THE MEASUREMENT AND CONTROL OF MOVING REACTION ZONES IN FIXED-BED REACTORS

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ABSTRACT

It is well known that exothermic reactions taking place in fixed-bed reactors can exhibit temperature profiles which slowly traverse the bed, either upstream or downstream, while the reactor is otherwise operating under steady - or near steady - state conditions. Theoretical and experimental studies demonstrate that in systems with decaying catalysts, a reaction zone moving in a direction counter to that of flow of fluid can be close to the optimal operating method for that system. The effects of various controls on the velocity of propagation and the position of ultimate steady-state (if any), have been studied. The chemical systems studied are the oxidation of carbon monoxide on a copper oxide catalyst, and the oxidation of carbon deposited on Alumina-Silica (i.e. the regeneration of a cracking catalyst). Studies are emphasised on the measurement of the moving reaction zone and methods of controlling the reaction zone velocity to achieve some objective. Propagation velocity has been measured with reasonable accuracy and reproducibility, and correlated as a function of feed and initial conditions. In a recent theoretical study, a model for predicting temperature and conversion profiles at any instant along an adiabatic catalytic reactor subject to catalyst decay was developed. This model was extended here to include the non-adiabatic behaviour of a reactor and simulated for comparison with the experimental studies. The model is described by a pair of non-linear, coupled, partial differential equations, and those have been solved by numerical techniques. The model predictions have been verified for the experimental systems studied.

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I dedicate this thesis to my wife, my son, and my daughter. I am thankful to my wife for having undertaken the difficulties of being married to a Ph.D student with stamina, sharing the successes and difficulties with an equal love during this long period of study.

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CHAPTER ONE

1.1 Introduction.

In recent years several workers have noted that propagating temperature profiles can be observed in fixed-bed tubular reactors in which strongly exothermic reactions are taking place (1-6). Depending upon the feed and controls, the profiles can propagate in either forward and reverse direction and can lead to a stable steady-state or to blow-out.

There has also been a substantial amount of work seeking to explain the above phenomenon by postulating various models of such system (7-11). These models differ considerably by the inclusion or omission of various contributing factors, including gas and solid conductivity, radiation, dispersion, the kinetics of the reaction, etc., but are still able to predict the observed behaviour of such systems.

To provide a more efficient method of operation a detailed analysis is presented on the effects upon transient behaviour of the reaction zone when several of the system parameters, such as feed velocity (u_o), feed concentration (C_{Ao}), feed temperature (T_o), and the peak temperature of the initially imposed temperature profile are varied.

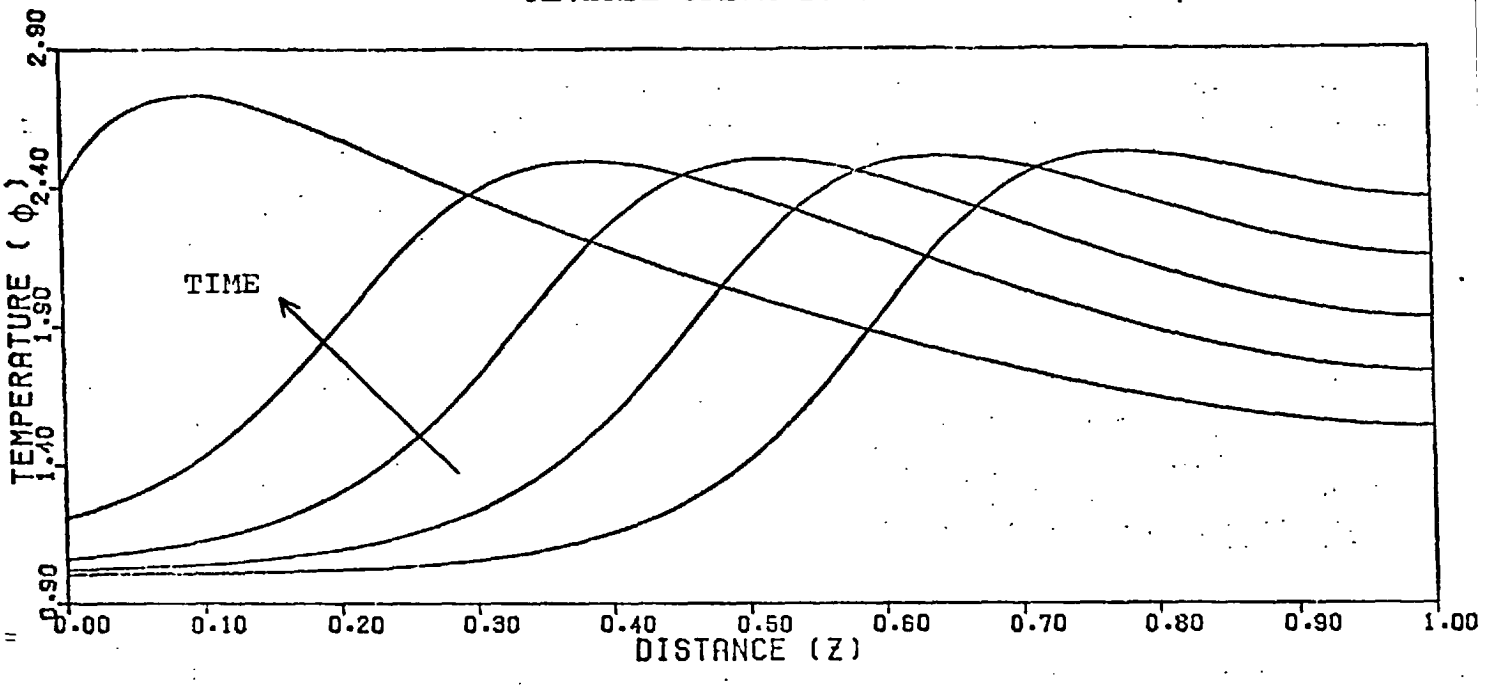
1.2 The Concept of Reverse Operation.

Reverse operation refers to the transient behaviour of a reactor in which a high temperature zone propagates, by conduction and or radiation through the solid phase of the fixed-bed, in a direction counter current to the flow of

the reactants. This is a naturally occuring phenomena which for an exothermic reaction can be induced by the external heating of the fixed-bed near the reactor exit and thereafter can be maintained without any form of external control. It is believed that for a wide variety of catalyst deactivation mechanisms, system subject to reverse operation can obtain increased time average performances through a more efficient utilization of the catalyst activity. With the conventional operation of a catalytic reactor, the reaction zone is either near the reactor inlet or distributed along the reactor axis and consequently if the catalyst deactivation mechanism is temperature sensitive or affected by a product of the main reaction the entire bed is exposed to the poisoning agent. Alternatively the reverse operation of a catalytic reactor involves the presence of a narrow high temperature reaction zone near the reactor exit with the remainder of the bed maintained cold and inactive. As the reaction zone is translated upstream the poisoning is restricted to the narrow reaction zone and the region of deactivated catalyst previously traversed; consequently, fresh catalyst remains until the reaction zone reaches the reactor inlet. Figures 1.1 and 1.2 represent the behaviour of a reactor undergoing reverse and conventional operation respectively. Reverse operation does not eliminate poisoning but does allow a more efficient use of the catalyst by reducing the active area available to the potential poisons.

One aspect of reverse operation which may be beneficial to industry is its application to the regeneration of carbon deposition in catalytic cracking and similar processes.

FIG. (1.1a) TRANSIENT BEHAVIOR OF THE TEMPERATURE PROFILE DURING REVERSE OPERATION.



(FROM THEORETICAL COMPUTATION OF CO OXIDATION)

$\Phi = T/T$ = Dimensionless temperature , T = 298°K

Z= l/L = Dimensionless distance

Y= Fractional conversion

FIG. (1.1b) TRANSIENT BEHAVIOUR OF THE CONVERSION PROFILE DURING REVERSE OPERATION.

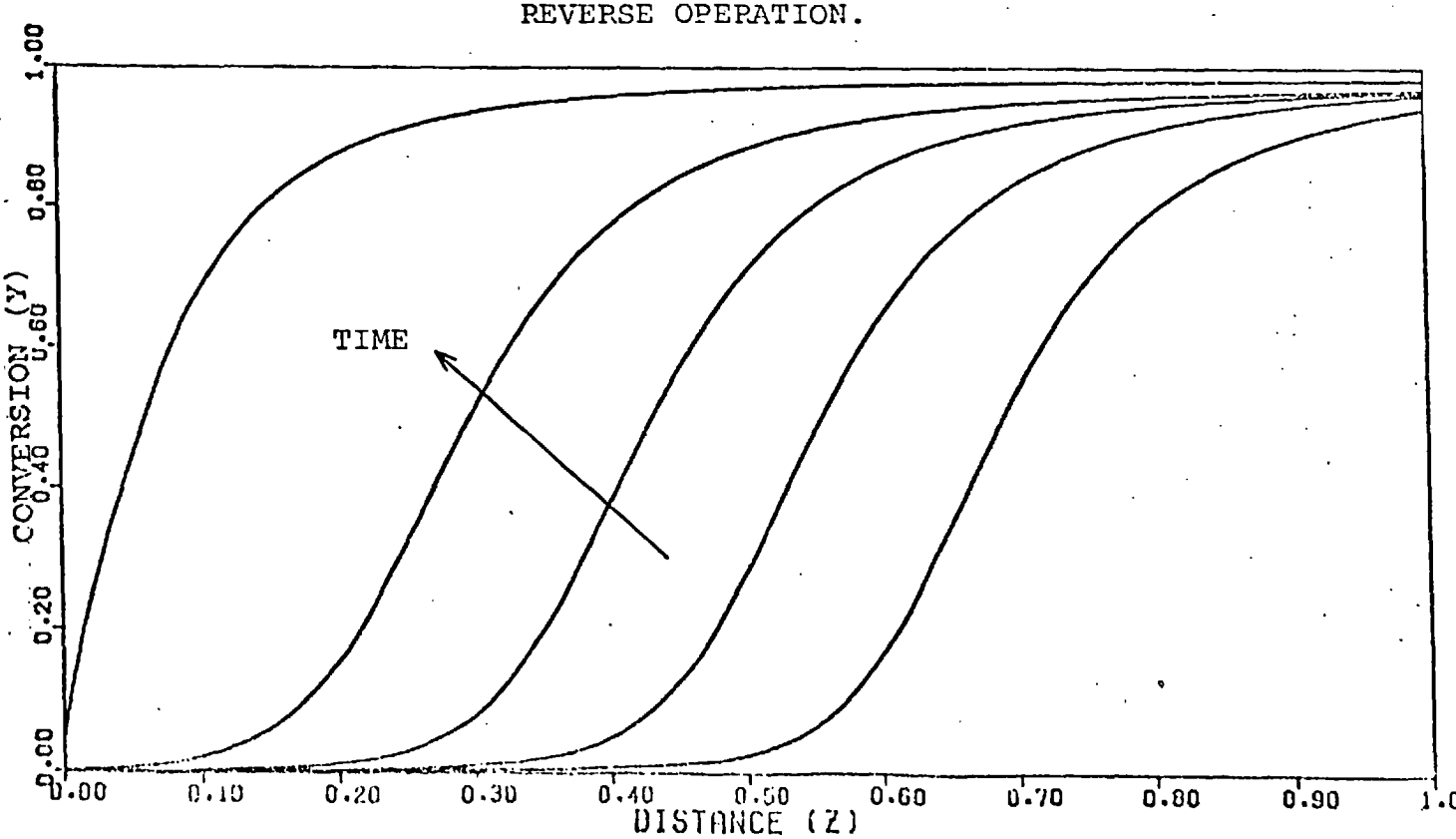


FIG.(1.2a) TRANSIENT BEHAVIOUR OF THE TEMPERATURE PROFILE DURING CONVENTIONAL OPERATION.

