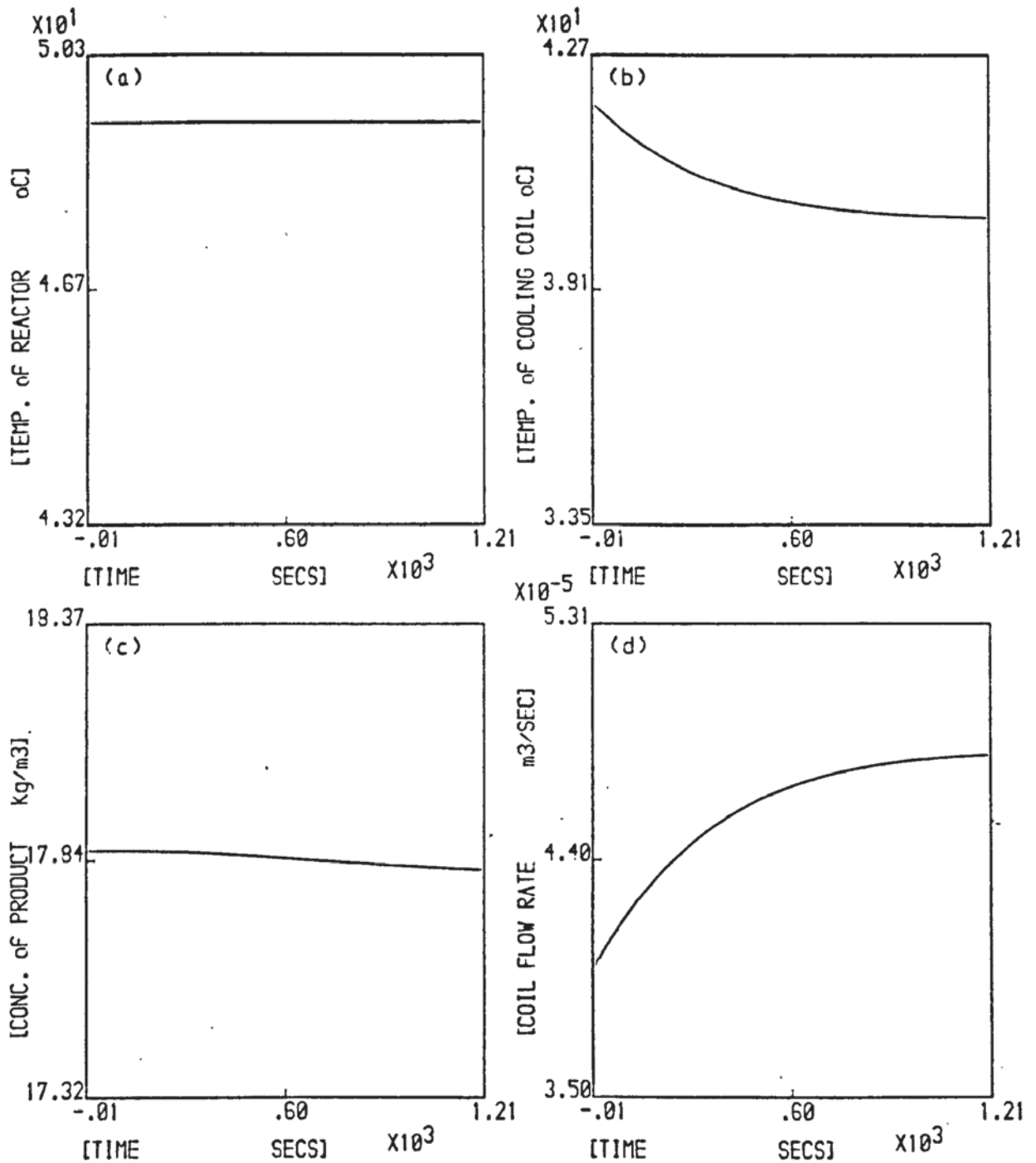


Step in temperature of liquid into cooling coil (-0.66 K). Proportional feedback control of reactor temperature. $K_c = 1.5E-06$
 Fig. A.6.1.44 Reactor Two. Experiment no:16

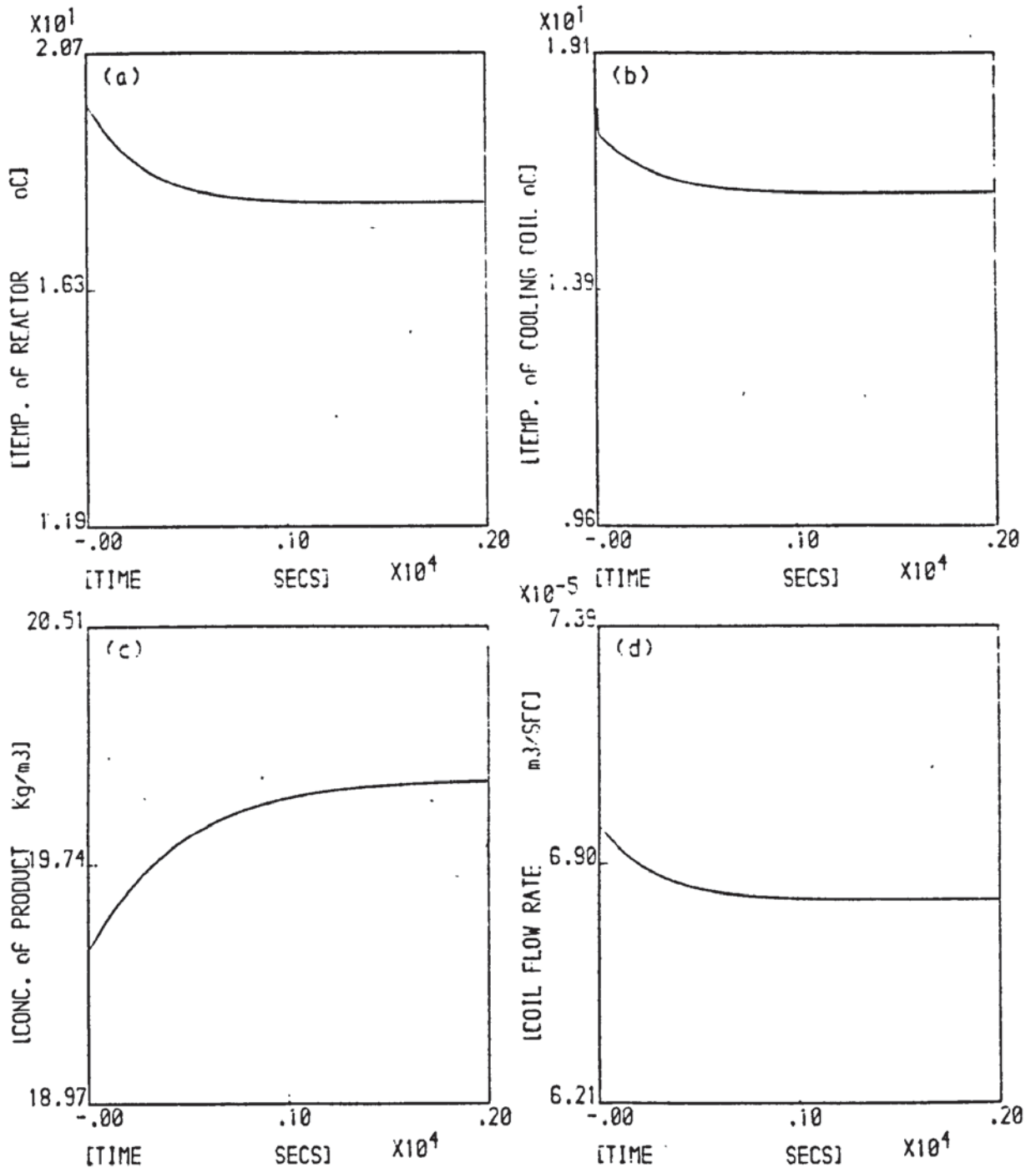


Step in feed temperature. No control of state variables. (2 K)

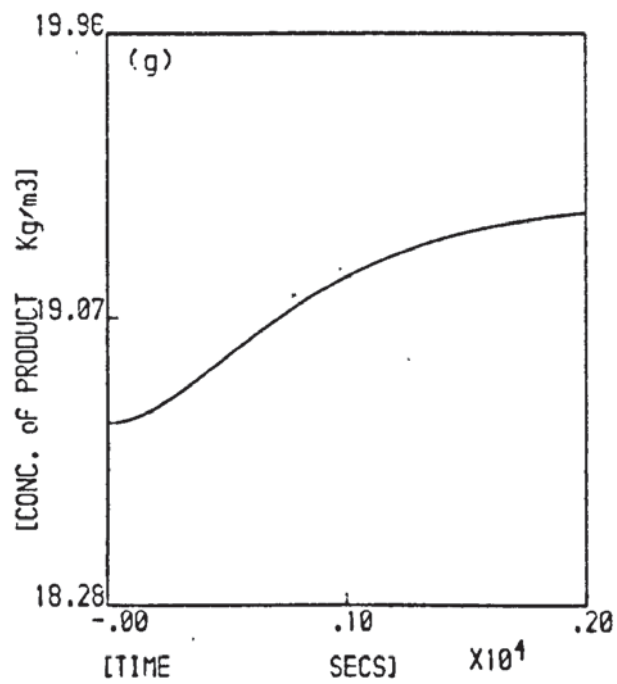
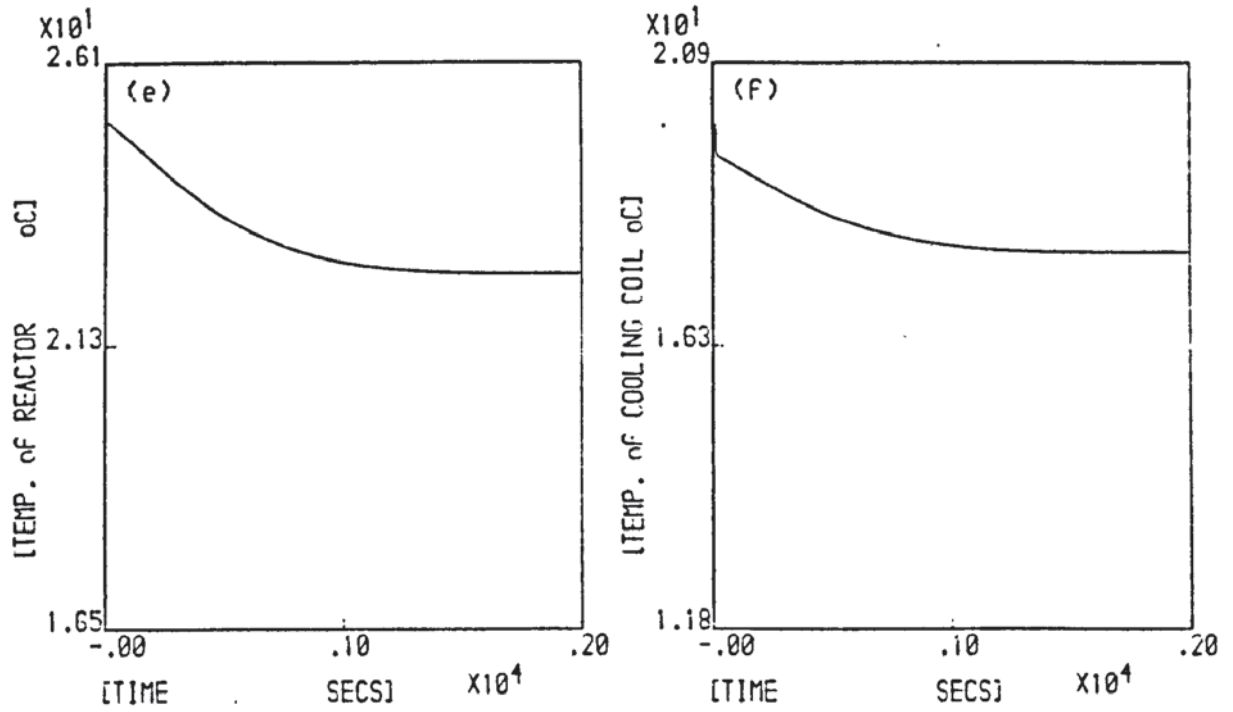
Fig. A.6.1.45 Reactor One. Experiment no:31



Disturbances from First reactor only.
 Feedback control of reactor temperature at
 unstable steady state. $K_c=1E-03$
 Fig. 1.6.1.45 Reactor Two. Experiment no:31

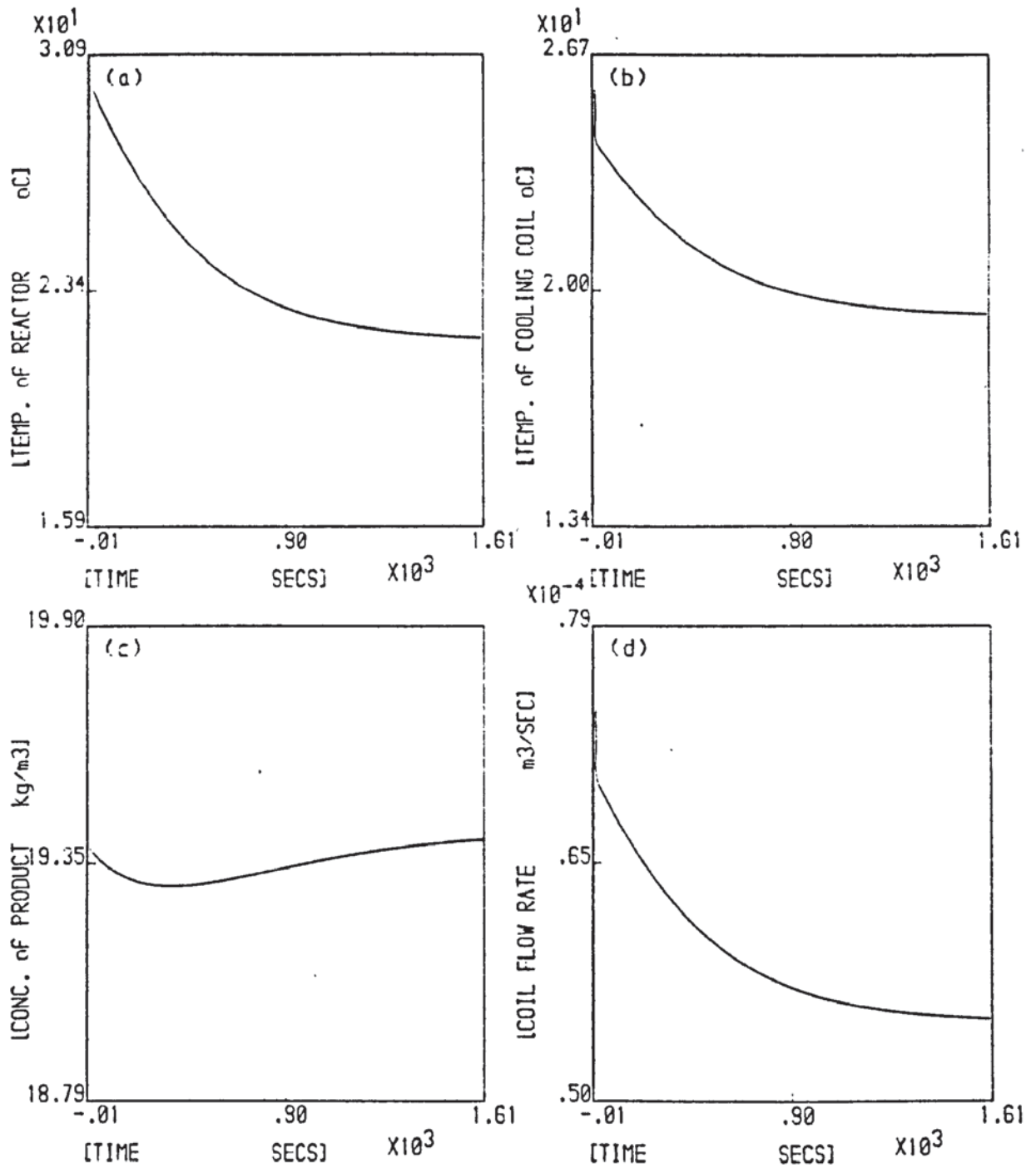


Step in feed concentration(0.5kg/m³) and temperature(1.3 K). Proportional Feedback control of reactor temperature. Kc=1E-06
 Fig. A.6.1.16 Reactor One. Experiment no: 4

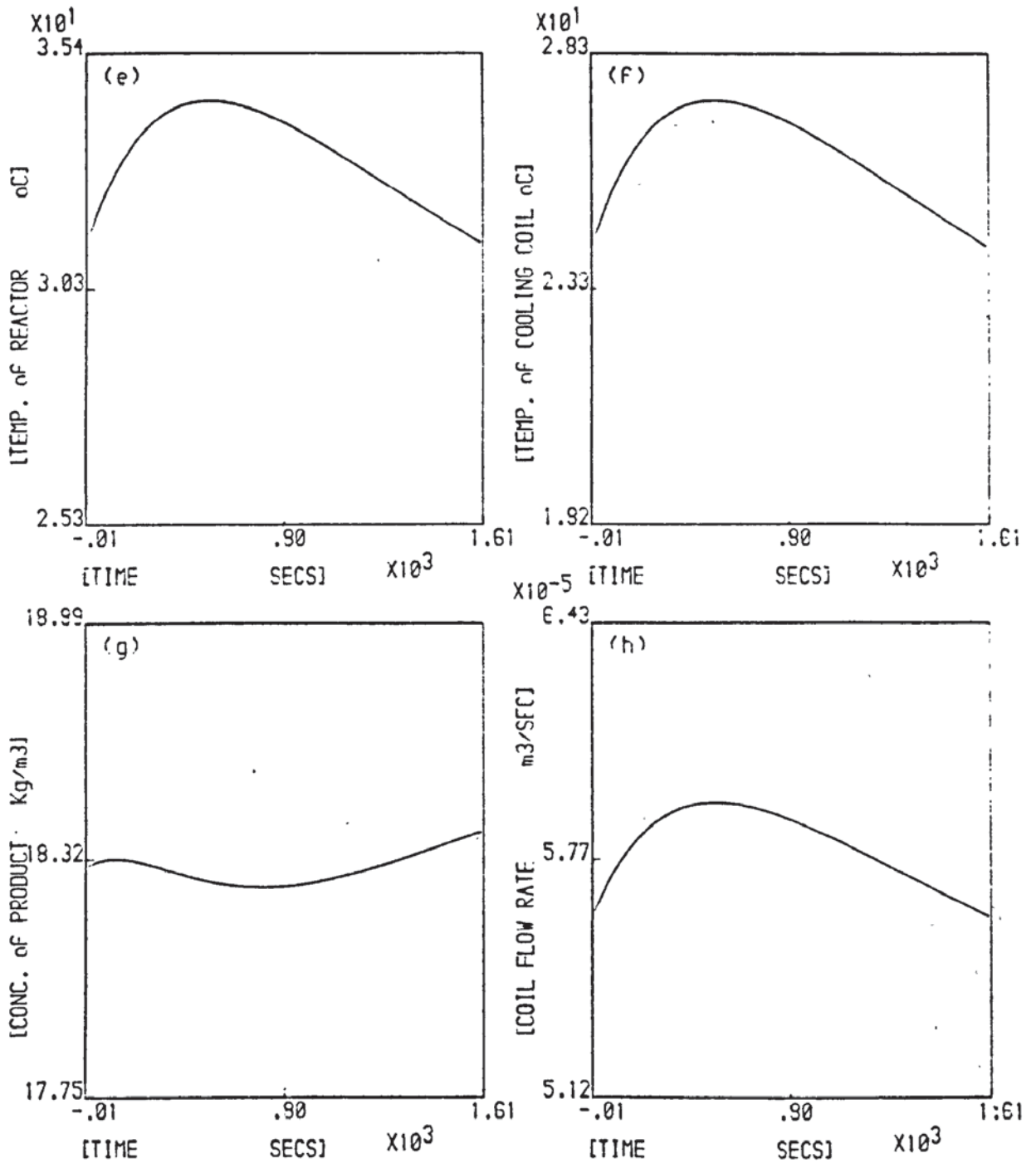


Step in temperature of liquid flowing into cooling coil (-1.23 K). No control of state variables.

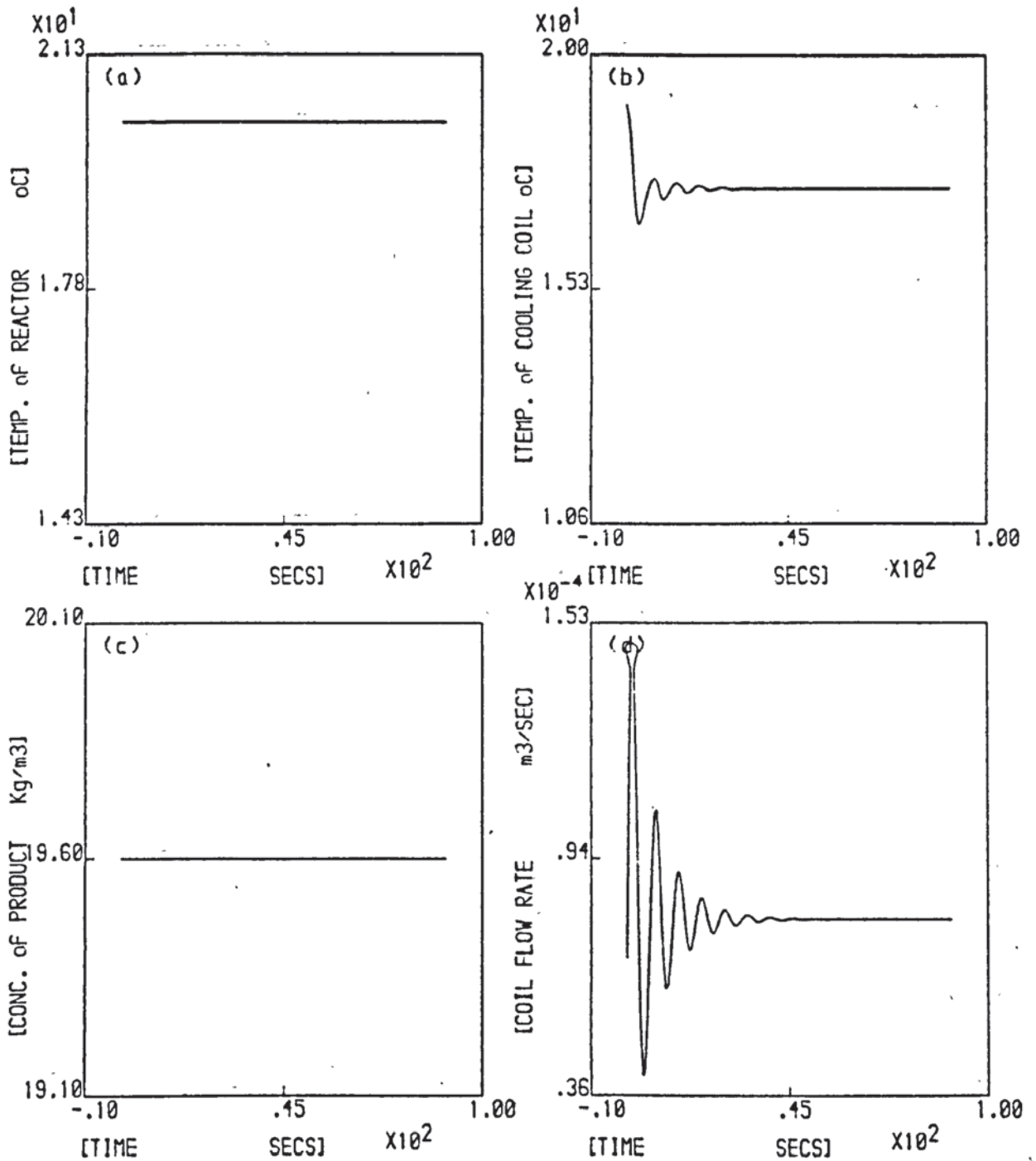
Fig. A.6.1.46 Reactor Two. Experiment no: 4



Initial perturbation in state variables.
 Proportional feedback control of coil
 temperature. $K_c = 3E-06$
 Fig. A.6.1.47 Reactor One. Experiment no:22



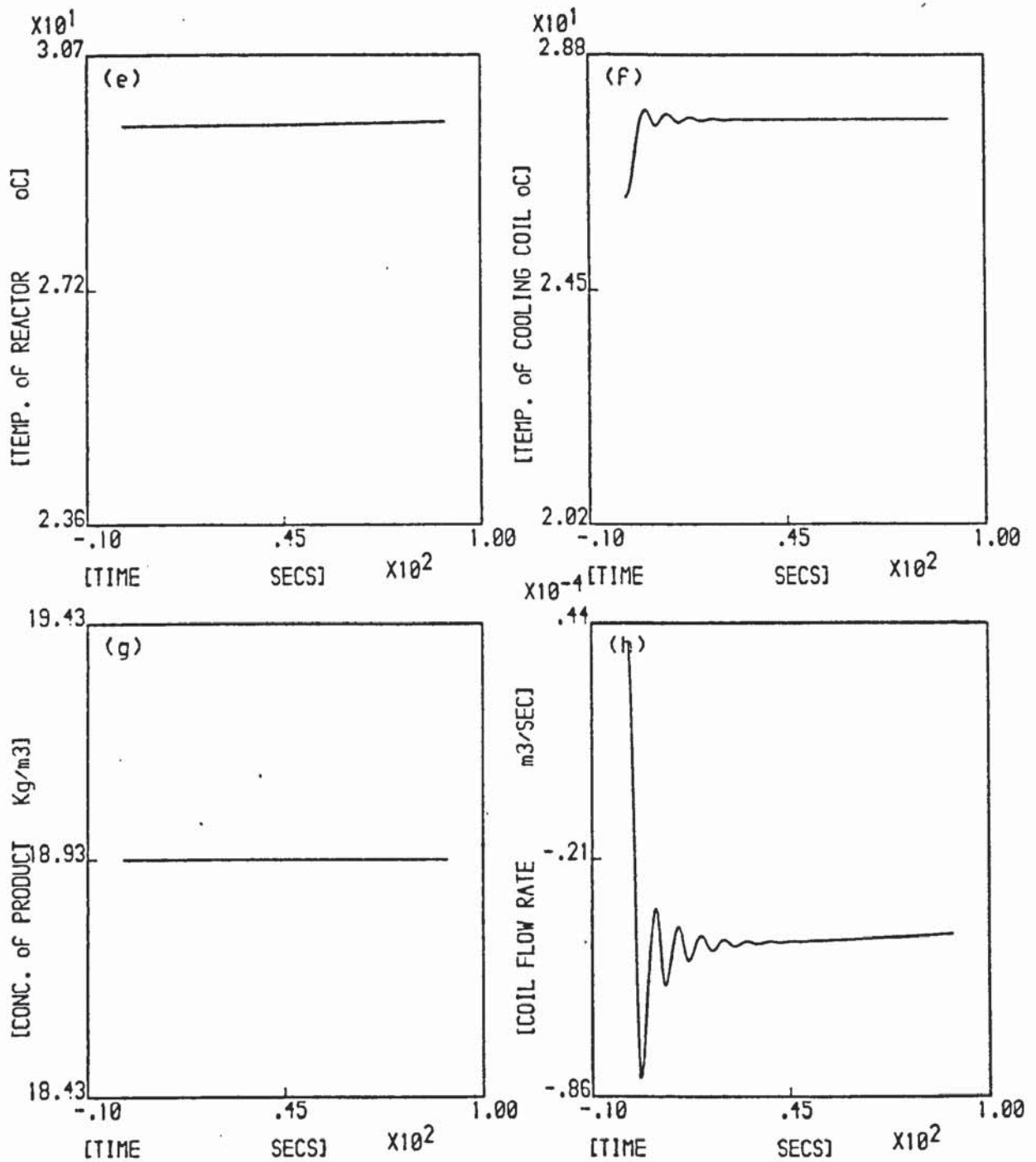
Initial perturbation in state variables.
 Proportional feedback control of reactor
 temperature. $K_c=1E-06$
 Fig. A.6.1:47 Reactor Two. Experiment no:22



Step in feed temperature (2.0°k). Proportional
Feedback control of reactor temperature.

$$K_c = 1.5E-02$$

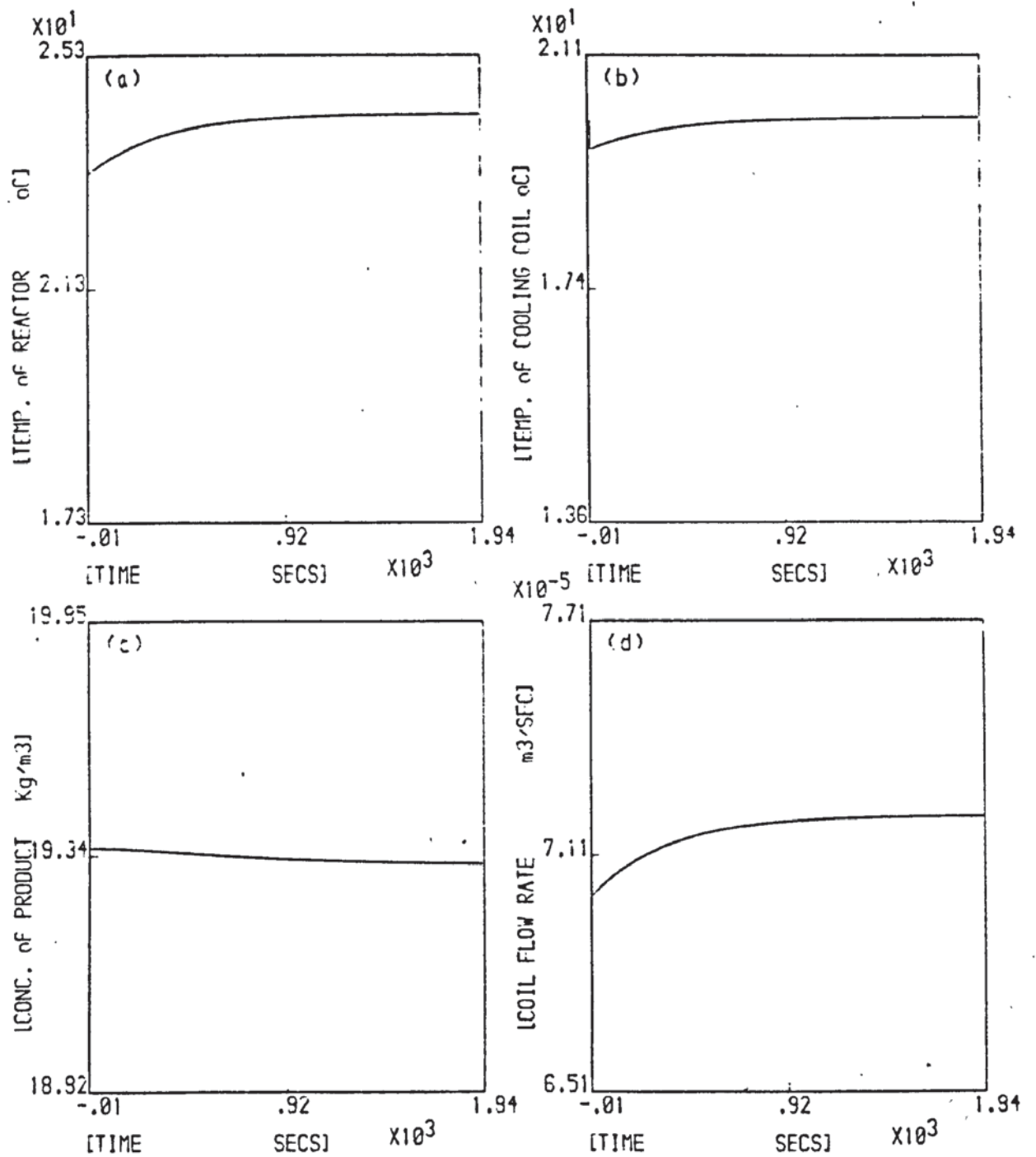
Fig. A.G.1.48 Reactor One. Experiment no:31



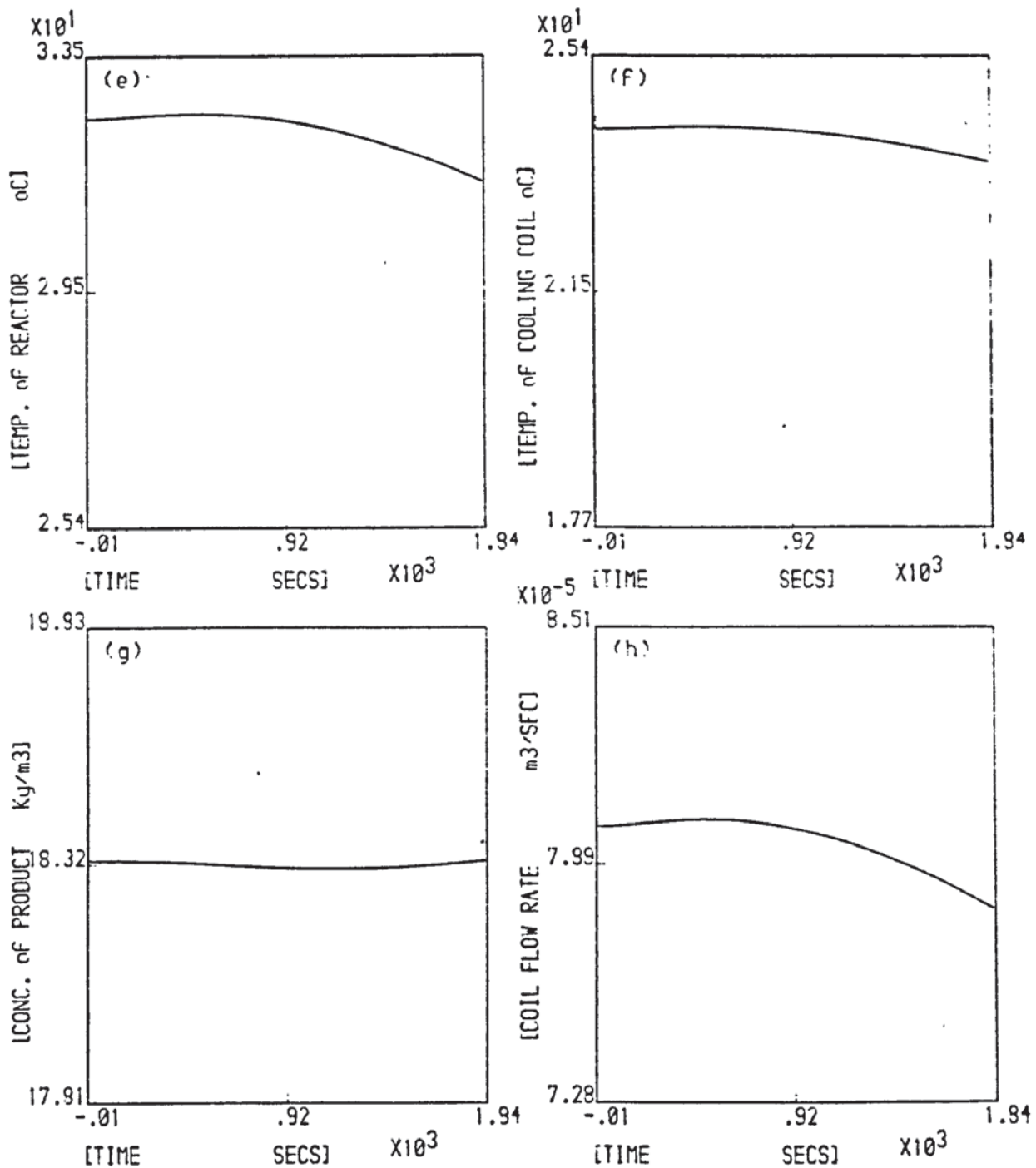
Disturbances from reactor one. Proportional
Feedforward & feedback control of coil temp.

$K_c=5E-05$

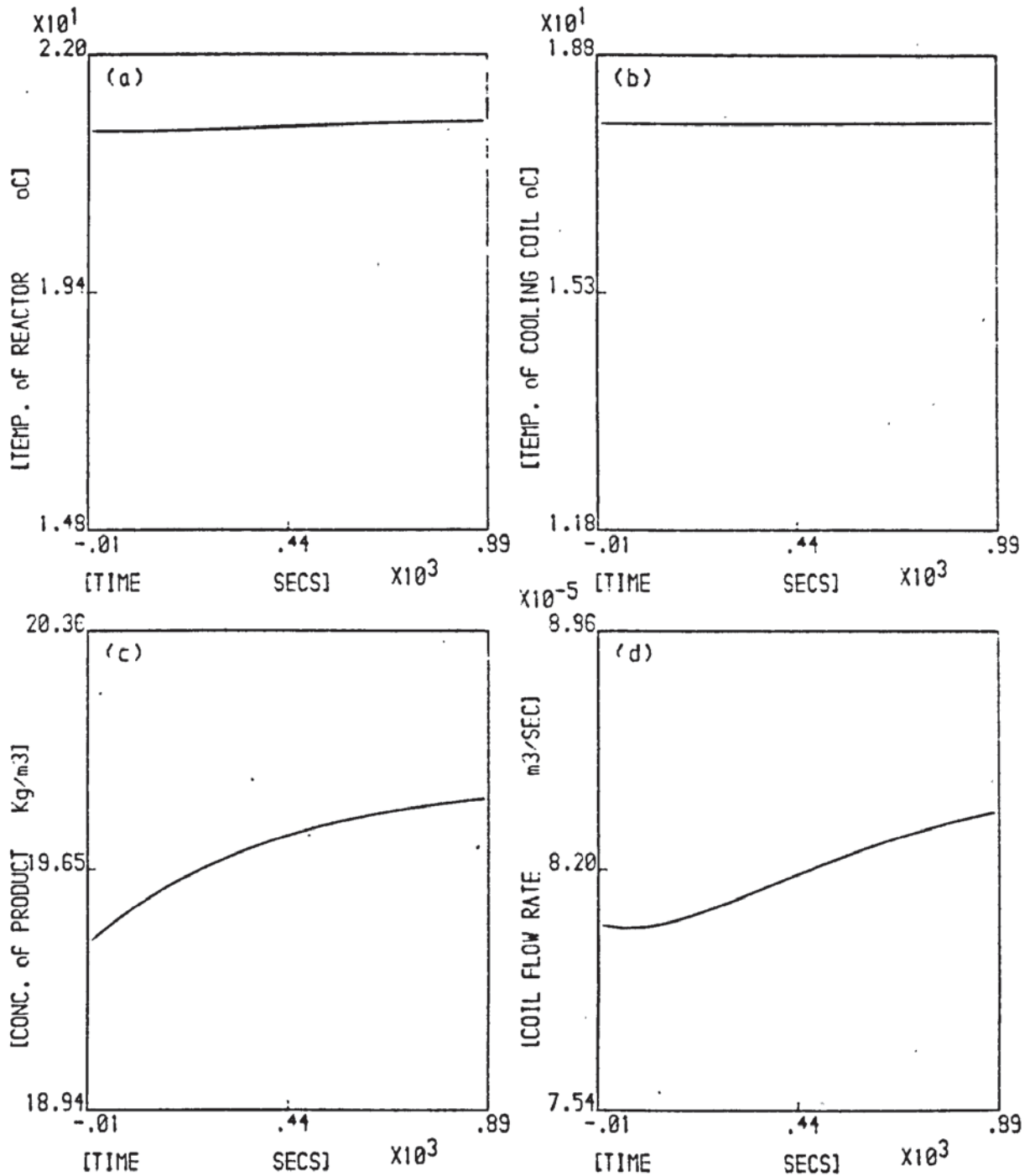
Fig. A.6.1.48 Reactor Two. Experiment no:31



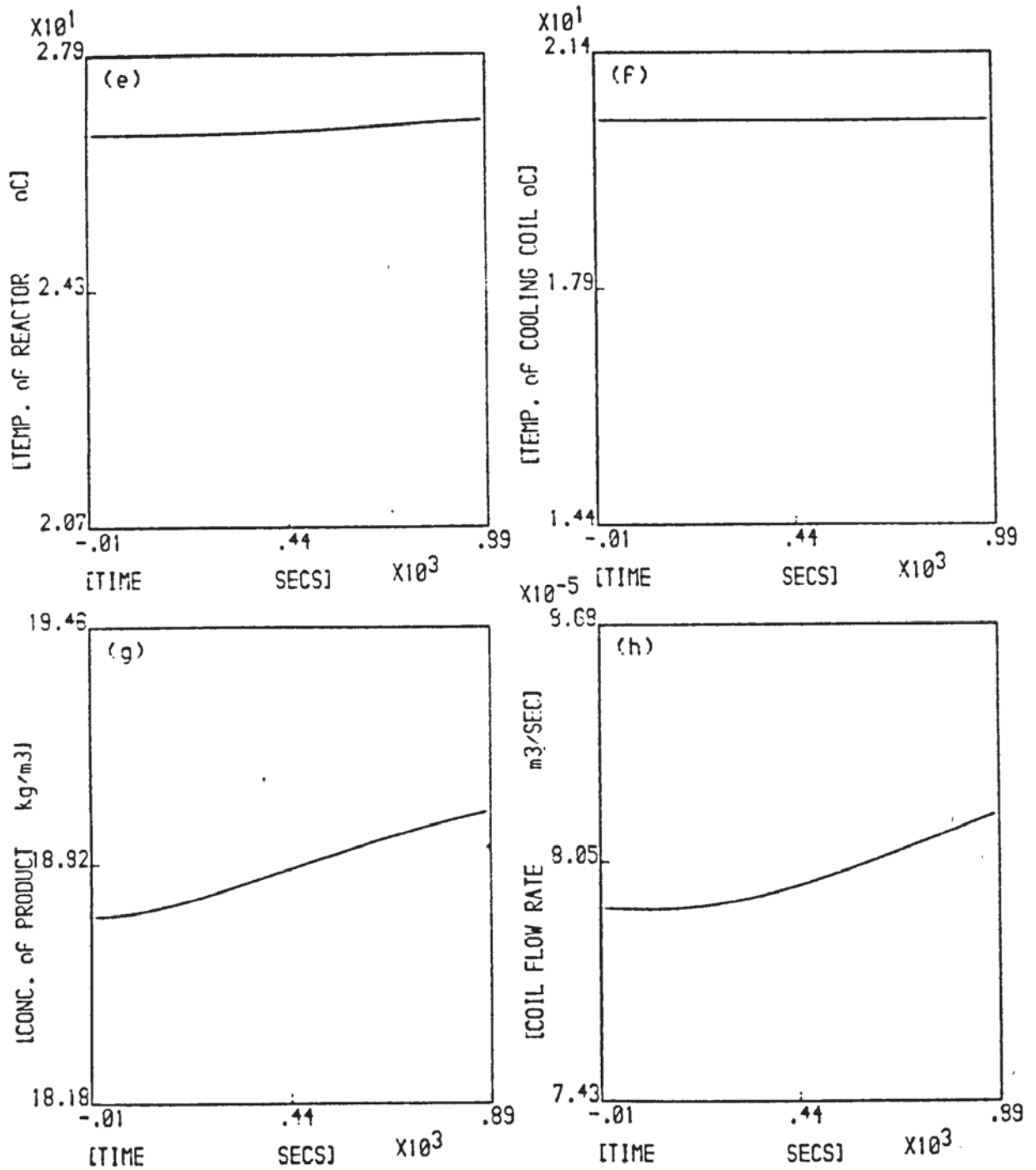
Step in feed temperature(2.76 K) and temperature of liquid feed into coil(-1.23 K). Prop. Feedback control of reactor temp. $K_c=2E-06$ Fig. 1.6.1.49 Reactor One. Experiment no:i5



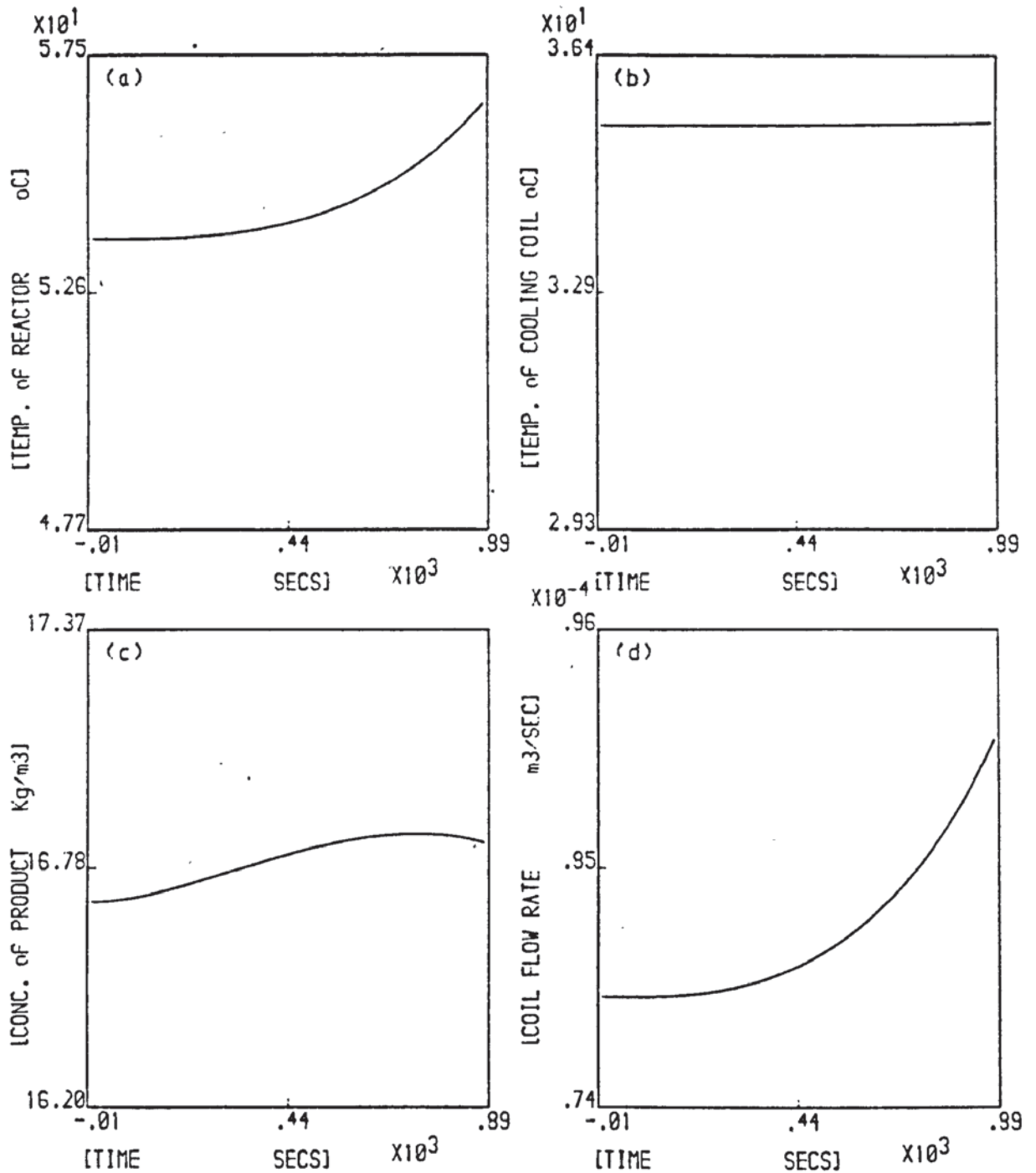
Step in temperature of liquid into coil (-.58K).
 Proportional feedback control of coil
 temperature. $K_c = 2E-06$
 Fig. A.6.1.49 Reactor Two. Experiment no:15



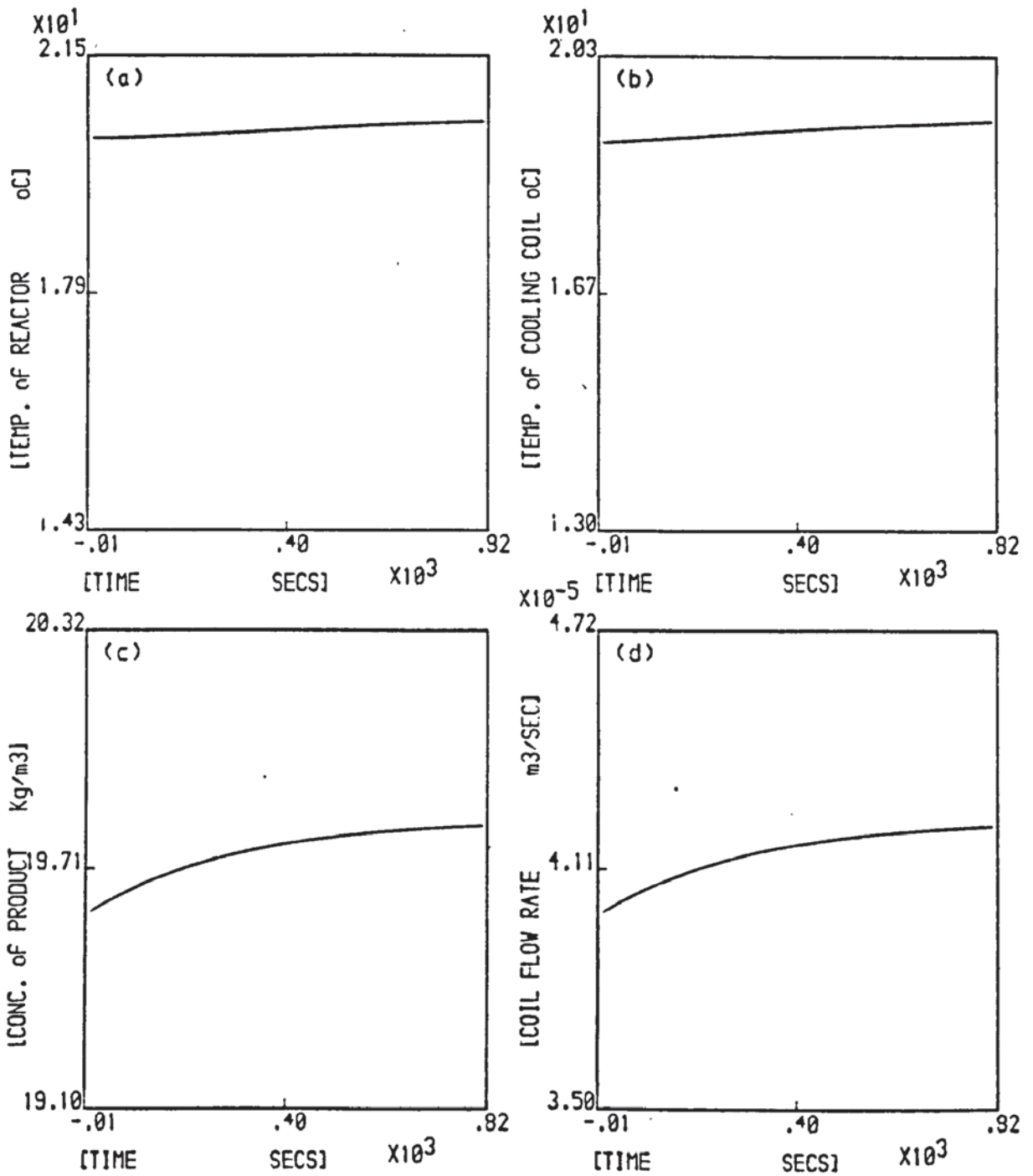
Step in feed concentration (0.5 kg/m^3) and liquid into cooling coil (-1.5 K). Proportional feedback control of coil temperature. $K_c = .3E-03$
 Fig. A.6.1.50 Reactor One. Experiment no: 7



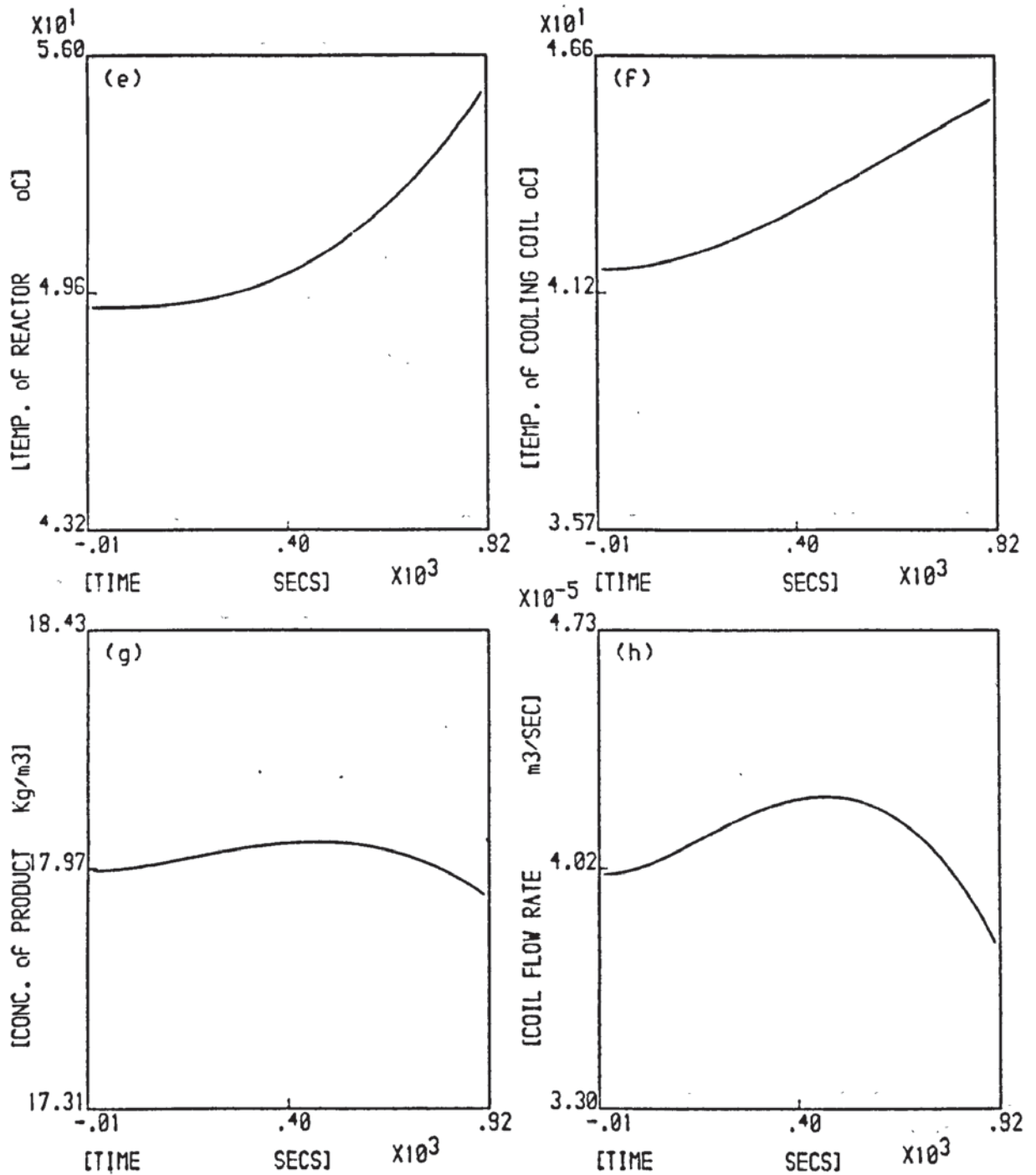
Step in temperature of liquid flowing into cooling coil (-0.5 K). Proportional feedback control of coil temperature. $K_c = 3E-02$
 Fig. 1.6.1.50 Reactor Two. Experiment no: 7.



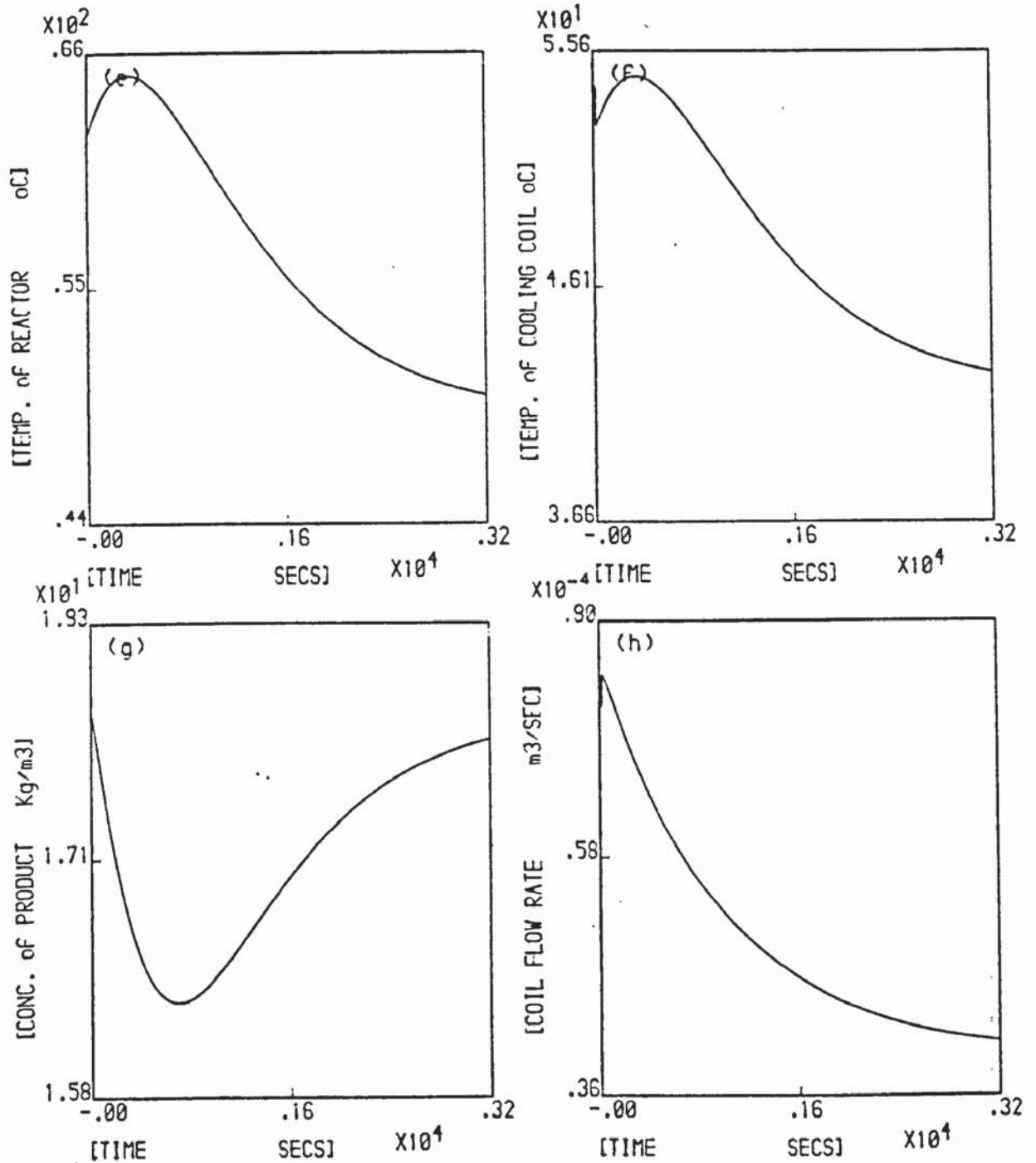
Proportional feedback control of coil temperature at unstable steady state. $K_c = 3E-04$.
 Step in cooling liquid inlet temperature (-.5K)
 Fig. A.6.1.51 Reactor Two. Experiment no: 7



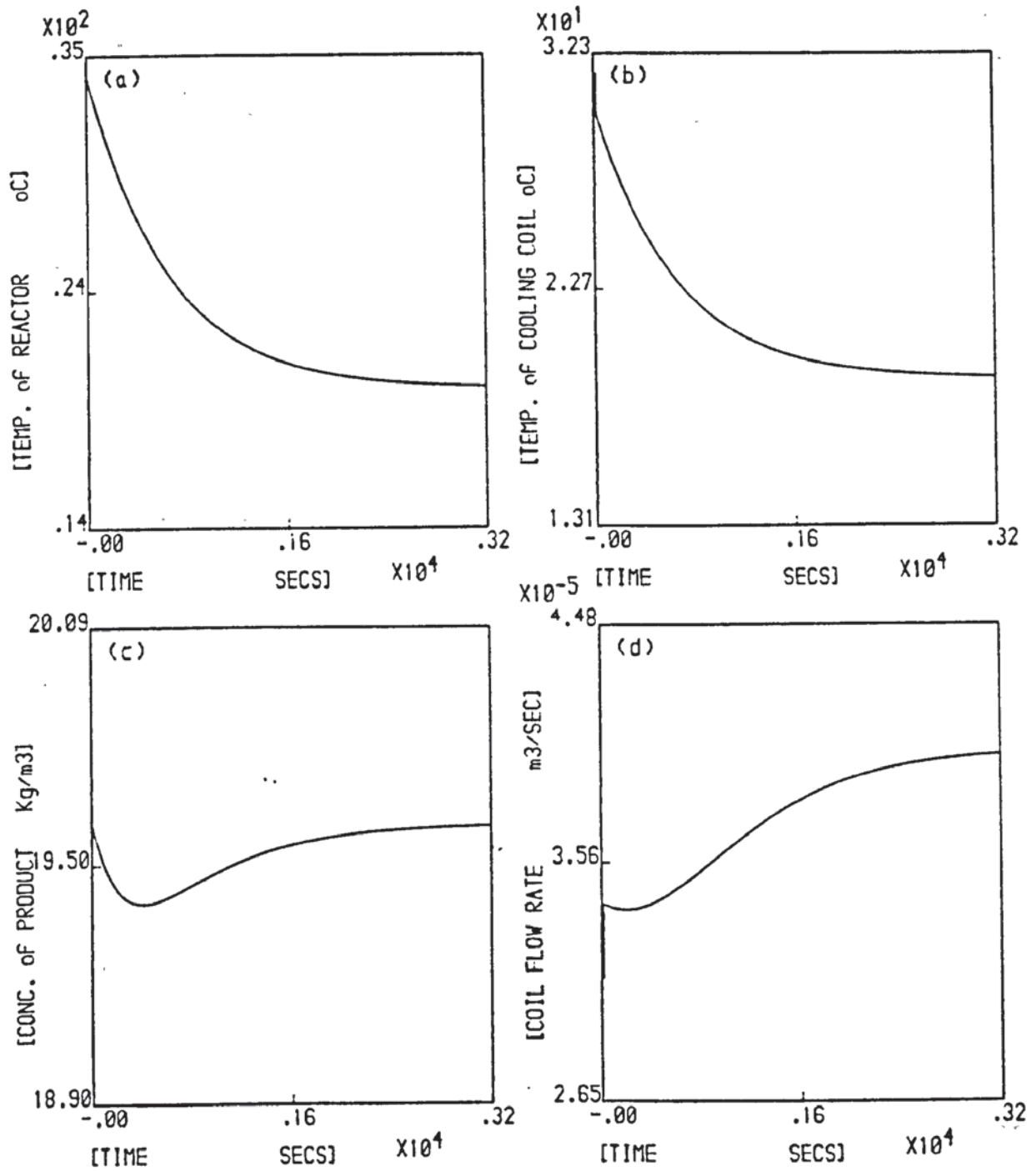
Step in feed concentration (0.25 kg/m^3).
 Proportional feedback control of
 reactant concentration. $K_c = 1 \text{E-}05$
 Fig. A.6.1.52 Reactor One. Experiment no:31



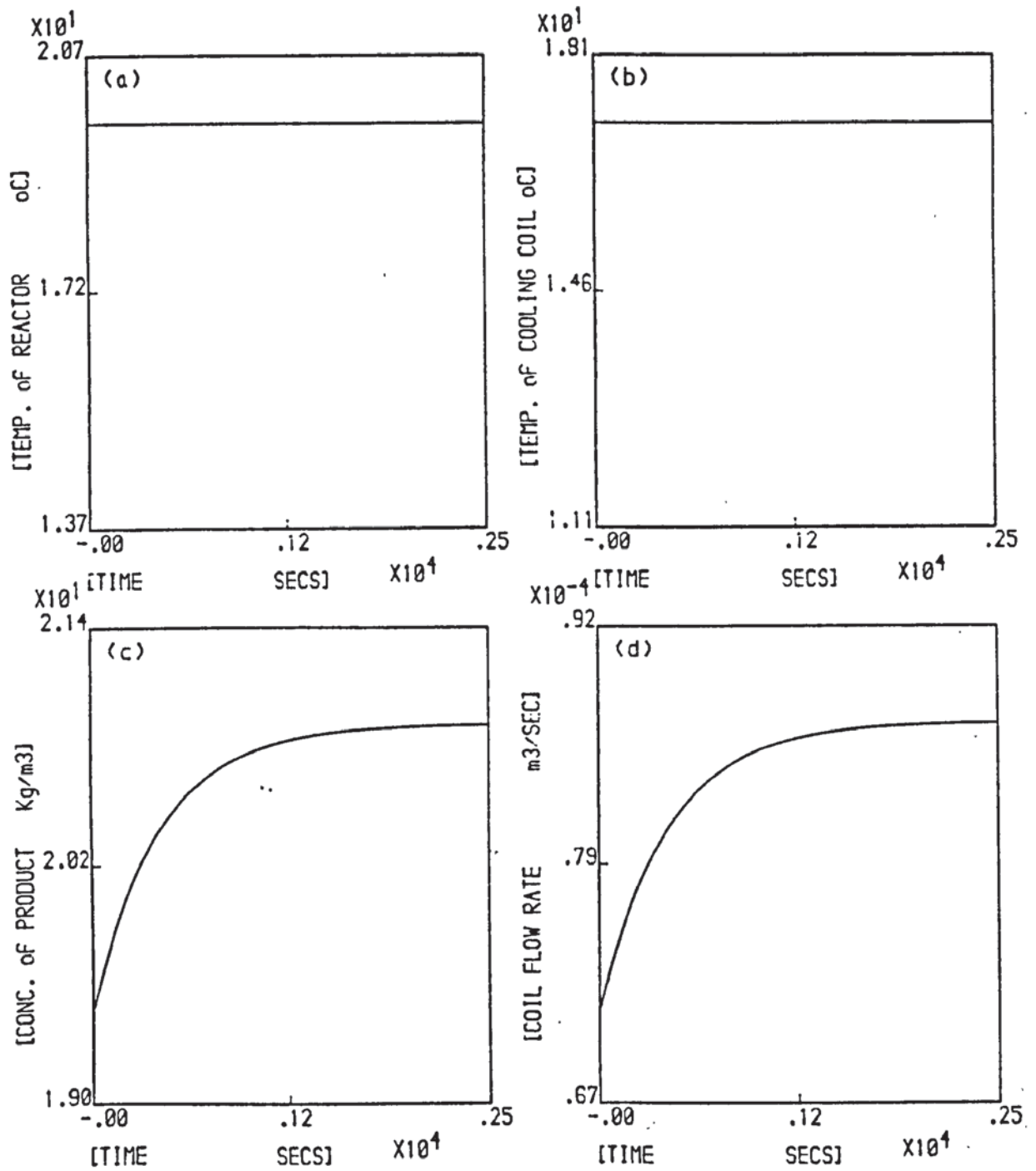
Disturbances from first reactor only.
 Proportional feedback control of reactant
 concentration at unstable state. $K_c=3.5E-05$
 Fig. A.6.1.52 Reactor Two. Experiment no:31



Initial perturbation in state variables.
 Noninteracting control of reactor temperature
 at unstable steady state: $\alpha_2=0.5$
 Fig. A.6.1.53 Reactor Two. Experiment no:31



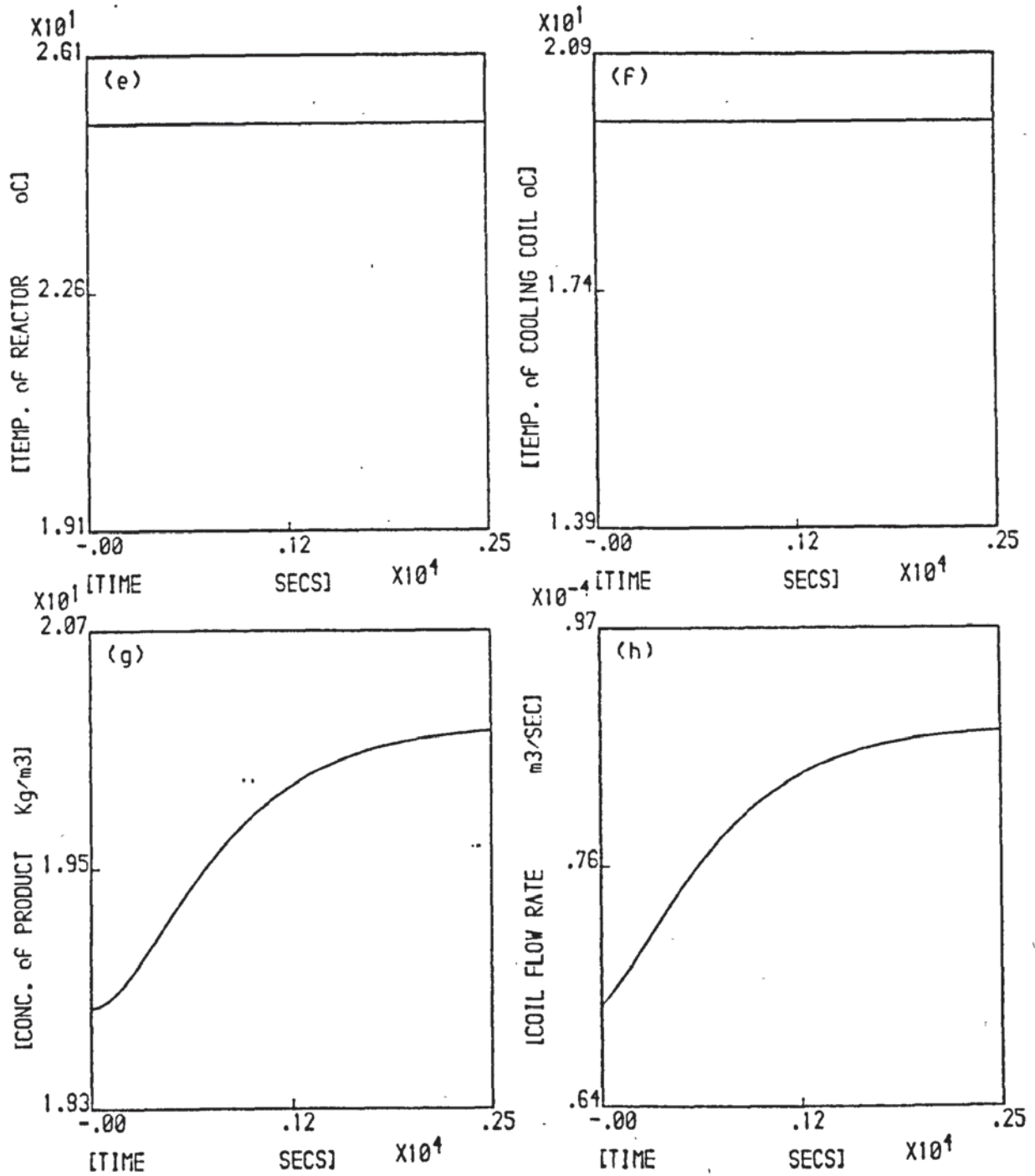
Initial perturbation in state variables.
 Noninteracting control of reactor
 temperature. $a_2=0.5$
 Fig. A.6.1.53 Reactor One. Experiment no:31



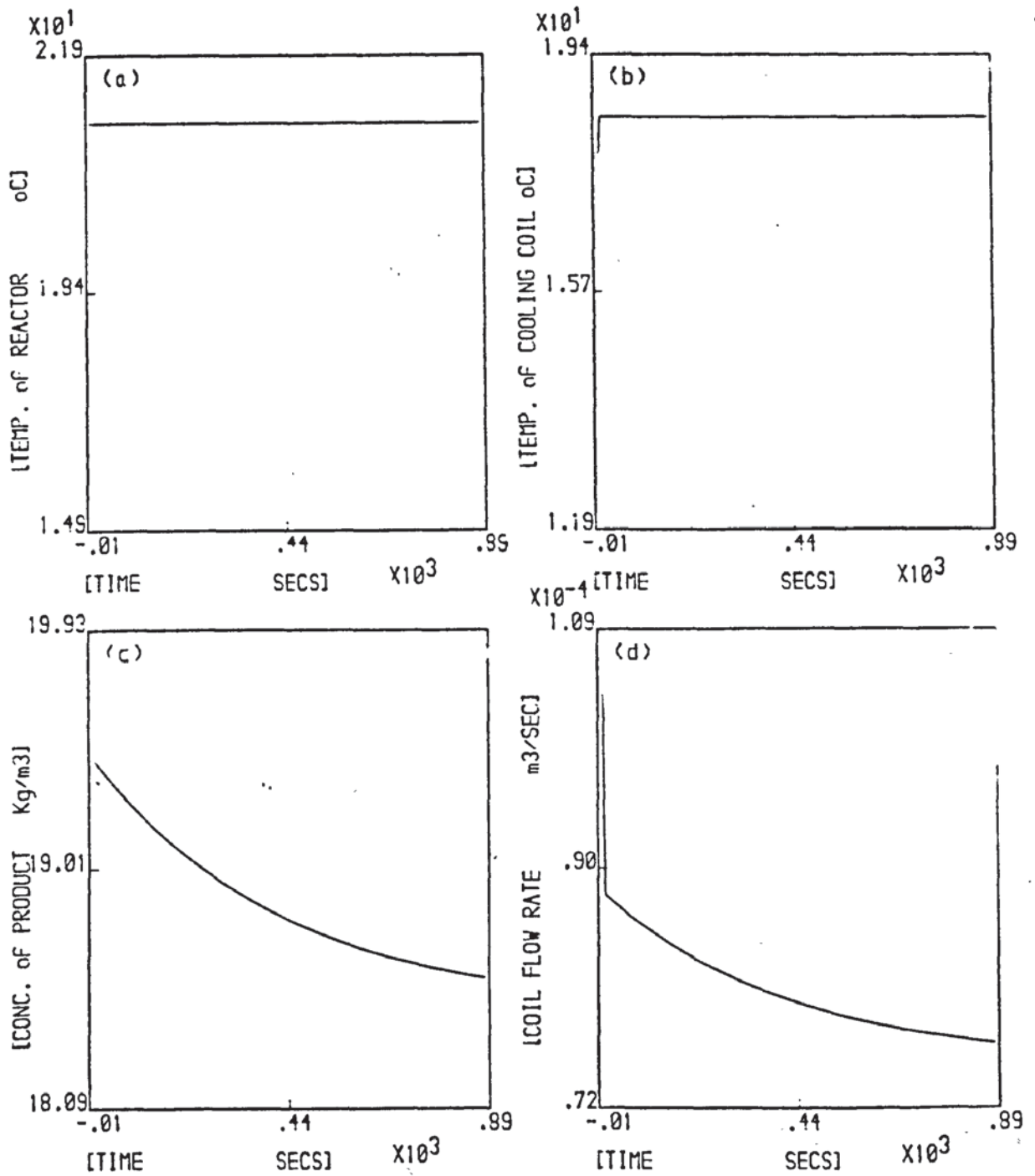
Step in feed concentration (1.5 kg/m^3).

Noninteracting control of reactor temperature

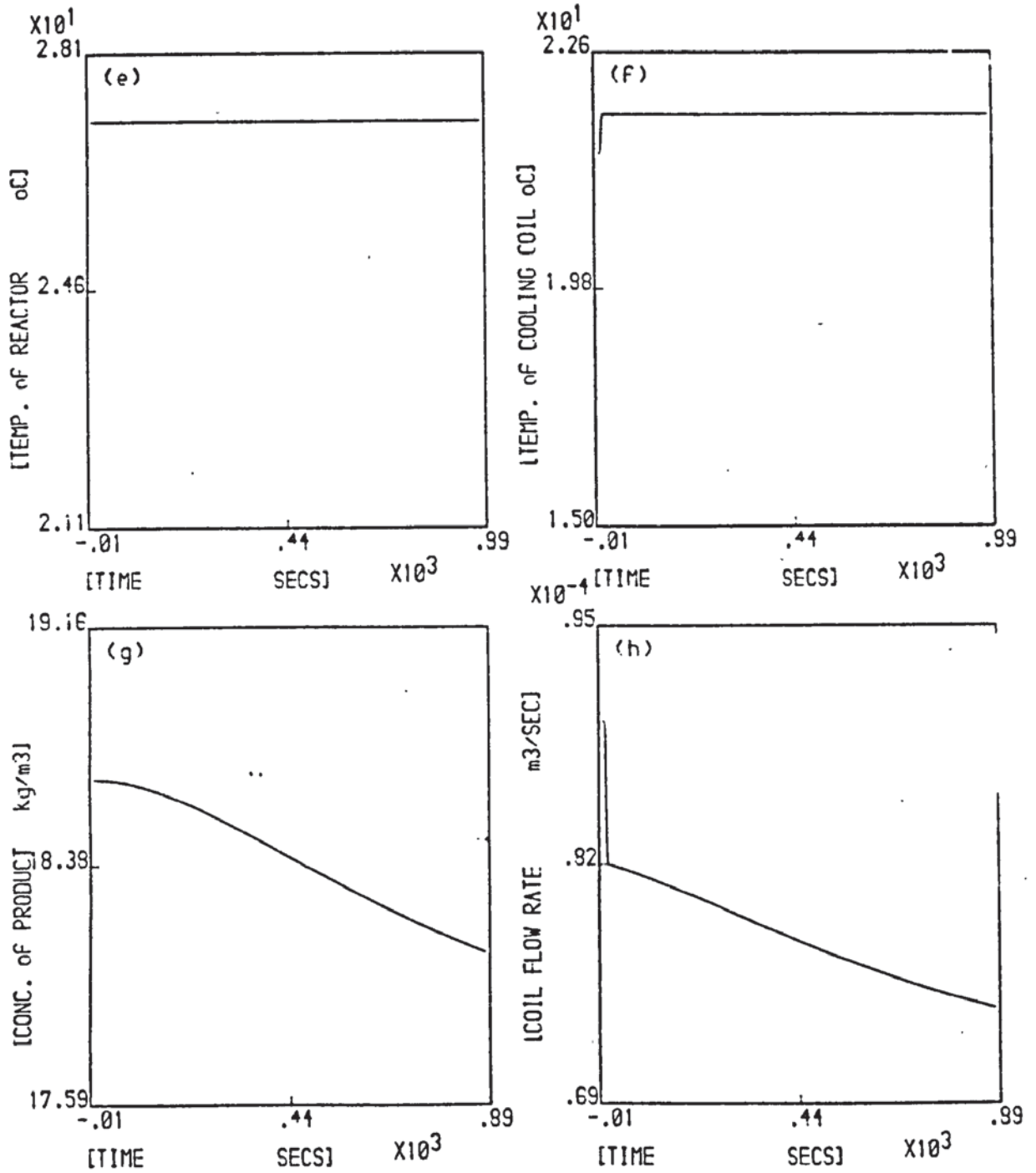
Fig. A.6.1.54 Reactor One. Experiment no:4



Disturbances in feed concentration from first reactor. Noninteracting control of reactor temperature.
 Fig. A.6.1.54 Reactor Two. Experiment no:4

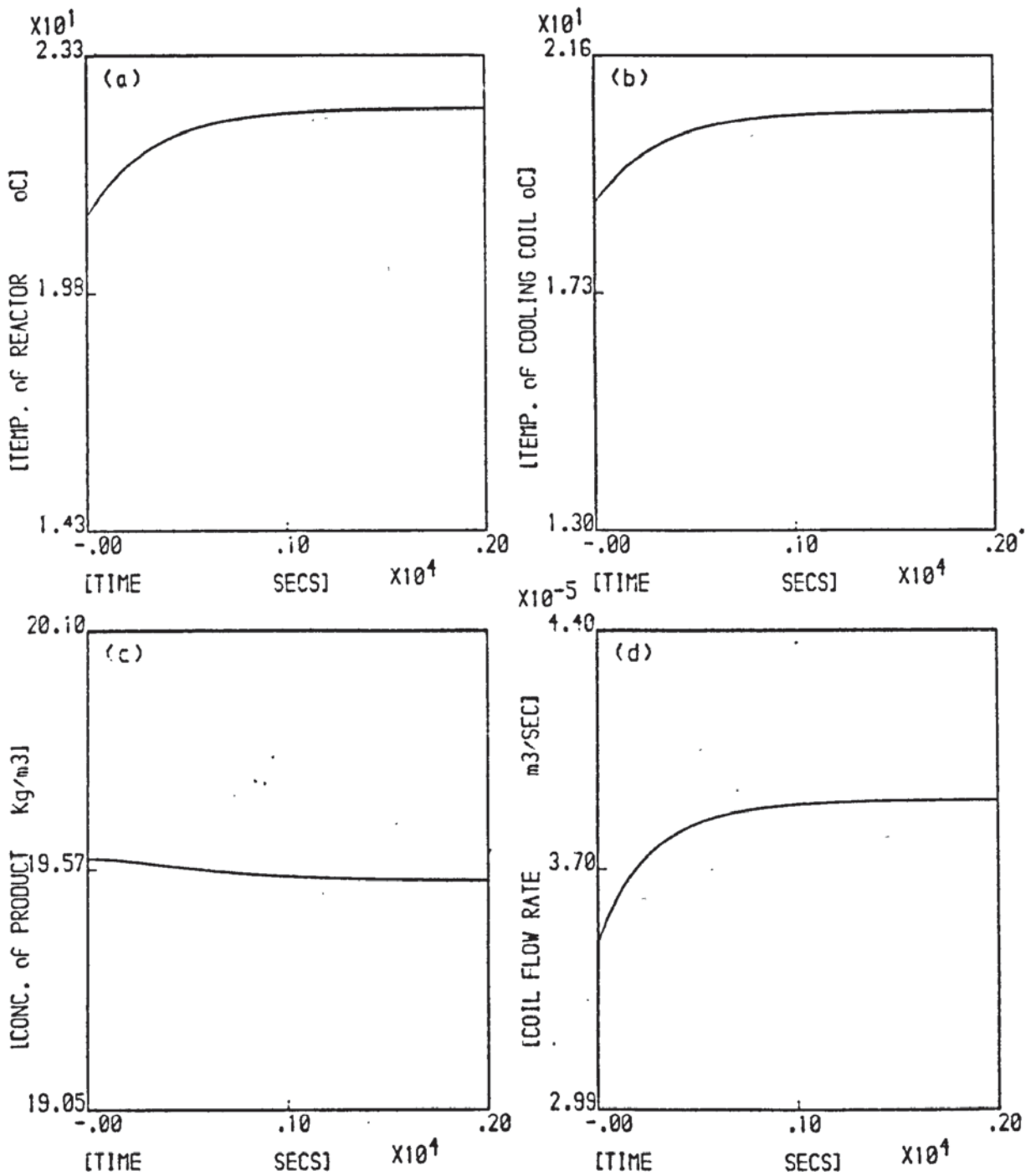


Step in Feed concentration (-1.0 kg/m^3) and temperature of liquid into cooling coil (1.5K)
 Noninteracting control of reactor temperature
 Fig. A.6.1.55 Reactor One. Experiment no:5



Step in temperature of liquid into cooling coil(1.5K). Noninteracting control of reactor temperature.

Fig. A.6.1.55 Reactor Two. Experiment no:5

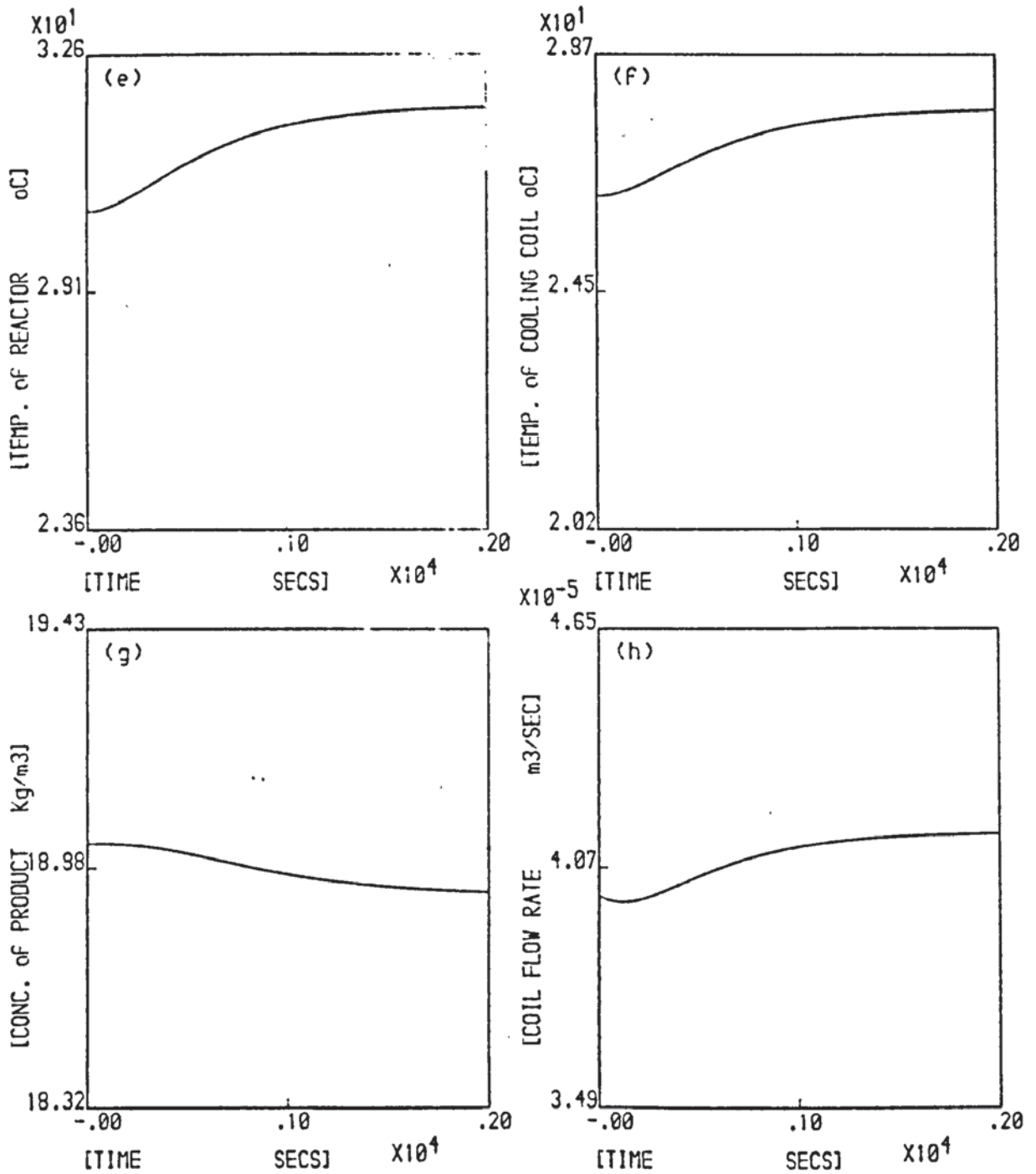


Step in Feed temperature(2.0K).