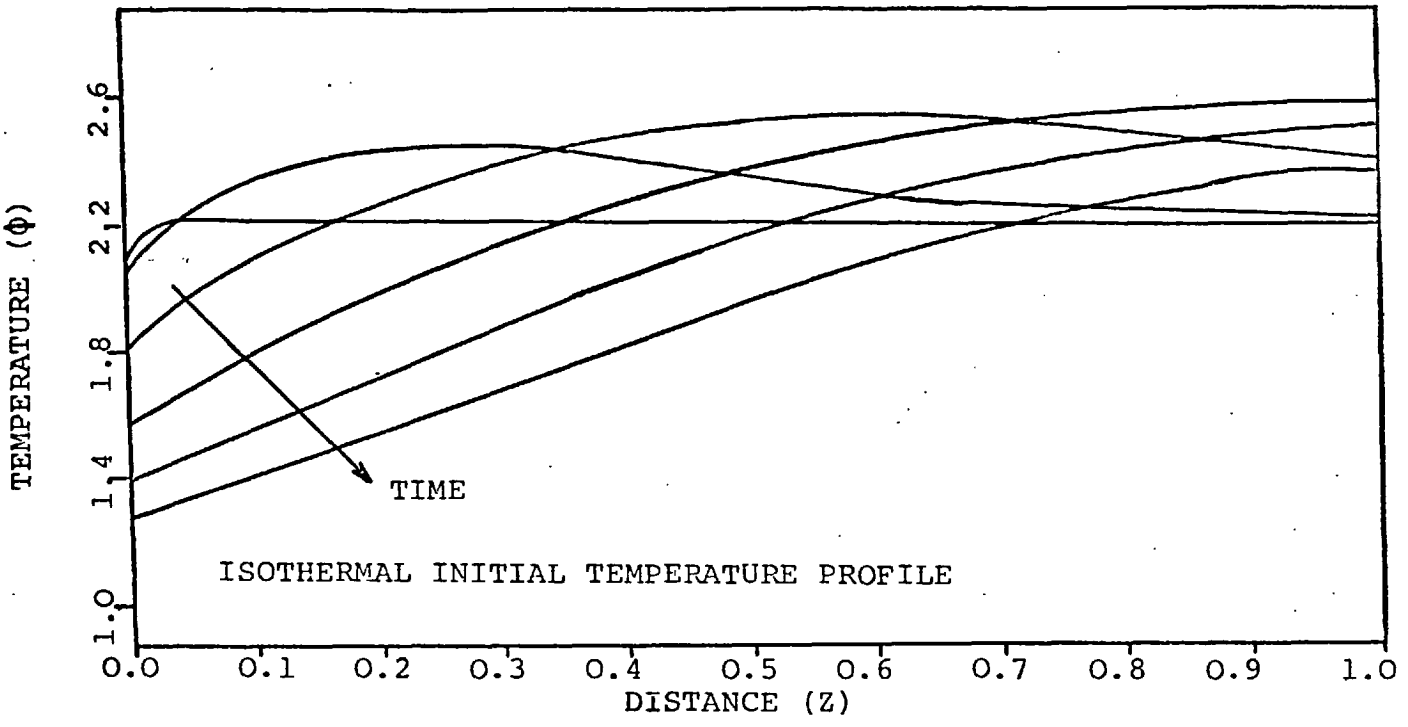
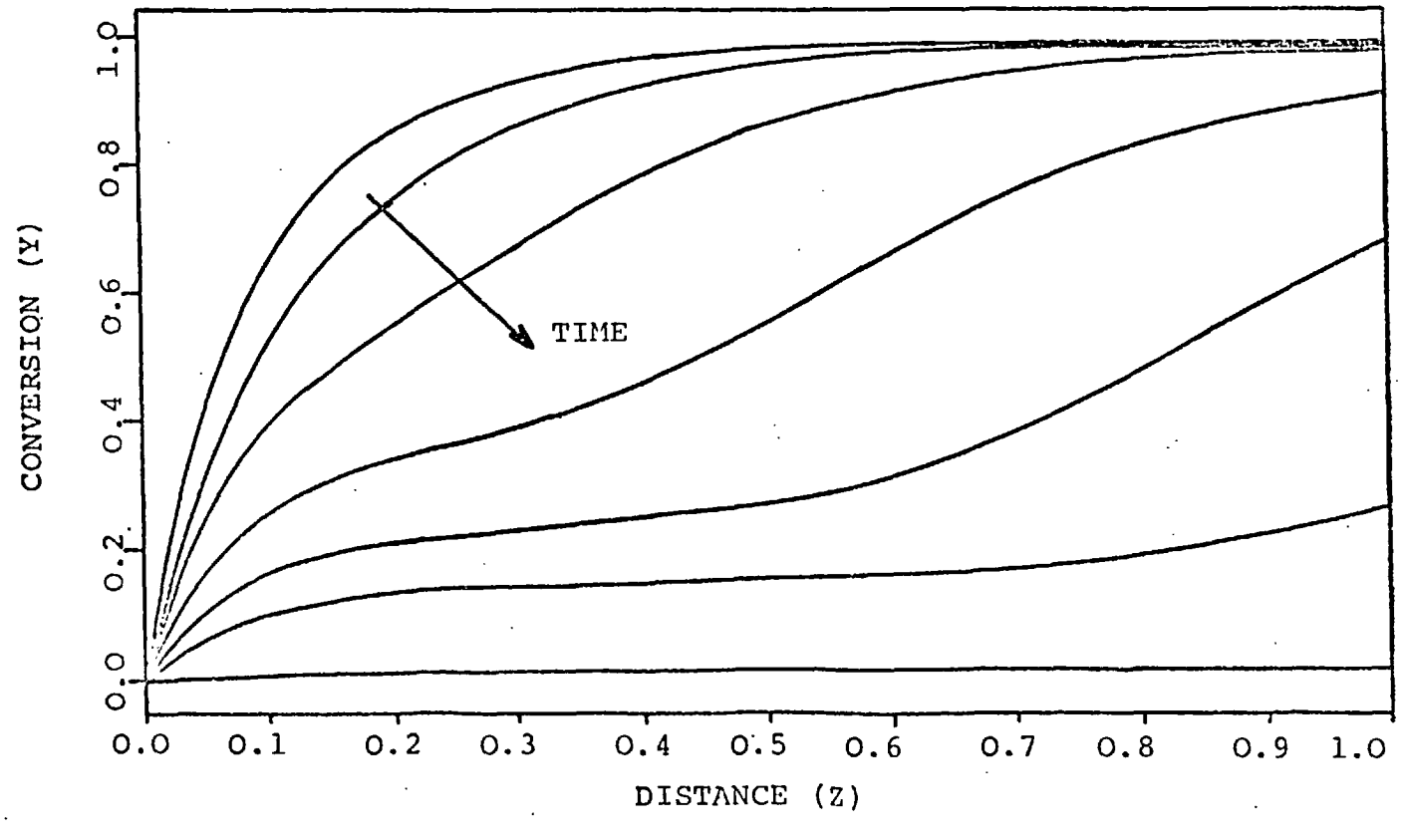


FIG. (1.2b) TRANSIENT BEHAVIOUR OF THE CONVERSION PROFILE DURING CONVENTIONAL OPERATION.



Many hetrogeneous reactions of industrial importance such as cracking, isomerization and dehydrogeneration of hydrocarbons are accompanied by a gradual decrease of catalyst activity which is reflected in a drop in conversion to the product of interest as the reaction proceeds. This deactivation of the catalyst in many cases caused by the deposition of carbonaceous substances, so-called "coke" which is formed by side reactions. This is called catalyst fouling, a phenomenon frequently encountered in the petroleum and petrochemical industry. In order to maintain production rates within the desired limits it is necessary to remove the deposit i.e. to regenerate the catalyst activity.

In catalytic processes, fouled catalysts are regenerated by burning the coke deposited on its surface with air. The operation is highly exothermic and must be conducted carefully to prevent the permanent deactivation of the catalyst. Estimation of possible overheating of catalyst must be made on regeneration, since this effect may influence the activity and mechanical strength of the catalyst. When the regeneration is conducted at high temperatures resulting from an increased air supply appreciable overheating is expected. Consequently if the process is not controlled properly the overheating causes the total deactivation of the catalyst through structural modification or sintering of the catalyst as a result of exposing the catalyst to extreme conditions. Sintering brings about essentially complete loss of surface area with a short time at 1273^{o}K with alumina-silica catalyst, 1120-1170^{o}K with clay catalysts, and about 1070^{o}K with magnesia-silica catalyst. At substantially lower temperatures

(870-970^{o}K) the loss of surface area is very small, but is considerably increased by the presence of steam. Hence in order to avoid the permanent deactivation of the catalyst, the supply of oxygen used during the regeneration process must be limited for a given system.

In catalytic cracking processes oil of a boiling point range higher than gasoline, is contacted with the catalyst at about 770^{o}K. The contact time is usually a few seconds, and the pressure 1 to 2 atmospheres absolute. During this stage a great number of reactions occur,predominantly cracking of carbon-carbon bonds. Cracking is accompanied by a host of reactions which are known to be catalyzed by strong acids: isomerization of paraffins and particularly of olefins formed by cracking of paraffins and naphthenes and by dealkylation of aromatics; transfer of hydrogen; transfer of alkyl groups from one aromatic molecule to another; some cyclization and some dehydrogenation. The extent of each reaction depends on the composition of the original oil, particularly the molecular weight and the structural characteristics of hydrocarbons present or formed by primary cracking. At this stage, the catalyst is rapidly being covered by a layer of coke. The origin and mechanism of coke formation have never been conclusively demonstrated. The coke deposition causes the gradual decrease of catalyst activity which is reflected in a drop in conversion to the product of interest as the reaction proceeds.

The coke formation is called catalyst fouling, physically blocking or plugging the pore entrances. The accumulation of coke on the catalyst will also increase the

pressure drop through the reactor, and this is the factor that frequently determines when the catalyst must be regenerated (12). Some examples of industrially important processes affected by fouling are presented in Table 1.1.

Deposition of carbonaceous material is formed within the catalyst particles, and must be burned off periodically to regenerate activity. The burning off need not be complete, for the catalyst has considerable activity even when fairly large amounts of coke are present. Typical curves showing activity at a given coke level, rate of coke formation, and the decline of activity within a process period are presented in Figures (1.3), (1.4) and (1.5) for fixed bed cracking. The burning off of coke, or regeneration, is a characteristic feature of the catalytic cracking process and largely determines the design of the plants.

A coke deposit deactivates the catalyst very effectively but the activity is substantially restored when the coke is removed by oxidation. For this purpose the catalyst is first treated with an inert gas, most often steam to liberate adsorbed heavy hydrocarboons (a procedure called "stripping"). Subsequently coke is burned off the catalyst with air. This procedure, called "regeneration" is carried out at a temperature of 800 to 820^{o}K. Following regeneration the catalyst is ready for the next cycle. It is probable that the surface of the catalyst is exposed to temperatures substantially higher than the measured temperature of the regeneration bed, and that these high surface temperatures contribute to the loss of surface and a progressive loss of activity of the catalyst in the units.

PROCESS	FEED	CATALYST	PRESSURE (atm)	TEMPERATURE (^{o}C)
STEAM-REFORMING	H_2O+CH_4 OR NAPHTHAS	Ni ON Al_2O_3,MgO OR MIXTURES THEREOF	3-40	450-1000
REFORMING	NAPHTHAS	Pt/Al_2O_3 or MoO_3/Al_2O_3	10-40	450-530
CRACKING	PETROLEUM FRACTIONS	SiO_2-Al_2O_3 ZEOLITES.	2-4	450-530
DEHYDRO-GENATION	LIGHT HYDRO-CARBONS	$Ca_8Ni(PO_4)_6$ Al_2O_3-Cr_2O_3,Fe_2O_3	1-3	550-650
FISCHER-TROPSCH	$CO+H_2$	$Fe_2C/Fe_3O_4/Fe$;also Co or Ni based.	17-25	220-350
DESULPHURISATION	NAPHTHAS	$CoO + MoO_3/Al_2O_3$	30-40	300-400
METHANATION	CO or $CO_2 + H_2$	Ni/Al_2O_3	1-30	230-450
DEHYDRATION	ALCOHOLS	Al_2O_3,SiO_2-Al_2O_3	1	250-350
WATER-GAS SHIFT	$CO + H_2O$	Fe_3O_4-Cr_2O_3	1-30	315-485

TABLE 1.1 INDUSTRIAL PROCESSES AFFECTED BY FOULING PROBLEMS.

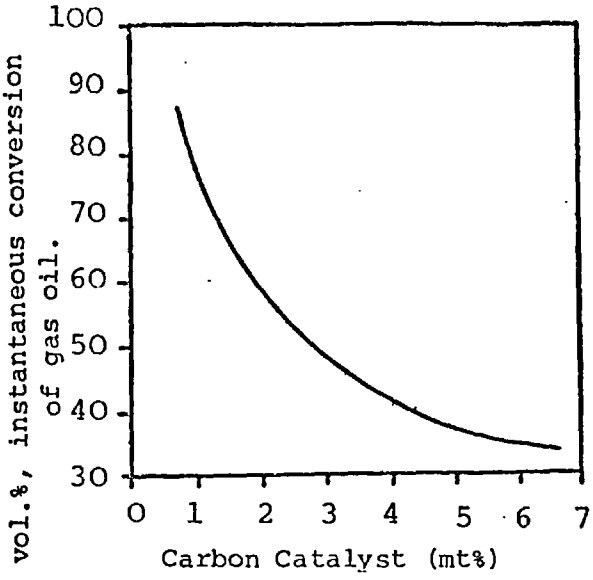


FIGURE (1.3)

Instantaneous conversion as a function of carbon on catalyst computed from data of Voorhies (13) for East Texas gas oil cracked over alumina-silica at 727°K.

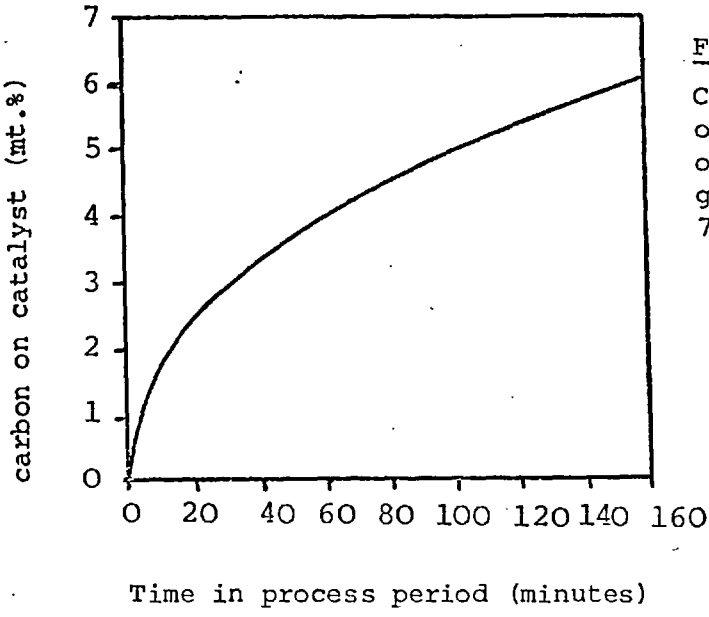


FIGURE (1.4)

Carbon on catalyst as a function of process period. From data of Voorhies for East Texas gas oil over alumina-silica at 727°K.

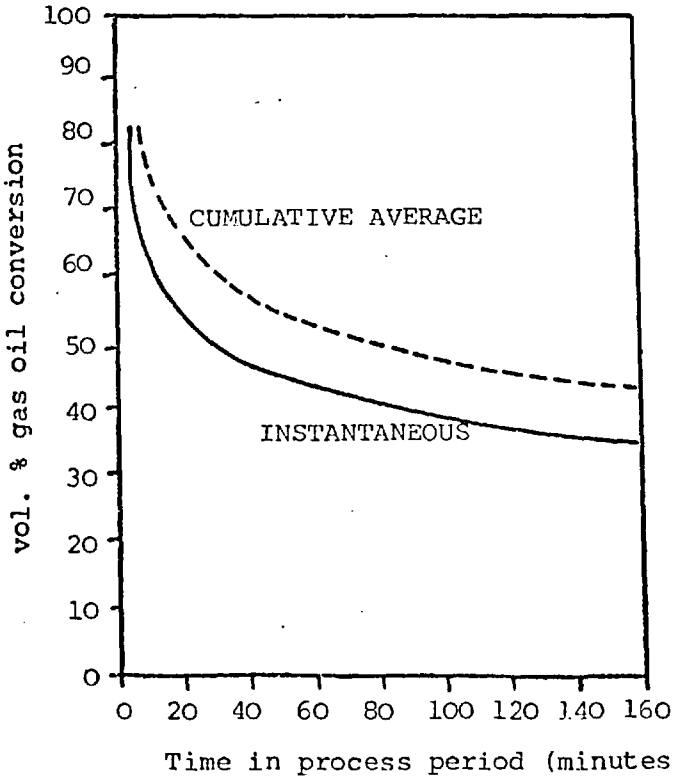


FIGURE (1.5)

Feed conversion as a function of process period. Data computed from Voorhies for cracking of East Texas gas oil over alumina-silica at 727°K.

The catalyst used is in the form of pellets or beads for one type of unit, or as a ground powder or microspheres for the so-called fluid bed units. The catalyst shapes and particle sizes are selected to suit the various methods used to circulate the catalyst through the unit.

In commercial operation a catalyst gradually deteriorates in physical properties and loses activity. Many of the reasons for such deterioration are known, but all the factors have not as yet been quantiatively evaluated. The loss of surface area and loss of activity occur by combined influence of heat and steam; contamination with heavy metals contained in oils or organometallic compounds or originating by corrosion of the units lead to an increase in coke production.

Synthetic alumina-silica catalyst manufactured in the early days of catalytic cracking contained 10 to 12 per cent alumina and were relatively dense materials. The composition was considered to be optimum, since it was generally observed that with an increasing alumina content the activity increased only slightly but the coke formation increased substantially. At least two different industrial groups studied alumina-silica catalysts of high alumina content but no advantage was shown (14).

Later improved catalysts with 18 to 30 per cent alumina content (so-called high alumina catalyst were developed. The first commercial high alumina catalyst was produced by the American Cyanamid Company in cooperation with Shell Development Company (14). As compared to older type low alumina catalysts, improvement in performance results to a large extent from the improved incorporation of 25 per cent alumina while at the same time increasing the pore

volume. In brief, high alumina catalysts have higher activity with the same product distribution and coke formation, a substantially greater activity stability, and are less prone to deterioration.

The regeneration process must be controlled carefully to avoid overheating and deactivation of the catalyst during the highly exothermic oxidation. The overheating of catalyst on regeneration, may influence the activity and mechanical strength of catalyst. When the process is conducted at low feed flow rate the quantity of heat evolved is therefore comparatively small, and significant heating should not occur. However, when the process is being operated with a high feed flow rate in the presence of considerable carbon deposition a high temperature takes place in the reaction zone resulting from the increase of heat liberation. The process thus begins to be limited by the amount of oxygen supply.

At the time of shut down the catalyst bed is at the high temperatures used to encourage the endothermic cracking reaction. Then the first step in a standard regeneration procedure is the introduction of an inert feed to cool partially the catalyst bed by convection after which a small concentration of oxygen can be allowed into the feed stream. As the oxygen initially oxidizes the carbon deposit near the reactor inlet the spent feedstream can only serve to raise the temperature of the remainder of the bed; consequently, oxygen concentration must be increased very gradually and only as the carbon concentration decreases. This is a very difficult procedure to control as it requires a dynamic balance between the oxygen concentration in the feed stream

and the temperature experienced in the bed; in other words it must ensure that the heat generated through the oxidation reaction is removed by convection.

Alternatively as it has been proposed in the present work, the regeneration can be conducted by the application of reverse propagation. If the cooling period is extended the reaction will be cooled from the inlet leaving a region of higher temperature near the exit. A preheated feed stream of air can then be introduced to the reactor, generating a reaction zone near the exit that propagate upstream by conduction through the solid phase along the reactor axis. The heat generated is therefore partially dissipated by conduction, the remainder is removed by convection.

1.4 Conditions for application of reverse operation.

Clearly the preliminary requirement is that the main reaction must be exothermic. For this reason all the experimental work on similar systems have been centred about oxidation reactions, from which it is possible to generate sufficient heat to ensure propagation at reactant concentrations that are attainable at atmospheric pressure.

The second condition requires that the catalyst must possess a relatively high activation energy so that with low inlet temperatures any significant reaction is precluded prior to the combustion zone.

It may be necessary to choose the diluent or support used for the catalytic agent for its coefficient of conductivity. Obviously too high a conductivity and the zone will disperse throughout the reactor. Alternatively,

too low a conductivity the reaction zone will be extinguished, and either the rate of deactivation will be faster than the rate at which fresh catalyst is exposed or the rate of convective heat transfer downstream will be much greater than the conduction upstream. In general the lowest conductivity in keeping with successful propagation is preferred as the temperature profile will then be closest to the ideal step function.

CHAPTER TWO

2. REVIEW OF THE LITERATURE.

2.1 Introduction.

This Chapter contains a theoretical and experimental review of the transient operation of reactors. Since studies of transient operations of reactors have been carried out with various objectives, emphasis is made here on the reverse operation investigations.

2.2 Previous Work on Similar Systems.

The earliest attempt to utilize a procedure similar to reverse operation was the experimental work of Reed et. al. (2) in which oil was recovered from tar sands by the in situ combustion of a fraction of the hydrocarbon deposit. As the heat generated by the oxidation of the hydrocarbon is sufficient to crack or vaporize the bulk of the immobile deposit, a highly upgraded oil can be produced from an exceedingly viscous deposit. If the reaction zone advances through the tar sand in the direction of the air flow the vaporized oil must flow into a relatively cold region; consequently, there is an upper limit on the viscosity of the oil that can be removed by this process.

On the other hand, if the reaction zone propagates in a direction opposite to the air flow the vaporized hydrocarbons flow through a region of the sand that has already been heated and which has had its liquid content eliminated. Therefore there is no upper limit to the viscosity of the oil;

indeed, the oil may be an entirely immobile semi-solid. The field application of the process does hinge on the existence of an adequate air permeability.

Reed, Warren and Price (15) simulated the reverse combustion of oil in tar sand, using as the basis for their work the adiabatic continuum model with axial diffusion effects in an infinite reaction region. The resulting partial differential equations were greatly simplified by physical approximations based upon flame propagation theory and the experimental observation of Reed et. al. (2).

During the experimental work it was noticed that the shape of the temperature and concentration profiles became independent of time and that they moved through the system at a constant velocity. Applying the quasi-steady state assumption, a moving co-ordinate system was introduced with a velocity equal to the velocity of propagation. This reduced the equations to a system of ordinary differential equations which were of a similar form to those of flame theory, but which differed in two significant respects. First, they are less closely coupled due to the presence of a large quantity of inert sand which absorbs and conducts the heat generated, making it impossible to assume equal effective mass and thermal diffusivities. Secondly, they are less general due to the absence of a fuel equation.

To make possible an explicit solution, the coupling of the equations is removed by a physical approximation to the source term. The approximation from the theory of flames, called the constant source of finite length, assumes the reaction rate is a function of temperature alone i.e. a zero order reaction. The constant rate version of the approximation assumes that above an ignition temperature the

rate is constant, until a maximum temperature is reached when the rate again becomes zero due to the depletion of reaction. A second version assumes that the reaction rate is a linear function of the temperature between the ignition and maximum temperatures. Despite the extensive simplifications obtained with these physical approximations, the resulting equations are able to represent the essential features of the reverse combustion.

Several mathematical artefacts were also presented, to allow numerical solutions to be developed for the quasi-steady state equations that required little computational effort. These numerical solutions are shown to be in closer agreement to the experimental data than the solution derived from the physical approximations that were presented above.

The experimental system of Reed et. al. (2) consisted of a stainless steel reaction tube filled with tar sands and fitted with thermocouples. The reactor was heated at one end by means of external heaters and air was introduced through the cold end. At the start of the combustion near the exit of the tube, external heating was stopped and the temperature profile recorded at regular intervals of time. Adiabatic conditions were not fully realized and often, if the temperatures generated beyond the working range, they were limited by external cooling. Even though the data lacked accuracy because of the experimental problems, some noteworthy conclusions were drawn which are listed below:

a) The velocity of propagation of the combustion zone was constant during a given run;

b) The average combustion zone velocity was found to be a linear function of the air flux;

c) Increasing the initial temperature profile caused an increase in the velocity of the reaction zone;

d) The average peak temperature attained during successful reverse combustion of most of tar sands could be adequately represented as a function of the air flux alone without being sensitive to the heat loss from the system.

The phenomena of "wandering combustion zones" in fixed bed reactors has been extensively studied both experimentally and theoretically by E. Wicke and D. Vortmeyer. Some of the essential results are presented in Wicke and Vortmeyer (1), Vortmeyer (16), Harting and Wicke (17) and Padberg and Wicke (3). The migration properties of the combustion zones have been investigated for several experimental systems based upon the catalytic oxidation reaction for either CO, C_2H_4 or C_2H_6. The emphasis was directed to the values of either the gas flow or reactant concentration that enabled the reaction zone to propagate in each particular axial direction. The characteristics of the transient behaviour were found to conform to the predictions from a model developed by analogy to the pure heat theory of flame propagation.

Wicke(18,19)and Wicke and Vortmeyer (1) carried out experimental investigations involving the oxidation of carbon monoxide with air over a platinum-carrier contact catalyst (0.3 weight per cent platinum on γ - $A\ell_2O_3$). These studies were conducted primarily to investigate the characteristics of the "wandering combustion zone". The investigation was entirely experimental and the observations included measuring the temperature inside and outside the catalyst pellets and determining the effective thermal conductivity of the system. Their study did not include the effect of the initial

reaction zone temperature on the velocity of reaction zone propagation. From the studies of Wicke and his co-workers, the following conclusions were drawn;

a) with exothermic reactions in adiabatic fixed bed reactors, characteristic unstable zones can occur which lead to ignition and quenching between the lower and higher operating conditions;

b) across a layer height of only a few catalyst particle diameters, there is almost complete conversion of the reactive mixture, accompanied by a steep temperature rise;

c) for a specific catalyst the effective axial thermal conductivity, which accounts for the propagation of the combustion zone, is a function of the gas flux only.

Wicke and Vortmeyer (1) have shown that the reaction zone may move through the tubular reactor in either axial direction. It was further demonstrated that the direction and velocity W of the zone depend heavily on the inlet gas velocity u_o and on the reactant concentration C_{Ao} . The experimental relationship is :

$$W = \alpha u_o^{0.77} \quad C_{Ao}^{0.5} - \beta u_o \qquad (2.1)$$

where α and β depend on other parameters of the system. Positive values of W denote movement against the gas flow while negative values indicate the reaction zone is being blown out of the reactor.

Vortmeyer and Jahnel (7 , 20) have simulated the "wandering combustion zones" investigated experimentally by Wicke and Vortmeyer (1) and Vortmeyer (16) with a homogeneous

one dimensional model that not only included second order mass and energy diffusion but also energy transport through radiation.

The reaction region is assumed to be infinitely long which allows a true quasi-steady state profile to be developed. This assumption enables the effects of various physical parameters upon the behaviour of the reaction zone to be investigated, without the result being influenced by the boundary conditions. Since the translation of the reaction zone was due to the energy transport and complete conversion was achieved within the reaction zone, the mass equation could be eliminated, once the quasi-steady state had been achieved by assuming a linear relationship between the conversion of the reactant and the temperature profile.

Vortmeyer and Jahnel (7) theoretical simulation included the effects of various physical parameters upon the velocity of propagation. They stated that such an investigation has many advantages, since it permits variation of parameters which are nearly impossible to change experimentally. Their results concerning the influence of these parameters on the velocity of reaction zones are as follows :

a) Since the radiative heat transfer supplements the conduction mechanism, the effect of its inclusion was to increase the velocity of propagation and slightly widen the propagation zone.

b) If the axial effective heat conduction was taken to be equal to

$$\bar{\lambda}^{e}_{ax} = \lambda_{axo} + 0.8\, u_o\, e_{go}\, \bar{C}_{pg}\, d$$

the exponents of correlation (2.1) is valid to be 0.77 for u_o and 0.5 for C_{Ao}. λ_{axo} , e_{go} , C_{pg} and d denote the gas heat conductivity, gas density at inlet temperature, the specific heat of gas and the catalyst particle diameter respectively.

c) Calculations with λ^e_{ax} = constant, results in a distorted curve with an exponent of 0.73 for feed velocity is obtained which is not in agreement with experimental evidence.

d) The axial mass diffusion processes are negligible in comparison with axial heat conduction.

e) Because conduction and radiation depend on catalyst particle diameter d, a slight influence of the particle diameter on the moving reaction zone velocity is noted. The functional relationship obtained between W and d is in the form,

$$W = \alpha' \; u_o^{0.77} \; C_{Ao}^{0.5} \; d^e - \beta u_o$$

an exponent e = 0.069 was found for the above correlation neglecting radiation, while inclusion of radiation the exponent is no longer constant. ($0.067 < e < 0.075$)

f) Different reaction kinetics do not change the exponents of u_o and C_{Ao} in correlation (2.1).

To assist in the design of an automatic control and shutdown system for the prediction of a commercial reactor from a developing hot spot, the spontaneous formation of a combustion zone was investigated by Berty et. al. (10). Of particular interest was the time lag before the reaction became uncontrolled and the subsequent rate of backward migration of the ignition zone. The numerical simulation

of the pilot plant studies which were based upon the oxidation of hydrocarbons , was able to predict the major characteristics of the observed transients.

In their work instead of the traditional continuum model, the one dimensional two phase cell model of Vanderveen Luss and Amundson (21) was used. The two phases of each cell can then be described by four ordinary differential equations in time. The assumptions that the reaction is wholly contained in the catalyst and that the cell to cell coupling is achieved solely through particle to particle radiative heat transfer are made. Intercell fluid transport properties are by convection with no axial dispersion and interphase mass and energy transfer is lumped into the approximate film coefficients.

The model was able to reproduce the most significant features of the experimentally observed transient zone with the shape of the profiles and the average rate of zone migration satisfactorily matching the experimental data. It should be noted that the number of spatial mesh points required to achieve sufficient accuracy (approximately sixty) is such that the model has approached the formulation of a continuum model spatially discretized by a differential difference approximation.

Eigenberger (8) modelled the "wandering combustion zones" of Wicke and Padberg (3) to investigate the multiplicity of steady states in catalytic fixed-bed reactors. A continuous two phase model similar to that of Liu and Amundson (22,23) was used except that it has been extended to account for the effect of heat conduction in the catalyst phase. It was assumed that heat conduction occurs only by direct contact

of the catalyst and any through the stationary fluid interstices was neglected. The fluid mass and energy balances are represented by first order hyperbolic partial differential equations coupled to the catalyst phase, where the reaction and conduction occur, by transfer terms. The effect of several boundary conditions for the catalyst phase at the inlet of the finite bed were investigated. These included the adiabatic condition, a boundary condition accounting for radiative heat loss from the catalyst phase at the reactor inlet and the introduction of inert packing before and after the inert bed. The first two of these conditions allowed the formation of a third steady state that could not be achieved with the latter boundary condition and which has not been isolated experimentally. The transient behaviour predicted was that of a reactor in which the reaction zone could propagate in either axial direction. Eigenberger (8) concluded that the foremost influence for this behaviour is the conduction of heat in the solid phase, and that the transient propagation of the reaction zone is primarily a transition from one state to another stable steady-state. The number of possible stable steady-states in a given configuration is also discussed. By allowing for heat conduction in the solid phase, the infinite number of steady-states predicted by early two-phase models (22) is reduced to two or three depending upon the exact configuration and the boundary conditions chosen.