Noninteracting control of reactor temperature

$$\alpha_2 = 1.0$$

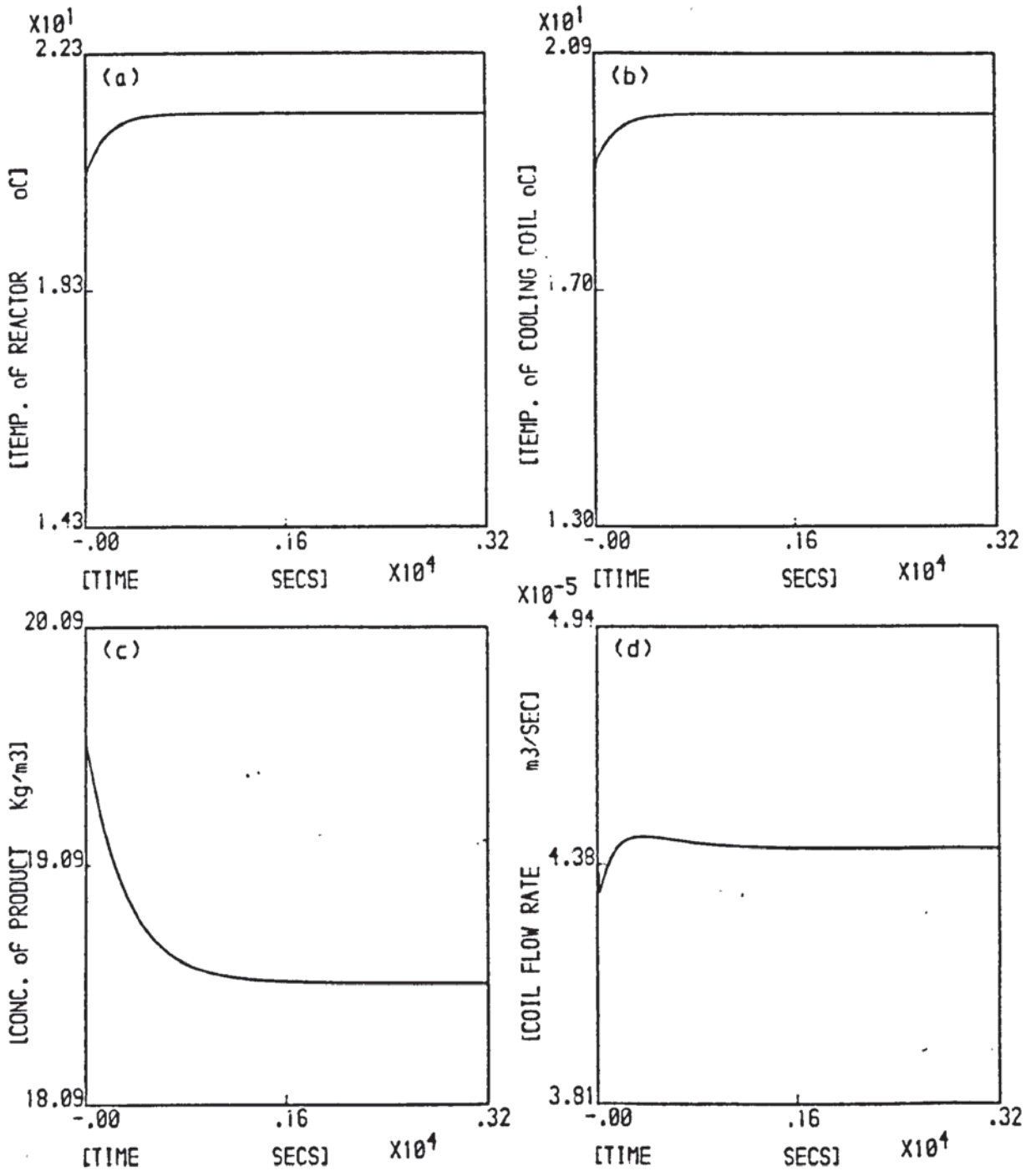
Fig. A.6.1.56 Reactor One. Experiment no:31



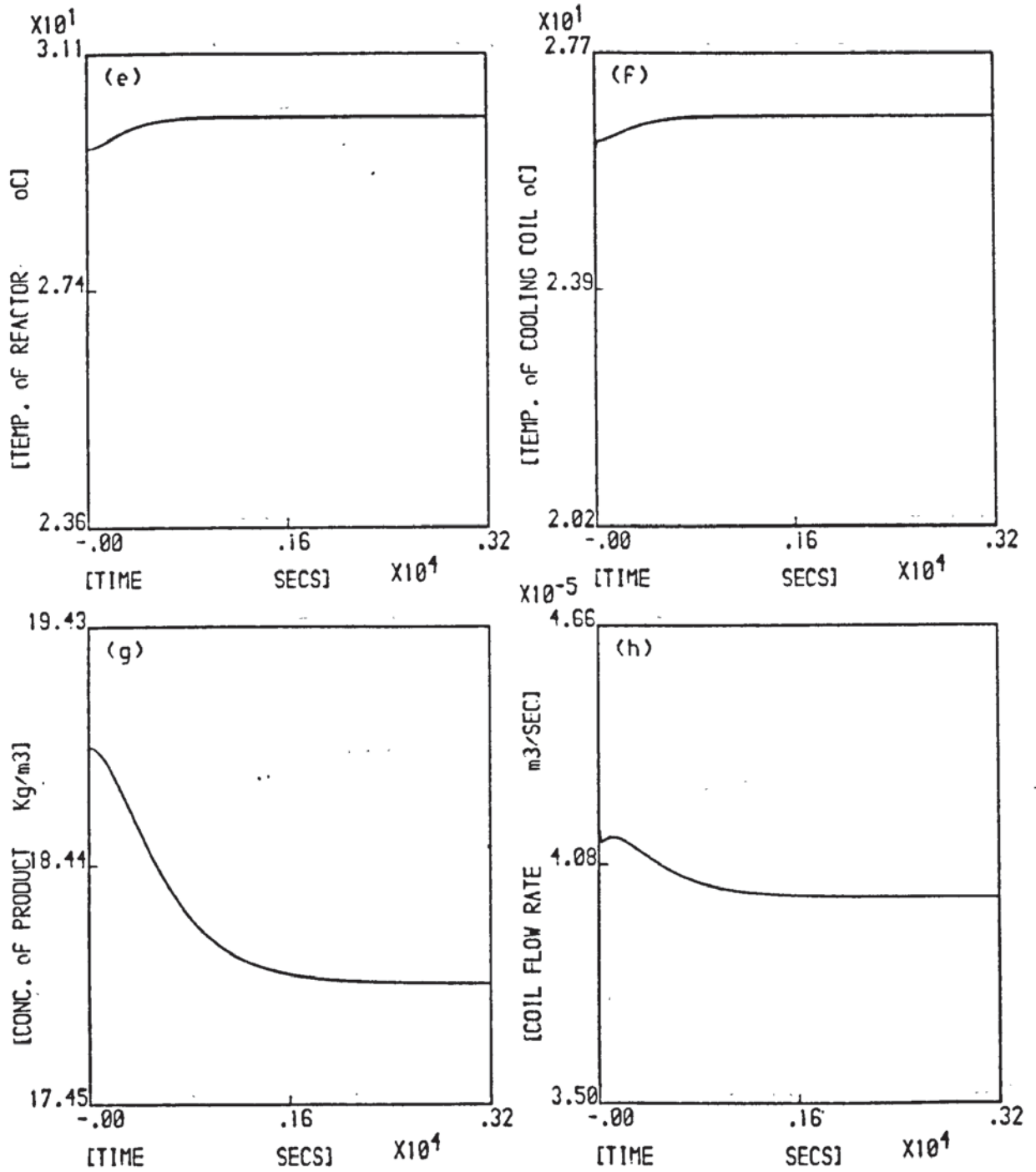
Disturbances from first reactor only.
 Noninteracting control of reactor temperature

$$a_2 = 1.0$$

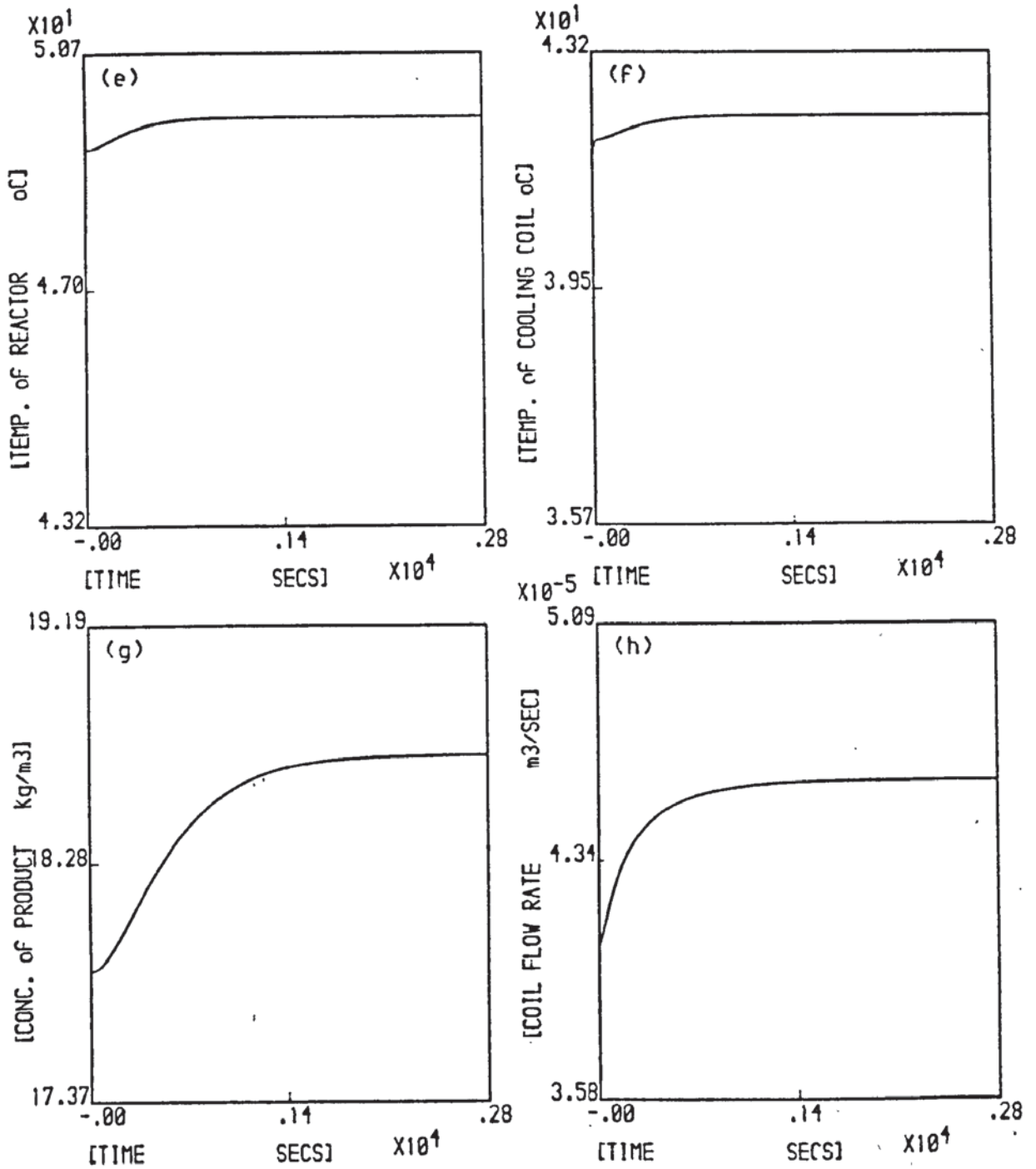
Fig. A.6.1.56 Reactor Two. Experiment no:31



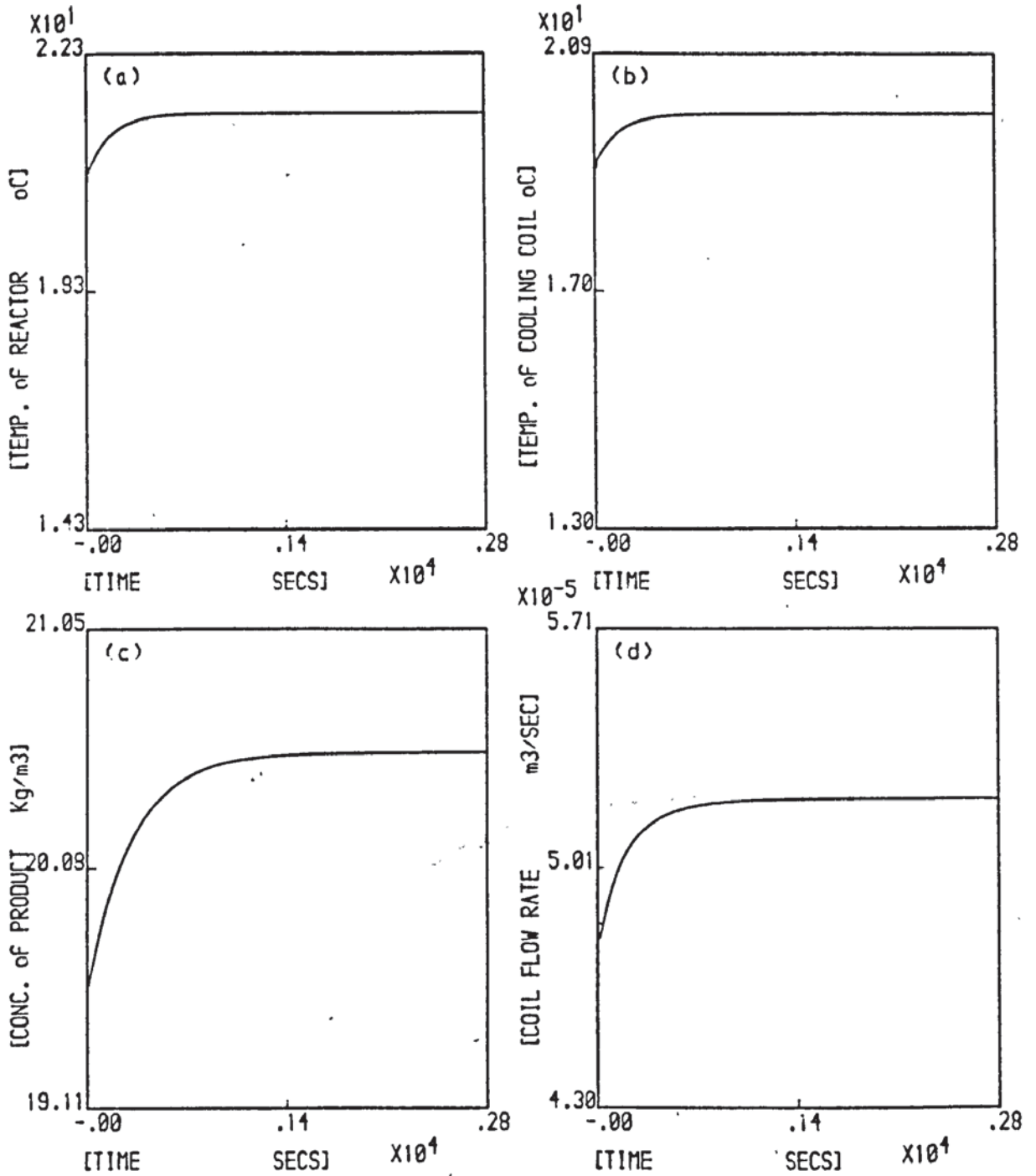
Step in feed concentration(-1.0kg/m³) and temperature(2.0K). Noninteracting control of reactor temperature. $\alpha_2=2$
 Fig. A.6.1.57 Reactor One. Experiment no:31



Step in temperature of liquid into cooling coil(0.5K). Noninteracting control of reactor temperature. $a_2=2$.
 Fig. 1.6.1.57 Reactor Two. Experiment no:31



Step in temperature of liquid into cooling coil(0.5K). Noninteracting temperature of control of reactor temperature. $\alpha_2=2.0$
 Fig. A.6.1.58 Reactor Two. Experiment no:31



Step in feed concentration(1.0kg/m³) and temperature. Noninteracting control of reactor temperature. $a_2=2.0$
 Fig. A.6.1.58 Reactor-One. Experiment no:31

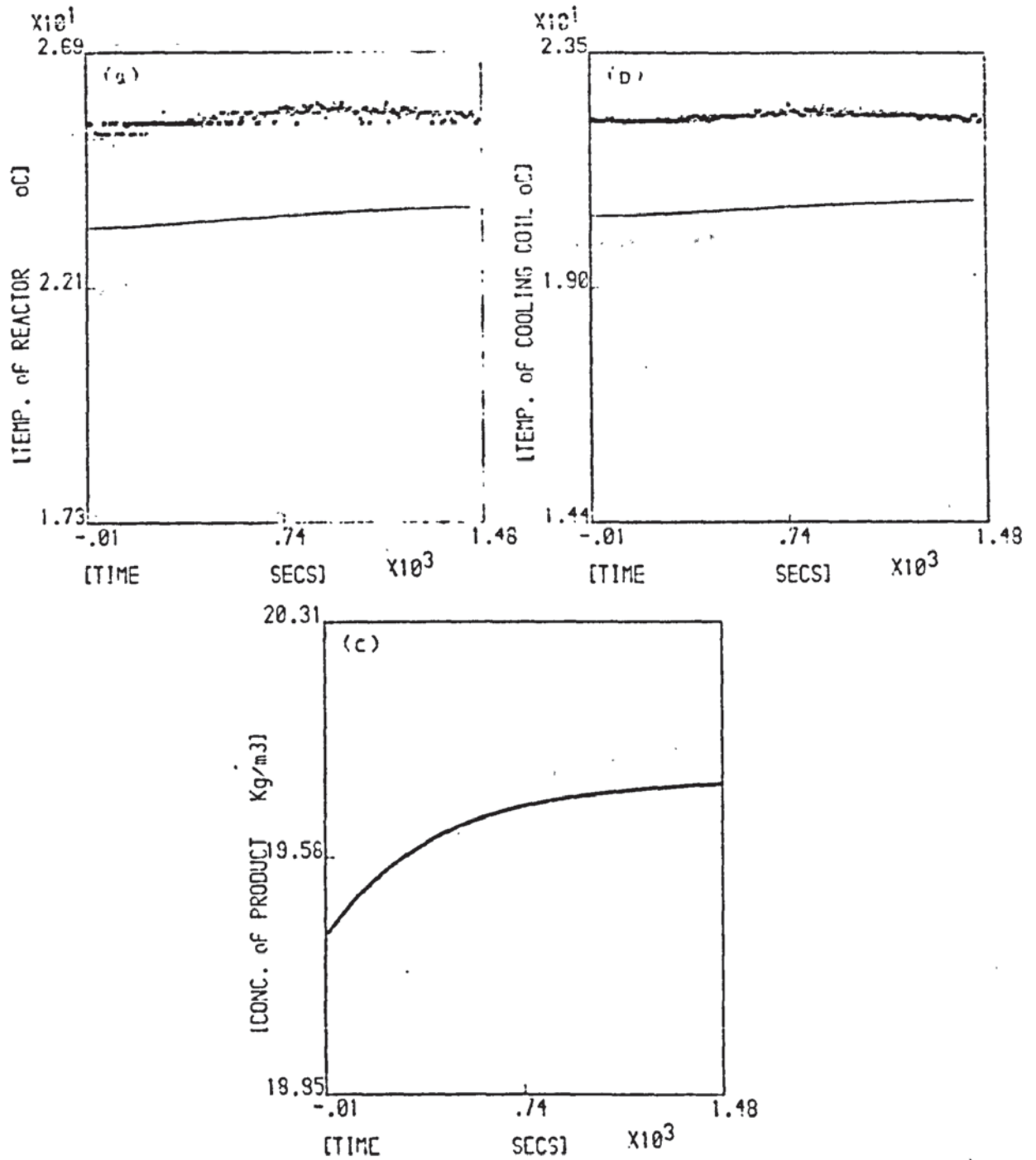


Fig A.6.2.1 Reactor One. Experiment no: 1

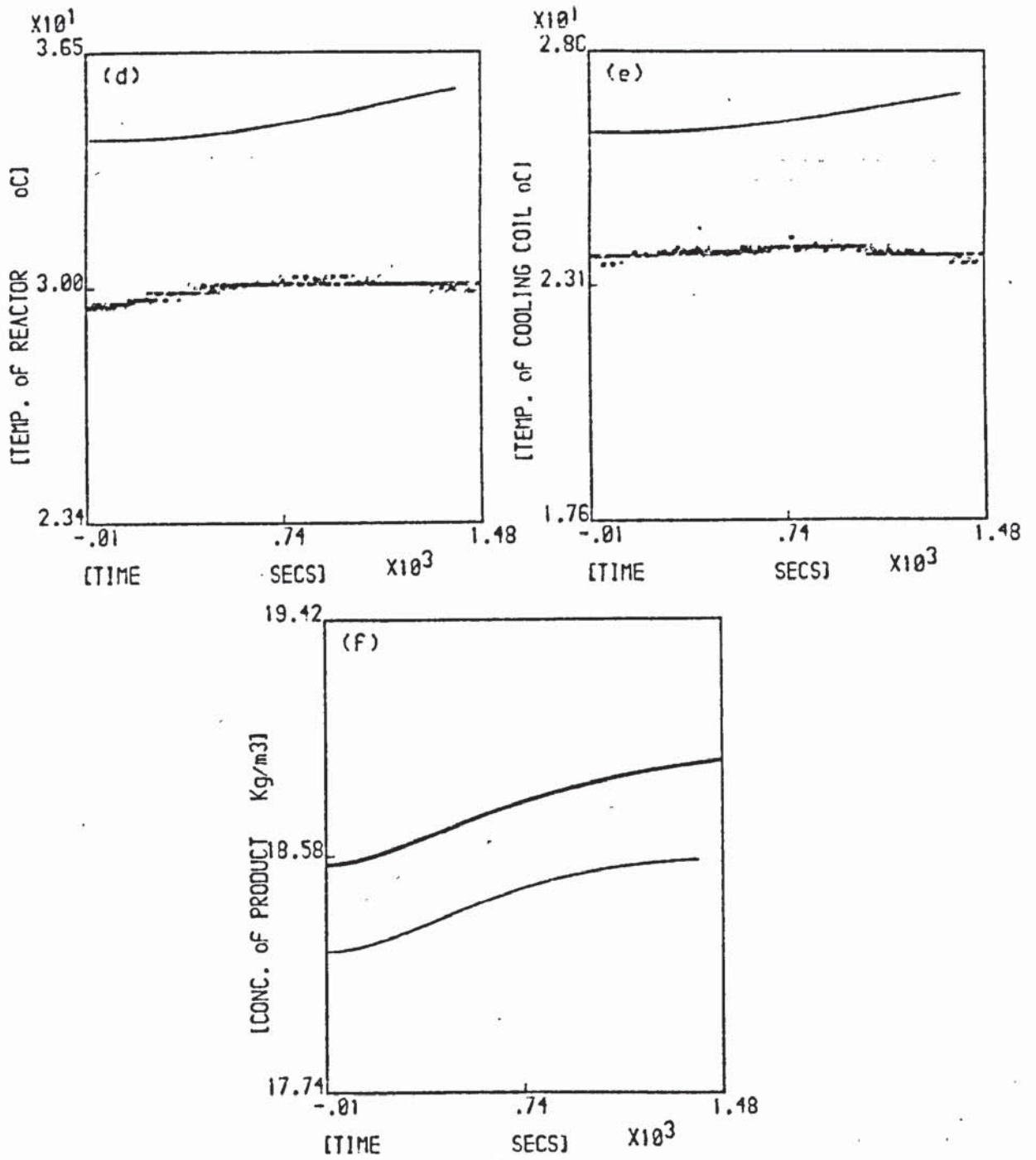


Fig A.G.2.1 Reactor Two. Experiment no: 1

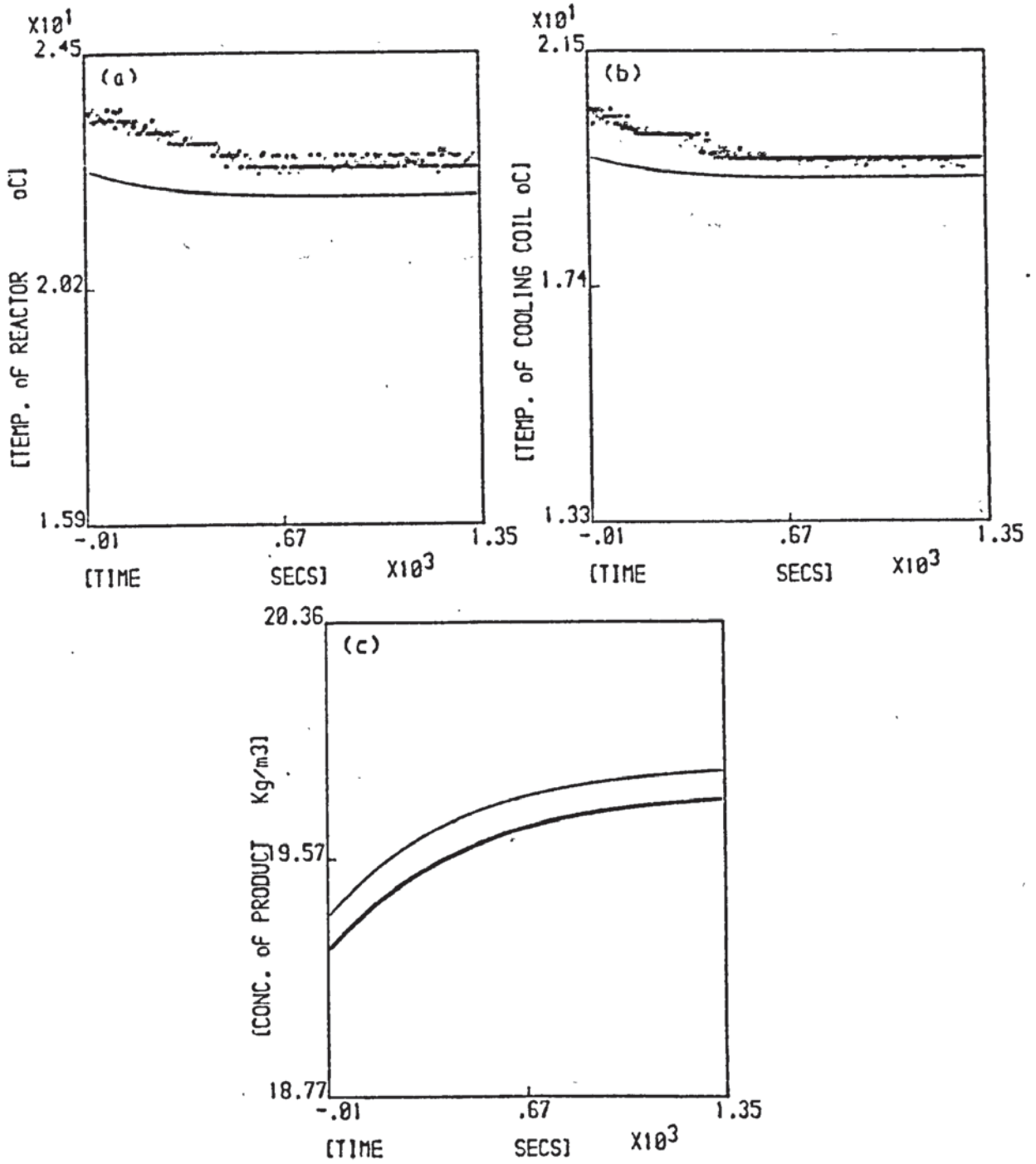


Fig A.6.2.2 Reactor One. Experiment no: 2

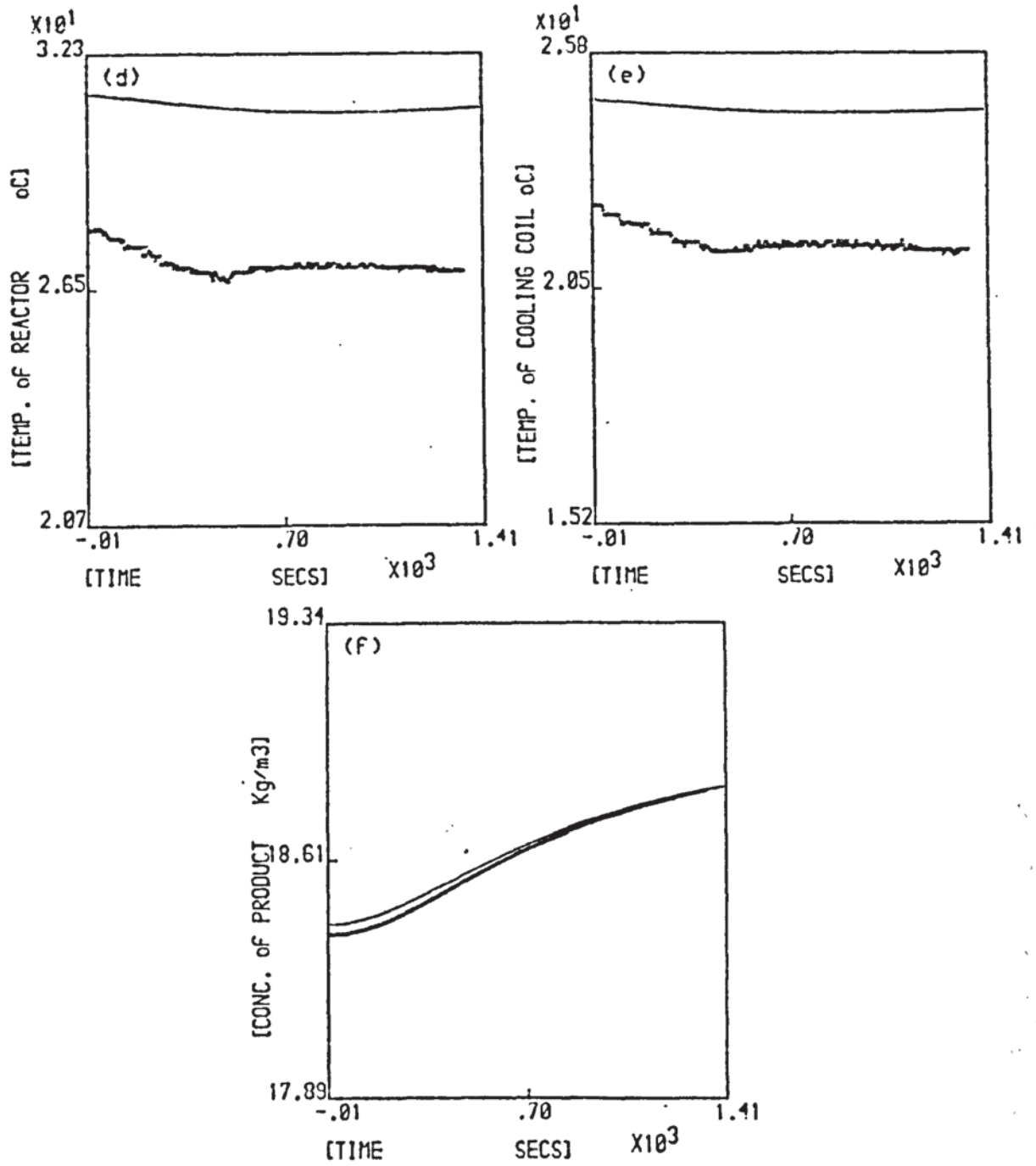


Fig A.6.2.2 Reactor Two. Experiment no: 2

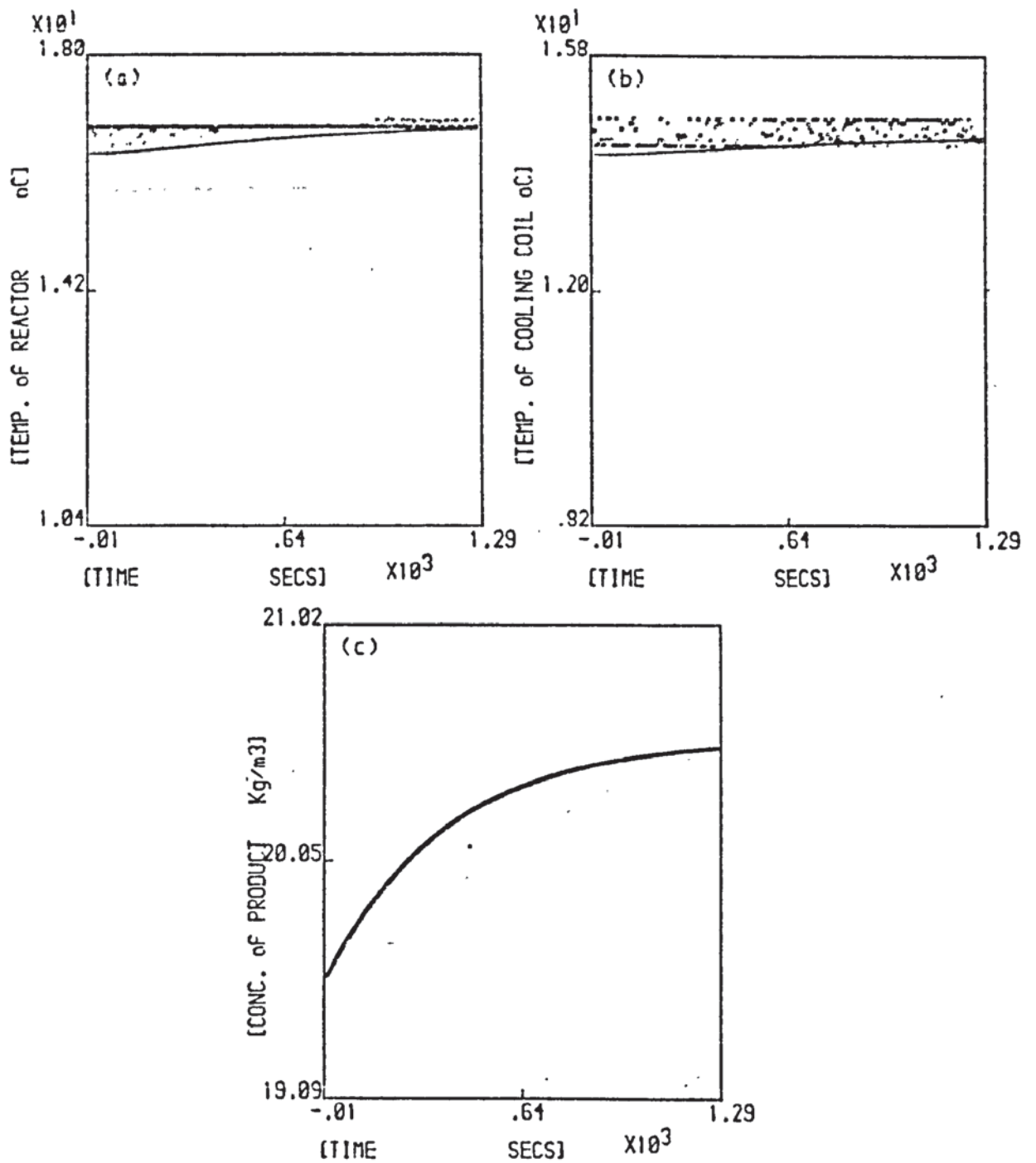


Fig A.6.2.3 Reactor One. Experiment no: 3.