Venkatachalam (25) applied the reverse operation to a catalytic reactor in which carbon monoxide was oxidized over a cupric oxide catalyst. Unfortunately the experimental results were so corrupted by heat loss, nearly fifty per cent of heat generated. In fact maintaining the adiabatic

conditions has proved to be a major experimental difficulty, with heat losses experienced by Berty et. al. (10) and overcome by Wicke and Vortmeyer (1) only by the construction of an oven that moved along the reactor axis with the ignition zone. As far as can be determined the sources of the heat loss suffered by Venkatachalam (25) were the connecting pipework, the large thermocouple shields and the compression fittings.

In the theoretical investigation of his experimental work on reverse operation, Venkatachalam (25) employed a one dimensional homogeneous model in which the sole mechanism for transporting energy upstream was conduction. The system equations and the inlet boundary conditions did not account for the fact that once past the entrance plane, only the void volume is available to the gas flow. This error effectively removes the conductive flux term from the Dankwerts boundary conditions used so that $\bar{T} \simeq \overset{+}{T}$ and weights too highly the convection and source terms in the energy equation. While an attempt was made to include the effect of gas expansion due to the large temperature rise, by allowing the gas velocity to be a linear function of temperature, the effect upon the concentration was neglected. The following conclusions outlined below are drawn from his work.

a) The model describes the experimental observations of Reed et. al. (2) on the reverse propagation of tar sand beds with an in-situ combustion of the oil present.

b) A higher initial ignition temperature increases the velocity of propagation of the reaction zone.

c) The average peak temperature during the reverse propagation and the average reaction zone velocity both vary

linearly with gas flux.

Earp and Kershenbaum (26) carried out a theoretical study on the optimal temperature profiles in a tubular reactor for several catalyst decay laws and demonstrated that in certain systems with decaying catalysts, a reaction zone moving in a direction counter to that of the flow of fluid can be close to the optimum operating method for that system. For the investigation of the transient behaviour of reverse operation a quasi-homogeneous, one dimensional model was developed in which the propagation of the high temperature zone was assumed to occur by conduction through the solid phase. Since the feed undergoes a severe temperature rise in the reaction zone, first order expansion effects were included in the second order non-linear partial differential equations that represented the mass and energy balances. Several catalyst deactivation mechanisms were considered of which only one was a function of present conversion. Using both quasi-linearization technique and finite difference technique a solution was generated for the complete model. When this solution was compared to that for a simplified model in which the accumulation of axial dispersion terms in the mass balance equation were neglected, there was a negligible difference. These approximations allowed the use of more accurate integration techniques, decreased the computation time required for a solution and reduced the mass balance equation to a first order hyperbolic form.

The optimal time and space dependent temperature history was generated for a tubular reactor represented by first order hyperbolic equation with different catalyst decay laws. The solution revealed that a critical parameter is the ratio

of the activation energy for the main reaction to that for the catalyst decay reaction. For the value of this ratio less than one, the optimal policy consisted of an isothermal or near isothermal reaction zone that occupied the entire active bed and whose temperature was slowly raised with time to counteract the loss in catalyst activity. However, where this ratio is greater than one, high reaction zone temperatures are preferred, so that for the same level of conversion the reaction zone need only extend over a fraction of the active bed. The optimal policy then consists of a short, high temperature reaction zone that can propagate along the axial direction as the previously exposed catalyst decays. The remainder of unused bed is kept at sufficiently low temperature to prevent any needless deactivation. Finally, Earp and Kershenbaum (26) demonstrated that for the system in which the decay law is independent of conversion, propagation in either co-current or counter-current direction was optimal. However with the introduction of the dependency upon conversion into the decay law the counter-current operation becomes the only true optimal policy.

CHAPTER THREE

3. MATHEMATICAL FORMULATION AND NUMERICAL SOLUTION FOR REVERSE OPERATED TUBULAR REACTORS.

3.1 Equations for reverse operation.

R.G. Earp (27) developed a model for the prediction of the temperature and concentration profiles for adiabatic catalytic reactors subject to catalyst decay. The model has been extended here to include the non-adiabatic behaviour of catalytic reactor (i.e. the heat losses from the system to the surroundings), and the electrical heat input to the system for the purpose of preheating the feed flow which is more nearly corresponding to the experimentation.

3.1.1 Assumptions.

The following assumptions will be made, that

a) A quasi-homogeneous one dimensional model is applied.

b) A single phase model is used in describing the behaviour of the reactor.

c) The dominant energy transport is to be conduction along the axis of the reactor.

d) The axial conduction and diffusion processes under transient conditions may be evaluated from the Fourier and Fick equations.

e) The catalyst is of uniform size and voidage.

f) The Danckwerts type boundary conditions are to be

used with the assumption that the free area normal to the flow is assumed equal to the voidage times the cross sectional area.

g) There is negligible pressure drop due to flow resistance.

Assumption (a) implies that the radial concentration and temperature effects can be neglected. This can be justified considering that the radius of the reactor is small and there is no appreciable heat transfer across the wall of the reactor.

Assumption (b) implies that there was no bulk gas concentration and temperature gradients. This indicates that the kinetics of the reaction is the rate controlling step, hence mass transfer within the catalyst may be neglected. On the other hand the gas flowrate is such that the local heat transfer coefficient is so great that there is negligible temperature gradient across the gas phase and the catalyst surface.

Assumption (c) indicates that the local heat transfer process is due to conduction only i.e. there is a negligible radiative heat transfer.

3.1.2 Differential mass and energy processes.

Within a differential volume of the reactor, the unsteady state of mass and energy balance on reactant A is:

$$(A)_{\text{Accumulated}} = (A_{IN} - A_{OUT})_{\text{by axial dispersion}} + (A_{IN} - A_{OUT})_{\text{by bulk flow}} - (A_{CONSUMED})_{\text{by reaction}}$$

Accumulation of energy = (Energy in-Energy out)-(Energy in-Energy out)

by conduction by convection

+ Reaction + Electrical heat input

- heat losses

Hence the differentical equations governing mass and energy transfers are :

$$\frac{\partial C'_A}{\partial t} = \frac{\partial}{\partial \ell} (C\, D_{AB} \frac{\partial X_A}{\partial \ell}) - \frac{\partial}{\partial \ell} (C'_A\, u') - r\,(T, C'_A, a') \qquad (3.1)$$

$$\frac{\partial}{\partial t} ((\rho C_p)_e T) = \frac{\partial}{\partial \ell} (-K_e \frac{\partial T}{\partial \ell}) - \frac{\partial}{\partial \ell} (u' \rho_g C_{pg} T)\varepsilon$$

$$+ (-\Delta H).\, r\,(T, C'_A, a')\varepsilon + \underset{(\text{IF ANY})}{Q'} - \frac{4U}{D_i} (T - T_a) \qquad (3.2)$$

With the boundary conditions

$$\text{at } \ell = o \quad u' C'_A - D_{AB}\, C \frac{\partial X_A}{\partial \ell} = u_o C_A = \frac{u_\ell C_A}{\varepsilon} \qquad (3.3)$$

$$u' \rho_g C_{pg} T\varepsilon - K_e \frac{\partial T}{\partial \ell} = u_o \rho_{go} C_{pgo} T_o \varepsilon \qquad (3.4)$$

$$\text{at } \ell = L \quad \frac{\partial C'_A}{\partial \ell} = O \qquad (3.5)$$

$$\frac{\partial T}{\partial \ell} = O \qquad (3.6)$$

3.1.3 Temperature effects and dimensionless variables.

Some modifications were necessary before equations 3.1 and 3.2 could be easily solved. Since the molar flowrate is independent of temperature, it is preferable to work in terms of moles and a dimensionless fractional conversion rather than in concentration. Although temperature expansion is usually neglected Earp (27) has shown that with the gas stream subject to a severe temperature rise in the reaction zone, the volume expansion will be significant (order of 100%) and that the linear and volumetric flowrate will not be constant. Therefore further assumptions are required for the mass and energy equations which are listed below:

a) The feed stream is dilute, so that the molar flowrate is to remain constant for the simple stoichiometry of CO oxidation. Using an air to CO ratio of 7:1, the effect of reduction in the number of moles is approximately 6%.

b) The perfect gas law is assumed to apply to the gas stream.

c) The thermodynamic properties will be represented by mean quantities. The mass Peclet number is assumed independent of the temperature. This is not strictly true but since dispersion represent a second order effect, little error is introduced.

3.1.4. Oxidation of carbon monoxide.

For the oxidation of carbon monoxide the stoichiometric equation is

$$C + \frac{1}{2} O_2 \rightarrow CO_2$$

(A) (B) (C)

$$r = K_o \; C'_A \; C'_B \; a' \; \exp\left(-\frac{E}{RT}\right)$$

Defining the fractional conversion of reactant A to be

$$Y = \frac{M_{Ao} - M_A}{M_{Ao}}$$

Then $$X_A = X_{Ao} \; (1-Y)$$

$$X_B = \frac{X_{Ao}}{2} \; (M-Y)$$

Applying the ideal gas law

$$C'_A = C_o T_o \; X_{Ao} \; \frac{(1-Y)}{T}$$

$$C'_B = C_o T_o \; \frac{X_{Ao}}{2} \; \frac{(M-Y)}{T}$$

$$u' = u_o \; \frac{T}{T_o}$$

Since it is assumed that the Peclet number is independent of temperature then

$$\frac{D_{AB}}{T} = \frac{Do}{T_o}$$

where M_A = molar flowrate of A (CO)

M_B = molar flowrate of B (O_2)

X_{Ao} = molar fraction of A at feed conditions

$M = \frac{2M_{Bo}}{M_{Ao}}$

D_o = mass diffusivity at feed conditions

3.1.4.1 Mass balance equation.

The mass balance equation 3.1 becomes

$$-\frac{\partial}{\partial t}\left(\frac{1-Y}{T/T_o}\right) = D_o \frac{\partial^2 Y}{\partial \ell^2} - u_o \frac{\partial Y}{\partial \ell} + a' K_o \frac{C_{Ao}}{2} \frac{(1-Y)}{T/T_o} \frac{(M-Y)}{T/T_o} \exp\left(-\frac{E}{RT_o} \cdot \frac{T_o}{T}\right) \qquad (3.7)$$

with the boundary conditions

$$Y - \frac{D_o}{u_o} \frac{\partial Y}{\partial \ell} = 0 \qquad \text{at } \ell = 0 \qquad (3.8)$$

$$\frac{\partial Y}{\partial \ell} = 0 \qquad \text{at } \ell = L \qquad (3.9)$$

Multiplying through by $\frac{L}{u_o} = \tau$ and using,

$\Theta = \frac{t}{\tau}$ = dimensionless time.

$a = a'/a_o$ = ratio of present catalyst activity to initial activity.

$z = \ell/L$ = dimensionless distance.

$\emptyset = T/T_o$ = dimensionless temperature.

$J = E/RT_o$ = dimensionless activation energy group.

$P' = \frac{u_o L}{D_o}$ = Peclet number for mass transfer.

$G_1 = \frac{a_o K_o L C_{Ao}}{2 u_o}$ = dimensioness reaction rate group.

so that equation 3.7 in dimensionless form becomes

$$-\frac{\partial}{\partial\Theta}\frac{(1-Y)}{\emptyset} = \frac{1}{P'}\frac{\partial^2 Y}{\partial z^2} - \frac{\partial Y}{\partial z} + aG_1(1-Y)(M-Y)\frac{\exp(-J/\emptyset)}{\emptyset^2} \qquad (3.10)$$

with the boundary conditions

$$\frac{1}{P'}\frac{\partial Y}{\partial z} - Y = 0 \qquad \text{at} \quad z = 0 \qquad (3.11)$$

$$\frac{\partial Y}{\partial z} = 0 \qquad \text{at} \quad z = 1 \qquad (3.12)$$

3.1.4.2 Energy balance equation.

For the energy equation $(\rho C_p)_e$, K_e , C_{pg} and $\rho_g u'$ are assumed independent of temperature so that equation 3.2 becomes

$$\frac{\partial(T/T_o)}{\partial t} = \frac{K_e}{(\rho C_p)_e}\frac{\partial^2(T/T_o)}{\partial \ell^2} - \frac{\rho_{go} C_{pg}}{(\rho C_p)_e} u_o \varepsilon \frac{\partial(T/T_o)}{\partial \ell}$$

$$+ \frac{(-\Delta H)}{(\rho C_p)_e} \frac{a_o K_o \varepsilon}{2} \frac{C_{Ao}^2 X_{Ao}^2}{T_o} \frac{(1-Y)}{\phi} \frac{(M-Y)}{\phi} a \exp\left(-\frac{E}{RT_o} \cdot \frac{T_o}{T}\right)$$

$$+ \frac{P''}{\pi/4 D_i^2 L_2} \cdot \frac{1}{(\rho C_p)_e T_o} - \frac{4U}{D_i (\rho C_p)_e} \cdot \left(\frac{T - T_a}{T_o}\right) \qquad (3.13)$$

with the boundary conditions

$$\frac{T}{T_o} - \frac{K_e}{u_o \rho_{go} C_{pg} \varepsilon} \frac{\partial}{\partial \ell} (T/T_o) = 1 \qquad \text{at } \ell = 0 \qquad (3.14)$$

$$\frac{\partial T}{\partial \ell} = 0 \qquad \text{at } \ell = L \qquad (3.15)$$

Defining the following dimensionless group

$$P = \frac{u_o L}{K_e/(\rho C_p)_e} = \text{Peclet number for axial energy transport.}$$

$$B = \frac{\rho_{go} C_{pg} \varepsilon}{(\rho C_p)_e} = \text{dimensionless convection group.}$$

$$Q_1 = \frac{(-\Delta H) K_o a_o C_{Ao}^2 L \varepsilon}{2 u_o (\rho C_p)_e T_o} = Gl \cdot \left(\frac{(-\Delta H) C_{Ao} \varepsilon}{(\rho C_p)_e T_o}\right)$$

$$U_1 = \frac{4U}{D_i} \frac{L}{u_o (\rho C_p)_e} = \text{dimensionless heat loss group.}$$

$$A = \frac{P''}{\pi/4 D_i^2 L_2} \cdot \frac{L}{u_o (\rho C_p)_e T_o} = \text{dimensionless rate of electrical heat input.}$$

so that equation 3.13 in dimensionless form becomes

$$\frac{\partial \phi}{\partial \Theta} = \frac{1}{P} \frac{\partial^2 \phi}{\partial z^2} - B \frac{\partial \phi}{\partial z} + Q_1 (1-Y)(M-Y) a \frac{\exp(-J/\phi)}{\phi^2}$$

$$+ A - U_1 (\phi - \phi_a) \qquad (3.16)$$

with the boundary conditions

$$\phi - \frac{1}{PB} \frac{\partial \phi}{\partial z} = 1 \qquad \text{at } z = 0 \qquad (3.17)$$

$$\frac{\partial \phi}{\partial z} = 0 \qquad \text{at } z = 1 \qquad (3.18)$$

3.1.5 Oxidation of carbon.

For the carbon oxidation the stoichiometric equation is

$$\underset{(D)}{C} + \underset{(E)}{O_2} \rightarrow \underset{(F)}{CO_2}$$

$$r = K'_o \; P_E \exp(-E/RT)$$

where

P_E = oxygen partial pressure = $C'_E RT$

The rate of reaction is assumed to be first order with respect to oxygen concentration, and zero order w.r.t. carbon concentration. This assumption is based on the presence of excess carbon.