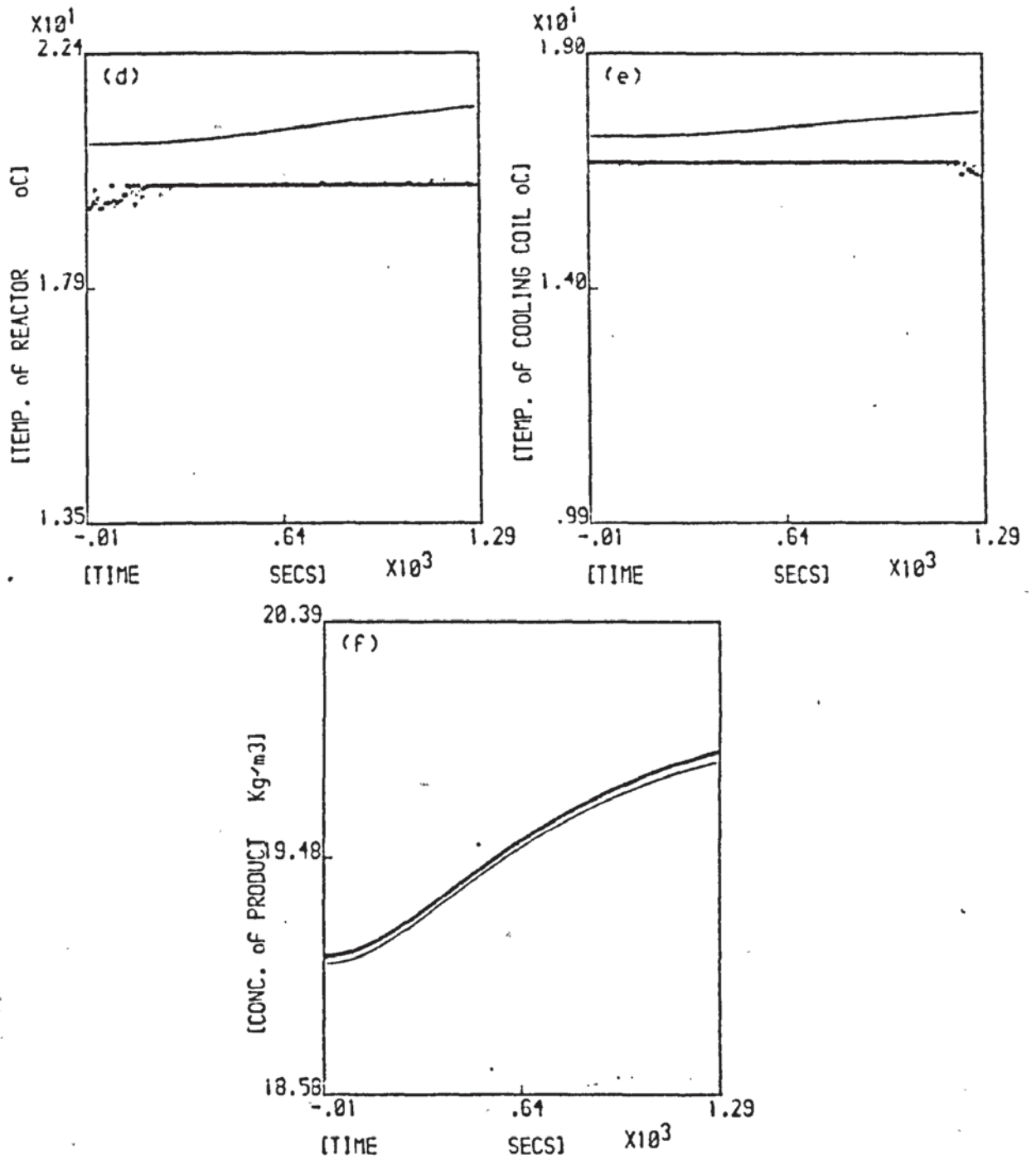


Fig A.6.2.3 Reactor Two. Experiment no: 3

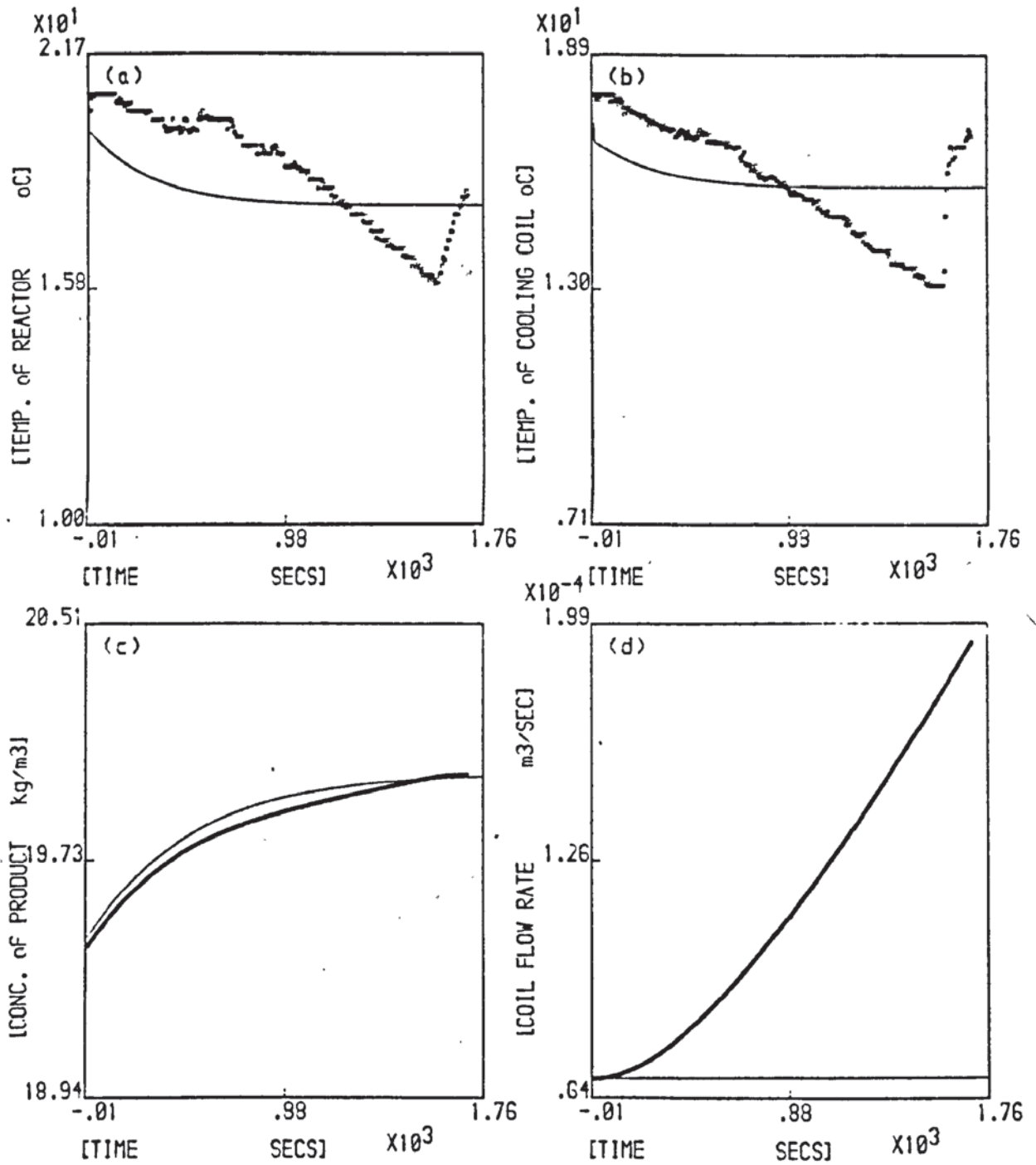


Fig. A.6.2.4 Reactor One. Experiment no: 4

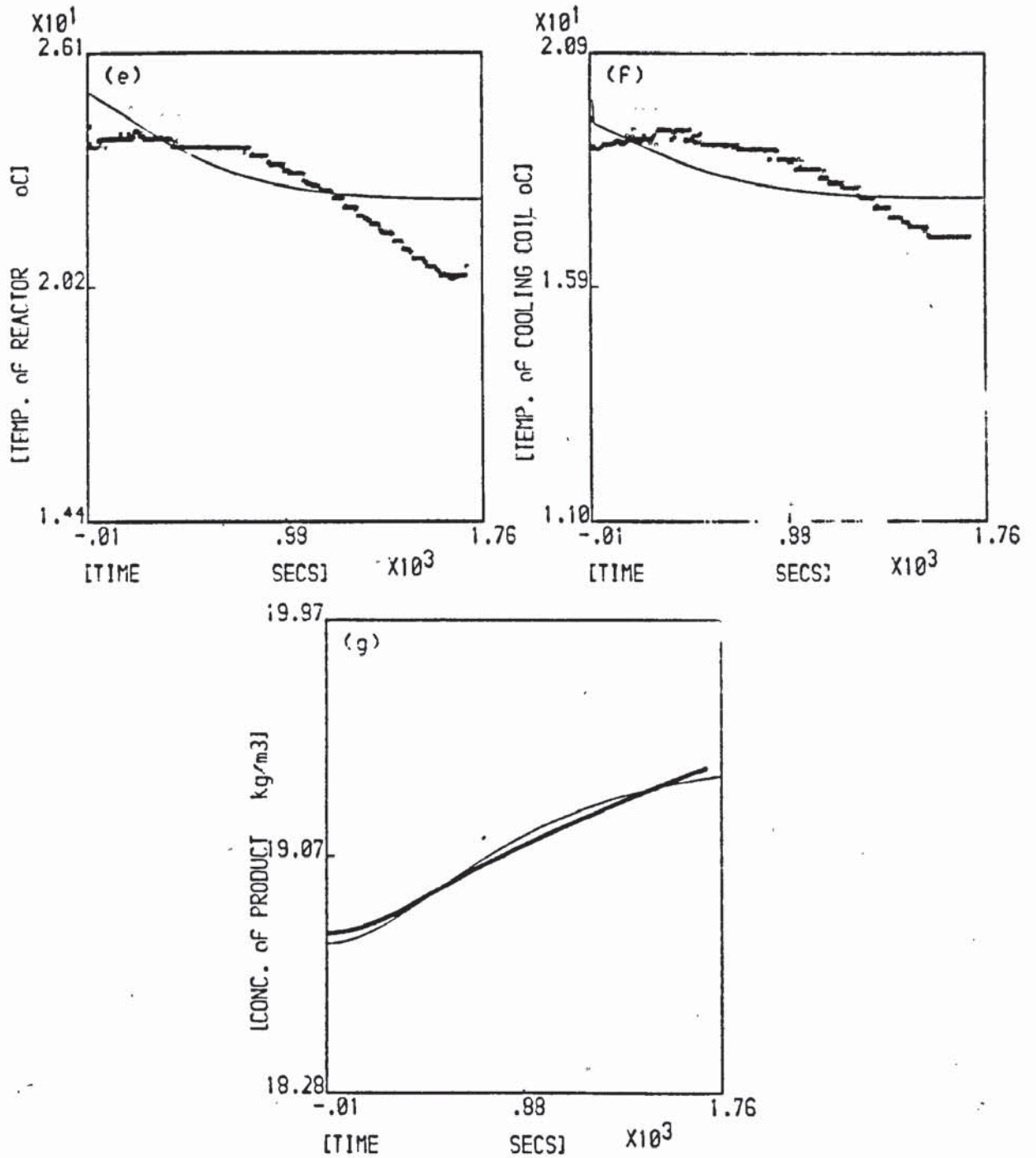


Fig. A.6.2.4 Reactor Two. Experiment no: 4

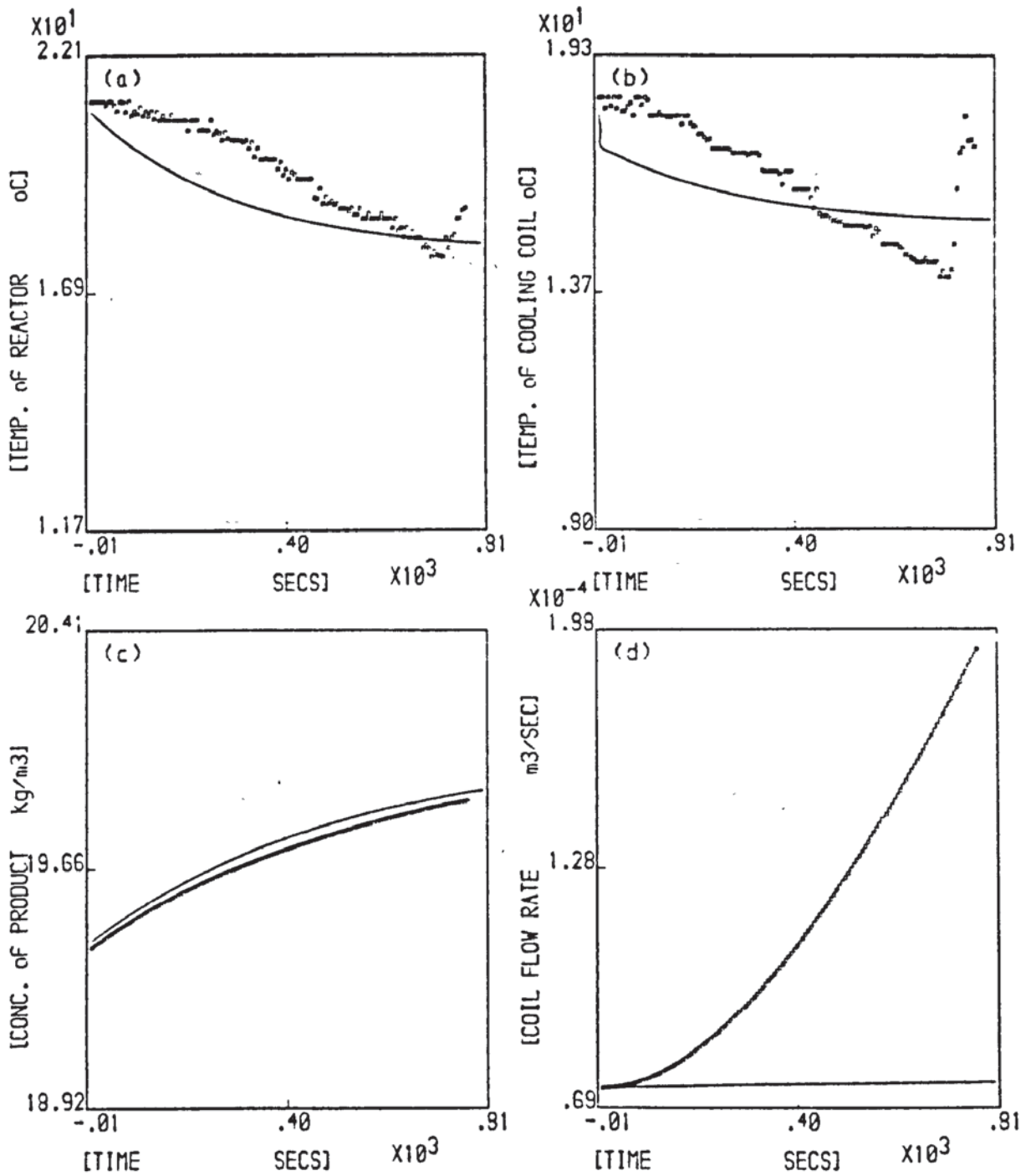


Fig. 1.6.2.5 Reactor One. Experiment no: 5

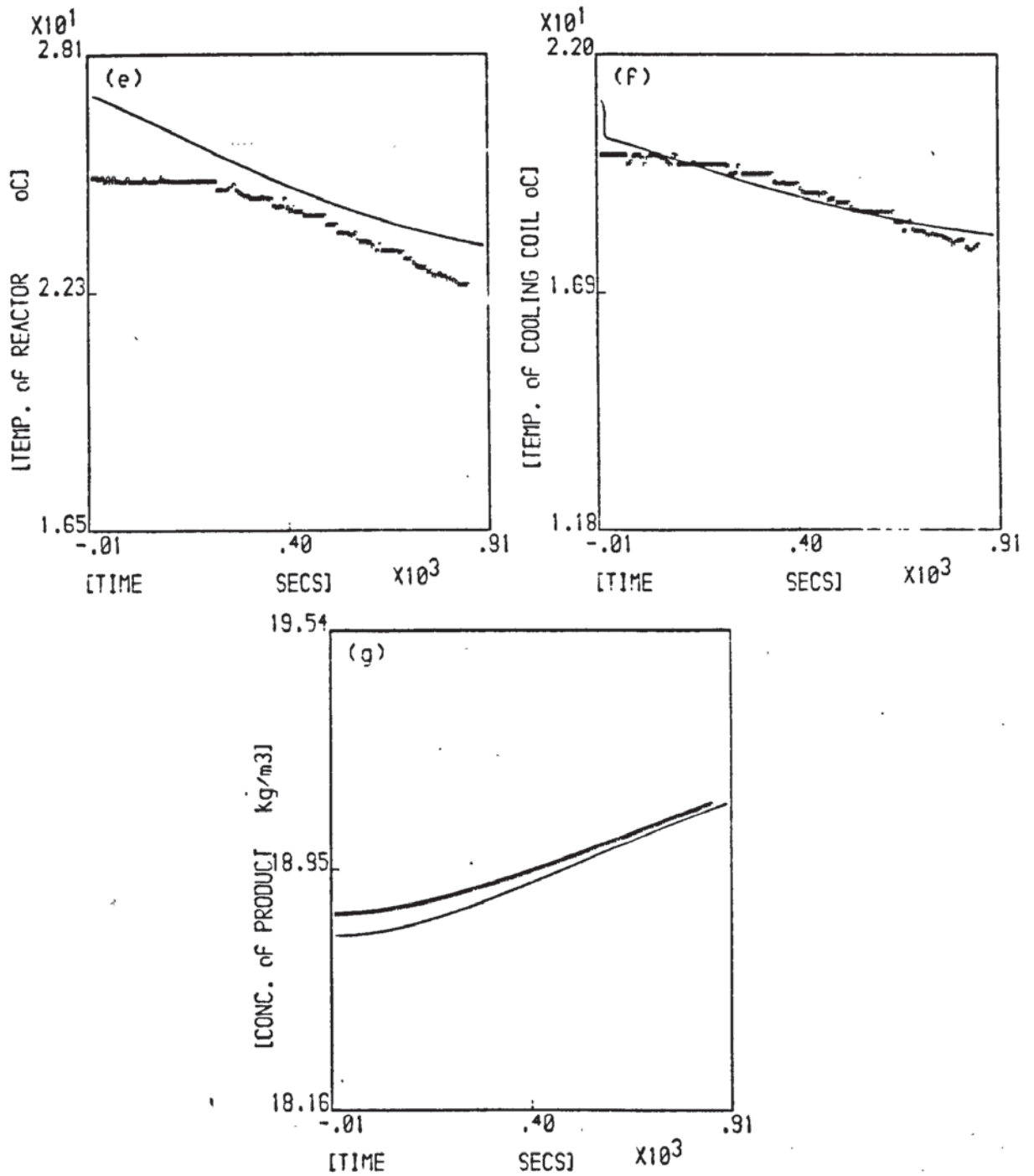


Fig. A.6.2.5 Reactor Two. Experiment no: 5

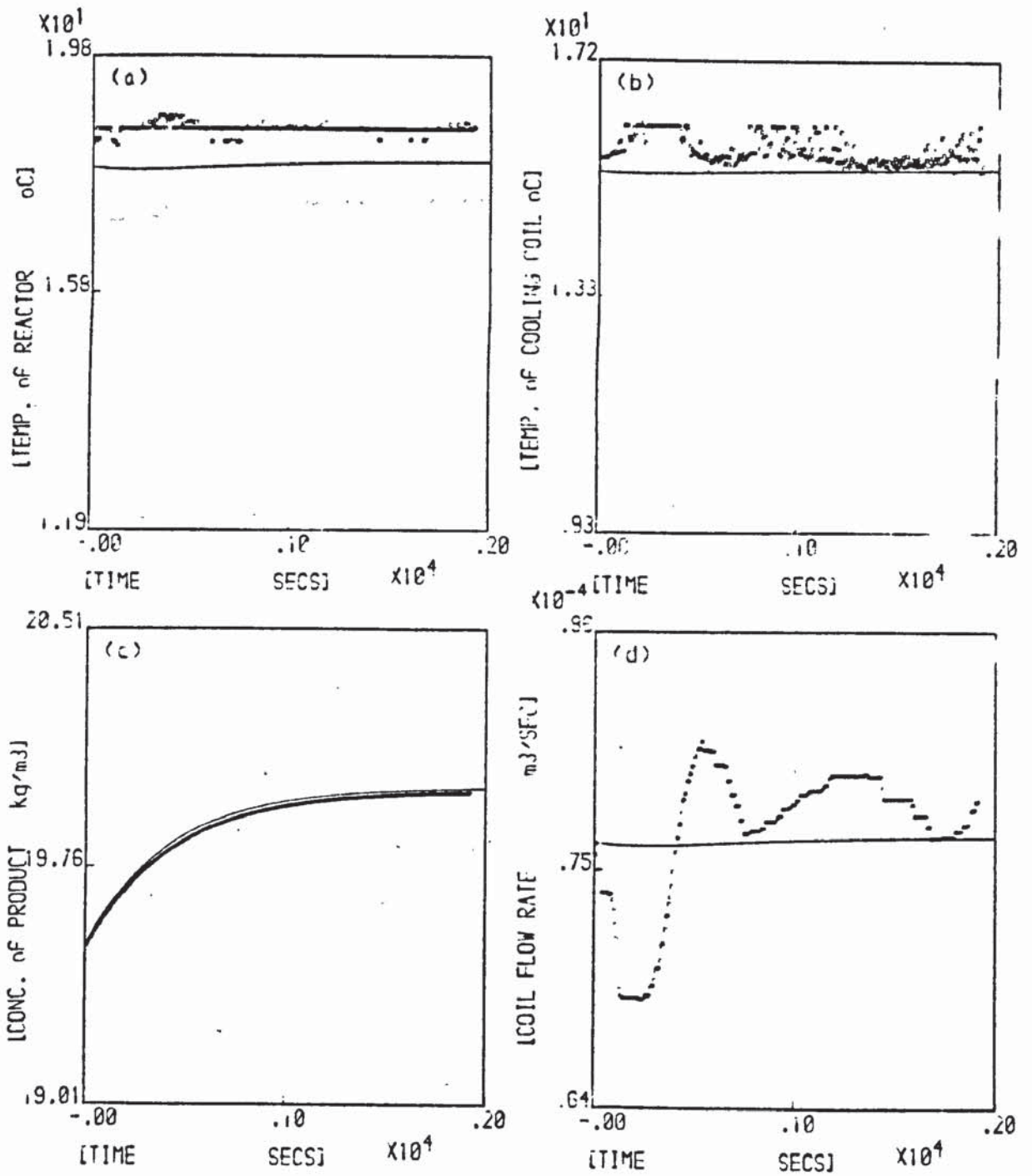


Fig. 4.6.2.6 Reactor One. Experiment no: 6

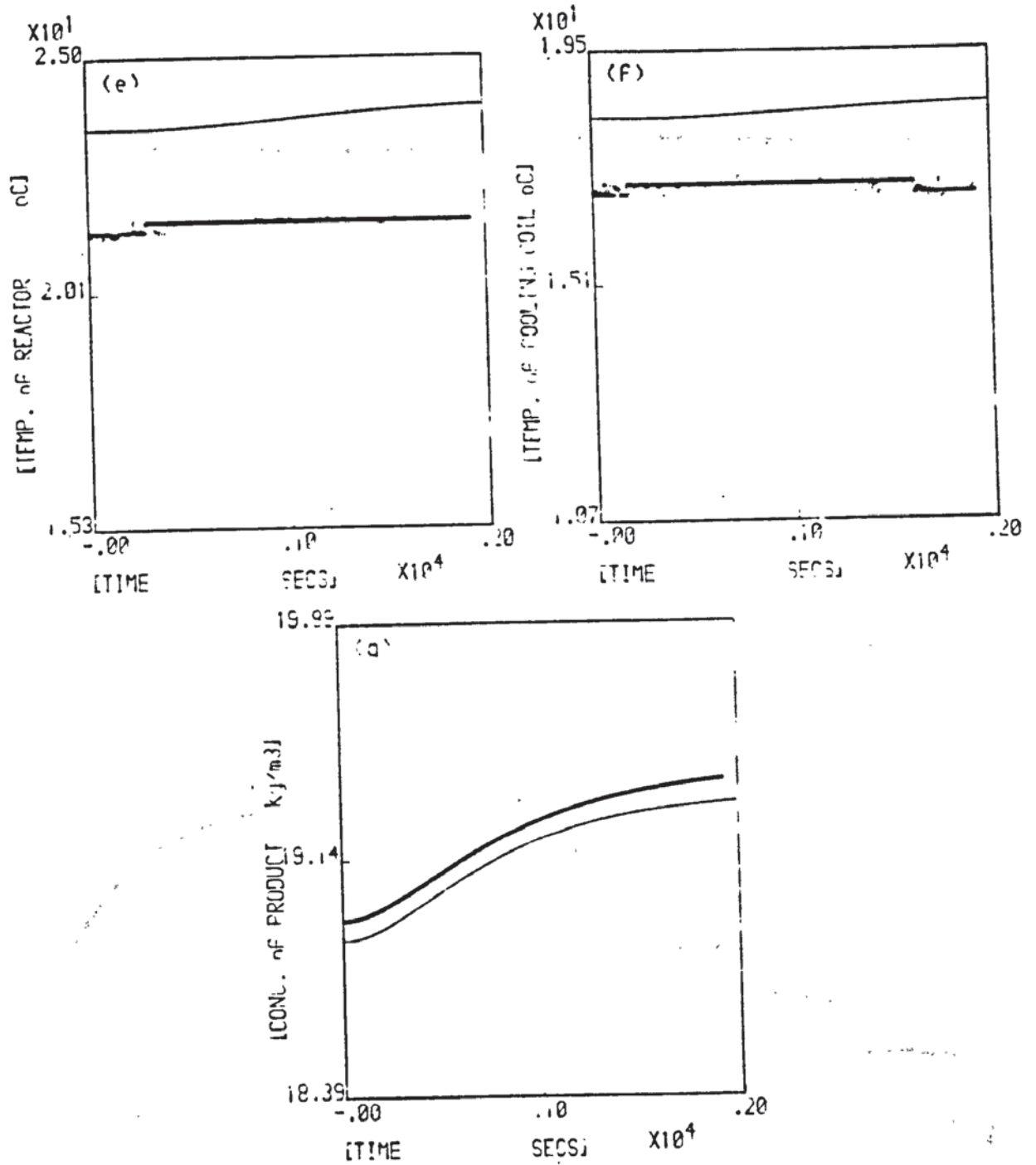


Fig. A.6.2.5 Reactor Two. Experiment no: 6

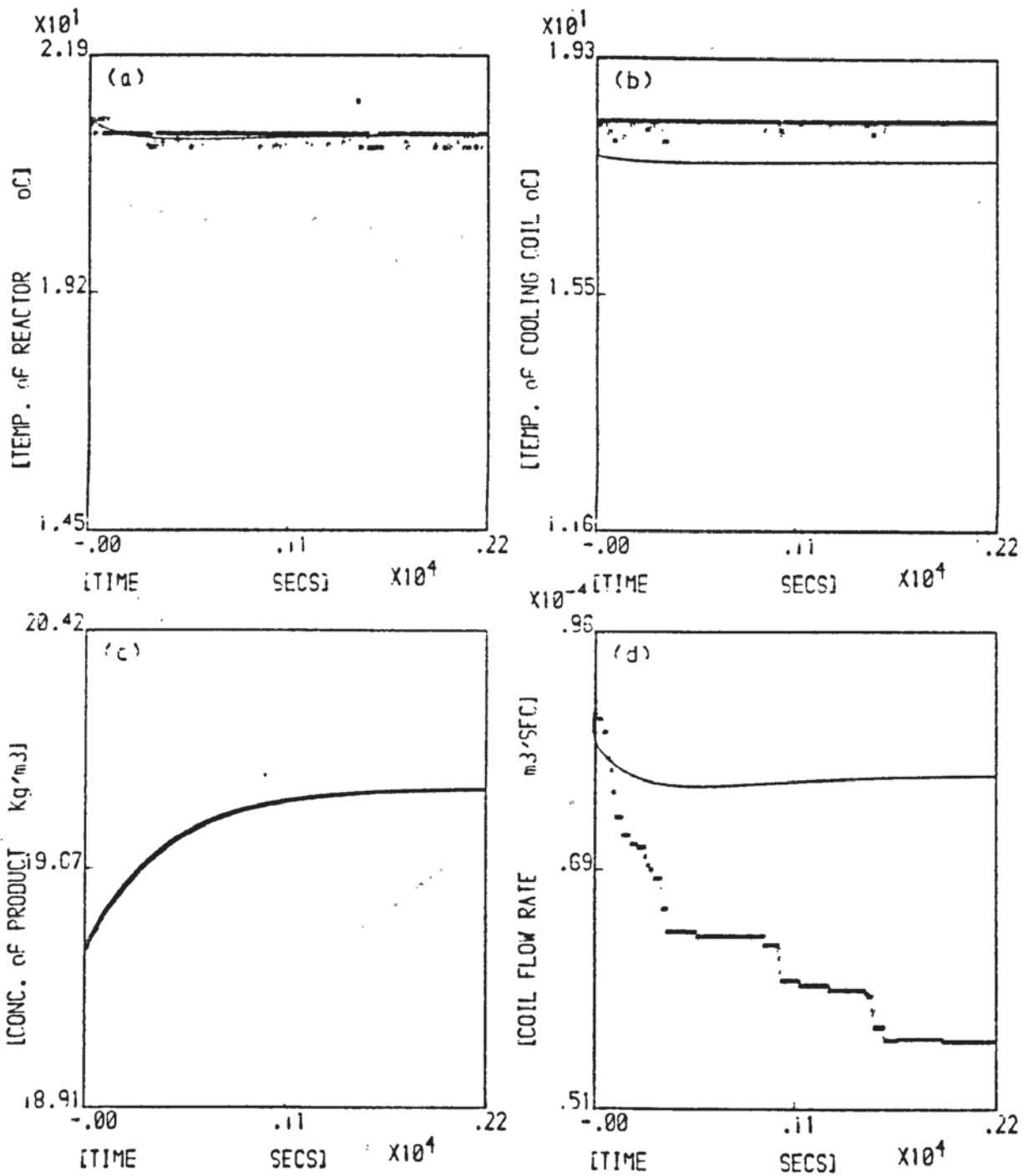


Fig. 1.6.2.7 Reactor One. Experiment no: 7

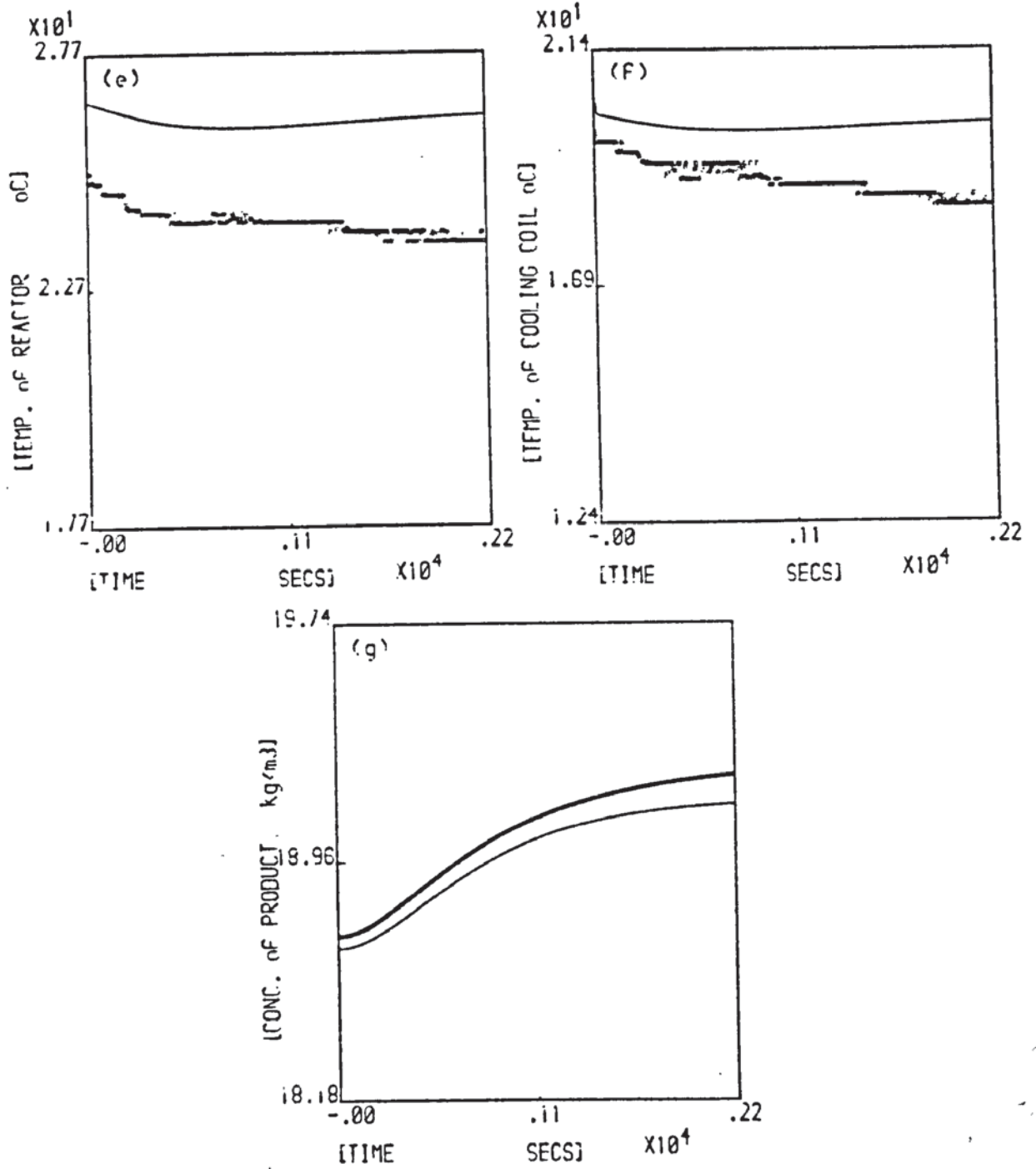


Fig. A.6.2.7 Reactor Two. Experiment no. 7

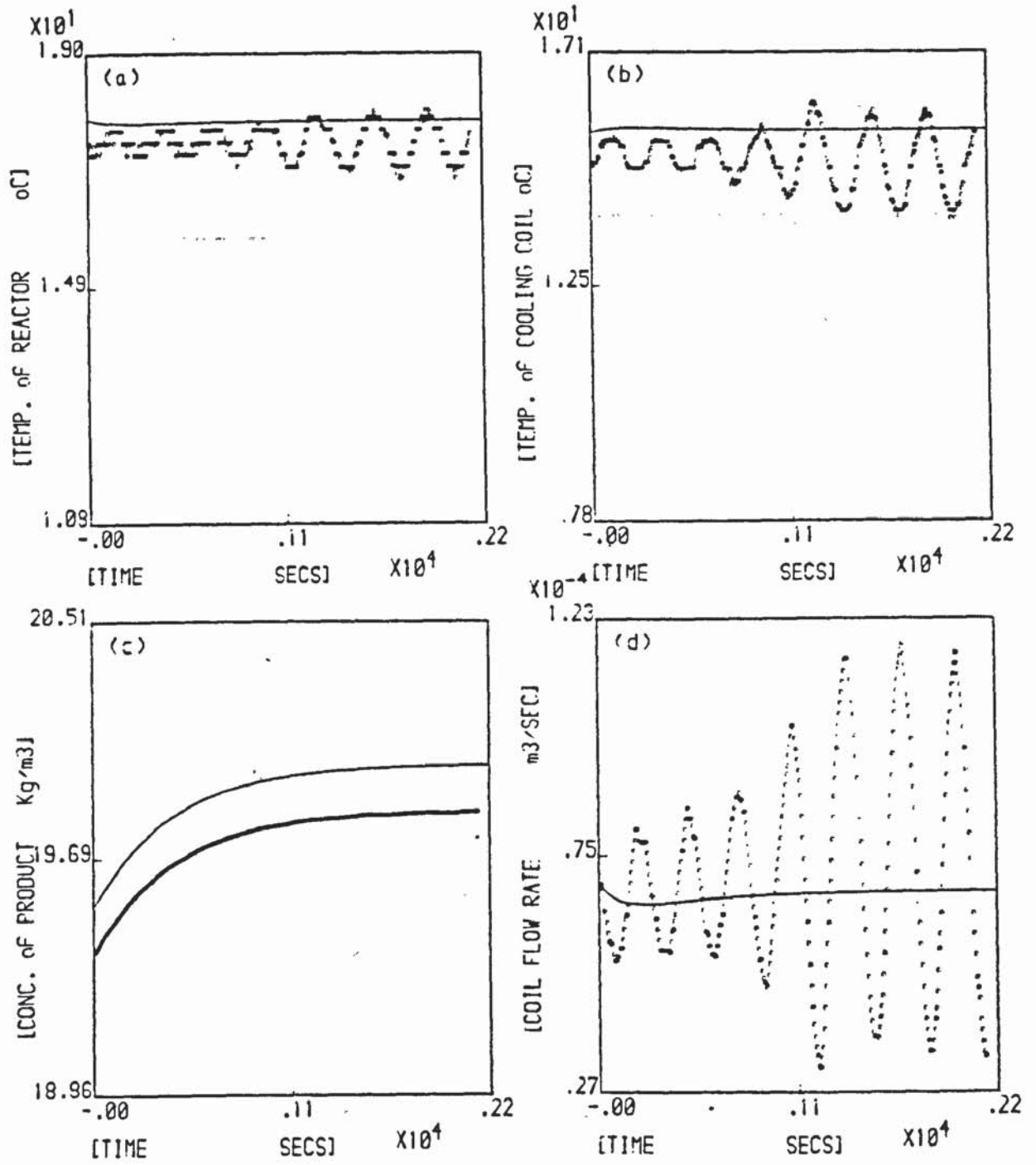


Fig. A.6.2.8 Reactor One. Experiment no: 9A

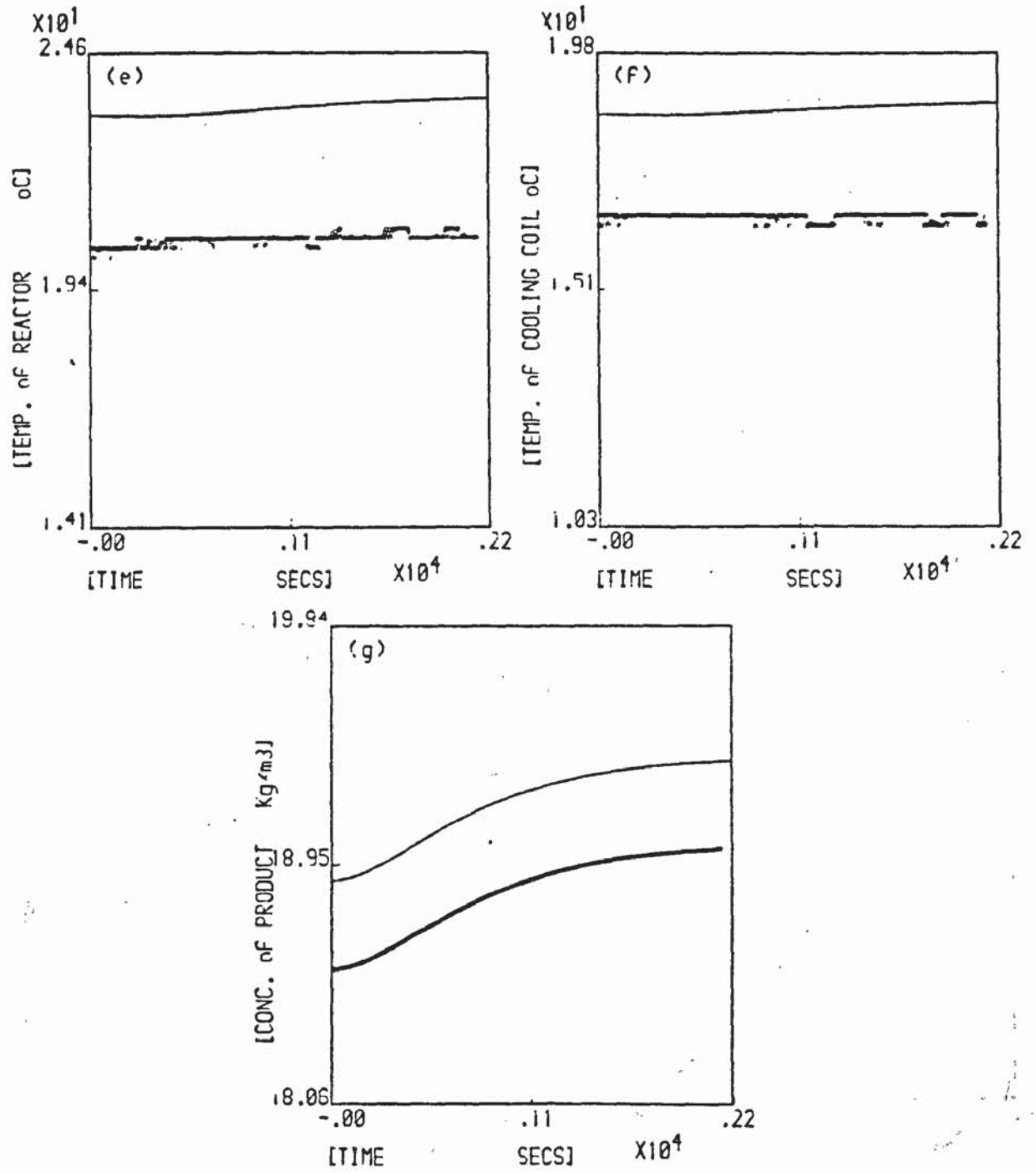


Fig. 1.6.2.9 Reactor Two. Experiment no: 9A

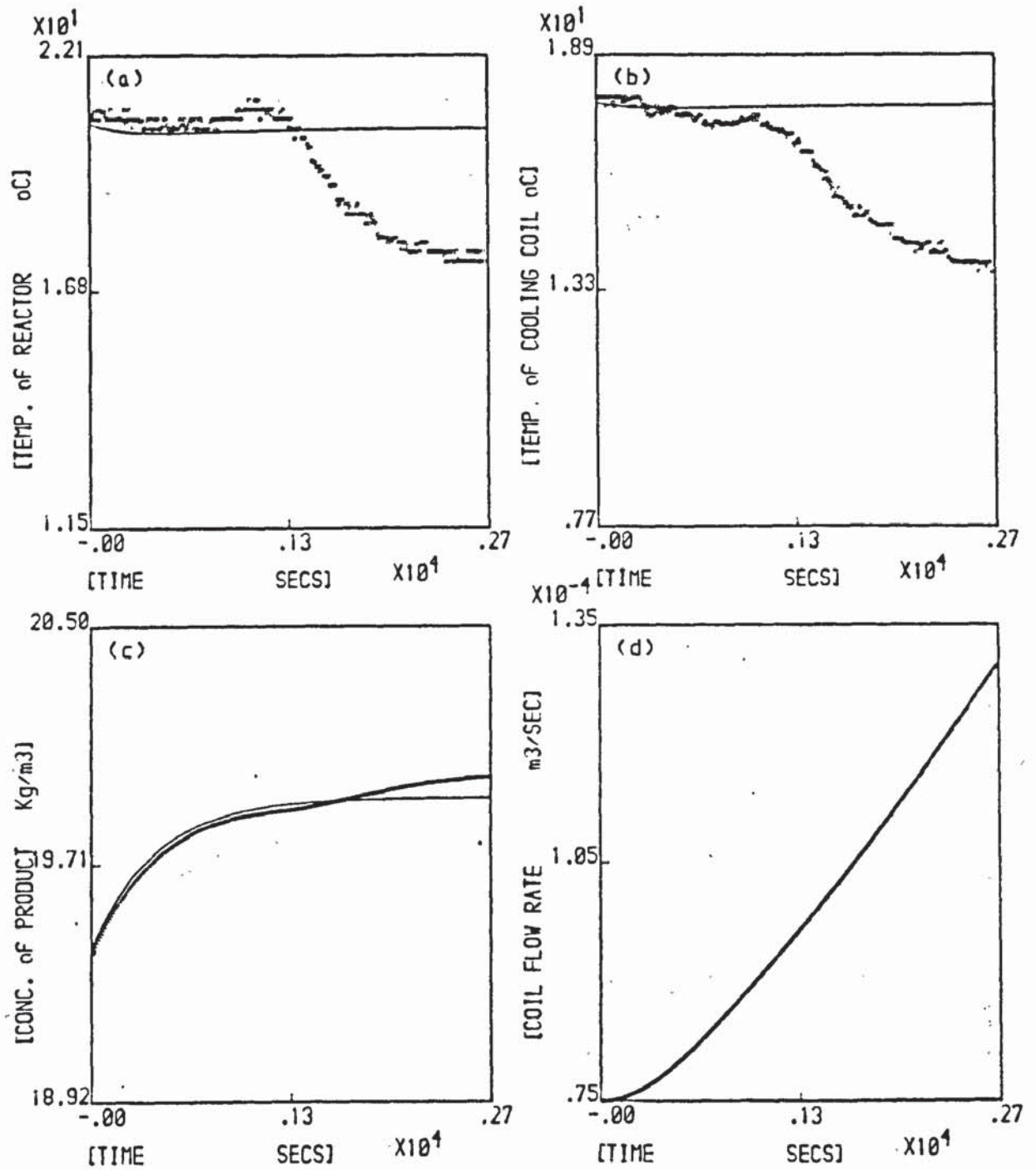


Fig. A.6.2.10 Reactor One. Experiment no: 10