3.1.5.1 Mass and energy balance equations.

Defining the fractional conversion of reactant E to be

$$Y_1 = \frac{M_{Eo} - M_E}{M_{Eo}}$$

using the same assumptions as before, and applying the ideal gas law, the equations in dimensionless form are as follows

$$-\frac{\partial\left(\frac{1-Y_1}{\phi}\right)}{\partial\Theta} = \frac{1}{P'}\frac{\partial^2 Y_1}{\partial z^2} - \frac{\partial Y_1}{\partial z} + G_2(1-Y_1)\frac{\exp(-J/\phi)}{\phi} \qquad (3.19)$$

and

$$\frac{\partial\phi}{\partial\Theta} = \frac{1}{P}\frac{\partial^2\phi}{\partial z^2} - B\frac{\partial\phi}{\partial z} + Q_2(1-Y_1)\frac{\exp(-J/\phi)}{\phi}$$

$$+ A' - U_1'(\phi - \phi_a) \qquad (3.20)$$

where

$$G_2 = \frac{K_2 L}{u_o}$$

$$Q_2 = \frac{(-\Delta H) K_2 \, L \, \varepsilon \, C_{Eo}}{u_o (\rho C_p)_e T_o} = G_2 \cdot \frac{(-\Delta H) \, \varepsilon \, C_{Eo}}{(\rho C_p)_e \, T_o}$$

$$A' = \frac{P''}{\pi/4 D_i^2 L_2} \cdot \frac{L}{u_o (\rho C_p)_e T_o} = \text{dimensionless rate of electrical heat input.}$$

$$U_1' = \frac{4U'}{D_i} \cdot \frac{L}{u_o (\rho C_p)_e}$$

3.1.6 Carbon burning rate.

It is important to know the burning rate of carbonaceous deposit accumulated on solid particles. This information is required for use in evaluating the mathematical model of regeneration. Literature reports of the burning rate of coke on cracking catalysts give widely different results, (28). Weisz and Goodwin (29) reported that for a given support, the rate of carbon burn off is largely independent of the source and structure of the catalyst. They further concluded that coke deposited on supports made of oxides of silica, alumina, and magnesia gives a minimum rate of burning at any given temperature and exhibits similar burning kinetics. Also the kinetics of coke burning on these supports showed both quantitative and qualitative resemblences to the combustion of pure graphite, and suggest the existence of a basic, uncatalyzed burning rate of such oxides. Gonzalez and Spencer (30) who worked on two different catalysts reported that the burning rates are affected by both the nature of the carbonaceous deposit and the surface of the

supporting solid. It is necessary therefore, to conduct laboratory experiment with the particular solid under study. However in the present work these studies were excluded, therefore the required information was obtained from literature (31).

The rate of carbon burning is represented by

$$\frac{dc}{dt} = - K_2 C'_E \exp\left(- \frac{E}{RT}\right) \qquad (3.21)$$

in dimensionless form

$$\frac{dc}{d\Theta} = - K_3 C_{Eo} (1-Y_1) \frac{\exp(-J/\phi)}{\phi} \qquad (3.22)$$

where $K_3 = \frac{K_2 L}{u_o}$

3.2 System Constants.

Tables 3.1 and 3.2 present the numerical values for various parameters used throughout this work which are based upon the oxidation of carbon monoxide over cupric oxide catalyst, and oxidation of carbon deposited on Alumina-Silica cracking catalyst respectively.

Gunn (32) has reported that for a particle Reynold's number greater than one the axial mass transport Peclet number P' based on the particle diameter is greater than or equal to 2.0, reaching, in the range $1 < Re < 20$, a maximum of 3.0.

For carbon monoxide oxidation over cupric oxide catalyst with the length to effective particle diameter ratio

of approximately 900, the Peclet number based on the reactor length will be assumed to be $2. \times 10^3$. With the length to effective particle diameter ratio of 300 for Alumina-Silica catalyst the Peclet number based on the reactor length will be assumed to be $8.\times10^2$. Since a relatively high value of Peclet number for axial mass transport (P') is used, Earp (27) demonstrated that the axial mass dispersion can be neglected for a Peclet number in this range despite the steep temperature gradients in the reaction zone. The use of the plug flow assumption reduced the computer time by one third. Vortmeyer and Jahnel (7) in order to show the generalized effect of mass diffusion have also performed calculations for P' (based on the particle diameter) = 1,2,3 and $P' = \infty$ and showed that there are only very small differences between the results for P'= 3 and $P' \to \infty$ ($D_o = 0$), and concluded that axial mass diffusion processes are negligible in comparison with axial heat conduction.

3.3 Numerical Solutions.

Equations 3.10 and 3.16 (also 3.19 and 3.20) are coupled, non-linear parabolic partial differential equations which can be solved by a variety of available numerical methods. The method adopted for numerical solution here, was the procedure carried by R.G. Earp (27). In that work several methods were tried, but the most efficient one was an iterative implicit technique which results from a quasi-linearization of the equations and subsequent application of the Crank-Nicholson algorithm for finite differences. The non-linear elements in equations arise

TABLE 3.1

SYSTEM CONSTANTS

CARBON MONOXIDE OXIDATION

$L = 0.6$ m

$\varepsilon = 0.48$

$\rho_{go} = 4.08 \times 10^{-2}$ K mol/m^3

$\rho_s = 6.4 \times 10^3$ Kg/m^3

$C_{pg} = 2.93 \times 10^4$ J/K mol ^oK

$C_{ps} = 4.438 \times 10^4$ J/K mol ^oK

$(\rho C_p)_e = 185.85 \times 10^4$ J/m^3 ^oK

$$B = \frac{\rho_{go} C_{pg} \varepsilon}{(\rho C_p)_e} = 3.07 \times 10^{-4}$$

$E = 3.6 \times 10^7$ J/ K mol

$R = 8.314 \times 10^3$ J/K mol ^oK

$\Delta H = -2.83 \times 10^8$ J/K mol

$K_o = 3.165 \times 10^6$ m^3/K mol s

$$J = \frac{E}{RT_o} = 4.33 \times 10^3 \quad (1/T_o)$$

$$G_1 = \frac{K_o L C_{Ao}}{2u_o} = 0{,}9495 \times 10^6 \quad (C_{Ao}/u_o)$$

$$Q_1 = \frac{G_1(-\Delta H C_{Ao} \varepsilon)}{(\rho C_p)_e T_o} = 2{,}343 \times 10^5 \quad (C_{Ao}^2/u_o)$$

$A = 0.0$

TABLE 3.2

SYSTEM CONSTANTS

CARBON OXIDATION

$L = 0.6 \quad m$

$L_2 = 0.45 \quad m$

$\varepsilon = 0.52$

$\rho_{go} = 2.0 \times 10^{-2} \quad K\ mol/m^3$

$\rho_s = 1.05 \times 10^3 \quad Kg/m^3$

$C_{pg} = 2.93 \times 10^4 \quad J/K\ mol\ ^oK$

$C_{ps} = 18.84 \times 10^4 \quad J/K\ mol\ ^oK$

$(\rho C_p)_e = 162.21 \times 10^4 \quad J/m^3\ ^oK$

$$B = \frac{\rho_{go}\ C_{pg}\ \varepsilon}{(\rho C_p)_e} = 1.88 \times 10^{-4}$$

$E = 10.969 \times 10^7 \quad J/K\ mol$

$R = 8.314 \times 10^3 \quad J/K\ mol\ ^oK$

$\Delta H = -3.882 \times 10^8 \quad J/K\ mol$

$K_2 = 0.92 \times 10^8 \quad s^{-1}$

$$K_3 = \frac{K_2 L}{u_o} = 0.552 \times 10^8 \ (1/u_o)$$

$$J = \frac{E}{RT_o} = 13.1934 \times 10^3 \ (1/T_o)$$

$$G_2 = \frac{K_2 L}{u_o} = 0.552 \times 10^8 \ (1/u_o)$$

$$Q_2 = \frac{G_2(-\Delta H\ C_{Eo}\ \varepsilon)}{(\rho C_p)_e\ T_o} = 68.694 \times 10^8 \ (C_{Eo}/T_o u_o)$$

in the reaction terms, and in the accummulation term of the mass equation. Linearization results where these terms are expanded in a Taylor's series about the previous estimate of them at any time or position and is led directly to an iterative calculation at each time interval, Lee (33). Because of the iterative nature of the solution, the usual procedure at this point is to uncouple the two equations by replacing $\emptyset$ in equation 3.10 and Y in equation 3.16 by their (known) values at the previous iteration. Then equation 3.10 need only be linearized with respect to conversion and equation 3.16 with respect to temperature.

The numerical algorithm used by Earp (27) is briefly outlined here. In any continuous function $F(\underline{x})$, non-linear with respect to variable $\underline{x}$, the quasi-linearization approximation is the expansion in a Taylor series about the previous estimate, at any time or position, neglecting second order and higher terms

$$F(\underline{x}^{n+1})_m = F(\underline{x}^n) + \left(\frac{\partial F}{\partial \underline{x}} \right)^n (\underline{x}^{n+1} - \underline{x}^n) \qquad (3.23)$$

where n denotes the n^{th} iteration at time step m. This leads directly to an iterative calculation at each time interval but if $\underline{x}^n$ is known then the right hand side of (3.23) will always be linear.

At this point there exists a choice between attempting to solve the entire coupled system as one or uncoupling the equations and solving each separately. Initially the equations will be uncoupled by setting the j^{th} variable

$x_j^{n+1} = x_j^n$ for $j \neq i$ in the i^{th} equation. Since $x_j^n \to x_j^{n+1}$ as the system of uncoupled equation converges, little additional error should be introduced. Thus equation i need only be linearized with respect to x_i.

In each iteration the state equations must be solved in some sequence and to reflect this the notation above should strictly be, $x_j^{n+1} = x_j^n$ for $j > i$ with x_j^{n+1} used for $j < i$ in the $(n+1)^{st}$ iteration. That is, the latest information is always used in the numerical evaluations; however, to avoid confusion the simpler notation will be used throughout.

Applying this partial linearization technique to the non-linear source term of equation 3.10 results in (CO oxidation over cupric oxide catalyst).

$$-\frac{\partial}{\partial\Theta}(1-Y^{n+1})/\phi^n = \frac{1}{P}\left[\frac{\partial^2 Y^{n+1}}{\partial z^2} - \frac{\partial Y^{n+1}}{\partial z}\right] + \xi_1^n (M-Y^n)^2 + (2Y^n - M - 1)\, Y^{n+1}). \qquad (3.24)$$

where $\xi_1^n = G_1 a^n \dfrac{e^{-J/\phi^n}}{\phi^{n^2}}$

Also applying this procedure to the source term, equation 3.16 becomes

$$\frac{\partial\phi^{n+1}}{\partial\Theta} = \frac{1}{P}\frac{\partial^2\phi^{n+1}}{\partial z^2} - B\frac{\partial\phi^{n+1}}{\partial z} + \xi_2^n\left(3\phi^n - J + \frac{(J-2\phi^n)}{\phi^n}\phi^{n+1}\right) - u_1(\phi^n - \phi_a) + A \qquad (3.25)$$

where $\xi_2^n = Q_1 a^n (1-Y^n)(M-Y^n)\dfrac{e^{-J/\phi^n}}{\phi^{n^3}}$.