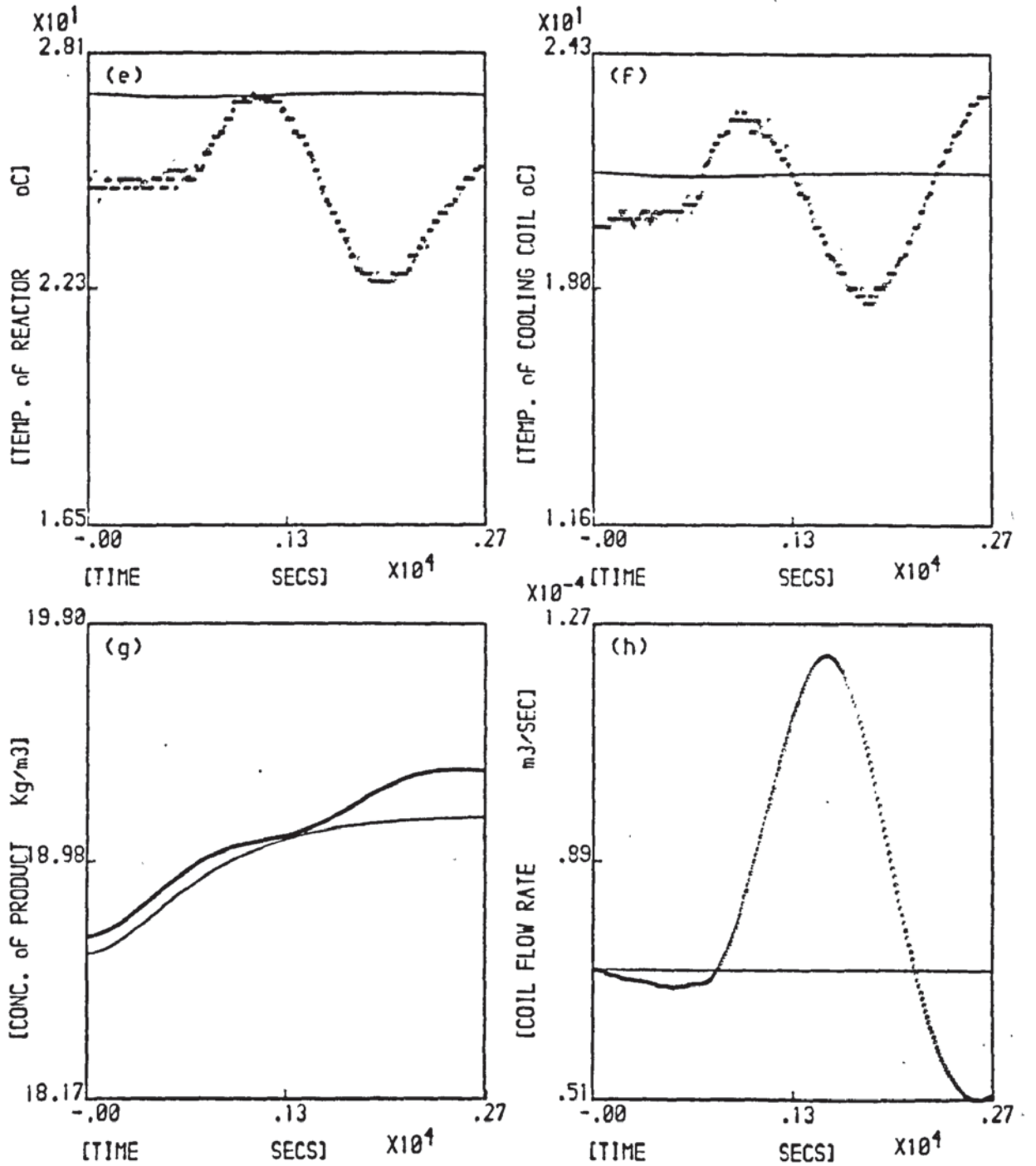


Fig. A.6.2.10 Reactor Two. Experiment no: 10

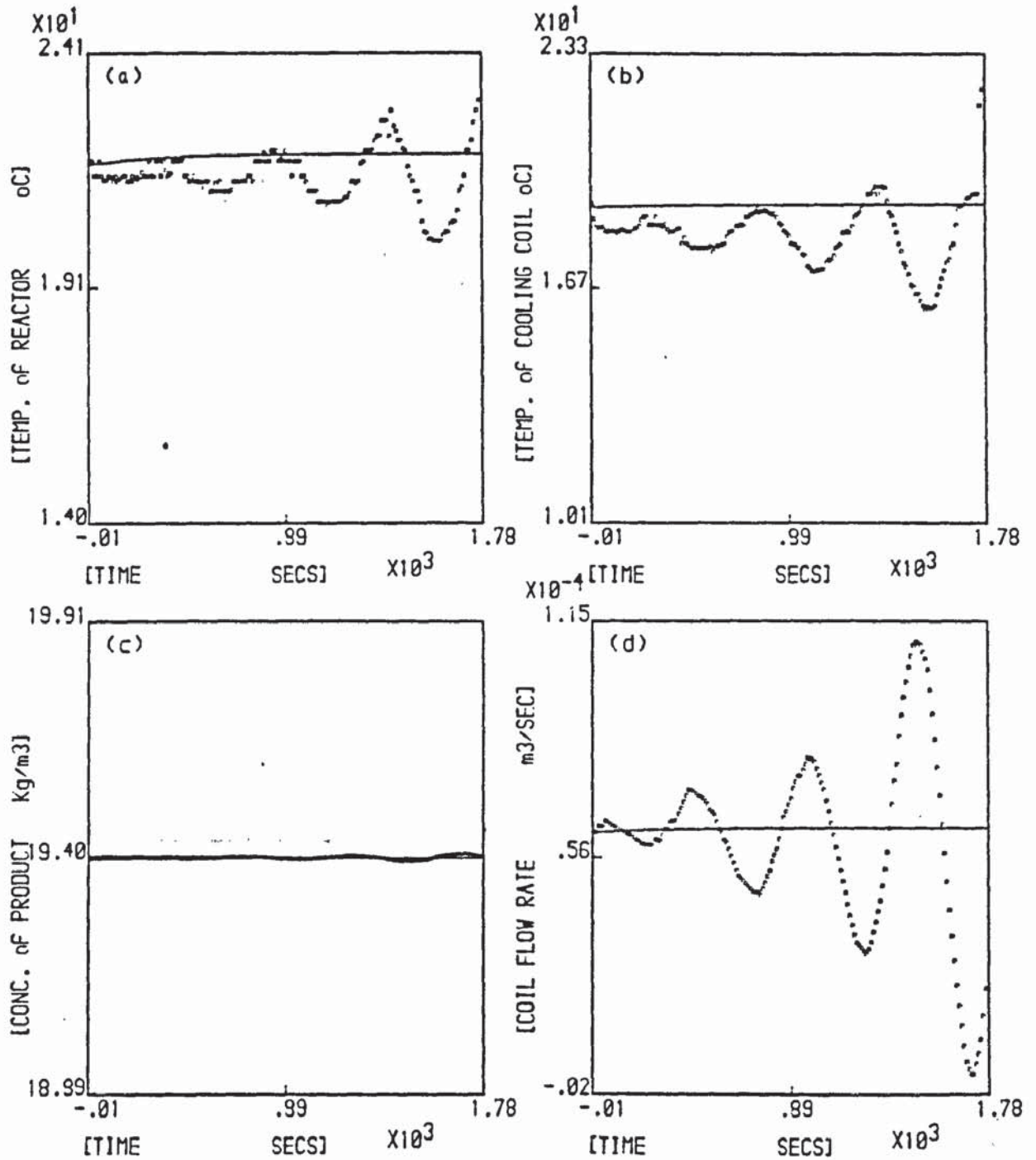


Fig. 4.6.2.11 Reactor One. Experiment no: 11

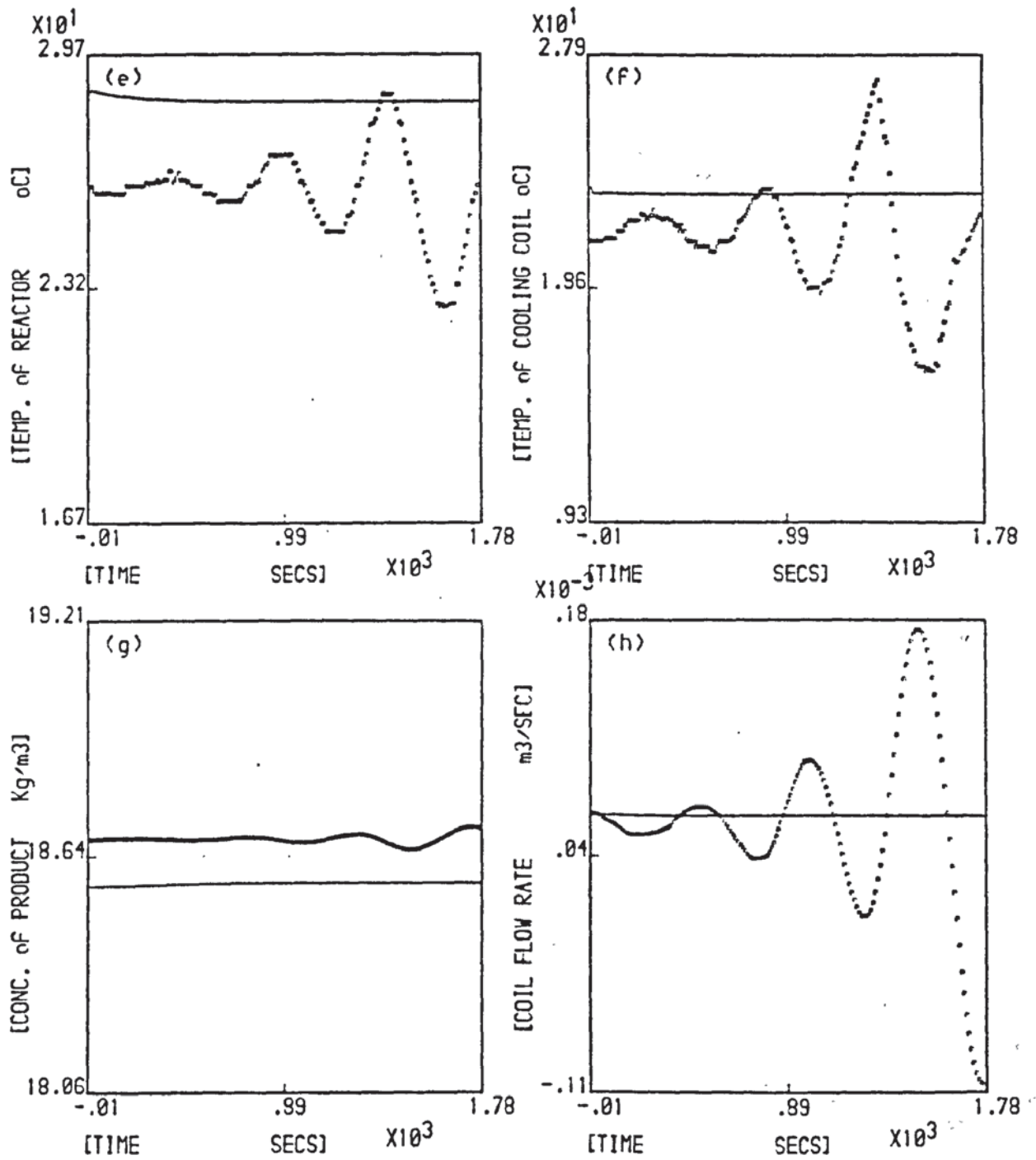


Fig. A.6.2.11 Reactor Two. Experiment no: 11

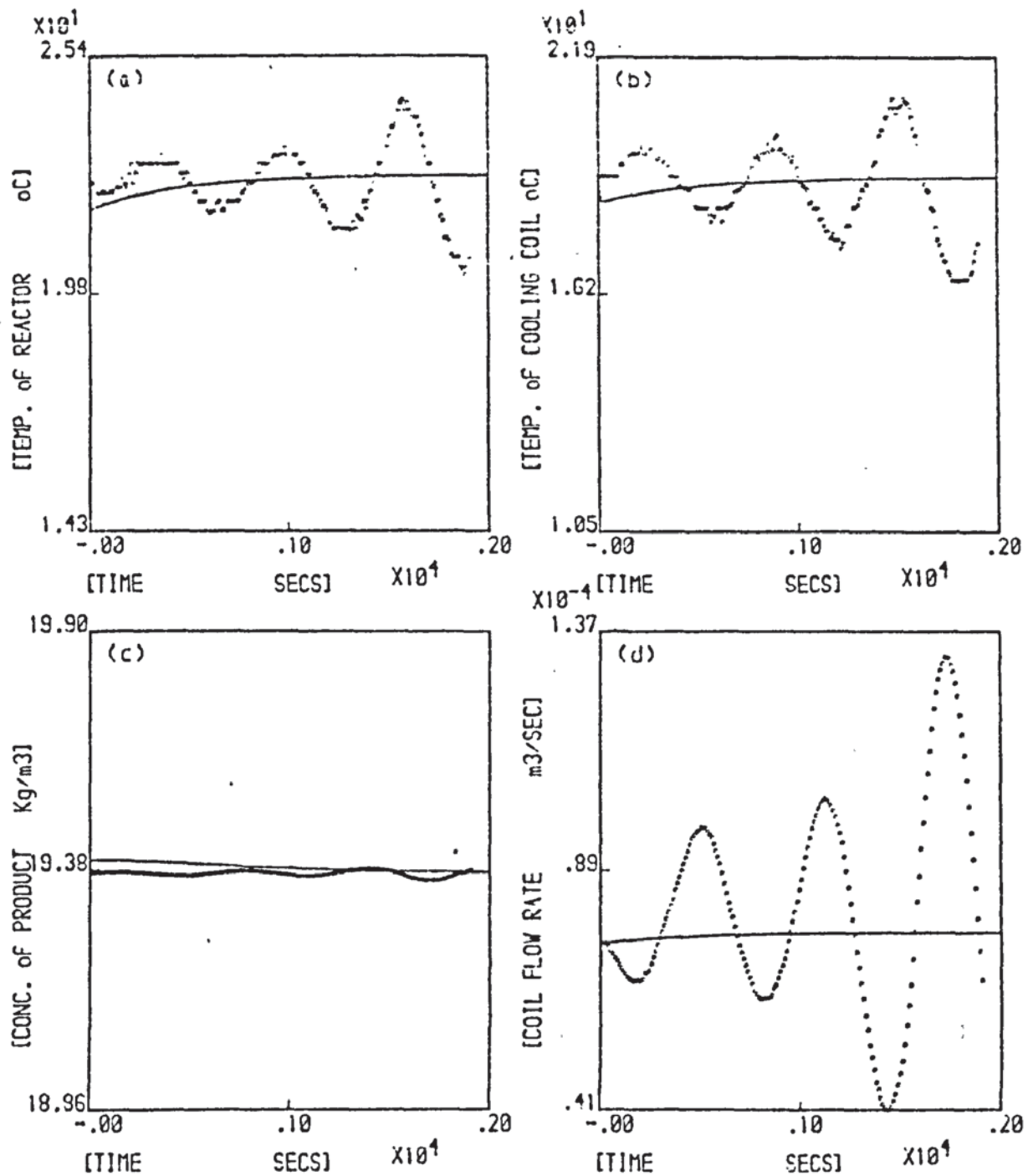


Fig A.6.2.12 Reactor One. Experiment no: 12

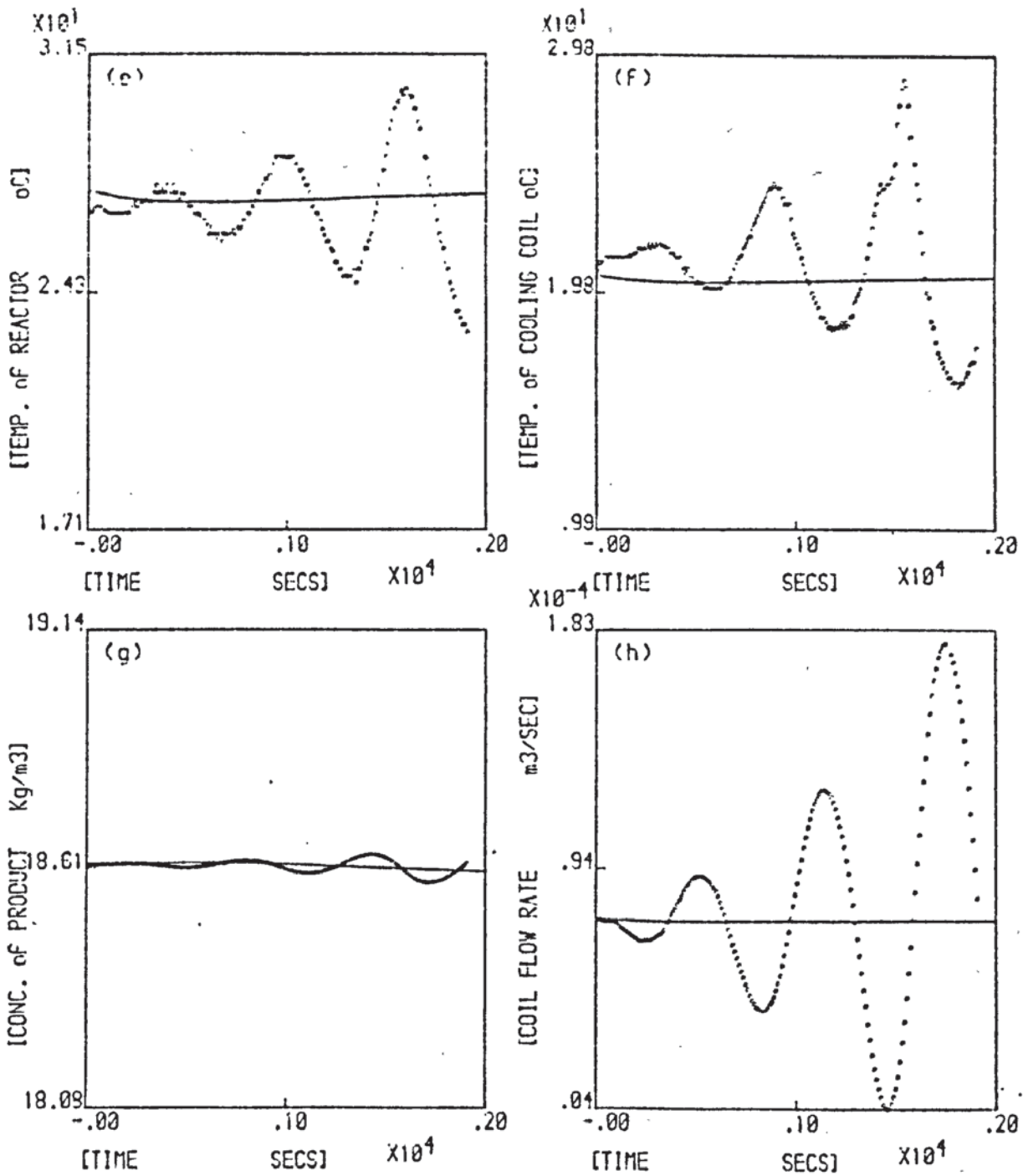


Fig A.G.2.12 Reactor Two. Experiment no: 12

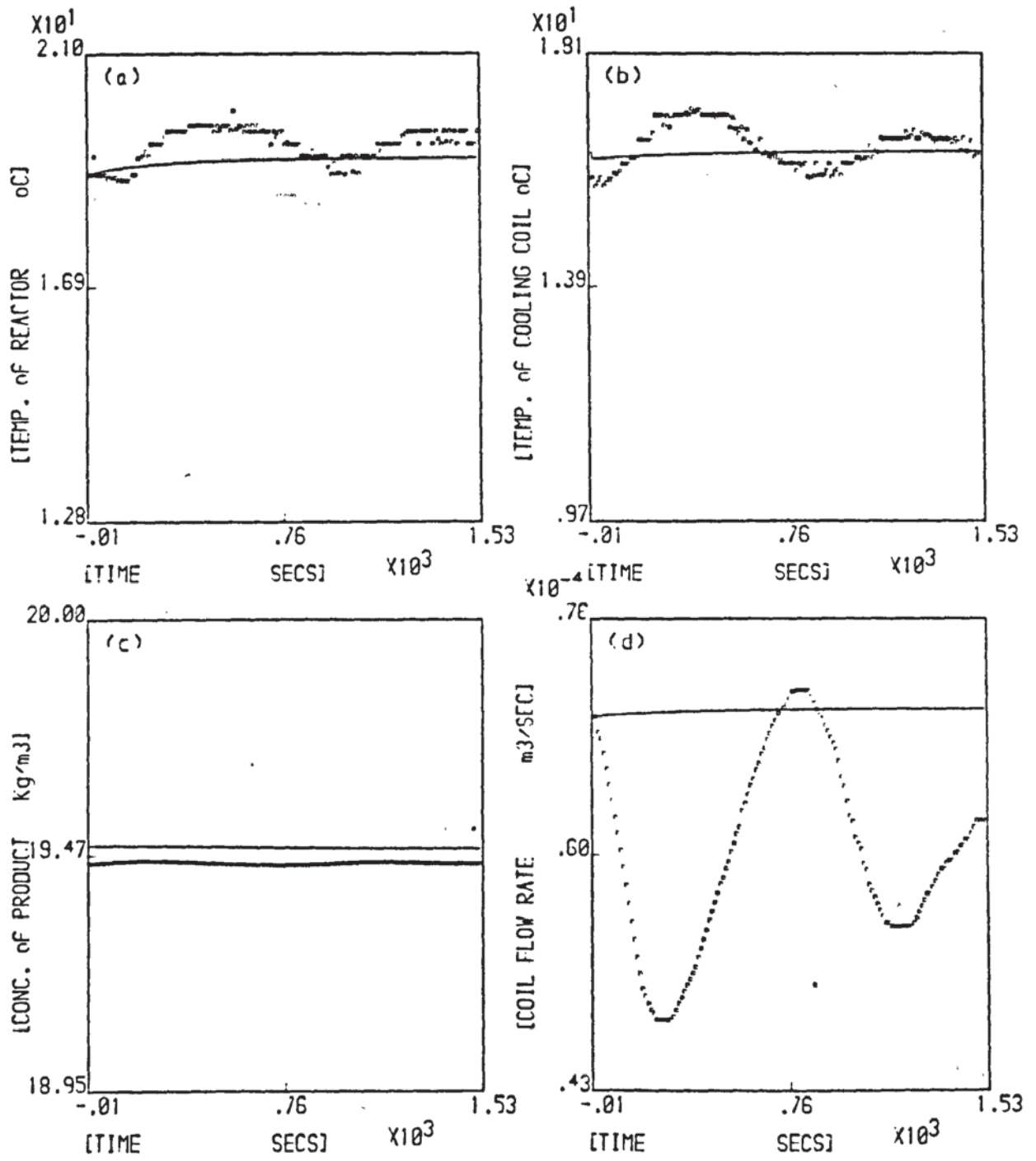


Fig. A.G.2.14 Reactor One. Experiment no: 14

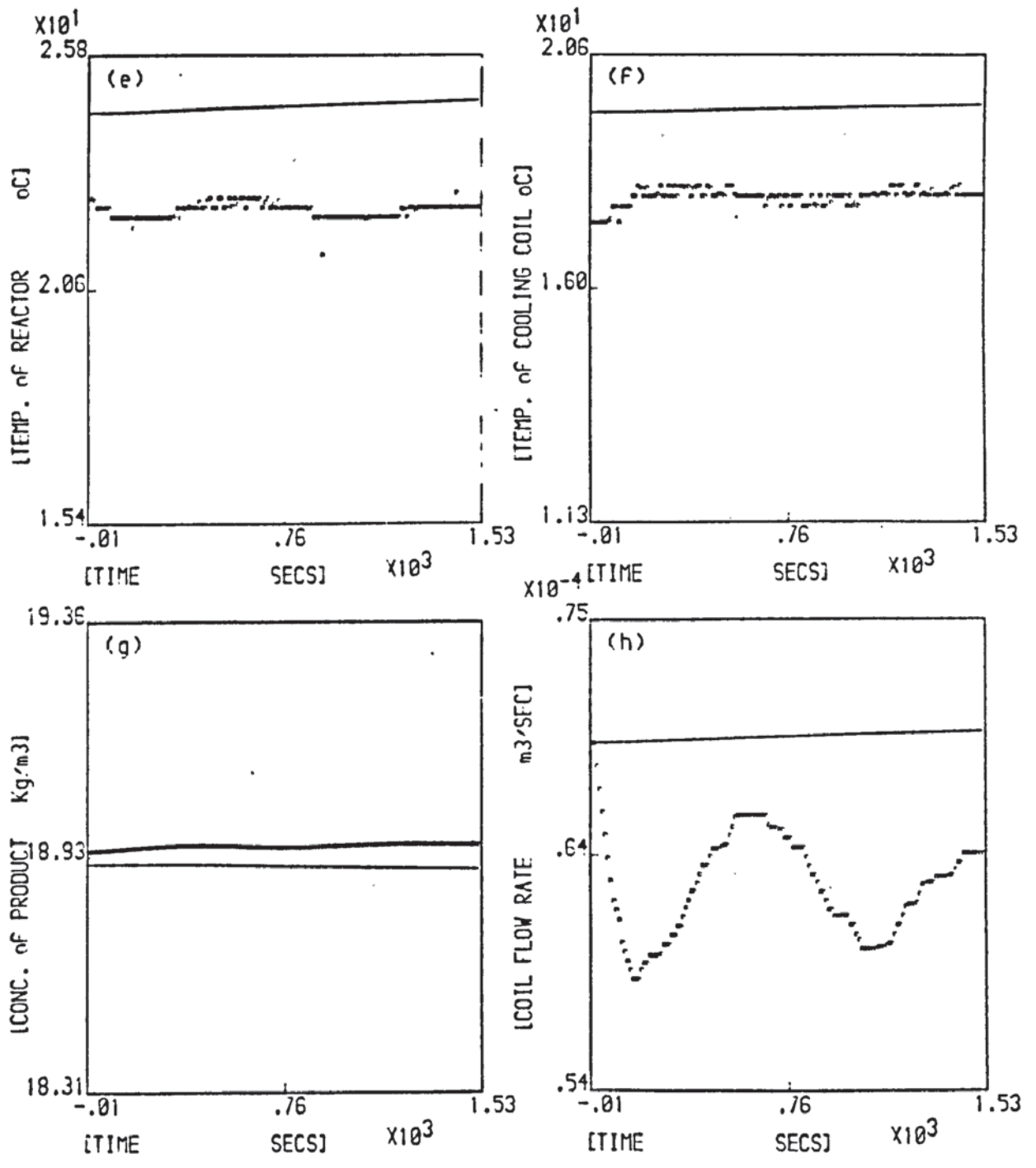


Fig. A.G.2.14 Reactor Two. Experiment no: j4

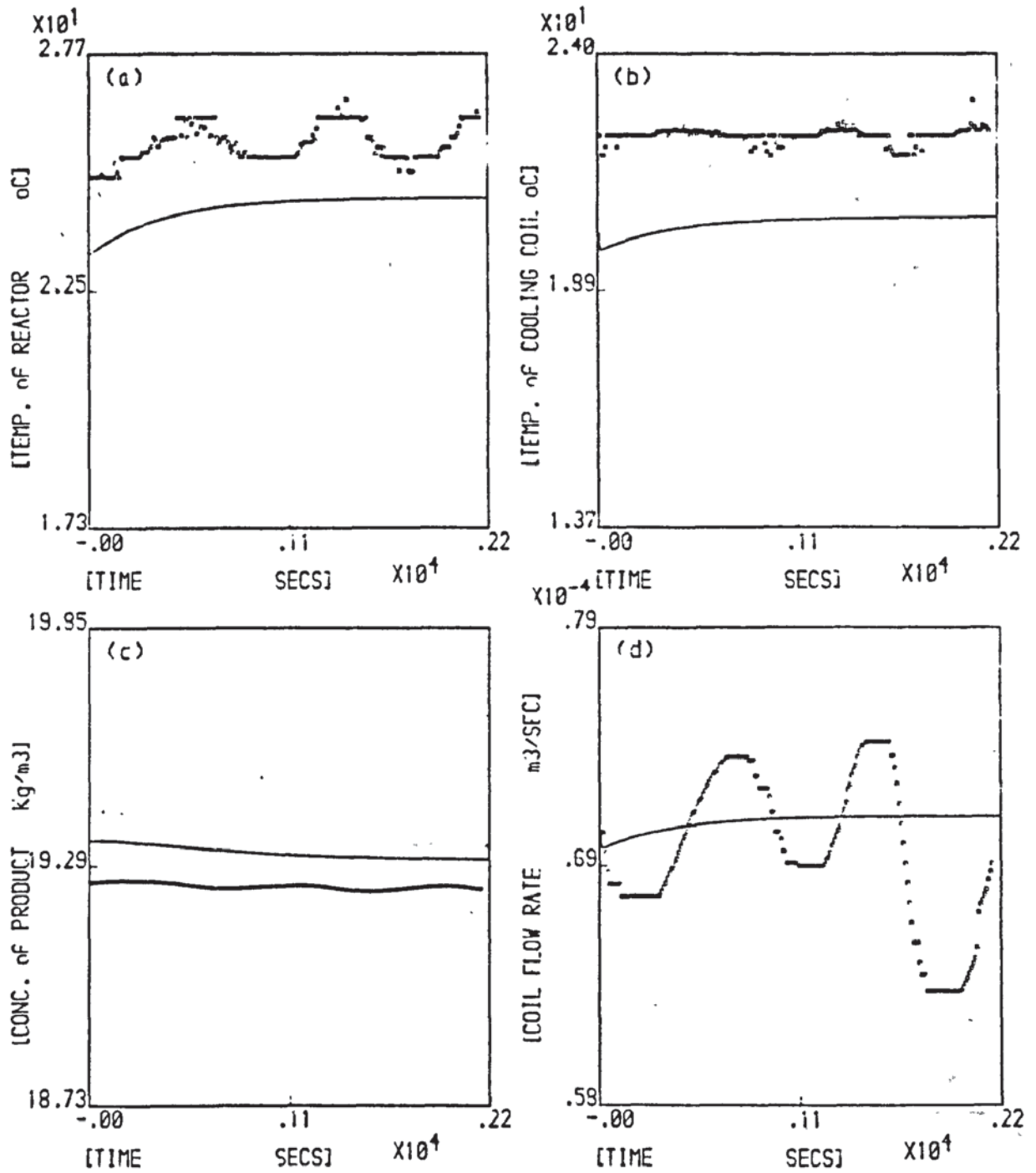


Fig. A.G.2.15 Reactor One. Experiment no: 15

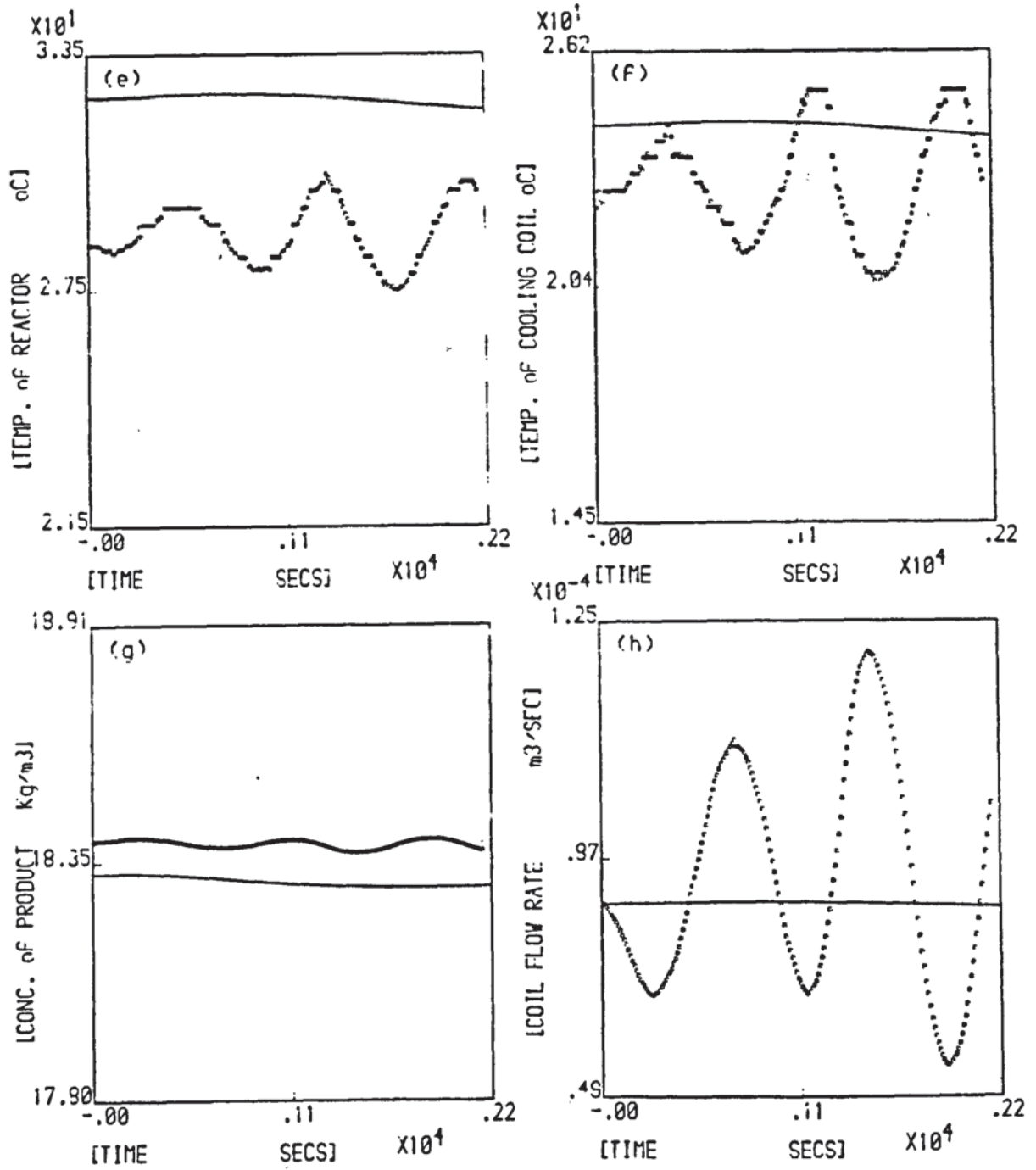


Fig. A.6.2.15 Reactor Two. Experiment no: 15

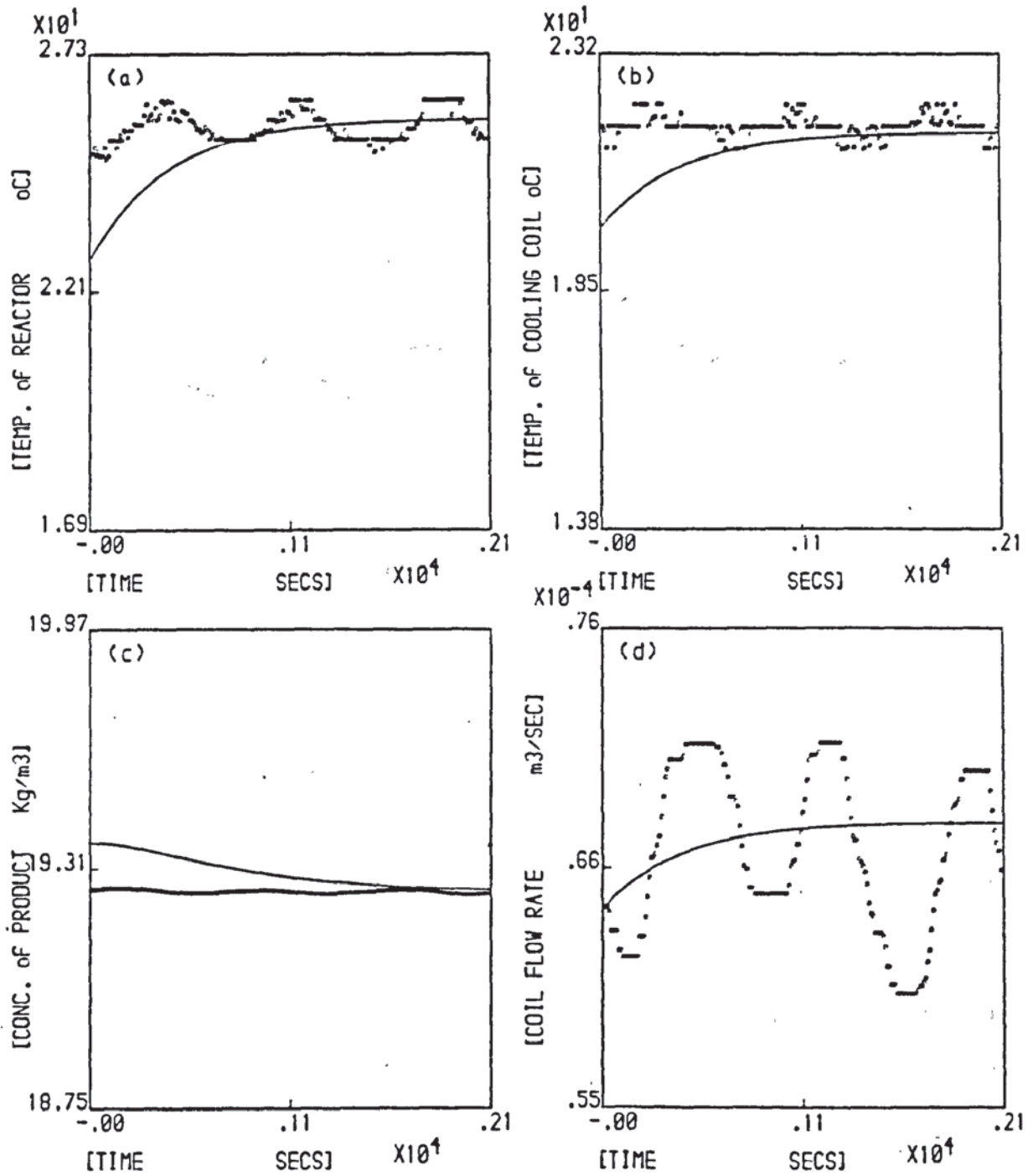


Fig. A.6.2.16 Reactor One. Experiment no: 16

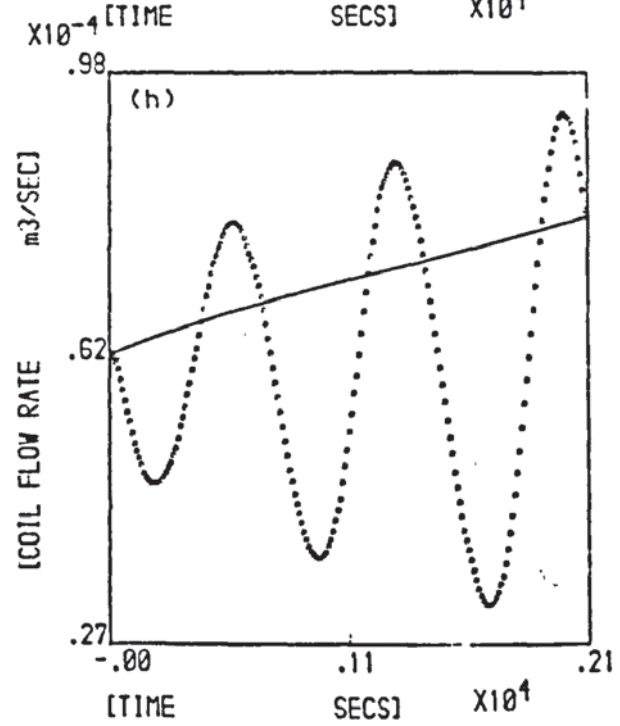
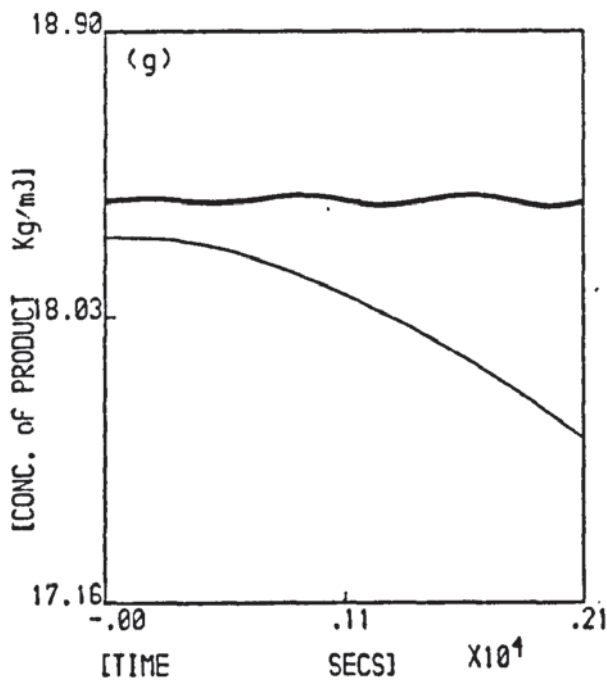
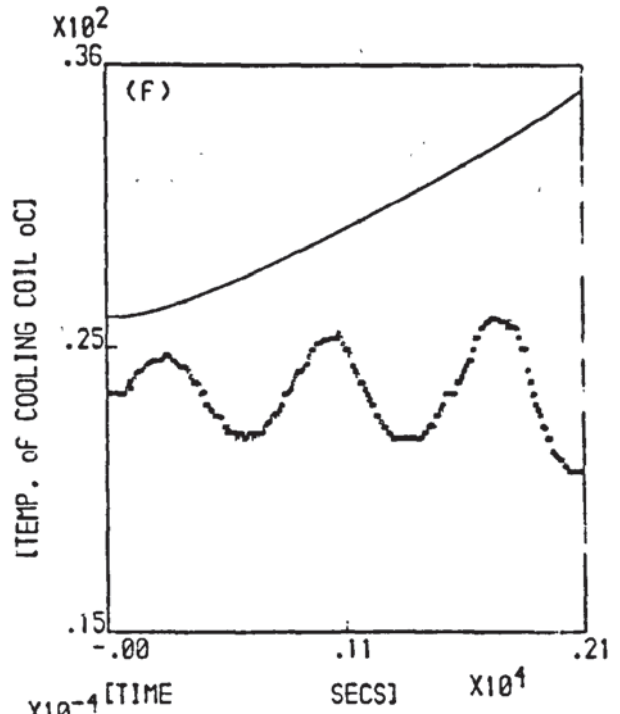
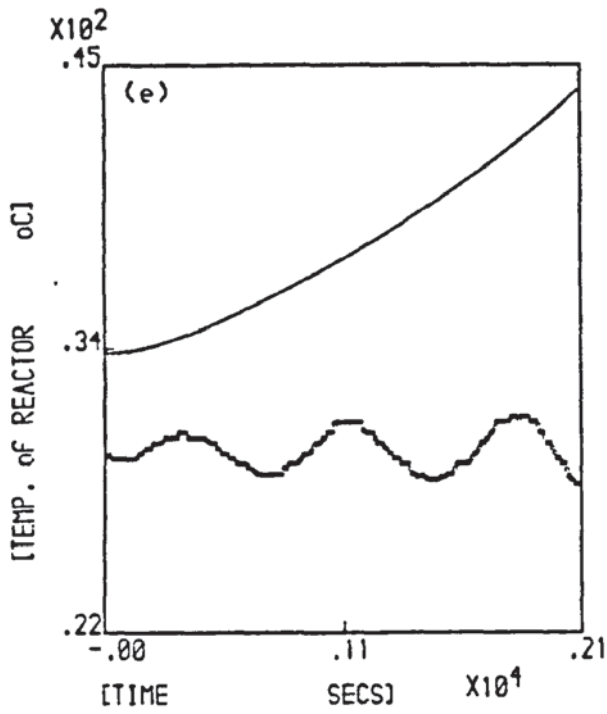


Fig. A.6.2.16 Reactor Two. Experiment no:16

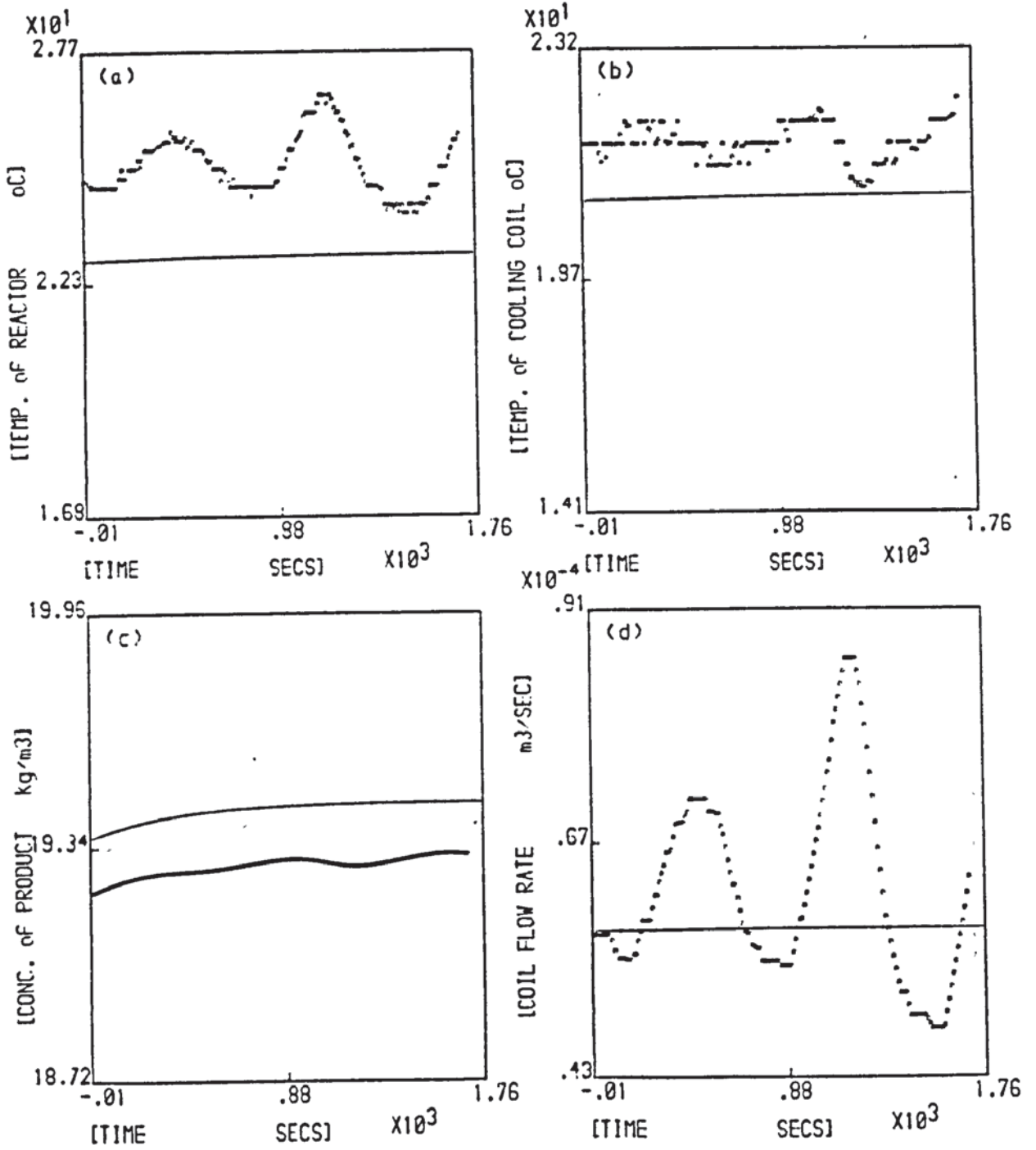


Fig. A.6.2.17 Reactor One. Experiment no: i7

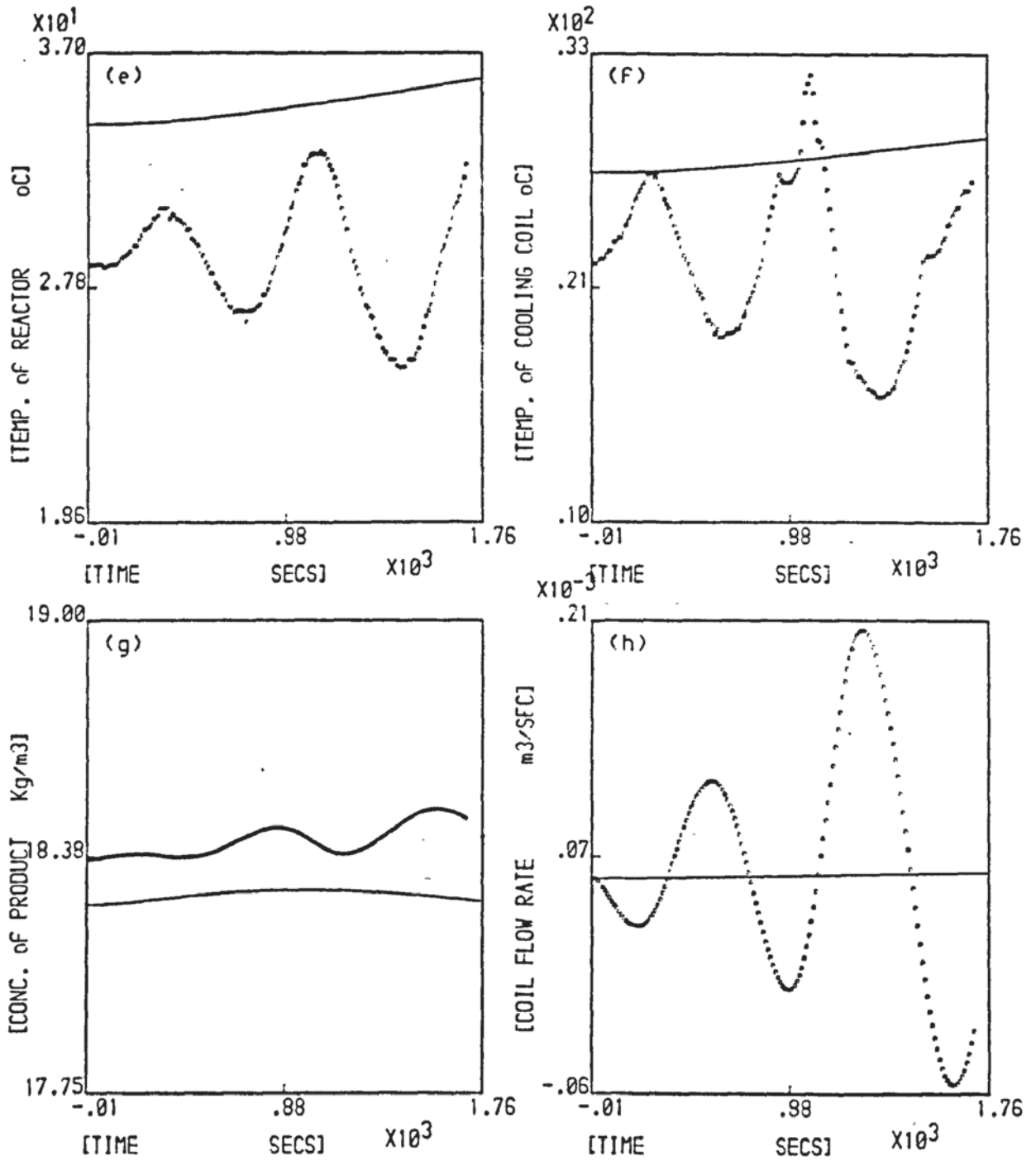
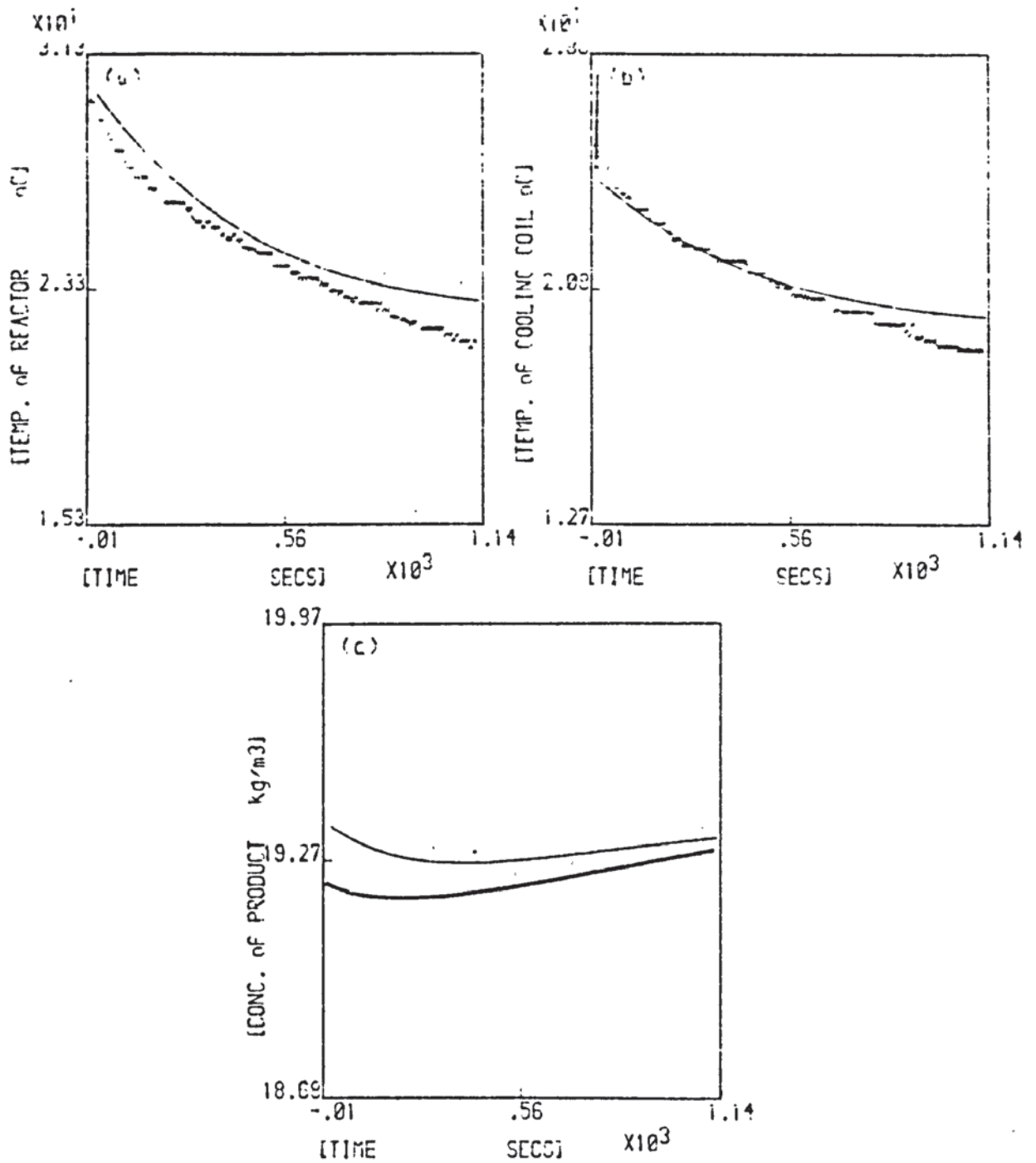


Fig. A.6.2.17 Reactor Two. Experiment no: 17



F.g A.G.2.18 Reactor One. Experiment no. 19

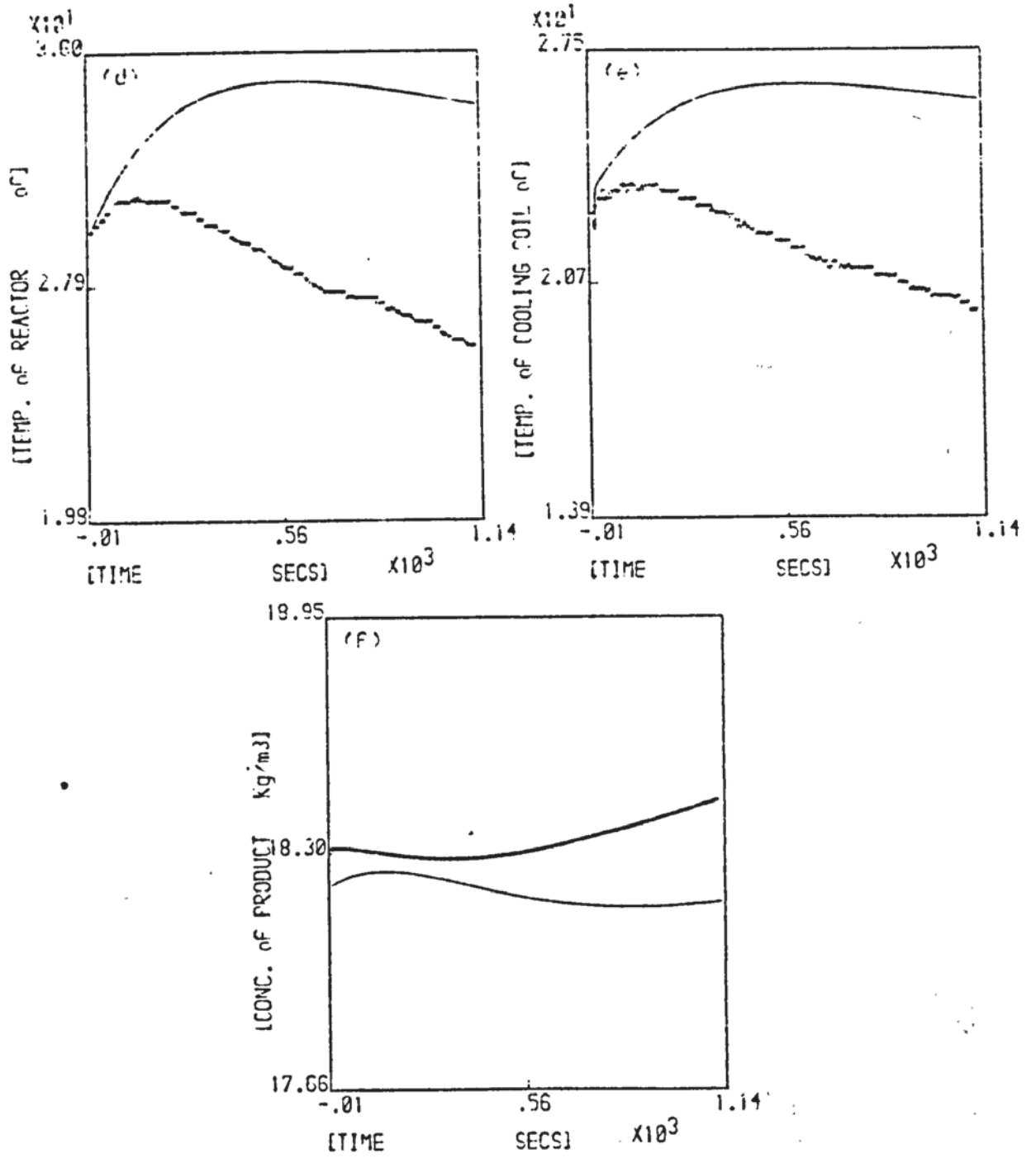


Fig A.G.2.18 Reactor Two. Experiment no: 18

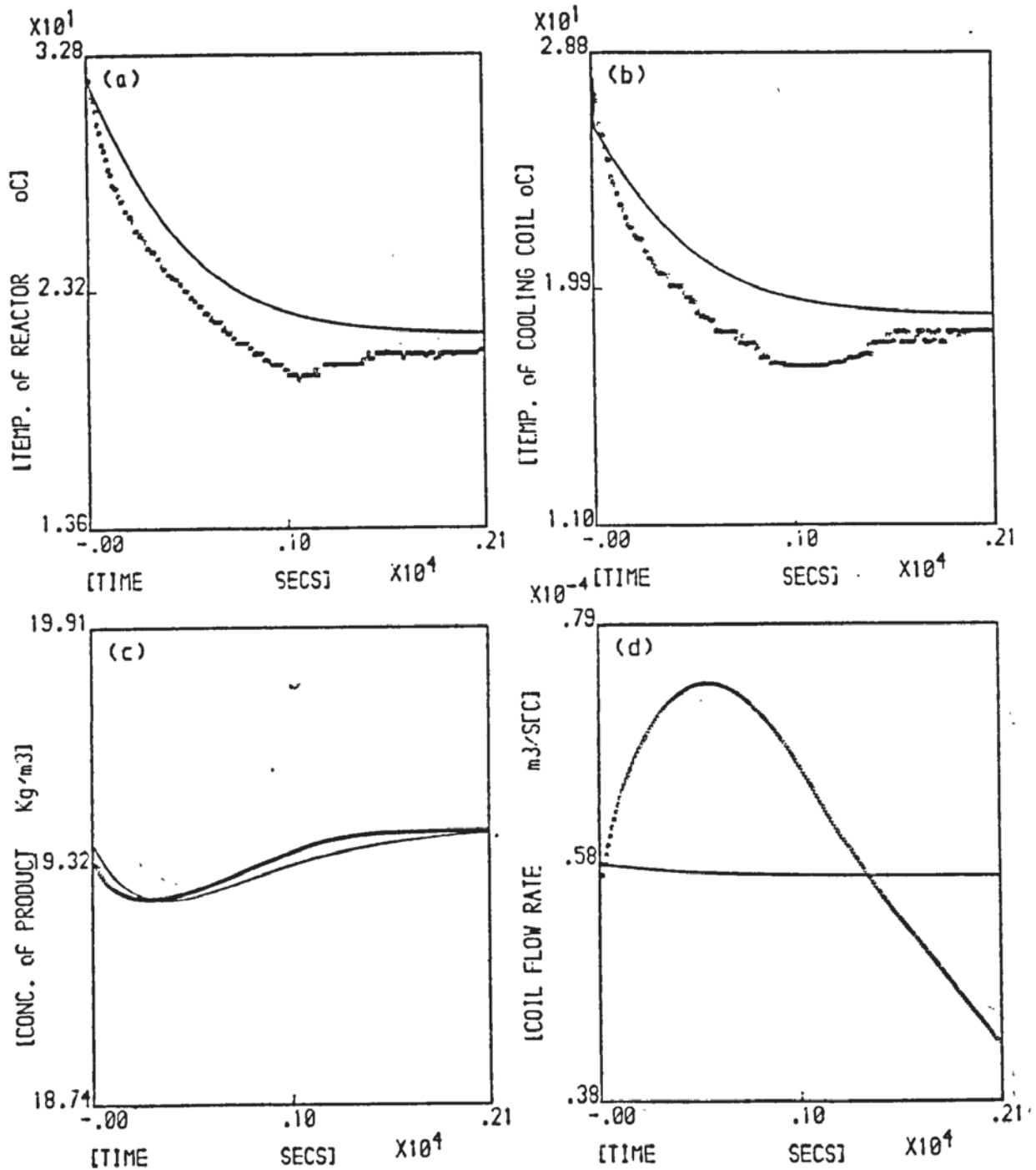


Fig. 1.6.2.19 Reactor One. Experiment no: 19

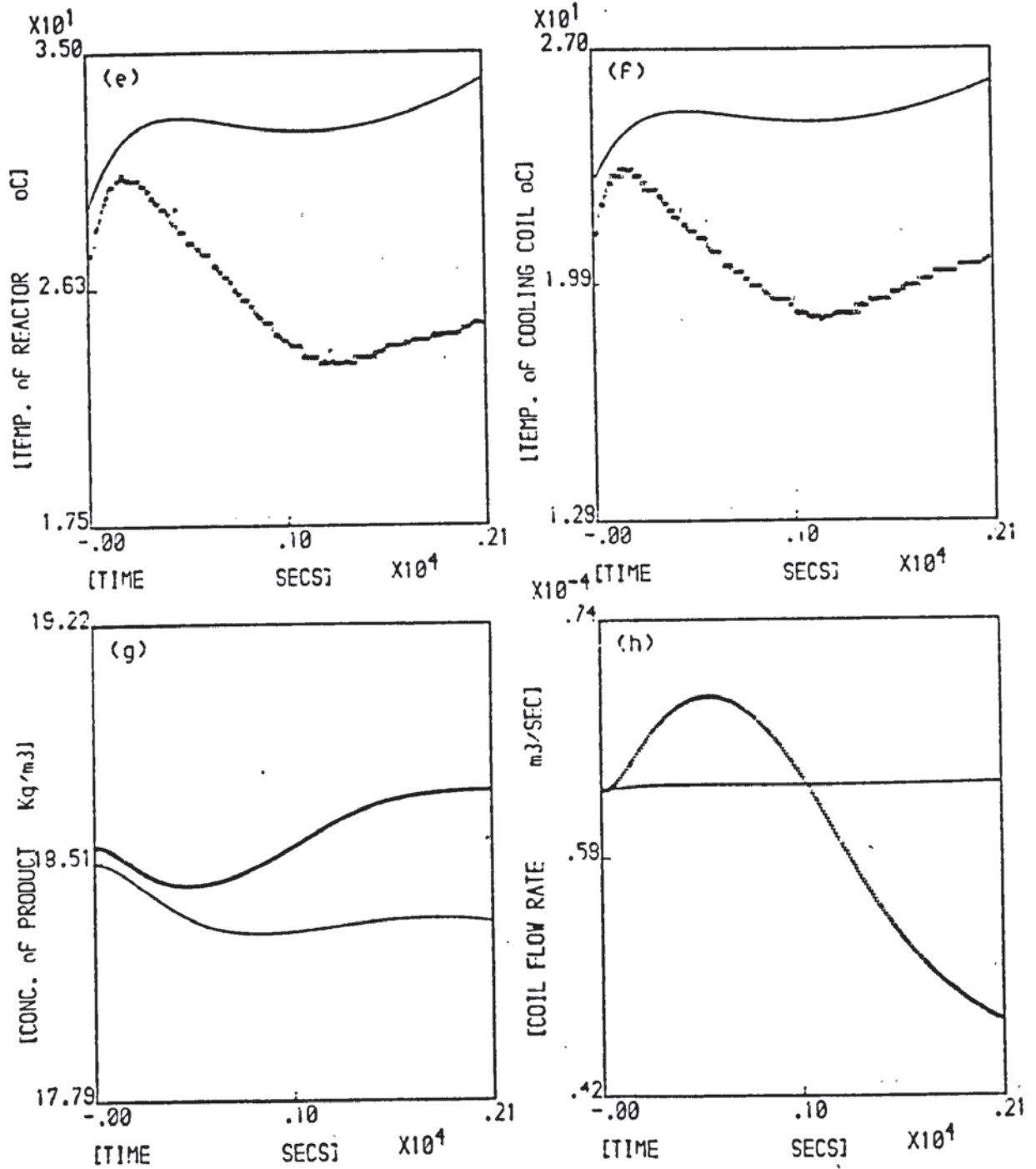


Fig. A.6.2.19 Reactor Two. Experiment no: 19

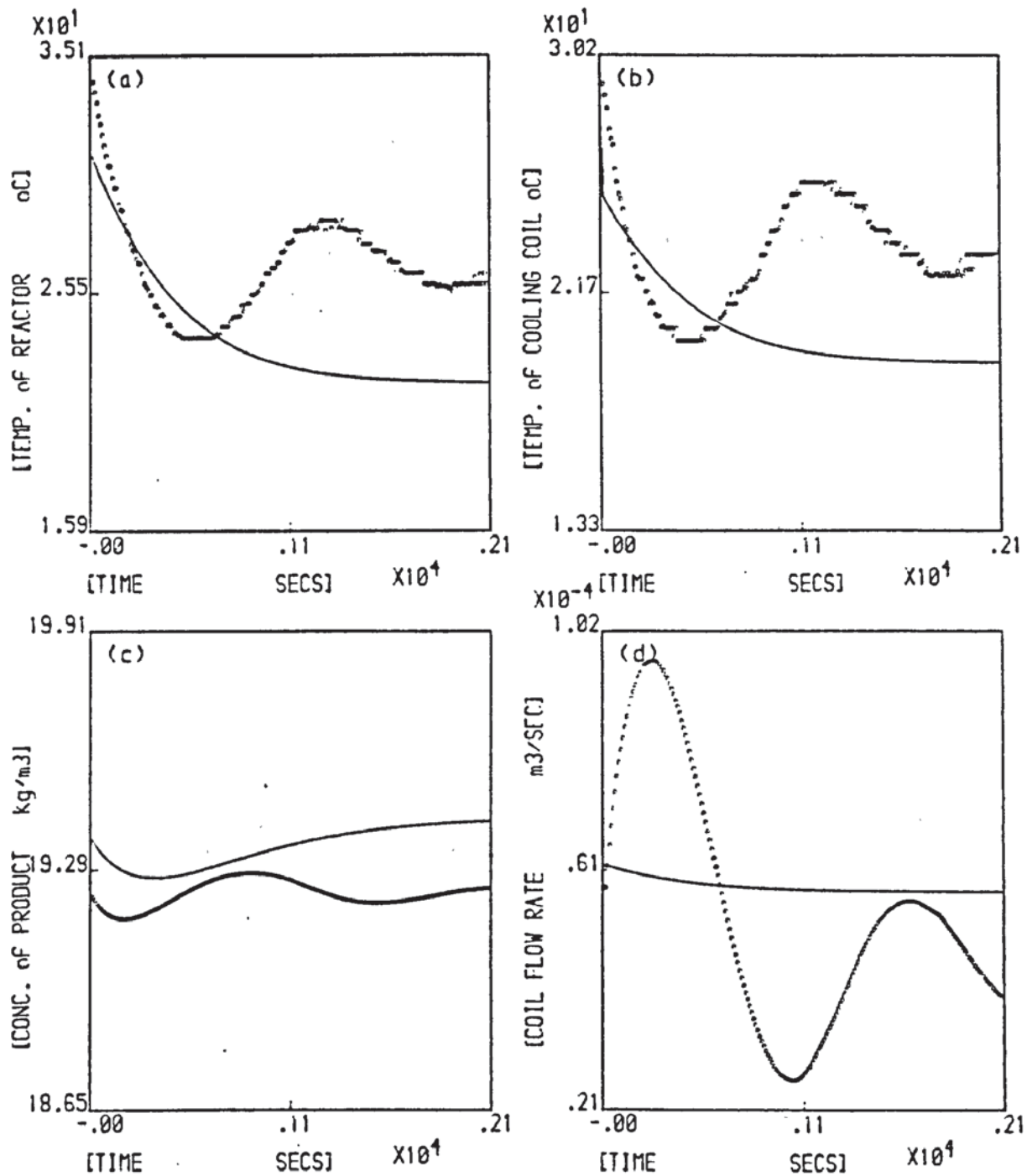


Fig. 1.6.2.20 Reactor One. Experiment no: 20

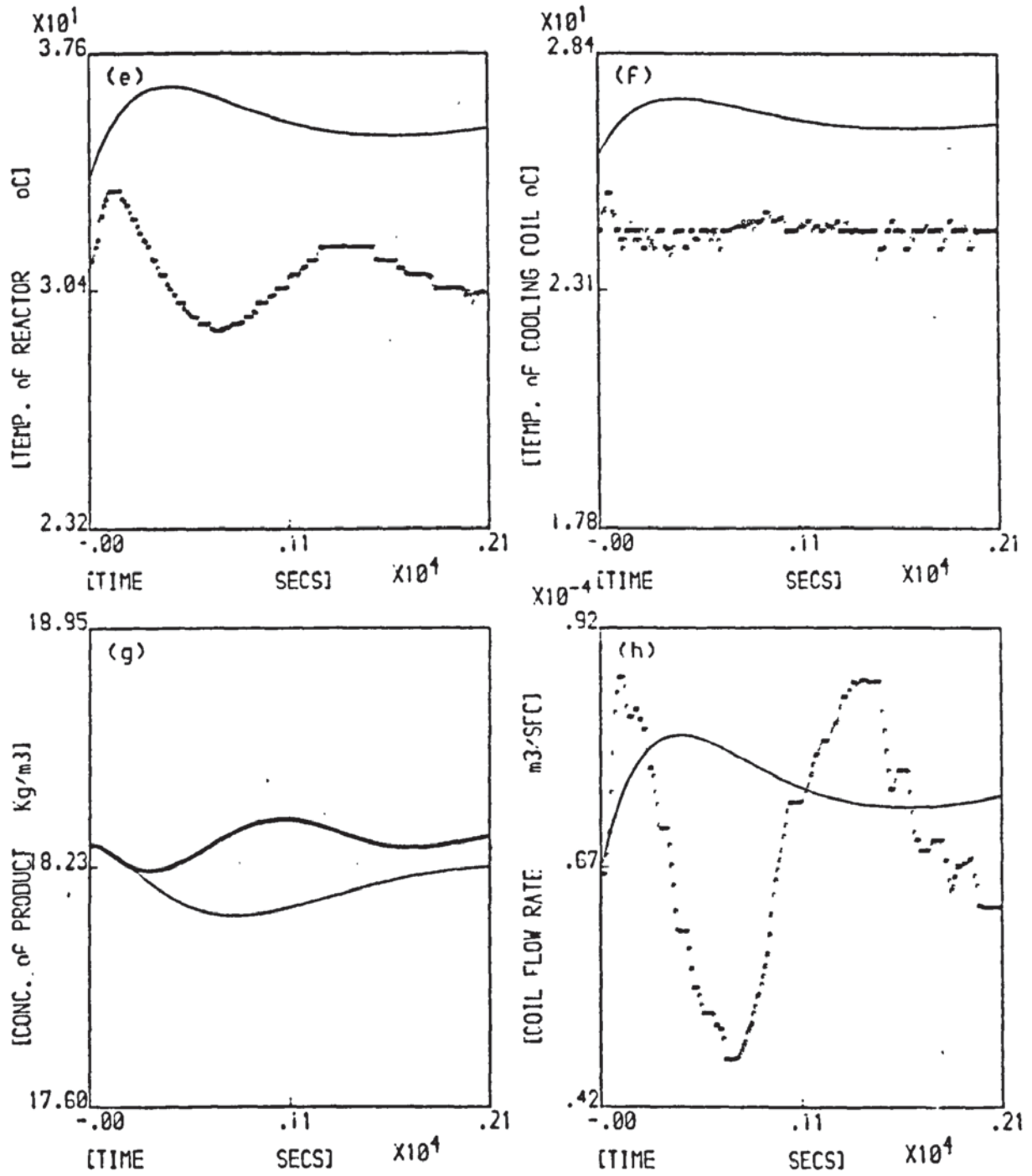


Fig. A.6.2.20 Reactor Two. Experiment no:-20

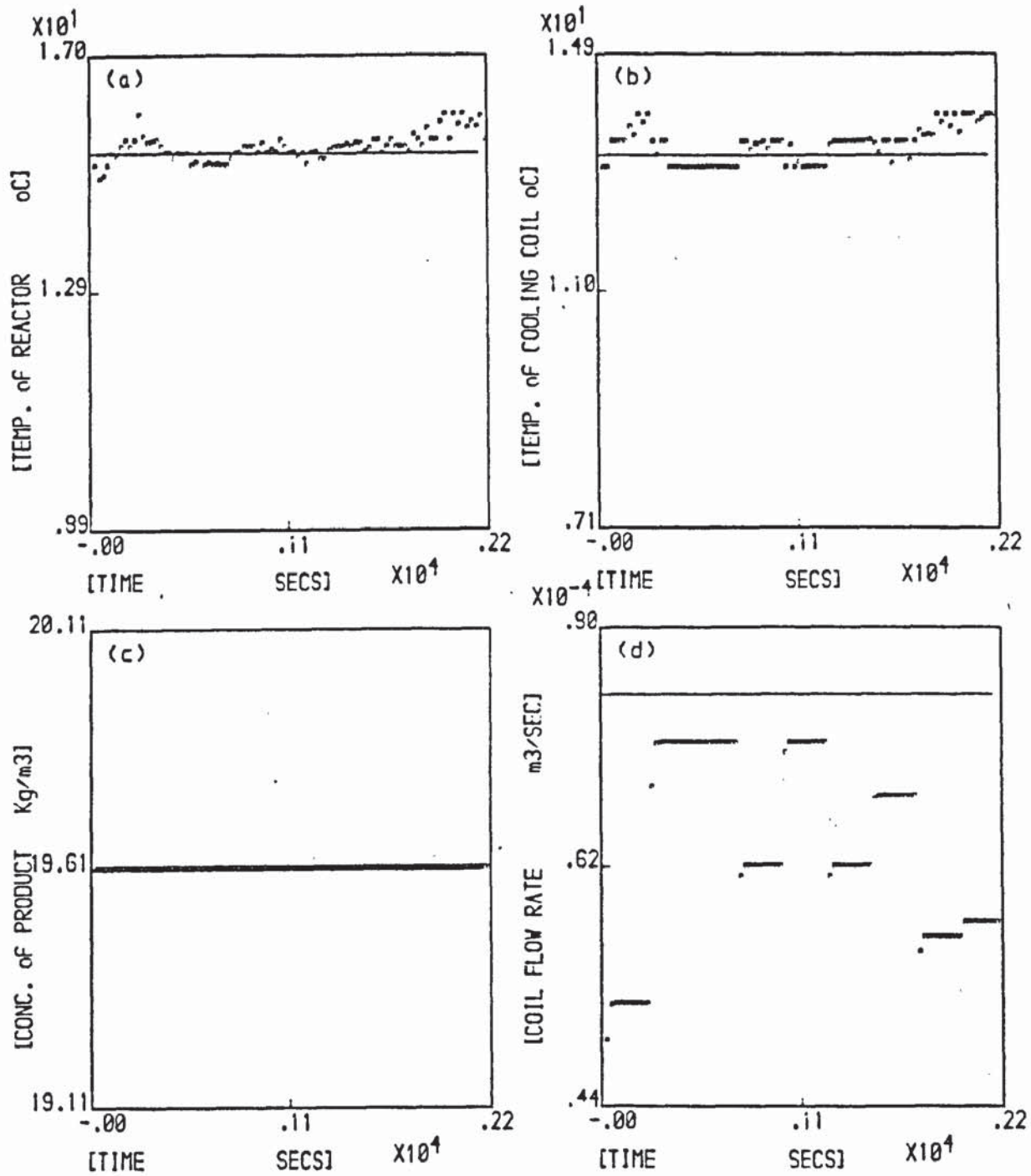


Fig. A.6.2.21 Reactor One. Experiment no:28

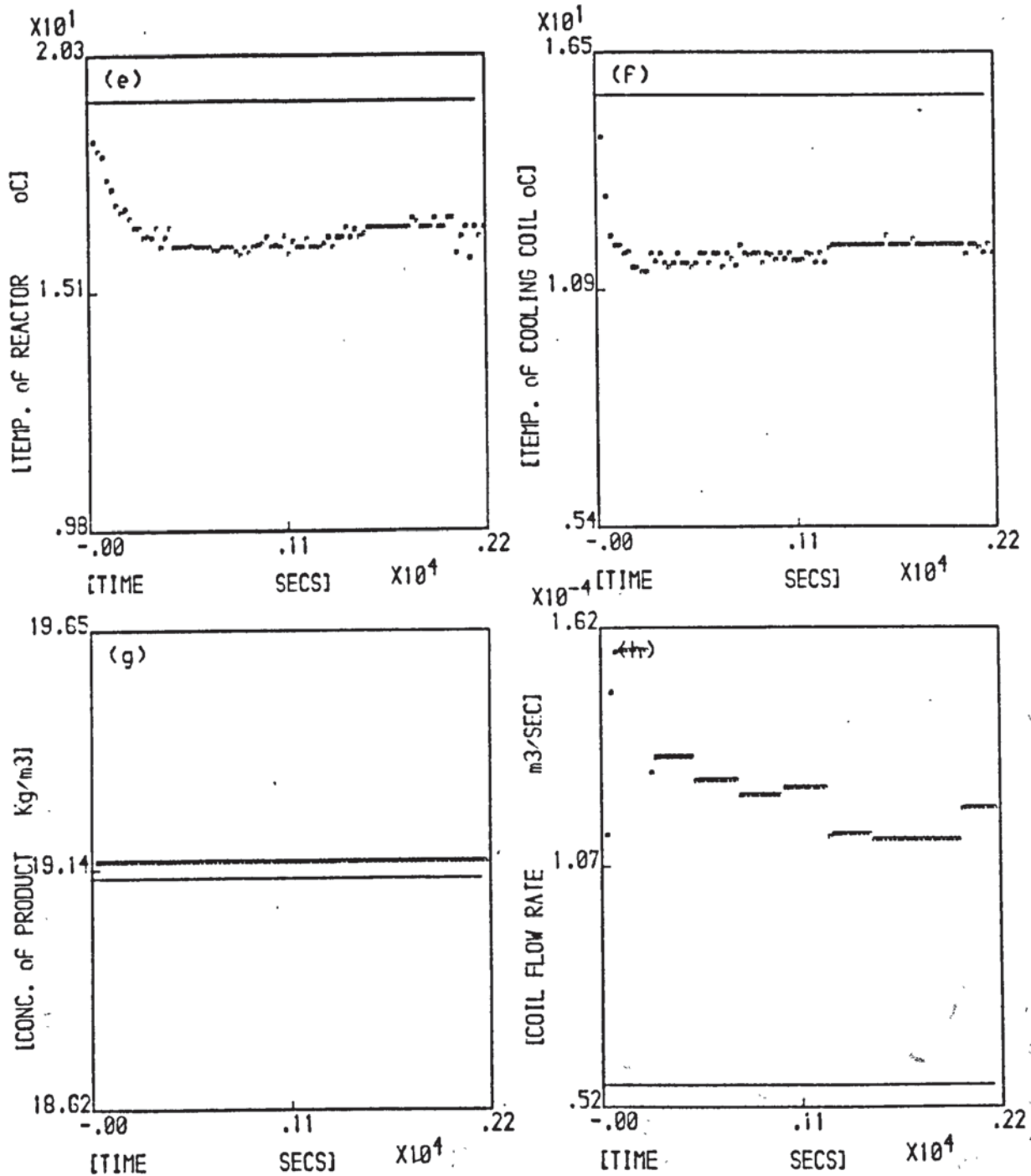


Fig. A.6.2.21 Reactor two. Experiment no:28.

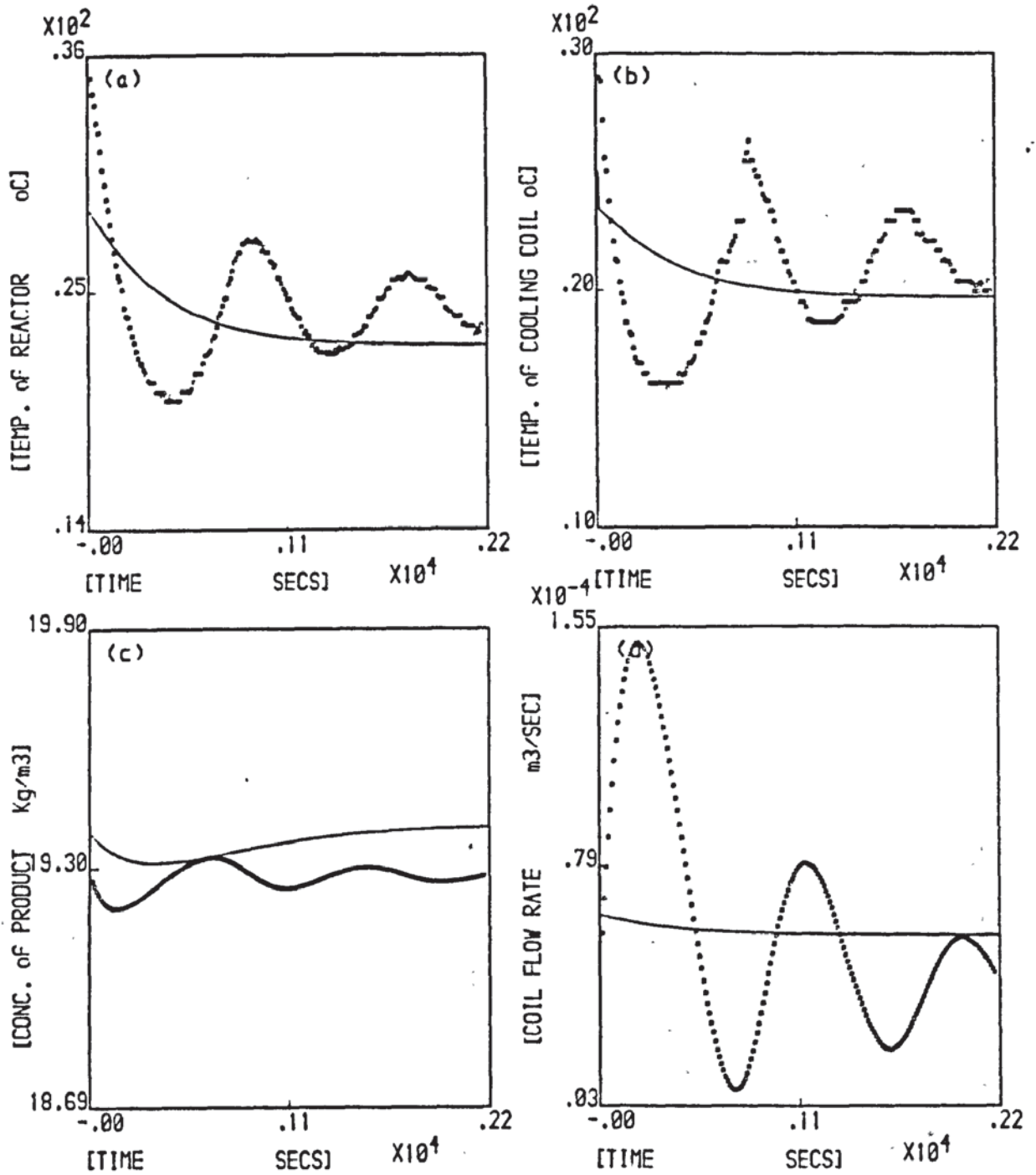


Fig. A.6.2.22 Reactor One. Experiment no:21

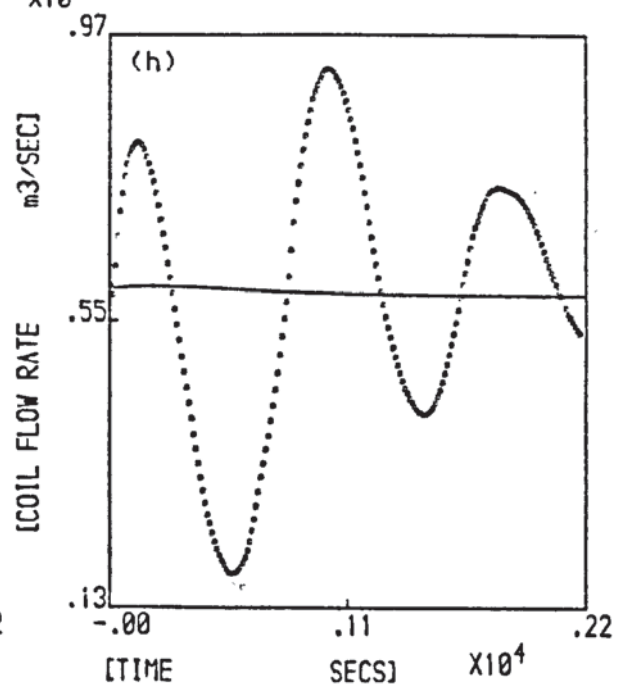
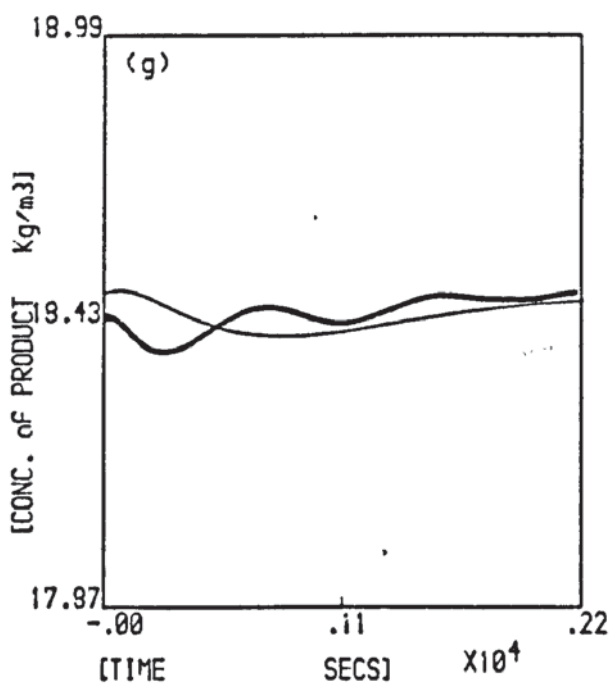
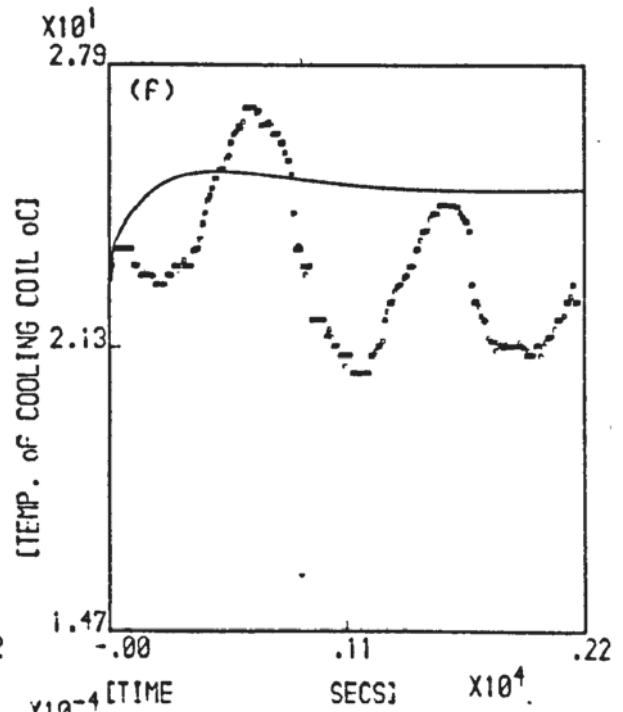
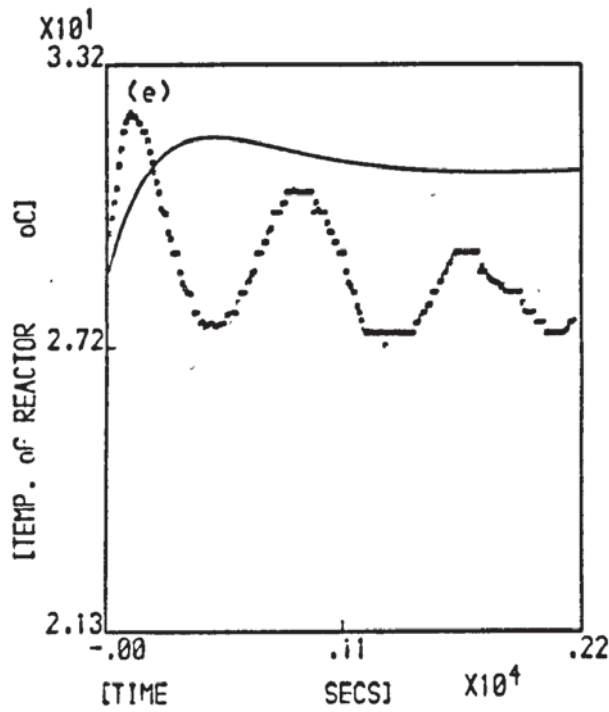