Applying the partial linearization technique to the non-linear source term of 3.19 results in (for carbon burning in regeneration process)

$$-\frac{\partial}{\partial\Theta}(1-Y_1^{n+1})/\phi^n = \frac{1}{P}\,\frac{\partial^2 Y_1^{n+1}}{\partial z^2} - \frac{\partial Y_1^{n+1}}{\partial z} + \xi_3^n\,(1-Y_1^{n+1}) \qquad (3.26)$$

where $\xi_3^n = G_2 . a^n \; \dfrac{e^{-J/\phi^n}}{\phi^n}$

Source term equation becomes

$$\frac{\partial\phi^{n+1}}{\partial\Theta} = \frac{1}{P}\,\frac{\partial^2\phi^{n+1}}{\partial z^2} - B\,\frac{\partial\phi^{n+1}}{\partial z} + \xi_4^n\left[(2\phi^n - J) + \left(\frac{J-\phi^n}{\phi^n}\right)\phi^{n+1}\right]$$

$$- U_1\,(\phi^n - \phi_a) + A' . \qquad (3.27)$$

where $\xi_4^n = Q_2\, a^n\,(1 - Y_1^n)\;\dfrac{e^{-J/\phi^n}}{\phi^{n^2}}$

If the time axis $0 \leq \Theta \leq \Theta_m$ is divided into intervals of s and the space axis $0 \leq z \leq 1$ is divided into γ equidistant intervals h, then

$f(\underline{x})_{r,m}$ denotes the value of $f(\underline{x})$ at a position $z = rh$ and at a time $\Theta = ms$. Allowing the notation $f(r,m) = f(\underline{x})_{r,m}$, then to the linear uncoupled partial equations 3.24 and 3.25 the following 6 point implicit formulae are applied.

$$\frac{\partial f^{n+1}}{\partial \theta}(r,m+\tfrac{1}{2}) = \frac{f^{n+1}(r,m+1) - f(r,m)}{s} \tag{3.28}$$

$$\frac{\partial^2 f^{n+1}}{\partial z^2}(r,m+\tfrac{1}{2}) = \frac{1}{2h^2}\,(f^{n+1}(r+1,m+1) - 2\,f^{n+1}(r,m+1) + f^{n+1}(r-1,m+1) + f(r+1,m) - 2f(r,m) + f(r-1,m)) \tag{3.29}$$

$$\frac{\partial f^{n+1}}{\partial z}(r,m+\tfrac{1}{2}) = \frac{1}{4h}\,(f^{n+1}(r+1,m+1) - f^{n+1}(r-1,m+1) + f(r+1,m) - f(r-1,m)) \tag{3.30}$$

$$f^{n+1}(r,m+\tfrac{1}{2}) = \tfrac{1}{2}\,(f^{n+1}(r,m+1) + f(r,m)) \tag{3.31}$$

Since the values at time step m are known, the superscript (n+1) which denotes the $(n+1)^{st}$ iteration has no meaning for $f(\underline{x})$ at the m^{th} time step. At any instant in time, the use of the finite difference formulae generates a system of linear algebraic equations for successive grid points. For example, substitution of equations 3.28 to 3.31 into equation 3.24 and its boundary conditions 3.11 and 3.12 yields for $0 \leq r \leq \gamma$

$$C_1 Y^{n+1}(r-1,m+1) + C_2\,Y^{n+1}(r,m+1) + C_3 Y^{n+1}(r+1,m+1) = -\,C_1 Y(r-1,m) - C_4 Y(r,m) - C_3 Y(r-1,m) - \Omega^n \tag{3.32}$$

with

$$C_1 = \left(\frac{1}{2Ph^2} + \frac{1}{4h} \right)$$

$$C_2 = \left(\frac{\alpha^n(r,m+1)}{2} - \frac{1}{Ph^2} - \frac{1}{\phi^n(r,m+1)s} \right)$$

$$C_3 = \left(\frac{1}{2Ph^2} - \frac{1}{4h} \right)$$

$$C_4 = \left(\frac{\alpha(r,m)}{2} - \frac{1}{Ph^2} + \frac{1}{\phi(r,m)s} \right)$$

$$\alpha^n(r,m+1) = \xi_1^n \left(2Y^n(r,m+1) - M - 1 \right)$$

$$\beta^n(m+1) = \xi_1^n (M - Y^{n^2}(r,m+1)$$

$$\Omega^n = \frac{\beta^n(m+1) + \beta(m)}{2} + \frac{1}{s} \left(\frac{1}{\phi^n(r,m+1)} - \frac{1}{\phi(r,m)} \right)$$

At the reactor boundaries the finite difference approximations of the boundary conditions are used to remove the imaginary points at r = -1 and r = γ+1 so that :

at r = 0

$$(C_2 - 2PhC_1)\, Y^{n+1}(o,m+1) + (C_3 + C_1)\, Y^{n+1}(1,m+1)$$

$$= - (C_4 - 2PhC_1)\, Y\,(o,m) - (C_3 + C_1)\, Y\,(1,m) - \Omega^n \qquad (3.33)$$

and at $r = \gamma$

$$C_1 Y^{n+1}(\gamma-1, m+1) + (C_2+C_3) Y^{n+1}(\gamma,m+1)$$

$$=-C_1 Y(\gamma-1,m) - (C_4+C_3) Y(\gamma,m) - \Omega^n \qquad (3.34)$$

An analagous set of equations can be obtained for the energy balance.

These finite difference approximations to the partially linearized state equations can be represented by two linear independent tri-diagonal matrix equations which can be solved by either a Gauss-Seidel or Gaussian elimination algorithm.

The best overall technique (from the point of view of accuracy and speed) appeared to be a Gaussian elimination for the conversion equation and Gauss-Seidel iteration for the temperature equation. The resulting solution were clear of oscillation, insensitive to P' and stable with increasing time axis mesh point s.

The spatial axis was divided into 100 equal intervals. The mesh points for the time axis were unevenly distributed, being much finer at the start (.1), but increased by a factor of 1.3 every 20 time step.

In the carbon oxidation simulation the solution indicated instability with increasing time axis mesh point. The instability in the solution was removed by allowing the mesh points to increase until a maximum of s=3.0 was reached.

The convergence cirterion for the time step iteration was set at a relative error of .001

CHAPTER FOUR

4. EXPERIMENTAL SYSTEM.

In this chapter, the experimental system for the measurement and control of the moving reaction zones subject to reverse propagation is discussed in detail. The reactions studied were oxidation of carbon monoxide over a cupric oxide catalyst, and the regeneration of the fouled cracking catalyst (Alumina-Silica). During the regeneration the deposit of carbon that causes the deactivation of the catalyst was removed through the oxidation to CO and CO_2.

4.1 Materials.

The catalyst used for the CO oxidation was cupric oxide, and as such provided the solid phase for the propagation of the reaction zone. The catalyst was in the form of thin cylindrical wires (2mm. long and 0.5mm diameter) with an equivalent diameter of 0.66mm. The catalyst was Baker reagent grade cupric oxide, number 1820. Impurities of the catalyst reported by the manufacturer in the form of carbon compounds (as C), nitrogen compounds (as N_2) and sulphur compounds (as SO_4) were less than 0.003%.

The catalyst was analysed for impurities using X-ray fluorescence spectroscopy. The impurities detected were iron, Fe, Calcium, Ca, and aluminium Al. Microprobe analysis were performed on the catalyst and the result indicated that the catalyst was not purely CuO and that it contained 13.2% by weight Cu_2O.

CO and air were the reactants for the oxidation reaction. The air used was dry and the CO was 99.5% pure (the impurities were mainly nitrogen and argon).

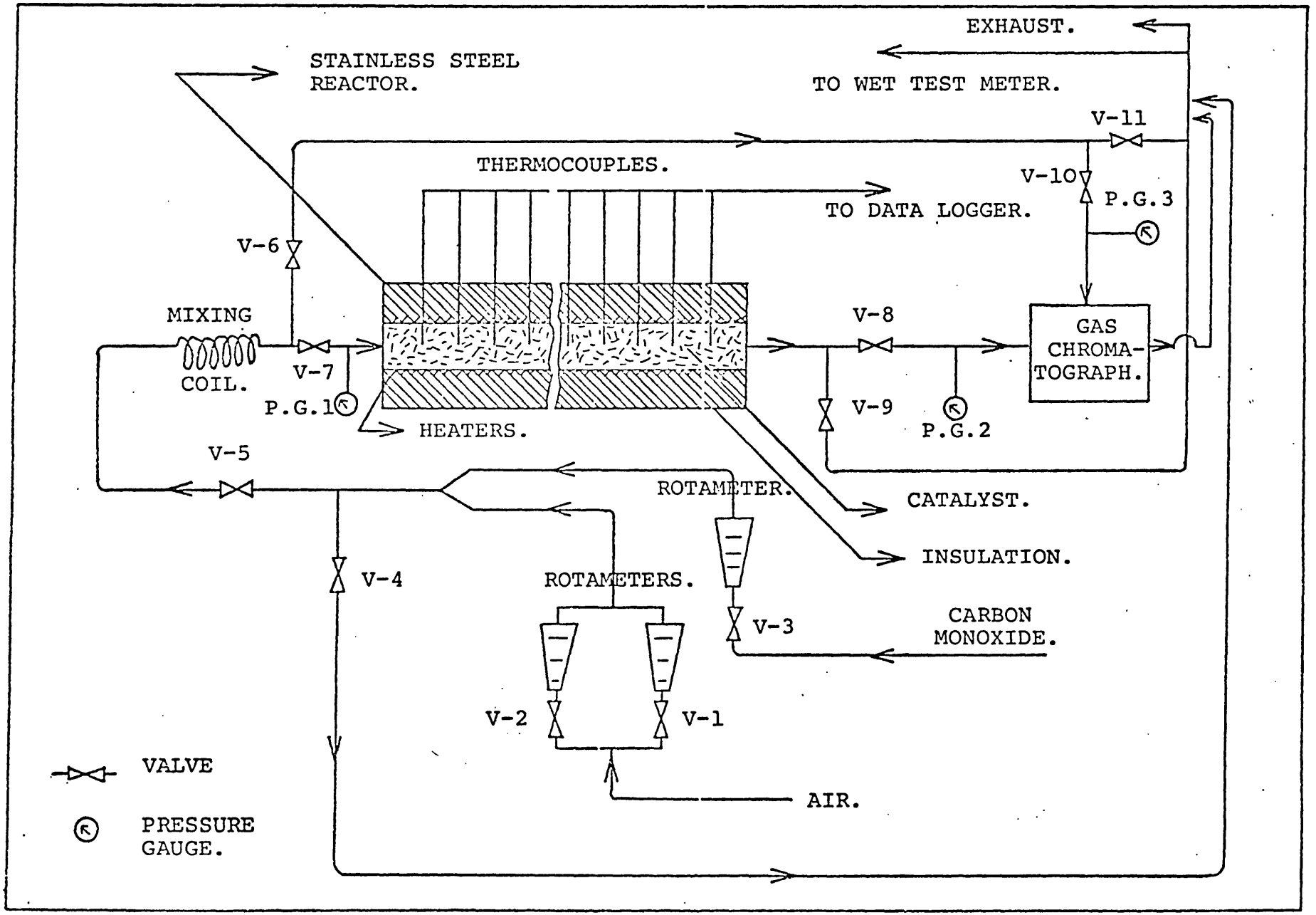
The cracking catalyst used for the regeneration was Alumina-Silica in the form of pellets. The catalyst was supplied by Joseph Crosfield & Sons Ltd., and contained 25% by weight of alumina, 74.4% Silica. The impurities in the form of sulphur compounds (as SO_4), sodium compounds (as Na_2O) and iron compounds (as Fe) were less than 1%.

4.2 Equipment.

Figure (4.1) is a schematic diagram of the experimental system. For carbon monoxide oxidation reaction, air and CO were metered through separate rotameters at room temperature. The gases were supplied from high pressure cylinders. The reactants were mixed thoroughly in the mixing coil before being introduced into the packed reactor. The effluent stream from the reactor could either be sent through a wet test meter (for flow rate measurements) or diverted to the exhaust. The stream could also be sampled for purposes of gas analysis in a gas chromatograph. Pressure gauges P.G.1 and P.G.2 measured the pressure drop across the packed reactor.

Stainless steel sheathed Chromel-Alumel thermocouples (1mm. diameter) were placed along the axis of the reactor at uniform intervals of 2.5 cm. Heating tapes wrapped around the outside of the reactor maintained the reactor at any desired temperature. Several inches of ceramic fibers (KAOWOOL) insulation wrapped around the reactor helped to minimize heat losses.

FIG. (4.1) SCHEMATIC OF THE EXPERIMENTAL SYSTEM.



Details of critical sections of the experimental system are discussed in turn.

The reactor was constructed of 18/8 stainless steel 0.93 Cm internal diameter, wall thickness of 0.085 cm, and 60 cm in length. Although thermal conductivity of stainless steel is high compared with other possible materials for construction of the reactor such as quartz, stainless steel provided flexibility in assembly, construction and ease of thermocouple installation. The unit was packed with the catalyst and sealed at the two ends with flange plates of 3.81 cm O.D. and 0.3175 cm thickness-type 18/8 stainless steel. 0.635cm O.D. tubing were welded to the end plates to serve as gas inlet and outlets. Annealed copper gaskets were used to seal the flanges. The sealing was achieved by means of six 4BA stainless steel cap screws evenly spaced on the flanges on a 2.46 cm diameter bolt circle. Stainless steel screen (200 mesh) was provided at the end of the reactor to prevent carry-over of the catalyst by the gases. Details of the reactor with end plates are shown in Figures 4.2 and 4.3.

Thermocouples were inserted through the wall of the reactor with the hot junction placed at the central axis of the reactor.

4.2.1 Electrical Power Input.

Four heavy duty flexible electrical heating tapes were wrapped around the reactor, providing four zones each of 15 cm. The power input to each heating tape was controlled by a separate autotransformer (variac). The heating tape on the exit section was used for the initial

FIG. (4.2) DETAILS OF THE REACTOR.

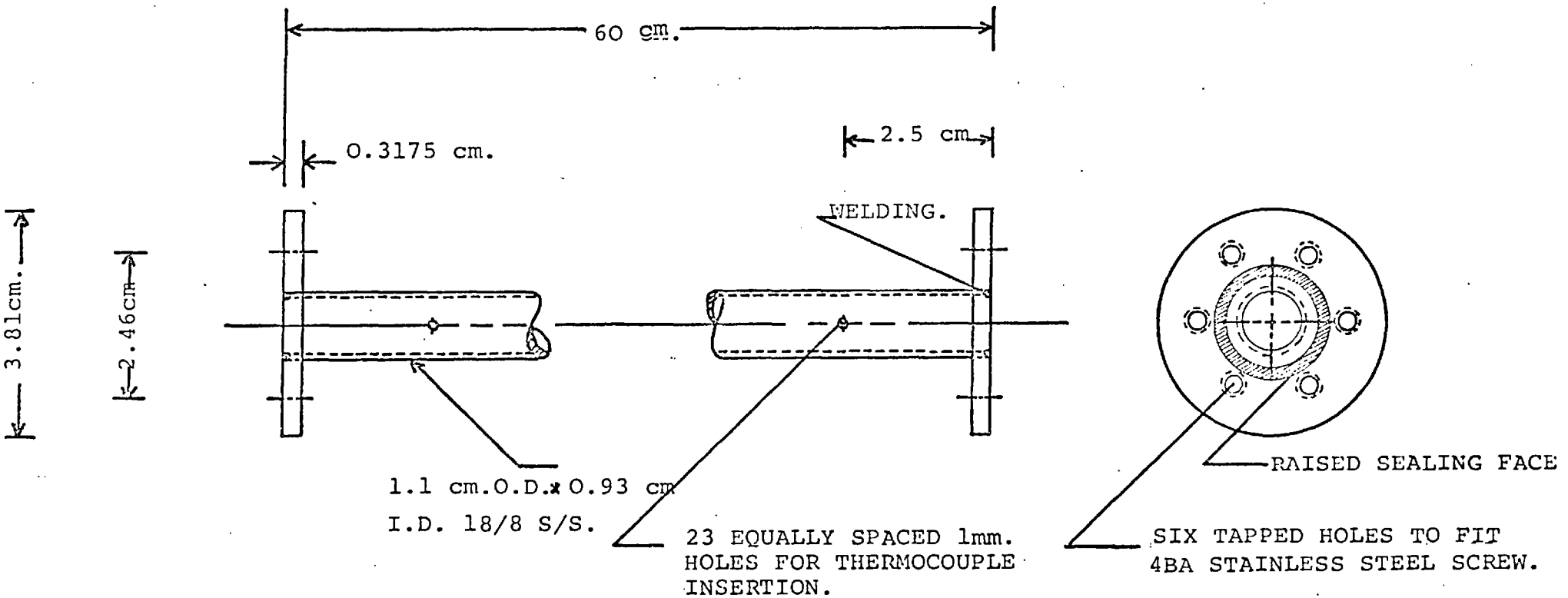
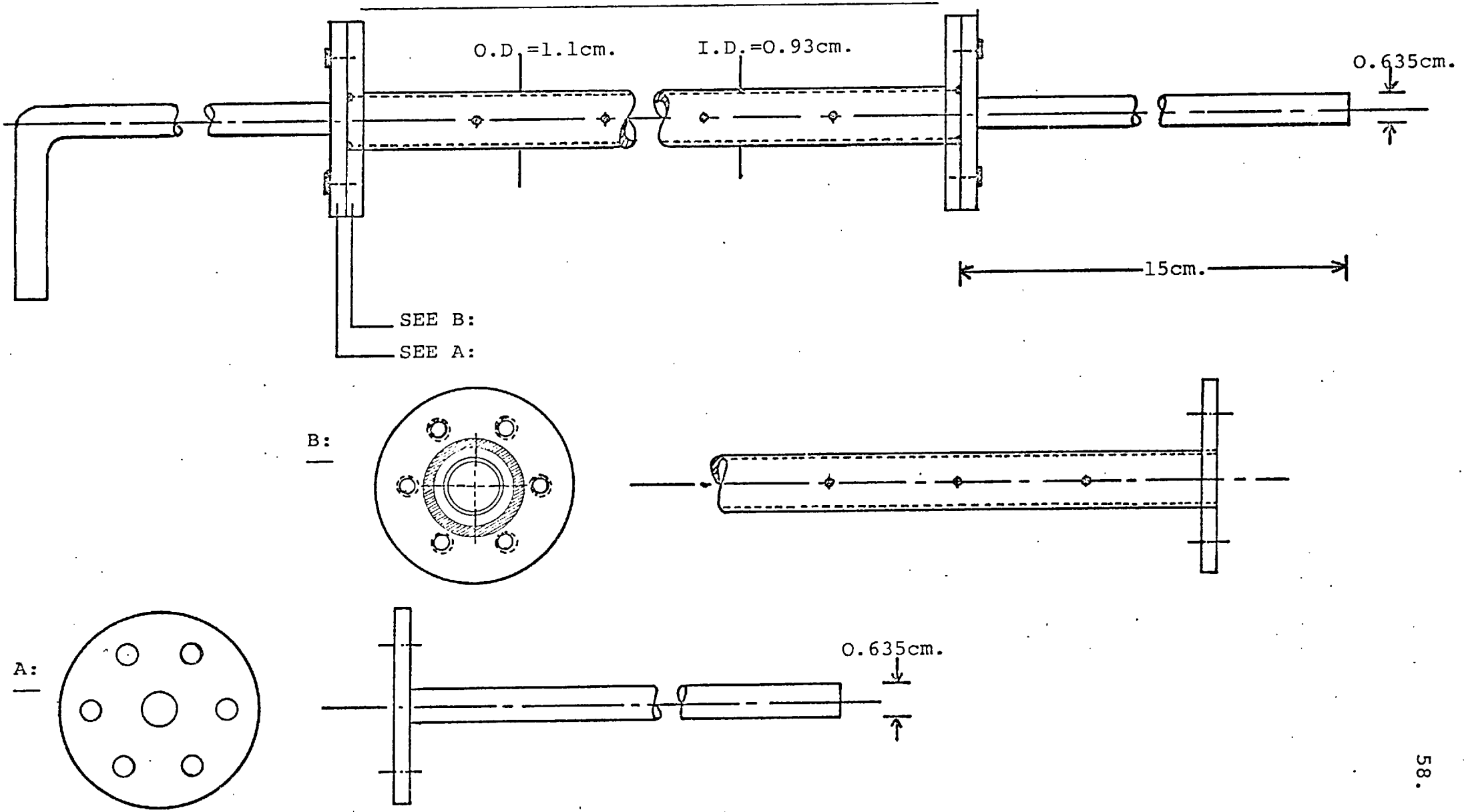


FIG. (4.3) DETAILS OF THE REACTOR END PLATES.



imposition of a temperature profile prior to each run. The purpose of the heaters were to heat up the reactor for the regeneration of the catalyst after each carbon monoxide run, and in the regeneration of Alumina-Silica catalyst to preheat the feed and were also used for the catalytic cracking. Two separate heating tapes were also wrapped round the inlet and outlet tubing of the reactor. The purpose of the former was for preheating the feed during the regeneration of cracking catalyst, and the latter to minimize the heat losses from the end flange.

The heating tapes used was type "ITQ high temperature isopads". These tapes utilize 98% quartz material which will withstand peaks of 800^{o}C. Terminations of the tapes were standard nickel, glass and asbestos insulated for robustness. Since the terminations were not designed to stand up to the high temperatures generated by the Quartz Tape they were taken out of the hot zone through the lagging.

4.2.2. Thermocouples.

Mineral insulated Chromel-Alumel Thermocouples were used in this work since this combination of alloy is capable of measuring temperature up to 1100^{o}C. The thermocouples were stainless steel sheathed 1mm in diameter and 25 cm in length with extension lead of 2m. They were placed inside along the axis of the reactor at uniform intervals of 2.5 cm and were brazed to the wall of reactor using 0.5 mm. Pd. alloy (Silver Pd. manganese) and high temperature brazing welding flux. Thermocouples were also placed on the mixing coil and the inlet of the reactor

for the feed and the inlet temperature measurement. The extension leads were connected to a data logger head unit.

4.2.3 Data Logger.

Temperature profile readings were taken automatically at an interval of one minute on a SOLARTRON Data Logger with output punched on paper-tape.

When measuring temperature with thermocouples, compensation for the effect of cold junctions is required. Therefore all the cold junctions are enclosed in an isothermal compartment so that they are kept at the same temperature. A resistance thermometer bridge senses the temperature of the compartment and generates a voltage proportional to the deviation from $0^{o}C$. This voltage when passed in series with the measurement circuit, compensates for the cold junction not being at $0^{o}C$.

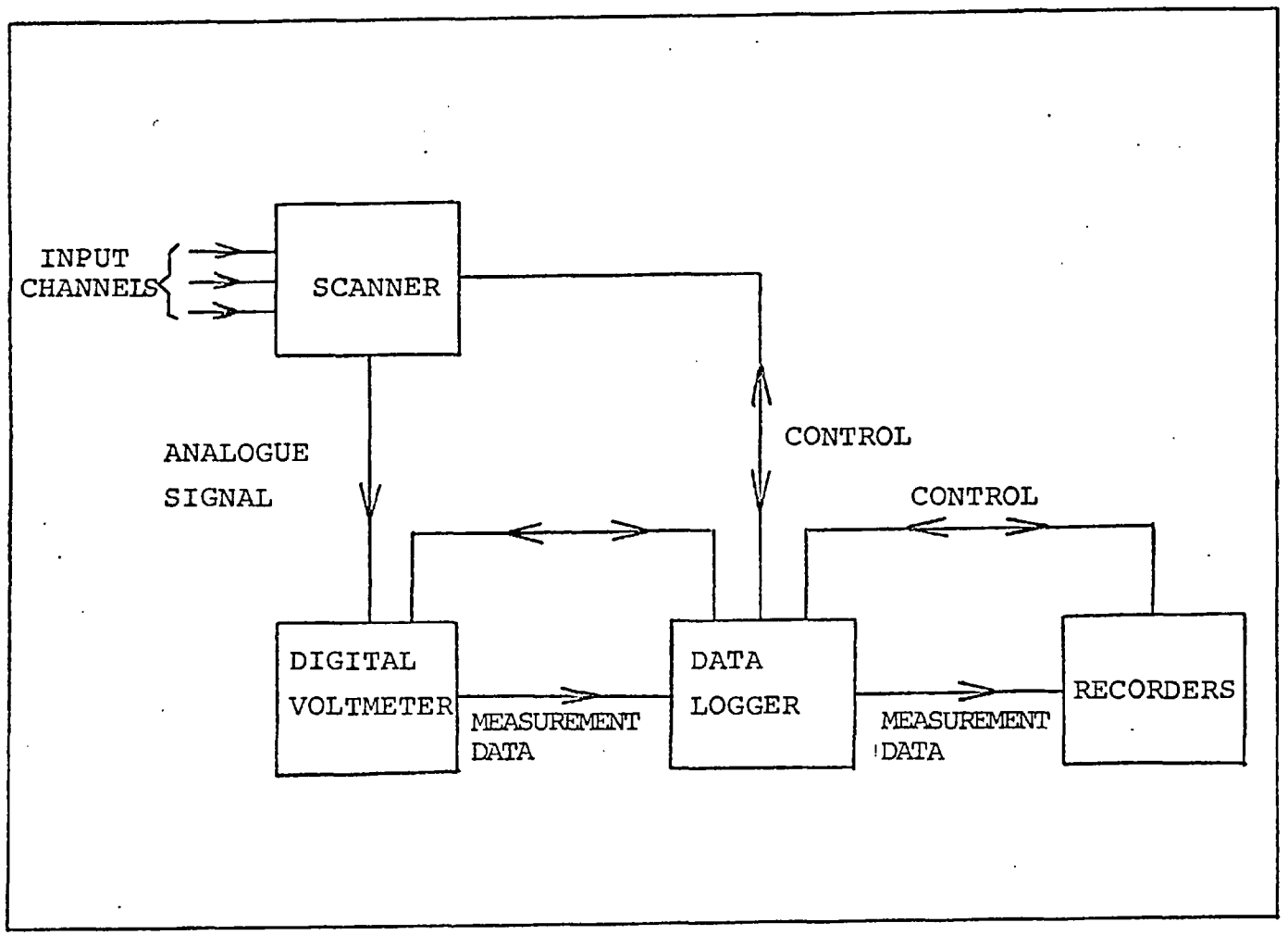
The digital clock built into the logger can initiate scans at present time intervals, and allows time at which measurements are made to be recorded.

The recorder chosen for the system was a Facit paper punch driver type 4070.

4.2.4. Gas Chromatography.

Analysis were performed on a servomex Gas Chromatograph. The samples were taken automatically from the reactor effluent and from inlet stream at suitable intervals. A thermal conductivity detector (Katharometer) was used with hydrogen as the carrier gas. The carrier gas flow was 90 cc/min and the column temperature was kept at $45^{o}C$. The signal from the Katharometer was attenuated and recorded on a

FIG. (4.4) BASIC LOGGING SYSTEM.



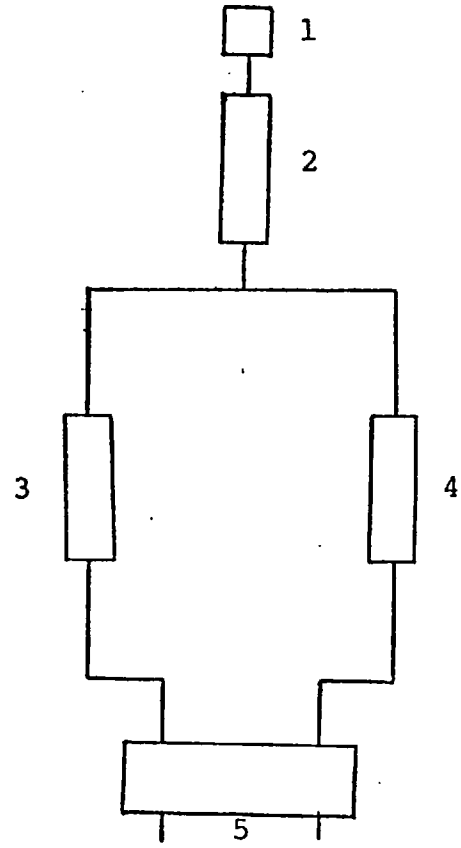


FIG. (4.5).

1=Gas sample valve

2=Primary column

1.5m x 4.8mm I.D. Stainless steel tubing packed with 50-80 ASTM mesh Poropak T

3=Secondary column

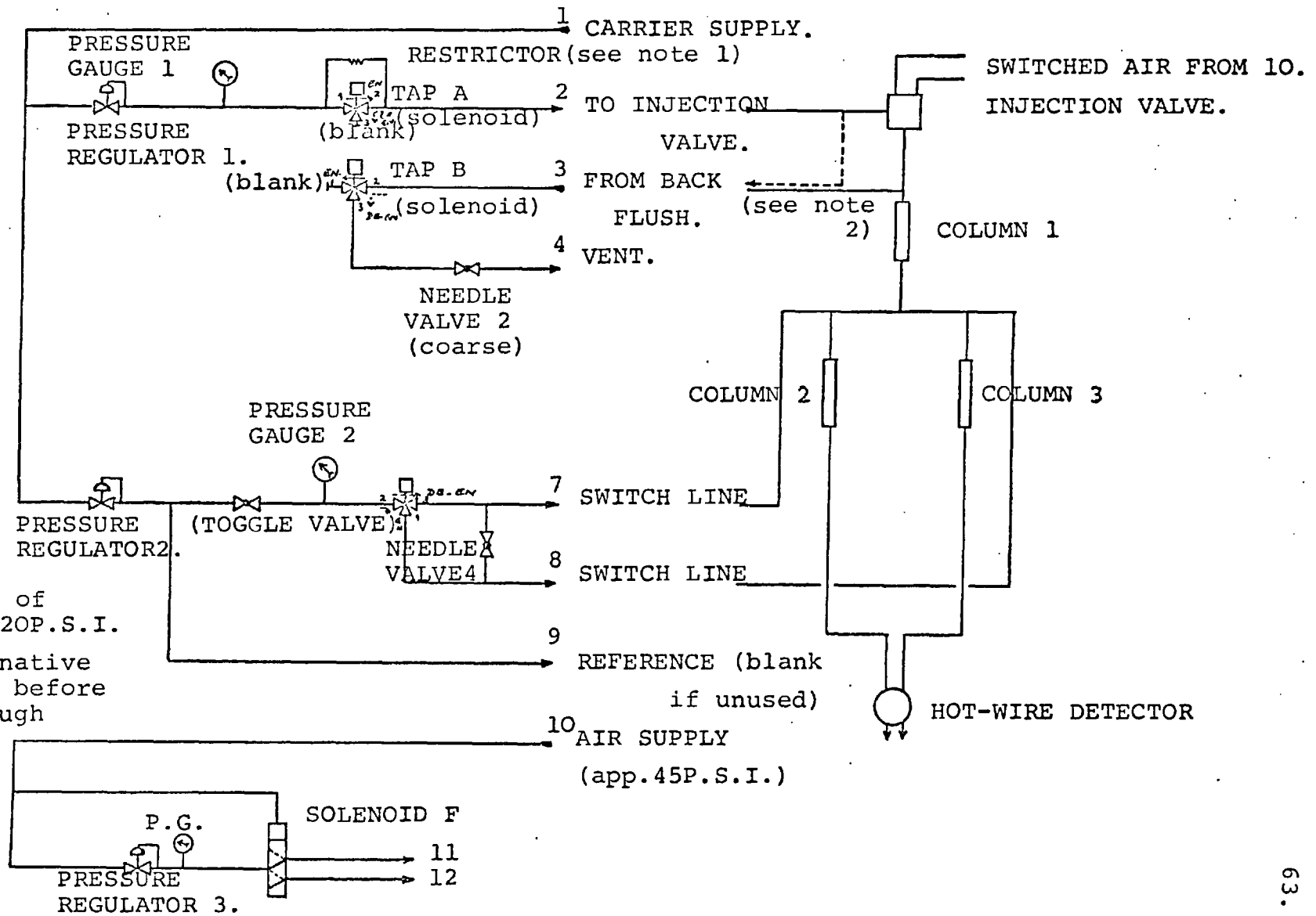
3.05mx4.8mm I.D. Stainless steel tubing packed with 50-80 ASTM mesh Poropak S

4=Secondary column

3.66mx4.8mm I.D. Stainless steel tubing packed with 44-60 BS mesh 13X molecular sieve activated as in text.