Fig. A.6.2.22 Reactor Two. Experiment no:21

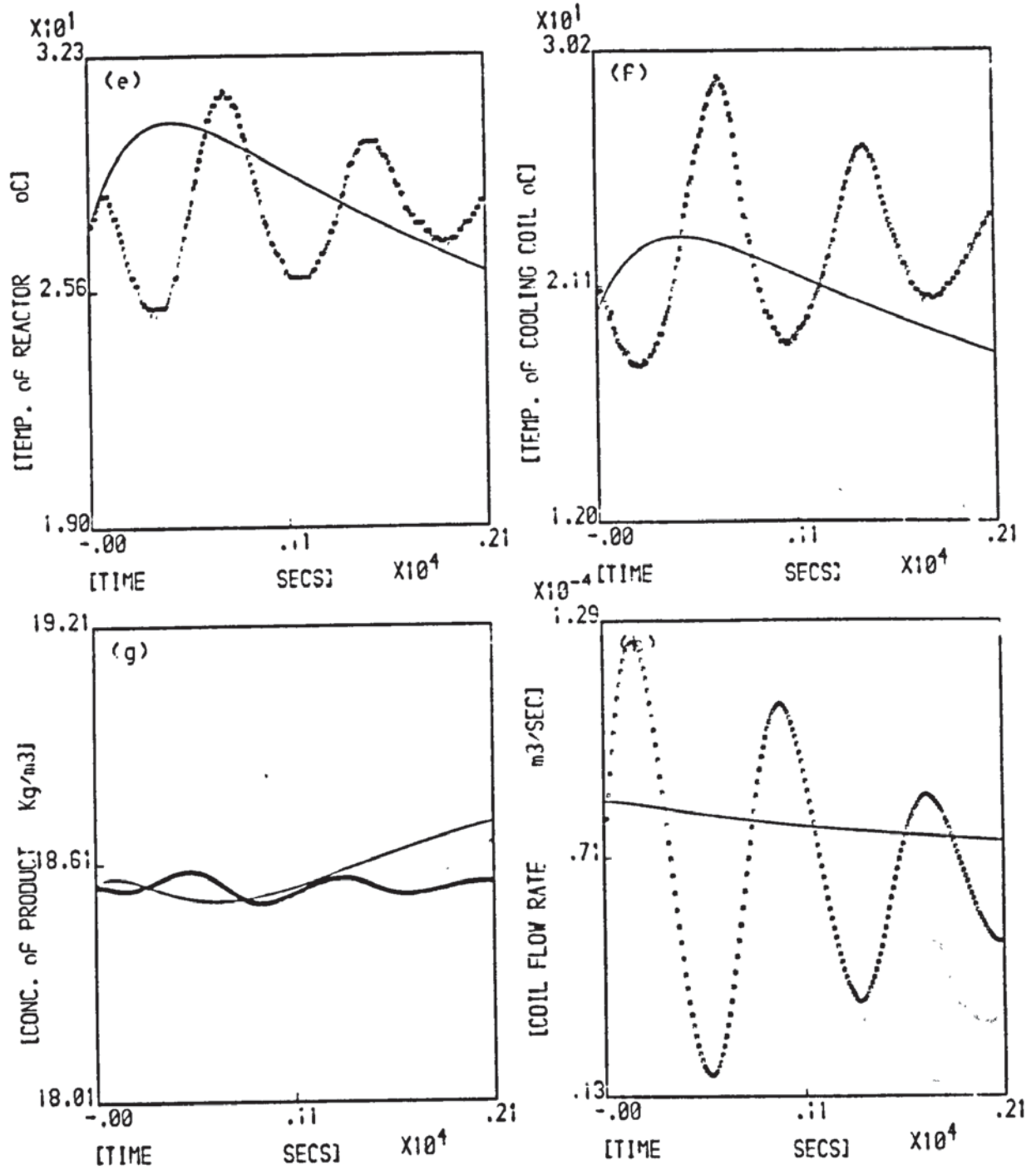


Fig. A.6.2.23 Reactor Two. Experiment no:22

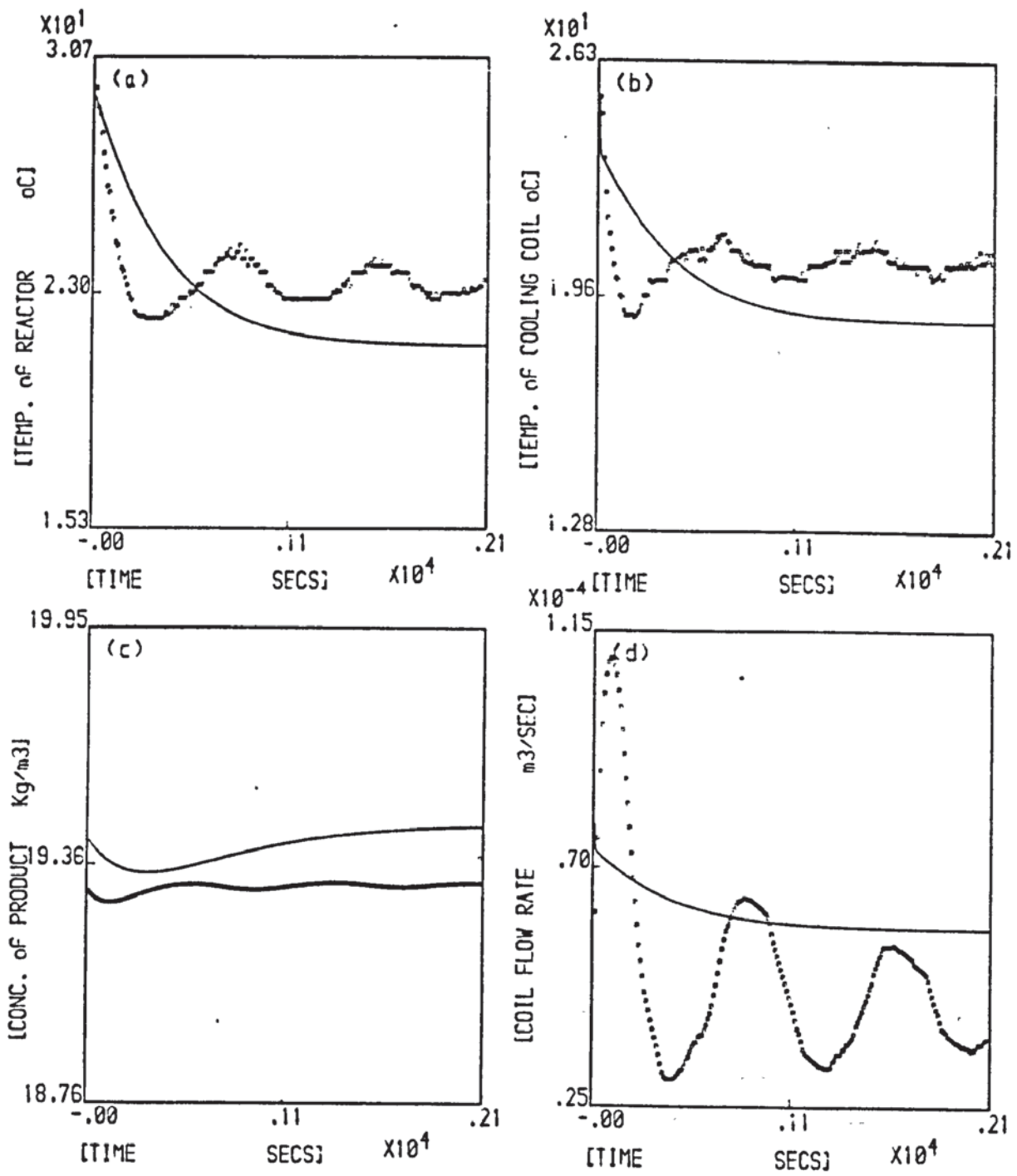


Fig. 1.6.2.23 Reactor One. Experiment no:22

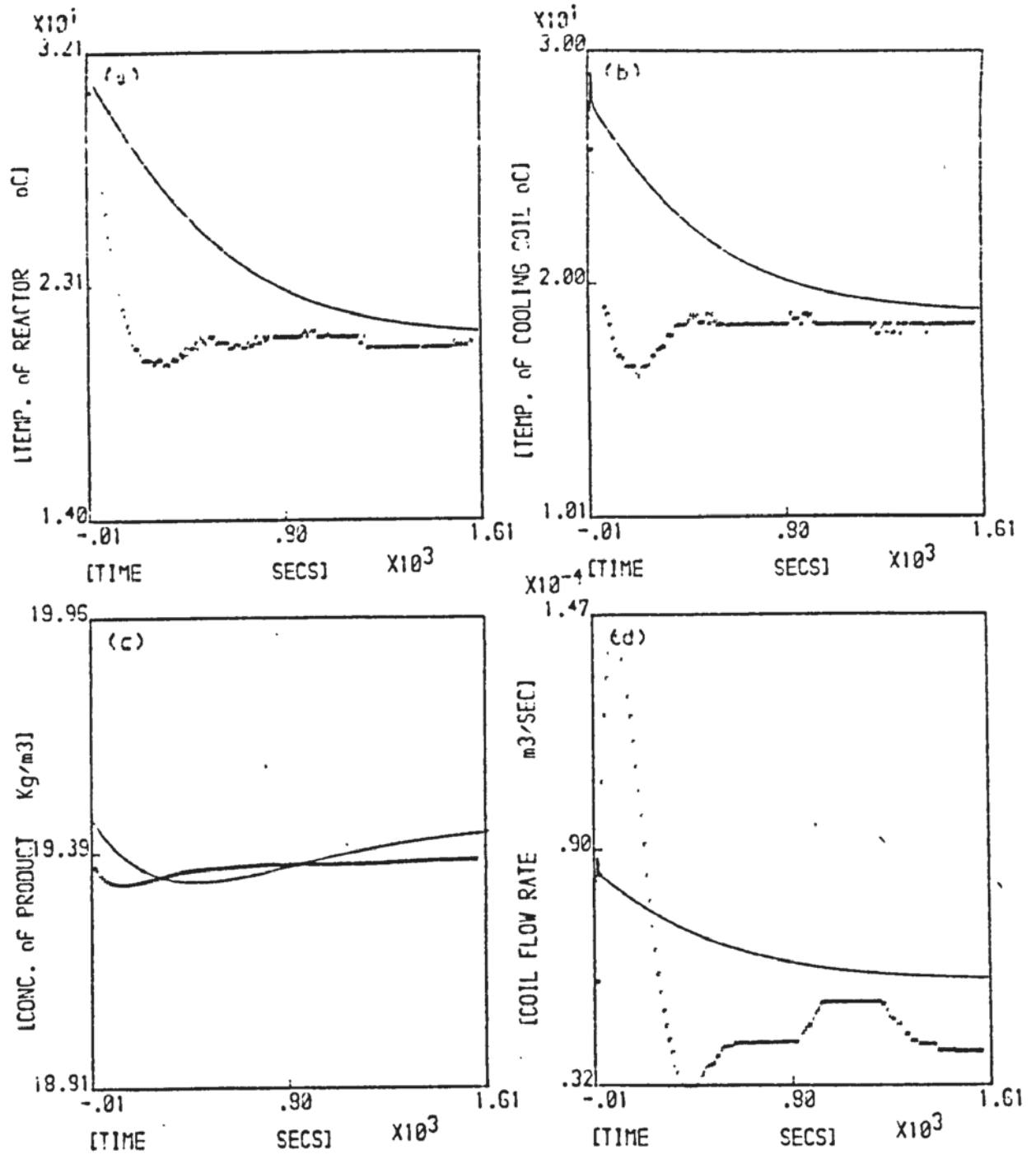


Fig. 4.6.2.24 Reactor One. Experiment no:24

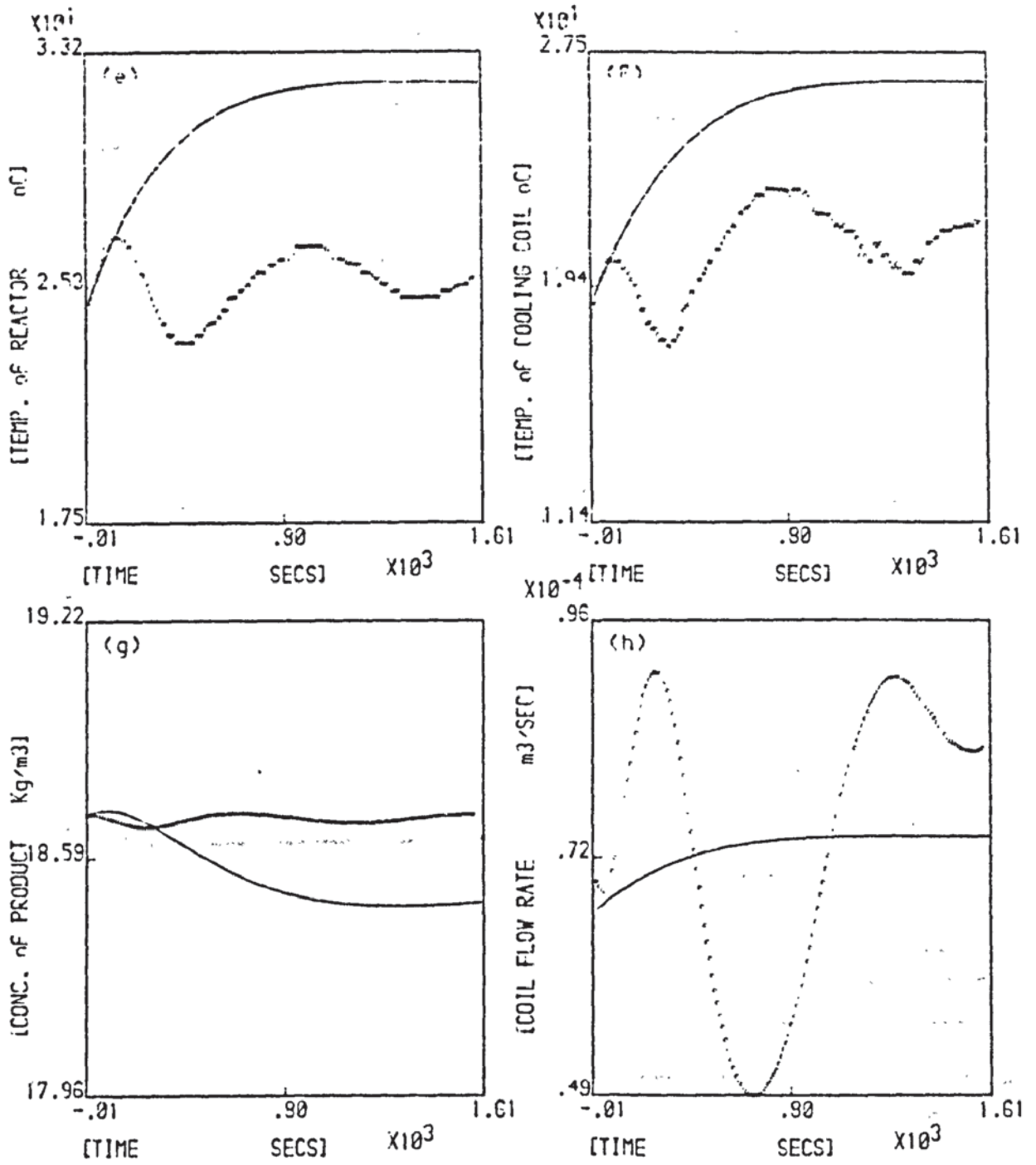


Fig. A.6.2.24 Reactor Two. Experiment no:24

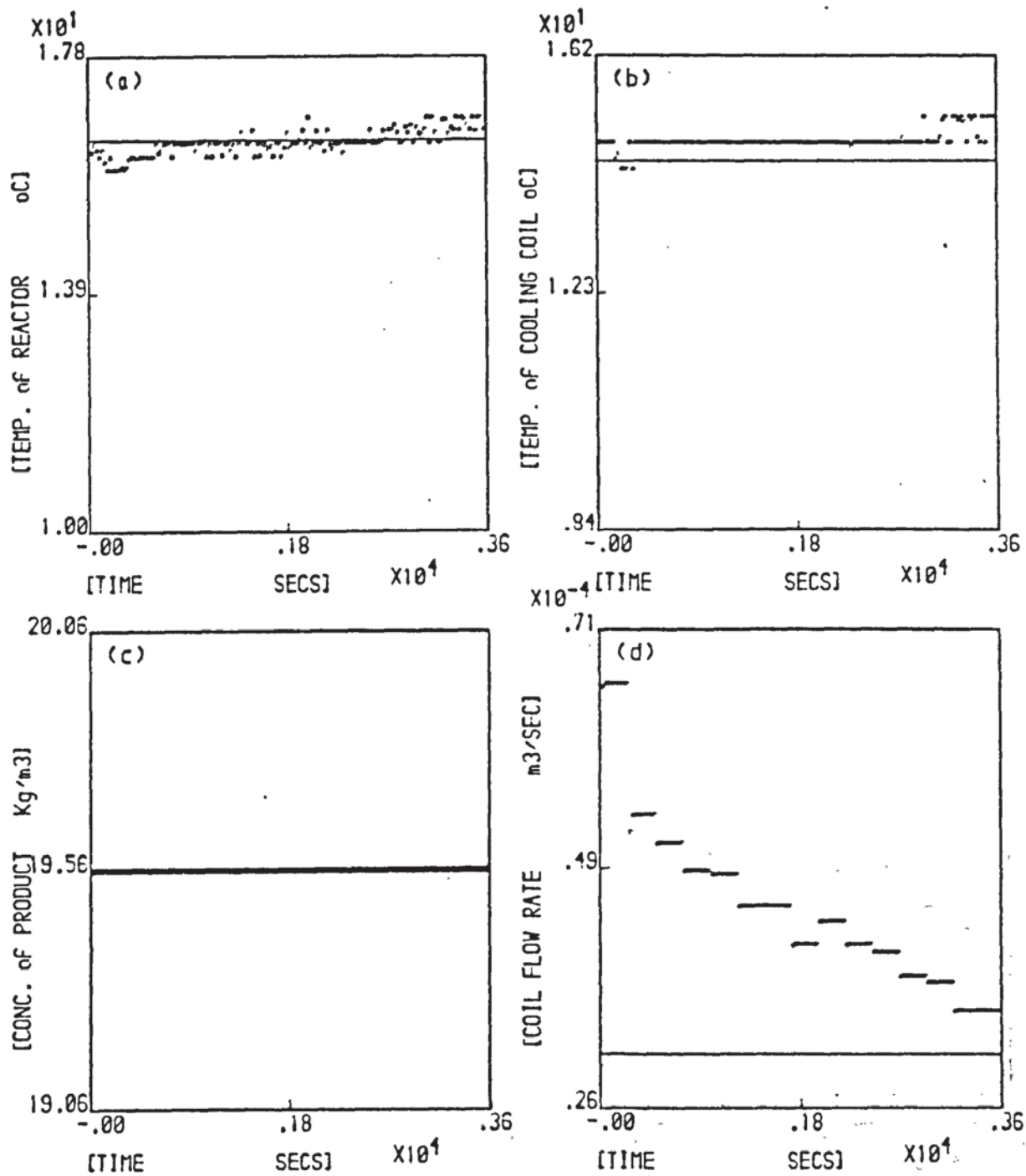


Fig. A.6.2.25 Reactor One. Experiment no:25

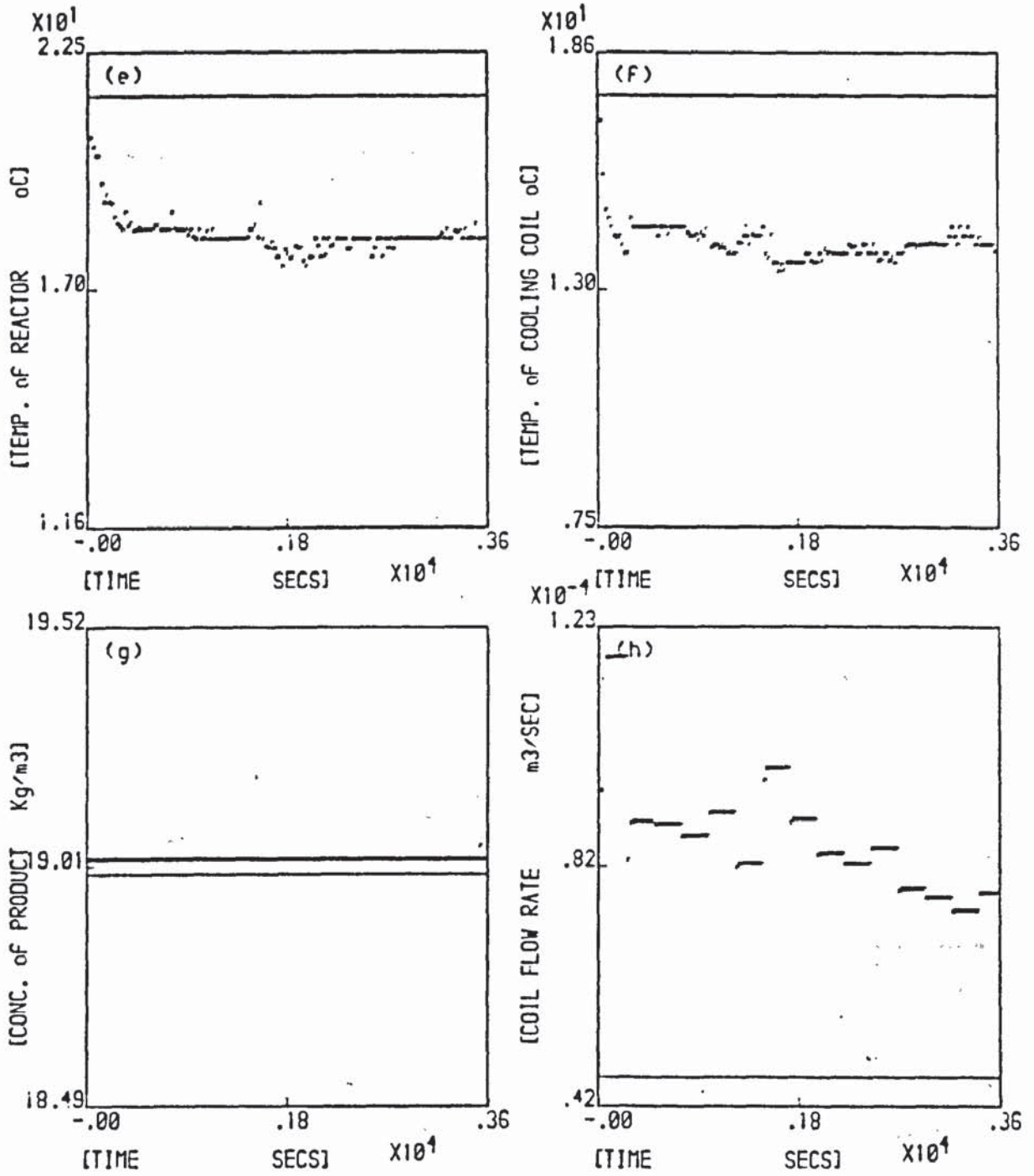


Fig. A.6.2.25 Reactor Two. Experiment no: 25

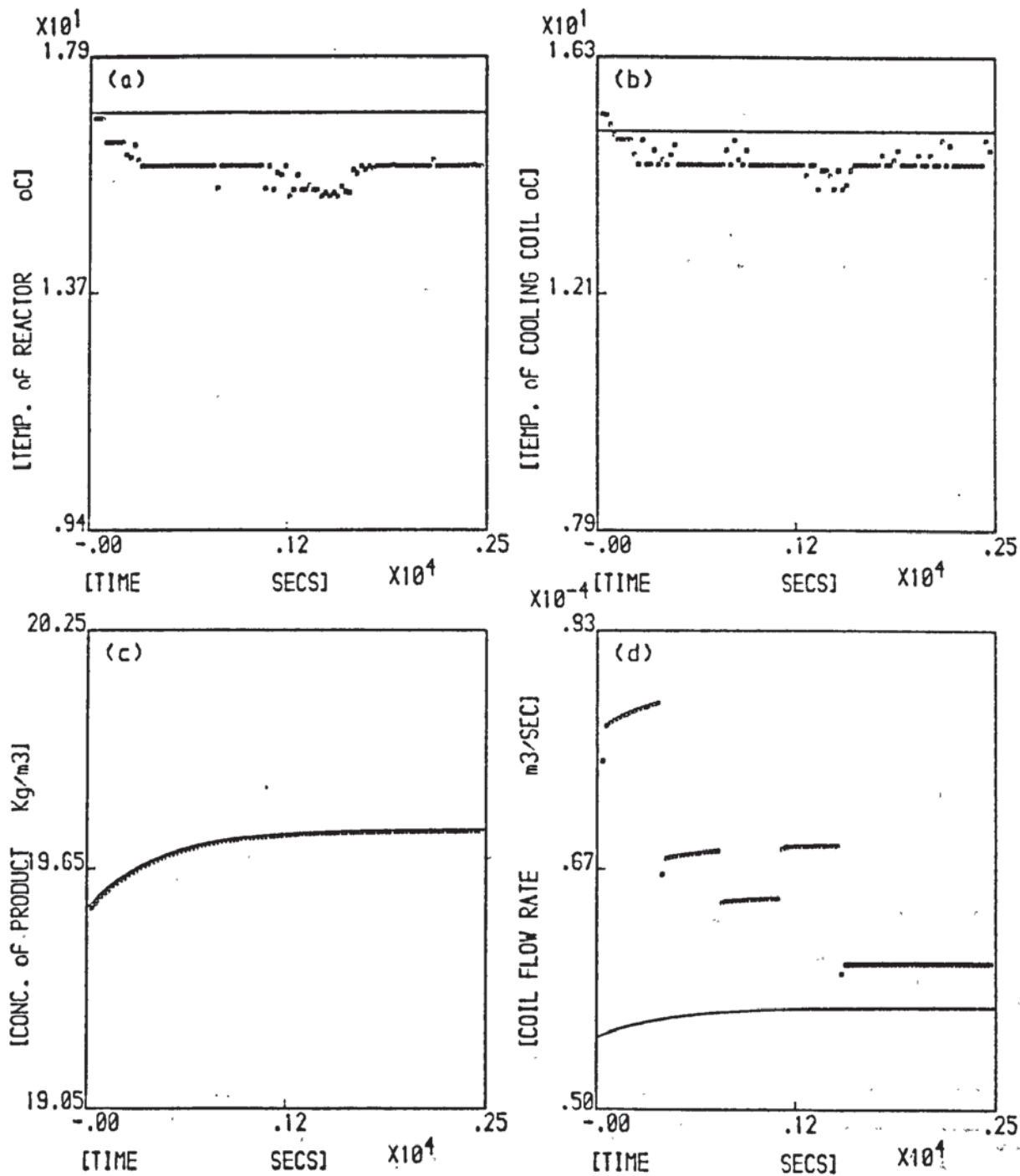


Fig. A.6.2.26 Reactor One. Experiment no:26

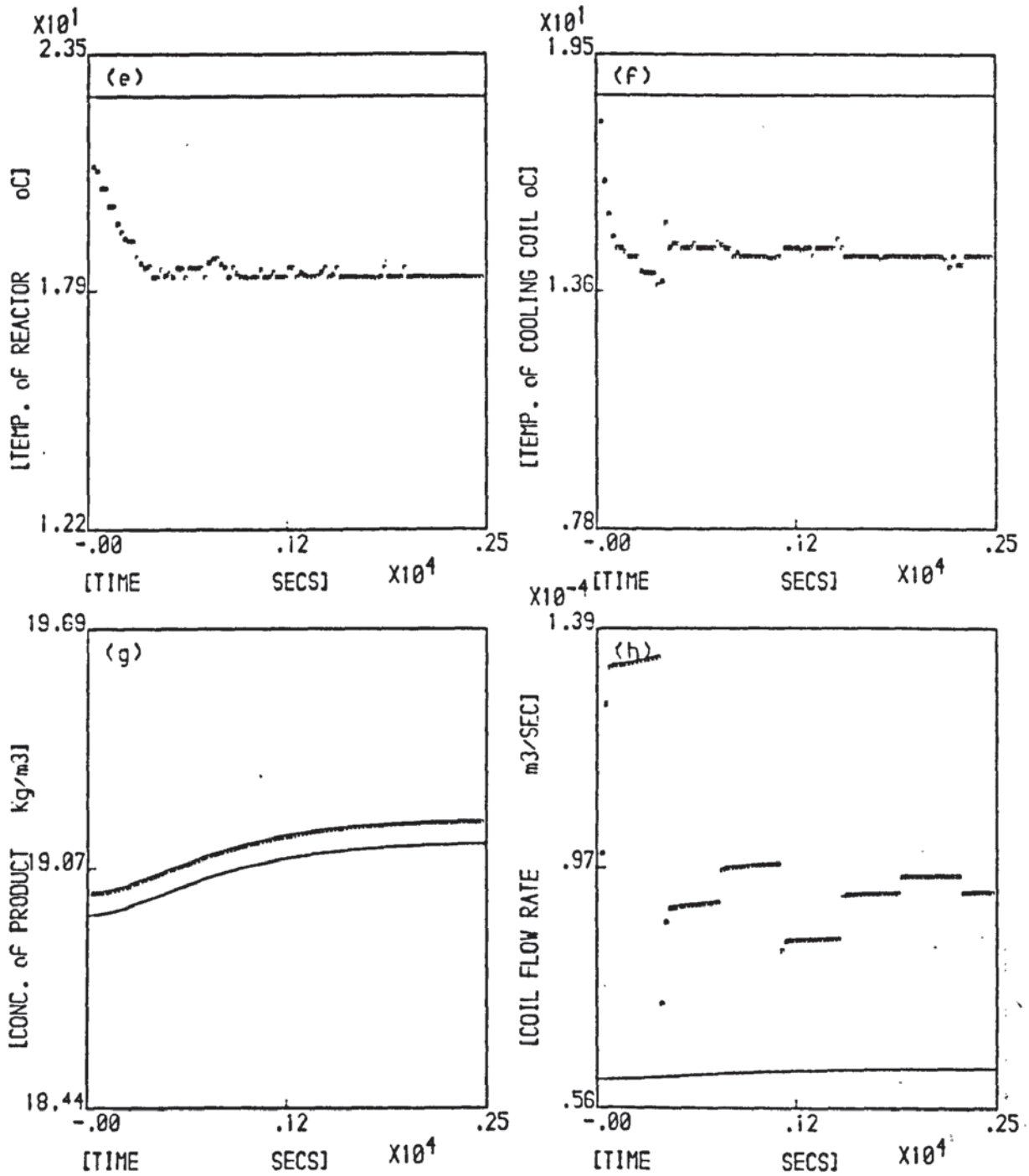


Fig. A.6.2.26 Reactor Two. Experiment no:26

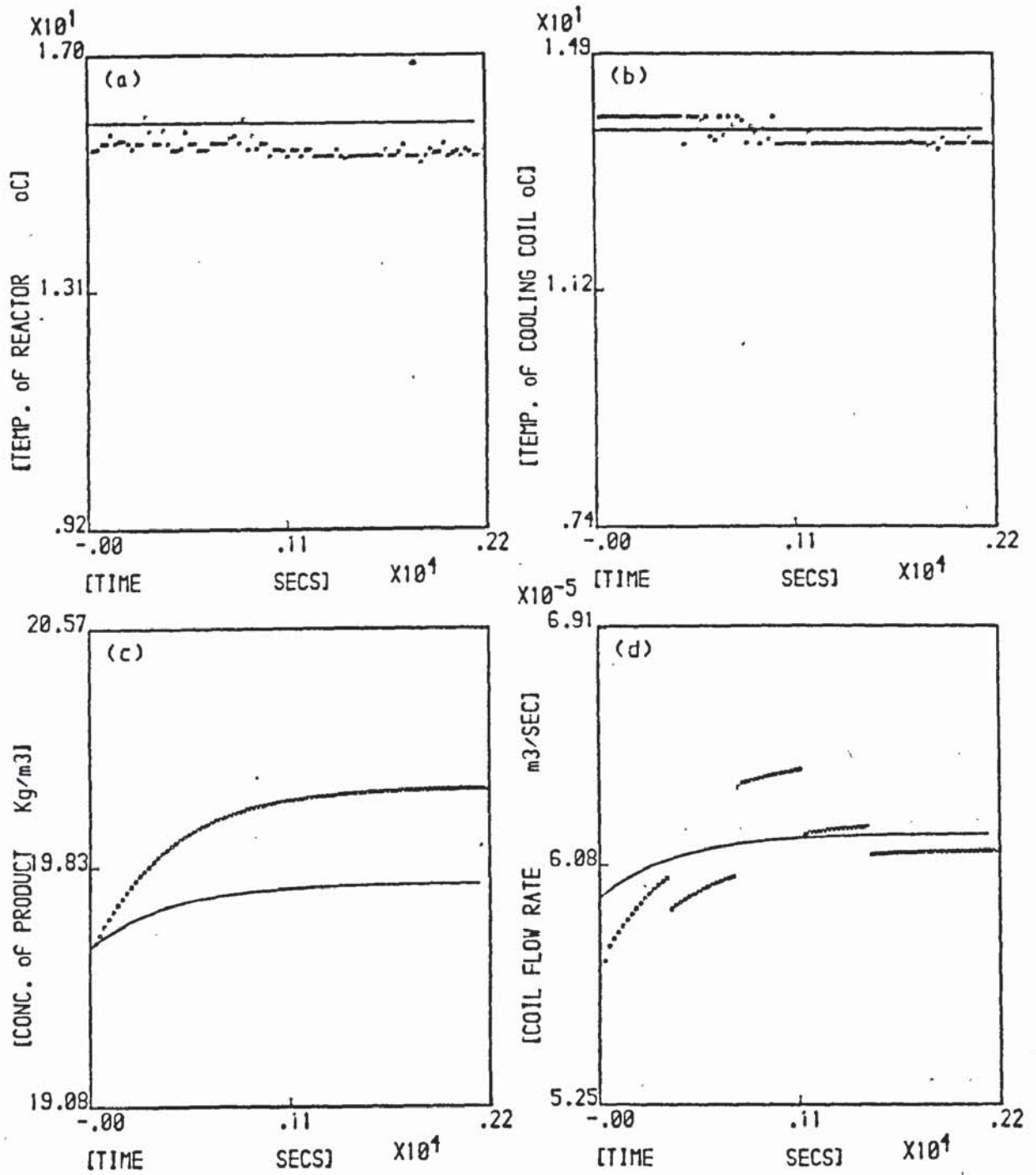


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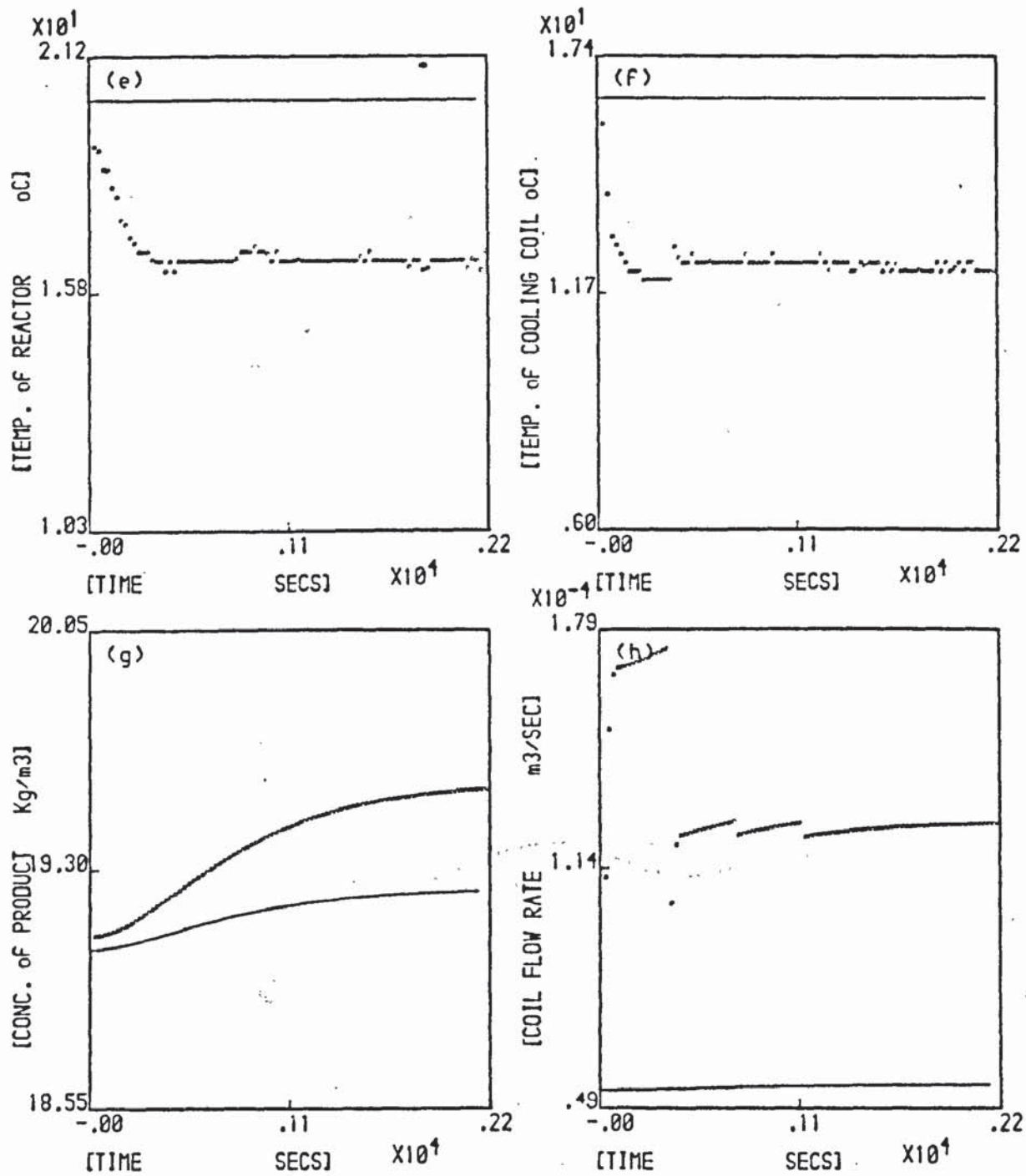


Fig. A.6.2.27 Reactor Two. Experiment no:27

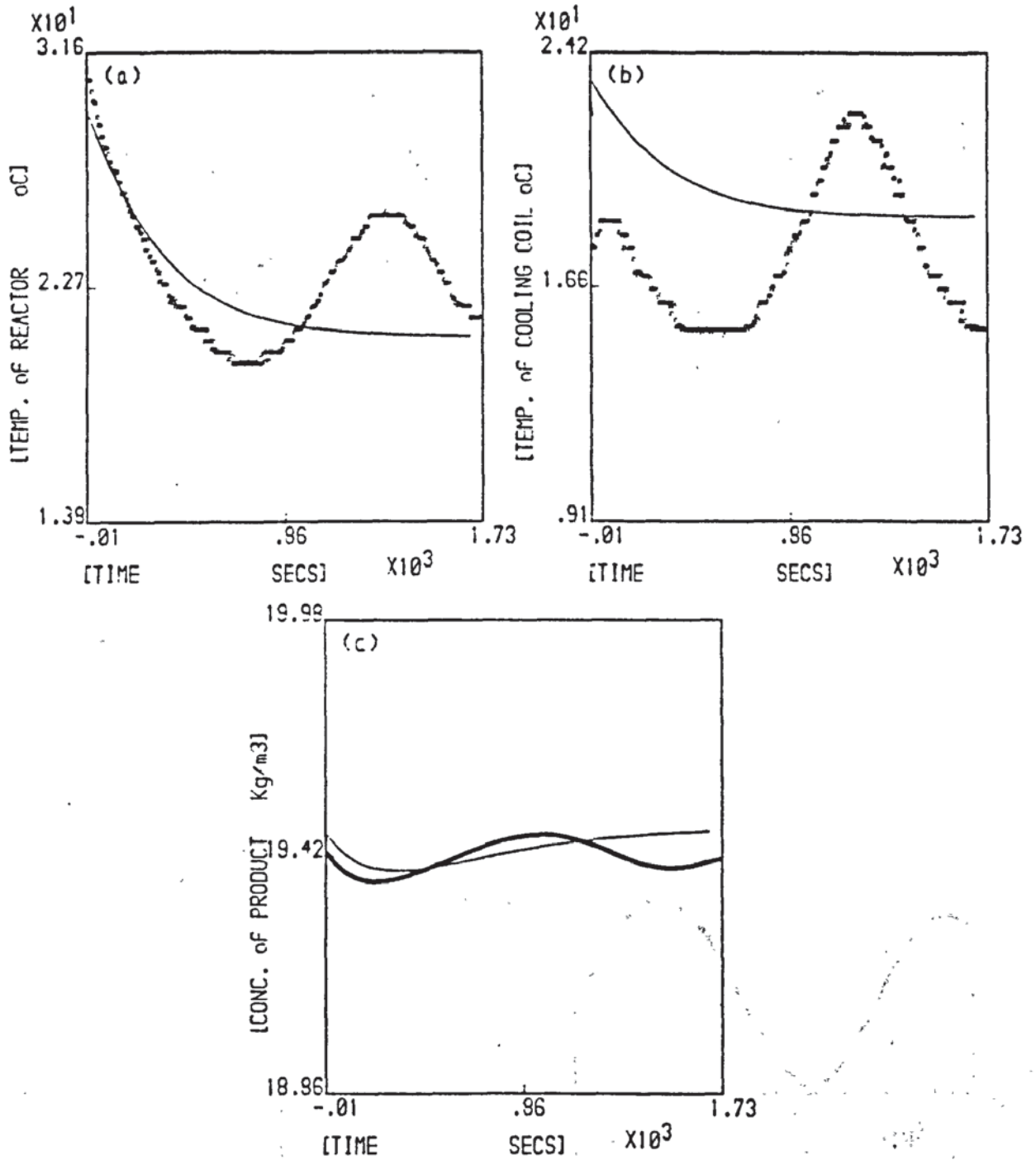


Fig. A.6.2.30 Reactor One. Experiment no:32

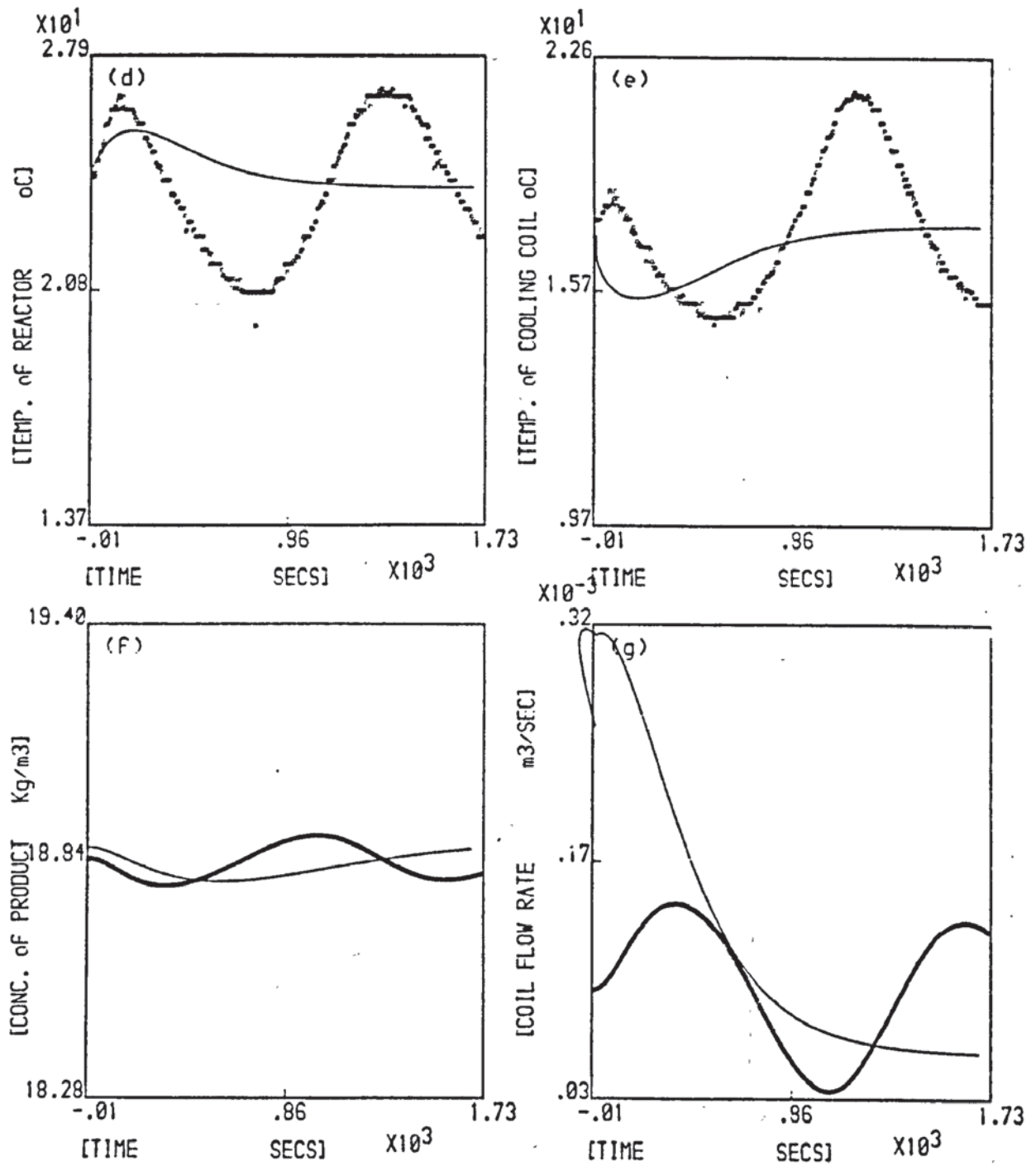


Fig. A.6.2.30 Reactor Two. Experiment no:32

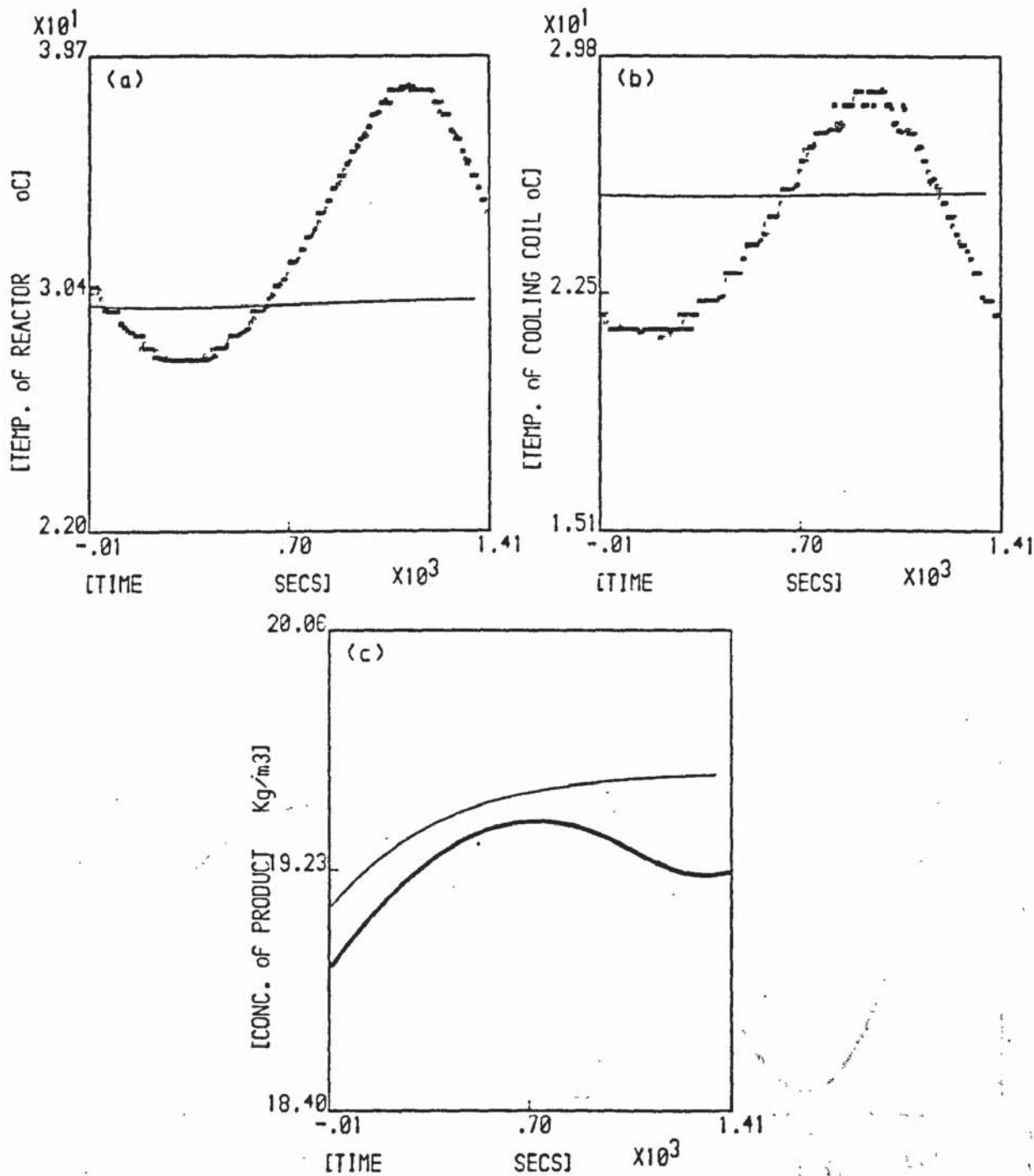


Fig. A.G.2.31 Reactor One. Experiment no:29

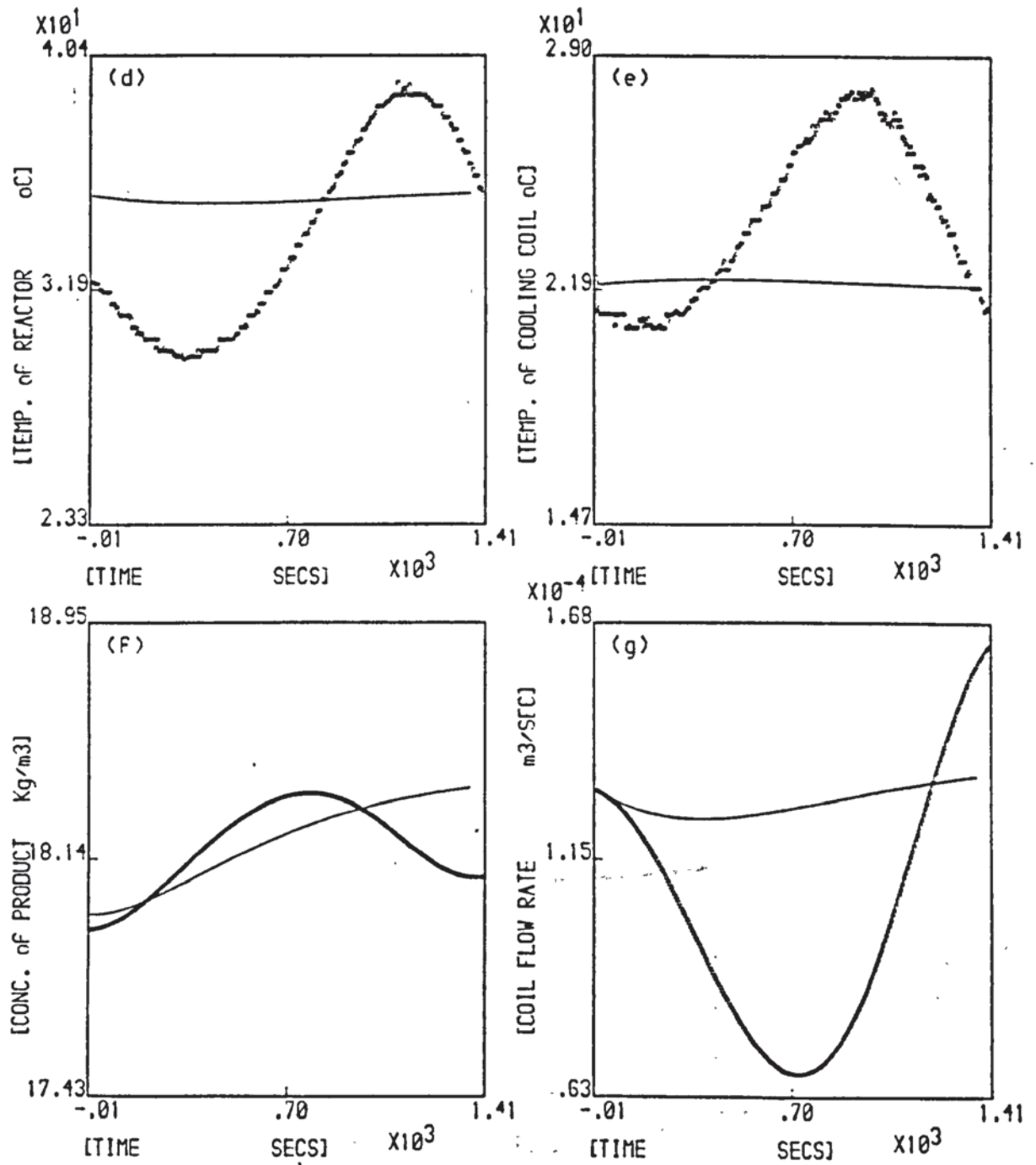


Fig. A.6.2.31 Reactor Two. Experiment no:29

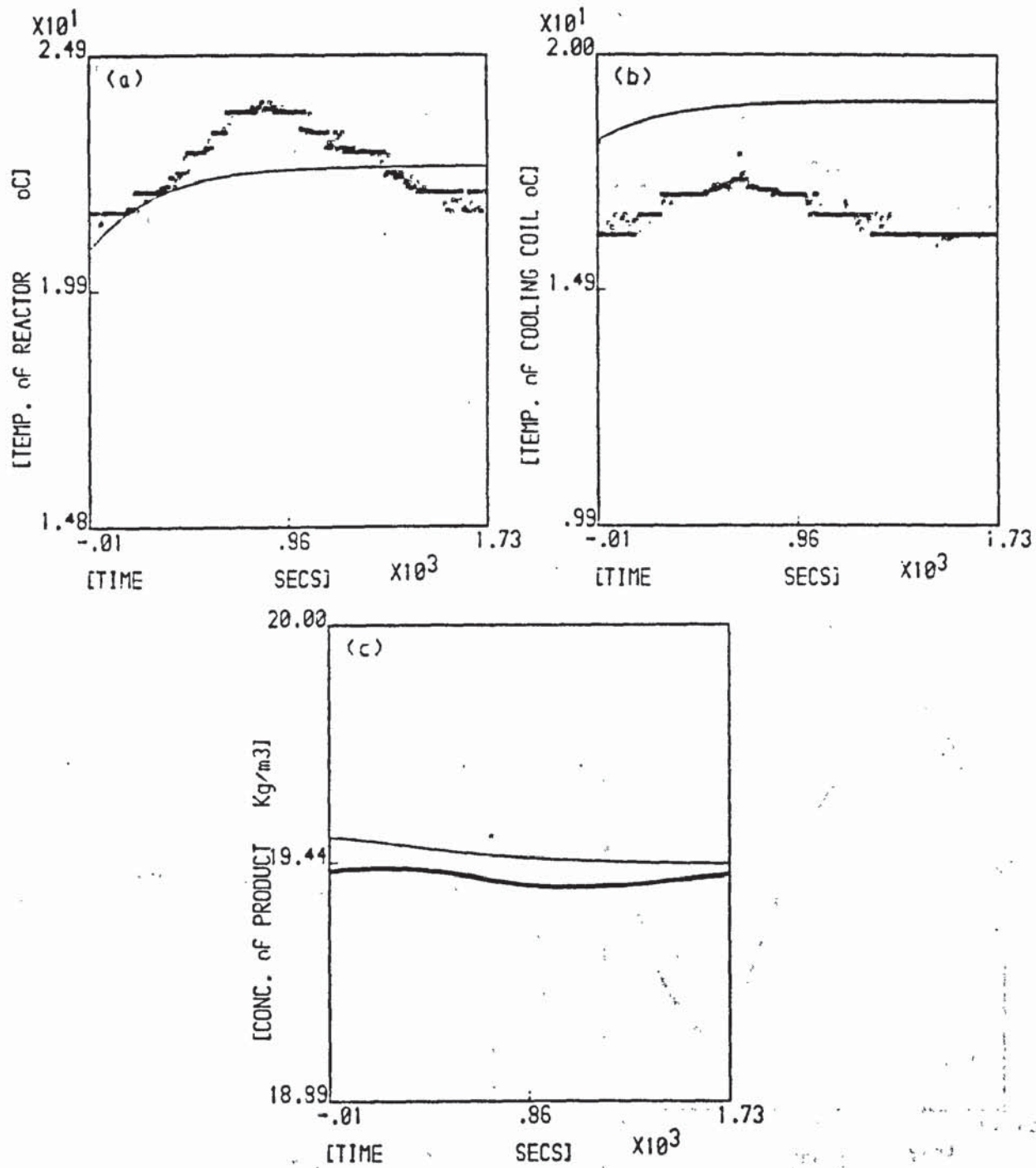


Fig. A.6.2.33 Reactor One. Experiment no:33

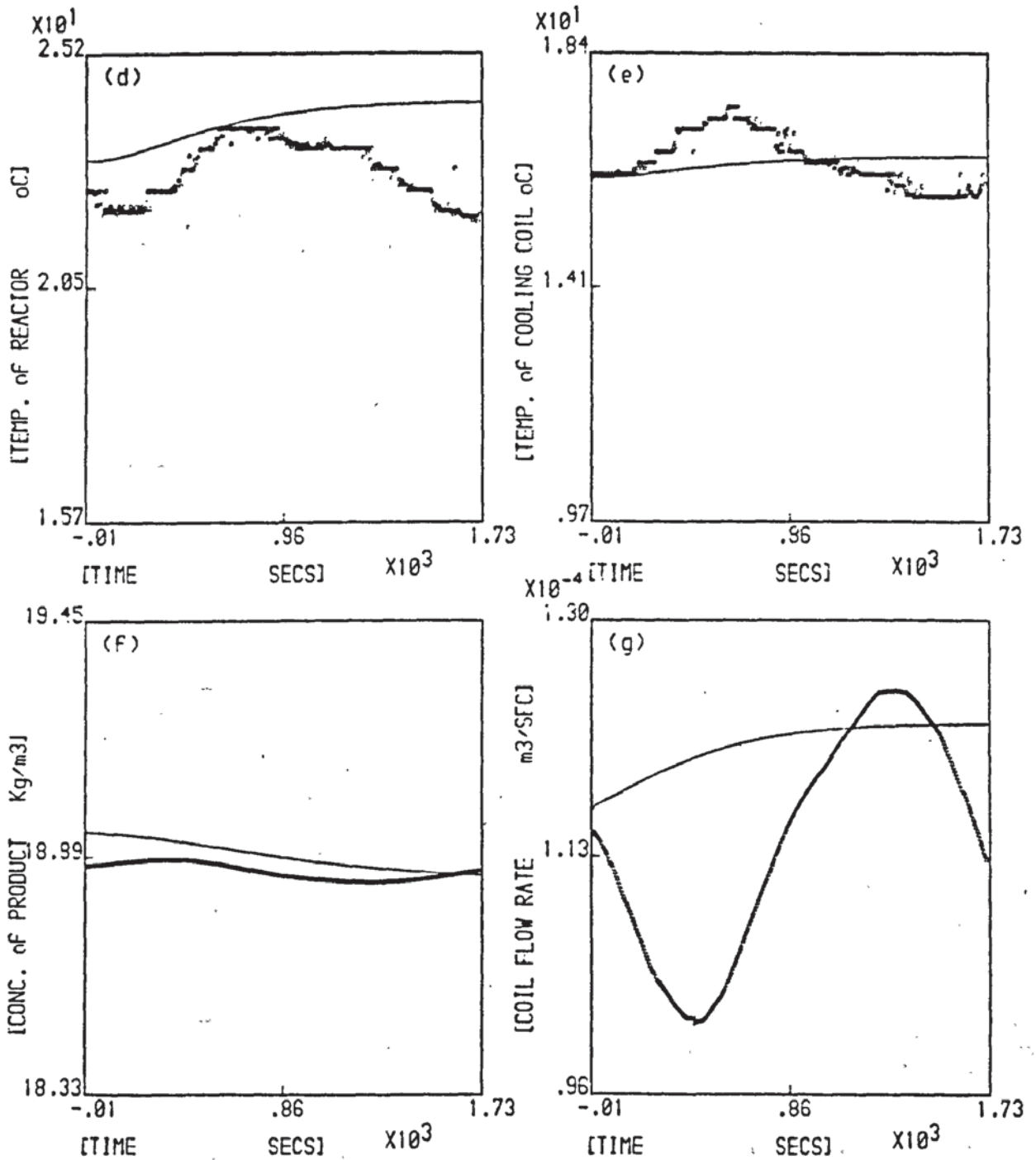


Fig. A.6.2.33 Reactor Two. Experiment no:33

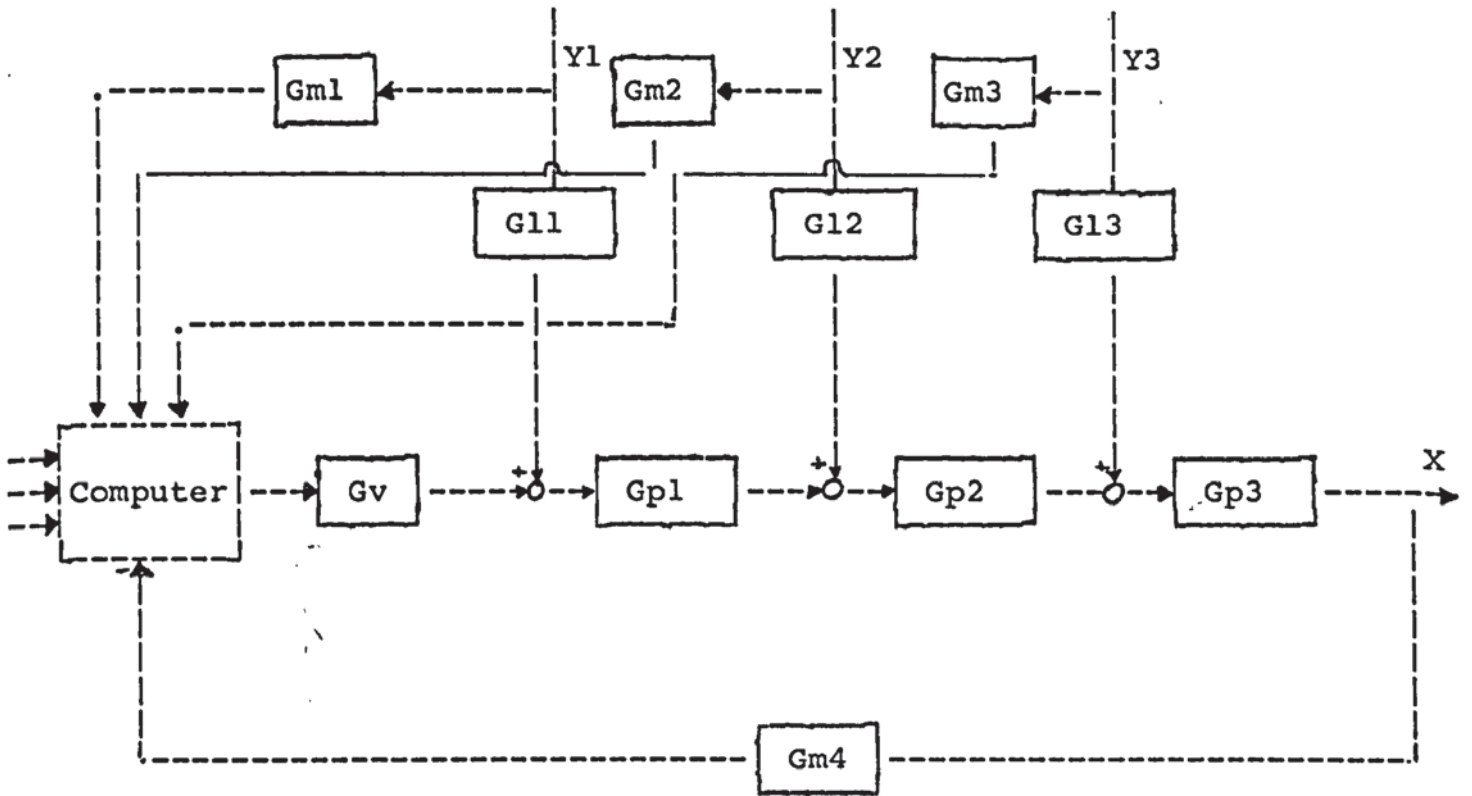


Figure 6.2
NONINTERACTING CONTROL OF REACTORS OUTLET TEMPERATURES.

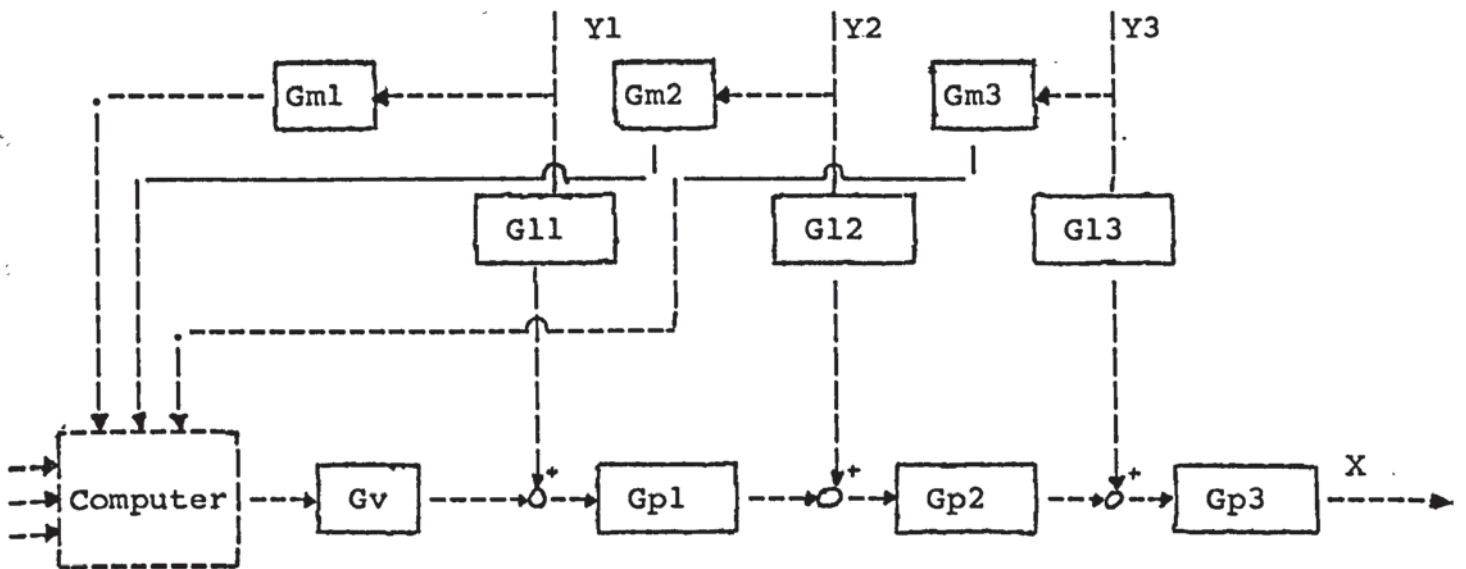


Figure 6.3
INVARIANCE CONTROL OF REACTORS AND COILS OUTLET TEMPERATURES.

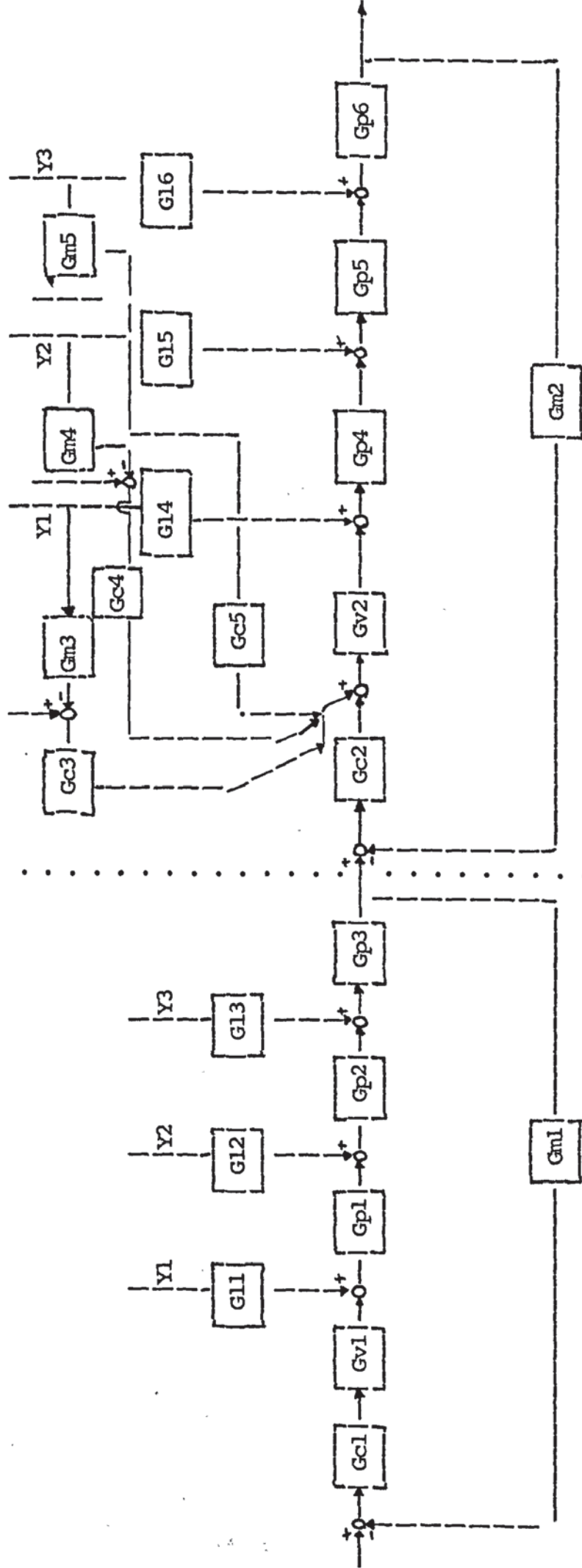


Figure 6.4
 FEEDBACK CONTROL OF STATE VARIABLES IN REACTOR ONE. FEEDBACK/FEEDFORWARD CONTROL OF STATE VARIABLES IN REACTOR TWO.

- KEY:
- Gv1, Gv2 valve transfer functions
 - Gp1 to Gp6 process transfer functions
 - Gm1 to Gm5 measuring element transfer functions
 - G11 to G16 load transfer function
 - Gc1 to Gc5 controller transfer function

A.7.1 SUBROUTINE SIX (SIMULATING REACTANT & PRODUCT CONCENTRATION)

```

SUBROUTINE UNCODY(X,XS,HS,Z)
DIMENSION SX(4,4),XS(4),Z(11)
COMMON /SV/ B,D1,G1,CS,TS,TY,CY,PV,FX(2)
EXTERNAL MEX,MAXI,MILL
G1=Z(1)
TS=Z(2)
CS=Z(3)
TY=Z(4)
CY=Z(5)
D1=Z(6)
PV=Z(7)
FX(1)=Z(8)
FX(2)=Z(9)
NF=INT(Z(10)+0.2)
B=Z(11)
IF(NF.EQ.1) CALL LINASS(MEX,2,SX,XS,ND,X,HS)
IF(NF.EQ.2) CALL LINASS(MAXI,4,SX,XS,ND,X,HS)
RETURN
END

```

```

SUBROUTINE LINASS(BONES,NIS,SX,XS,ND,X,HS)
REAL SX(4,4),PS(4),HS,X,XS(4)
COMMON /SV/ B,D1,G1,TS,CS,TY,CY,PV,FX(2)
INTEGER NIS,M,J,I
EXTERNAL BONES
PS(1)=XS(1)
PS(2)=XS(2)
PS(3)=XS(3)
PS(4)=XS(4)
CALL D0INT(X,PS,NIS,HS,SX,BONES)
XS(1)=PS(1)
XS(2)=PS(2)
XS(3)=PS(3)
XS(4)=PS(4)
RETURN
END

```

```

SUBROUTINE MEX(PT,PS,X,ND)
REAL PT(4),PS(4),X
COMMON /SV/ B,D1,G1,TS,CS,TY,CY,PV,FX(2)
PM=EXP(PX(1)/(1.+G1*FX(1)))
PT(1)=PV-PS(1)-D1*PS(1)*PM
ZM=EXP(FX(2)/(1.+G1*FX(2)))
PT(2)=(PS(1)-PS(2))-D1*PS(2)*ZM
RETURN
END

```

```

SUBROUTINE MAXI(PT,PS,X,ND)
REAL PT(4),PS(4),X,S1,S2
COMMON /SV/ B,D1,G1,TS,CS,TY,CY,PV,FX(2)
FW=FX(1)+TS
WF=EXP(FW/(1.+G1*FW))
S1=EXP(TS/(1.+G1*TS))
PT(1)=PV-PS(1)-D1*((PS(1)+CS)*WF-CS*S1)
PT(2)=PS(1)
ZW=FX(2)+TY
ZF=EXP(ZW/(1.+G1*ZW))
S2=EXP(TY/(1.+G1*TY))
PT(3)=(PS(1)-PS(3))-D1*((PS(3)+CY)*ZF-CY*S2)
PT(4)=PS(3)

```

RETURN
END

A.7.2 SUBROUTINE SEVEN (GRAPH).

```
      SUBROUTINE OLGRA(T,C,D,E,G,X,Q,R,V)
      REAL T,A(4),C(4),D,E(4),F(4),G,X(4),Q,R,V(6)
      DIMENSION I(4),K(4)
C     M CONTROLS INITIAL ENTRY VALUES TAKEN FROM BASIC.
C     M1 CONTROLS NUMBER OF POINTS.
C     IF M.EQ.M1=1 PROGRAMME CLEARS SCREEN.
C     V(1)=A(1) IS THE INITIAL CONC. (ORIGIN OF Y-AXIS).
C     V(2)=A(2) IS THE Y-AXIS
C     V(3)=A(2) IS THE Y-AXIS FOR J1>2
C     V(4)=A(3) IS THE TOTAL SCANNING TIME
C     V(5)=A(1) IS THE INTIAL TEMP. (Y-AXIS FOR J>2)
      A(1)=V(1)
      A(2)=V(2)
      A(3)=V(4)
      A(4)=V(5)
      M=INT(Q+0.2)
      M1=INT(R+0.2)
      IF(M1.EQ.1) GO TO 35
      IF(M1.EQ.2) GO TO 40
      IF(M.EQ.1) GO TO 50
      J1=0
10    J1=J1+1
      IF(J1.GE.3) A(2)=V(3)
      IF(J1.GE.3) A(1)=V(6)
      CALL VWINDO(A(4),A(3),A(1),A(2))
      CALL SWINDO(I(J1),J,K(J1),L)
      CALL POINTA(S1,F(J1))
      CALL DRAWA(T,X(J1))
      F(J1)=X(J1)
      IF(J1.LT.4) GO TO 10
      S1=T
20    M=M+1
      Q=FLOAT(M)
      IF(M1.EQ.1) GO TO 40
      IF(M.NE.M1) RETURN
      DO 30 I1=1,5
30    CALL BELL
      CALL FINITT(I(4),K(4))
      RETURN
35    CALL ANCHO(24)
      RETURN
40    CALL ANCHO(25)
      RETURN
50    CALL ANCHO(29)
      CALL INITT(0)
      S1=0.0
      J=INT(D+0.2)
      L=INT(G+0.2)
      DO 60 M2=1,4
      IF(M2.GE.3) A(2)=V(3)
      IF(M2.GE.3) A(1)=V(6)
      I(M2)=INT(C(M2)+0.2)
      K(M2)=INT(E(M2)+0.2)
      F(M2)=X(M2)
      CALL VWINDO(A(4),A(3),A(1),A(2))
      CALL SWINDO(I(M2),J,K(M2),L)
      CALL MOVEA(A(4),A(1))
```



```

CALL DRAWA(A(4),(A(1)+A(2)))
CALL DRAWA(A(4)+A(3),(A(1)+A(2)))
CALL DRAWA((A(4)+A(3)),A(1))
CALL DRAWA(A(4),A(1))
60 CONTINUE
GO TO 20
END

```

A.7.3 SUBROUTINE FIVE (CONTROLS OUTPUT DEVICES)

```

SUBR SU89
REL
SU89 DAC **
JST VAL
SNZ
JMP SU8          JMP TO SN4 ROUTINE
JST VAL
SNZ
JMP PLD1         JMP TO PUNCH
HLT              PAUSE
PLD2 IRS SU89
JMP* SU89        RETURN
PLD1 JST PLD      PUNCH LEADER
JMP PLD2
PLD EQU '5432
SU8 JST VAL      SNSW4 ROUTINE
SNZ
JMP *+3
IRS* PFLG
JMP *+3
CRA
STA* PFLG
JMP PLD2
PFLG XAC PFLG
VAL DAC **       ARGUMENT ROUTINE
LDA* SU89
STA TEMP
LDA* TEMP
IRS SU89
JMP* VAL
TEMP BSZ 1
END

```

A.7.4 SUBROUTINE FOUR (RECORDS PROGRAMME EXECUTION TIME)

```

SUBR ITIM
REL
ITIM DAC **
LDA* ITIM
STA DMY
IRS ITIM
LDA* DMY
SNZ
JMP TER
LDA* ITIM
STA DMY1
LDA TIM
SUB CONS
OCP '220
JST* C&12
JST* H&22
DMY1 DAC **

```

```

        JMP      OUT
DMY    BSZ      1
TIM    EQU      '61
C£12  EQU      '675
H£22  EQU      '654
TER    LDA      CONS
        STA      TIM
        OCP      '20
OUT    IRS      ITIM
        IRS      ITIM
        JMP*     ITIM
CONS   DEC      -32760
        END

```

A.7.5 LIBRARY ROUTINE POINTERS

```

        SUBR     ABS
        SUBR     L£22
        SUBR     H£22
        SUBR     N£22
        SUBR     S£22
        SUBR     A£22
        SUBR     D£22
        SUBR     M£11
        SUBR     M£22
        SUBR     C£12
        SUBR     EXP
        SUBR     SQRT
ABS    EQU      '5470
L£22  EQU      '5554
H£22  EQU      '5560
N£22  EQU      '5576
S£22  EQU      '5753
A£22  EQU      '5760
D£22  EQU      '6035
M£11  EQU      '6163
M£22  EQU      '6204
C£12  EQU      '6247
EXP    EQU      '6563
SQRT  EQU      '6677
        END

```

A.7.6 MEMORY MAP OF SUBROUTINES CALLED FROM BASIC.

```

*LOW    00000
*START  00720
*HIGH   37610
*NAMES  11434
*COMN   37651
*BASE   37636
*BASE   36733
*BASE   31775
*BASE   32757
*BASE   33765
*BASE   30771
*BASE   34771
*BASE   35772
*BASE   27773
*BASE   26710
*BASE   25574
IOMOD   00720
PFLG    00756

```

ABS	05470
L£22	05554
H£22	05560
N£22	05576
S£22	05753
A£22	05760
D£22	06035
M£11	06163
M£22	06204
C£12	06247
EXP	06563
SQRT	06677
HADIOS	25000
SUB3	25433
IFLG	25473
MYSR	26603**
ERCL	26624
ITIM	26710
SU89	26742
UNCODY	27000
LINASS	27266
MEX	27422
MAXI	30000
DOINT	31000
F£AT	31450
IFIX	31532
IDINT	31532
INT	31532
C£21	31542
OLGRA	32000
FINITT	33000
SWINDO	33014
BELL	33042
VWINDO	33050
MOVEA	33110
POINTA	33130
DRAWA	33160
ANCHO	33224
NEWLIN	33260
CARTN	33266
LINEF	33326
V2ST	33352
CLIPT	34000
LVLCHT	35000
MODCHK	35034
REVCOT	35062
WINCOT	35170
PCLIPT	35306
PARCLT	35366
INITT	35506
NEWPAG	35656
VECMOD	36000
PNTMOD	36052
XVCNVT	36110
IOWAIT	36362
TOUTPT	36426
MOVABS	36444
ANMODE	36464
MOD	36506
FLOAT	36534
D£11X	36544
D£11	36544

F&ER 36614
 F&HT 36624
 ARG& 36662
 AC1 36702
 AC2 36703
 AC3 36704
 AC5 36706
 TKDASH 37000
 TKTRNX 37651
 SV 37753
 MR

A.7.7 I/O MOD

	REL	
	ENT	IOMOD,AA
	ENT	PFLG
AA	SS3	
	JMP	*+3
	CRA	
	STA	'105
	LDA	'406
	JMP*	*+1
	OCT	4143
BB	IRS	'105
	CRA	
	STA	'106
	JST*	*+2
	JMP*	*+2
	OCT	3056
	OCT	4575
CC	LDA	PFLG
	SZE	
	JMP	*+3
	SS4	
	JMP	*+3
	OCP	2
	IRS	'106
	JST*	*+2
	JMP	*+2
	OCT	3047
	OCT	4212
DD	IRS	'105
	CRA	
	STA	'106
	JMP*	*+1
	OCT	5245
PFLG	BSZ	1
	ABS	
BASE	EQU	'767
	ORG	BASE
	DAC	AA
	DAC	BB
	DAC	CC
	DAC	DD
	ORG	'4142
	JMP*	BASE
	ORG	'4574
	JMP*	BASE+1
	ORG	'4211
	JMP*	BASE+2
	ORG	'5244
	JMP*	BASE+3

END

A.7.8 ADT1-8 TABLE

*ADT1-8 RELOCATION

*

ORG '4757
STA '761
ORG '4761
STA '762
ORG '4763
STA '764
STX '763
ORG '4766
STA '766
ORG '5006
OCT 764
STA '764
IRS '762
ORG '5023
LDA '764
ORG '5025
ADD '762
ORG '5027
STA '765
ORG '5034
STA '757
SUB '765
ORG '5037
STA '760
LDA* '757
STA* '760
IRS '757
IRS '760
ORG '5045
SUB '757
ORG '5050
LDA '756
ORG '5061
SUB '765
ORG '5065
LDA '767
ORG '5070
STA '757
ORG '5074
IRS '757
ORG '5076
LDA '771
ORG '5100
STA '757
ORG '5104
IRS '757
ORG '5112
LDA '762
ORG '5114
LDA '761
ORG '5123
LDA '766
ORG '5126
LDX '763
END