5=Katharometer detector

FIG.(4.6): SCHEMATIC OF THE AUTOMATIC SAMPLING SYSTEM.



NOTES.

1) Restrictor allows bleed of 500 ± 100 Ml s/Hr.air at 20P.S.I.

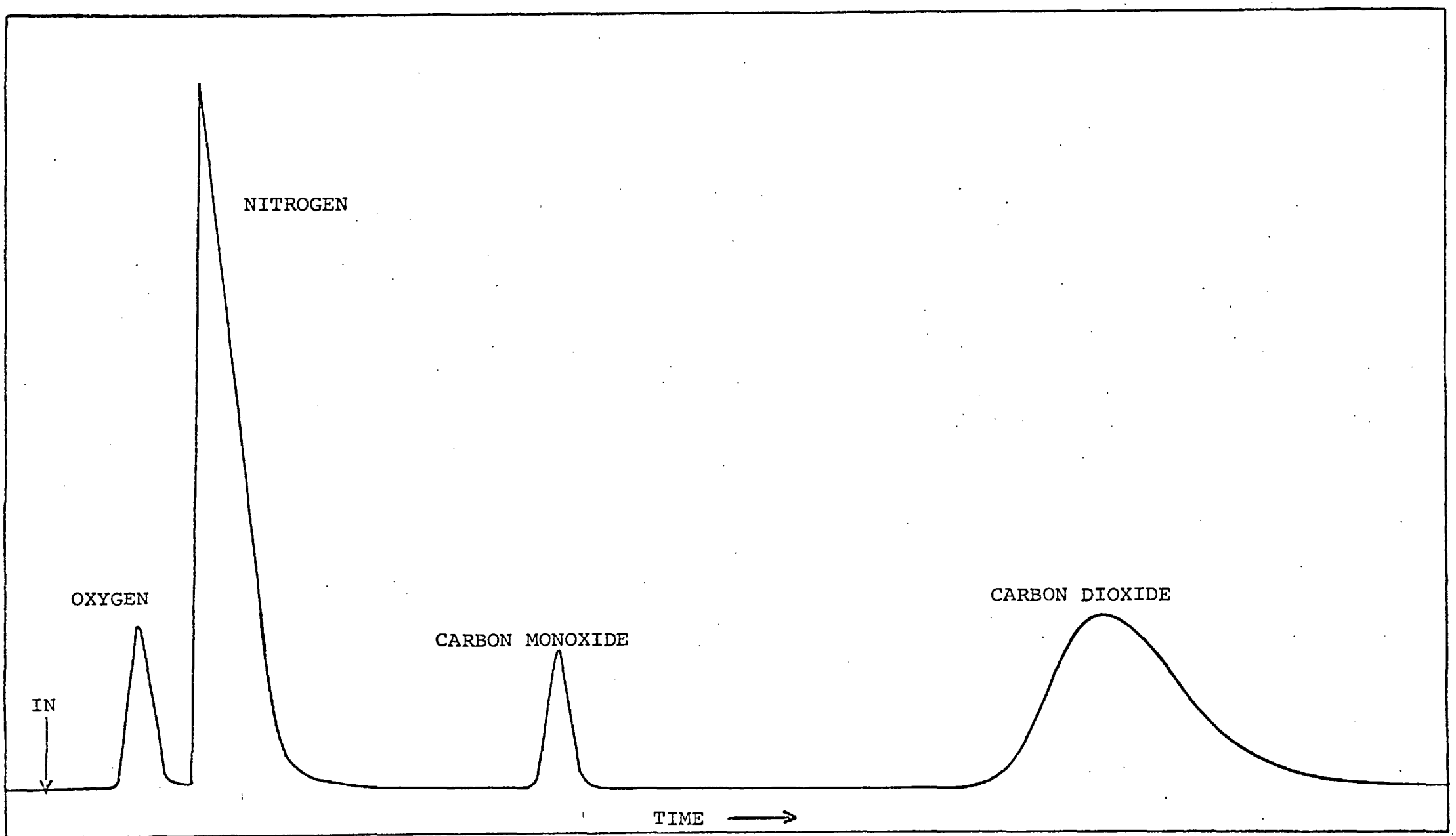
2) Dotted lines show alternative positions of back-flush before injection valve or through injection valve.

Vitatron UR402 linear integrating recorder.

The system adopted uses three columns connected together as illustrated in Fig. (4.5). The primary column of Poropak T serves to separate the light components (O_2,N_2 and CO) as a group from heavier fraction CO_2. The light components are routed from the primary column to a 13X molecular sieve secondary column for separation and subsequent detection by one arm of the Katharometer bridge. Immediately after the light components have emerged from the primary column the effluent flow is diverted to the other secondary column (Poropak S) where CO_2 is detected by the other arm of the Katharometer bridge. The operation of column switching system is discussed in detail in Appendix A. The columns are sized (for detail see Fig. 4.5) so that the detection of components eluting from the molecular sieve column is complete before the CO_2 component emerges from the Poropak S column connected to the other arm of the bridge.

The achievement of this objective lies in the use of sparingly activated 13X molecular sieve. Before packing into the column the molecular sieve is washed in distilled water and fines removed by decantation. It is then dried at 100-120^{o}C overnight. When packed in the column it is activated for 4 hours at 175^{o}C. In this state the rapid elution of the permanent gases is achieved in the order O_2 , N_2, CO. The rapidity of elution enables the detection of carbon monoxide to be completed before the emergence of CO_2 from the Poropak S column. Moreover in this state the molecular sieve column can be stored in the laboratory without deterioration and,kept in the chromatograph, rarely

FIG. (4.7) SCHEMATIC OF SAMPLE CHROMATOGRAM.



requires reactivation.

4.2.4.1 Programme Controller P.C. 260.

The P.C. 260 is an automatic sequence timer. It controls the switching functions of the flow switch 241 by means of microswitches activated by a punched programme card.

The following instruments are the complete units used for the gas chromatography.

Flow switch unit F.S. 241
Oven type A.O. 221
Temperature controller T.C. 201
Katharometer Control unit 197
Sample valve type 220
Microkatharometer 158
Vitatron recorder UR402

The calibration of individual gases was carried out by injection of known amount of gas, the calibration being plotted in terms of number of counts read off from the integrator, corrected for base-line counts and multiplied by the attenuation factor and divided by factor given for synchronizing particular chart speed and dial setting of the recorder. The values obtained were linear for all the gases over the range of concentration used in the present work. The retention times for the components are listed on Table (4.1).

TABLE (4.1) RETENTION TIMES FOR GAS CHROMATOGRAPY.

COMPONENT	RETENTION TIME (Sec.)
O_2	45
N_2	55
CO	85
CO_2	150

4.2.5 Insulation.

In an attempt to maintain adiabatic conditions the reactor was insulated with ceramic fiber (KAOWOOL) capable of withstanding 1400^{o}C. The heating tapes were first fitted and then several rolls of insulation totalling 1 foot in diameter were placed around the reactor unit. The insulation was kept in position by means of soft copper wires wound around the insulation.

4.3 EXPERIMENTAL PROCEDURE.

4.3.1 Cupric Oxide Catalyst.

The catalyst chosen for carbon monoxide oxidation was CuO. Initially the catalyst was supplied by Hopkin and Williams. The catalyst was packed in a batch reactor and heated over a stream of air at 730^{o}K for the purpose of regeneration for a period of 4 hours. The caralyst was tested for its efficiency to oxidise the carbon monoxide using air at a temperature of 700^{o}K. The chromatographic analysis of the product indicated that carbon dioxide was

not produced. The catalyst was further regenerated by air for various length of time, however no improvement was observed concerning the formation of carbon dioxide.

The second batch of catalyst was supplied by B.D.H. and the above experiments were conducted on this sample. The resulting observations were exactly identical. It is probable that both samples from Hopkin and Williams and B.D.H. were produced by the same manufacturer.

The third batch of catalyst was supplied by Baker (U.S.A). Oxidation was carried out in the presence of this catalyst by the same procedure as mentioned above. The Chromatographic analysis showed 100% conversion of carbon monoxide. Hence the Baker catalyst was chosen for the carbon monoxide oxidation to study the reverse propagation of the reaction zone.

On the first attempt of investigation of the moving reaction zone, the zone travelled upstream to the entrance of the reactor with a uniform velocity of propagation and 100% conversion of carbon monoxide. On the completion of this experiment the catalyst was regenerated over a stream of air for the restoration of its activity at a temperature of $730^{o}K$. It was decided to duplicate the same experiment for its consistency. However on the duplication of the experiment with the same feed conditions the product analysis indicated 60% conversion of CO, and the reaction zone velocity was reduced considerably. The experiment was repeated further several times and on each occasion a further drop in conversion of CO and the velocity of propagation was observed. Since it was demonstrated that this behaviour is due to the loss of activity of the catalyst and that on

regeneration with air the activity of the catalyst was not restored to its original value, the regeneration was carried out using oxygen. However this method did not improve the catalyst behaviour.

The reactor had to be heated up during the regeneration, and also in the exit section for imposition of a temperature profile prior to each run. For this purpose four heating tapes were used. The power input to each heating tape was controlled by a separate variac. On heating normally these variacs were switched to the desired voltage for the appropriate temperature required. Since this caused a fast heating up of the reactor, it was decided to alter the procedure of heating up by a lower voltage through the variacs at the start. The desired voltage was then increased in several steps. By operating this method the reactor was heated up in a much slower manner.

The investigation was followed using the slow heating up of the reactor. This procedure offered absolute improvement in carbon monoxide conversion, however the rate of propagation was still reduced on duplication of the experiment.

As it was thought that the cause of deterioration of the catalyst may be due to the impurities on the surface of the catalyst (such as S) it seemed worthwhile to regenerate the catalyst by passing hydrogen over the heated reactor. A hydrogen flow of 100 cc/min was introduced to the reactor at a temperature of 700^{o}K for a period of eight hours. On duplication of several experiments the product analysis showed 100% conversion of carbon monoxide and consistency in the rate of propagation of the reaction zone was observed.

The combination of slow heating up of the system and regeneration of catalyst by hydrogen resulted in restoration of the activity of the catalyst. In order to be certain that hydrogen regenerated the catalyst some experiments were conducted without hydrogen regeneration which resulted to the same problem i.e. reduction in the rate of propagation of the reaction zone.

Therefore prior to each run the catalyst was heated up slowly, followed by a regeneration of the catalyst by a hydrogen flow of 100 cc/min for a period of eight hours. Upon treatment with hydrogen, the metal was obtained.

Sample No.1	Hopkin and Williams.
Sample No.2	B.D.H.
Sample No.3	Baker
Sample No.4	Baker (deteriorated in process)

The above catalysts were analysed for the impurities by X-ray fluorescence spectroscopy. The impurities detected by this method were Fe, Ca and Al. The last two metals appeared to be in almost identical concentration in all four samples. There was twice as much Fe in the Baker material, (both samples) as in the H & W and B.D.H.; the latter two contained identical concentrations.

The Baker material, both samples, consists mainly of CuO, with some Cu_2O. On the other hand the reverse was the case with the H & W and B.D.H. which appeared to be identical materials, i.e. these two materials consist mainly of cuprous oxide with some cupric oxide. The latter two on grinding became brown in colour; the Baker material a dark grey.

Although all samples were black they were really inhomogeneous. The surfaces of all consist of CuO and Cu_2O increased inwards. The H & W and B.D.H. materials have not been so throughly oxidised in manufacture as the Baker. It is suggested that the inefficiency of the two former is due to their higher content of Cu_2O and further that the loss of efficiency of the Baker material may be due to the thermal effects resulting in some reduction of the outer surface of the granules. This was difficult to detect by E.S.C.A. due to difficulty of presentation to the technique. Electron proble microanalysis were carried out on the samples 3 (as received), and 4 (deteriorated). The analysis indicated that minimal but significant reduction has occured during the process. The cuprous oxide content increased from 13.2 weight % in sample 3 to 13.7 weight % in sample 4. An earlier, electron probe microanalysis had suggested that sample 4 appeared to have been completely reduced to Cu_2O. This result, on investigation, was obtained in examination of one grain only.The portion used in chemical analysis were about 0.25 grams, each consisting of many grains. Accordingly in the further electron probe microanalysis several grains of each samples were used. There can be no doubt that the odd grains, few and far between in the catalyst bed do become completely reduced to Cu_2O.

Chemical analysis for carbon content of samples 3 and 4 indicated the absence of carbon in sample 3, whereas 0.015 weight % were found in sample 4.

4.3.2 Carbon Monoxide Oxidation.

The reactor was heated at the exit section by means of external heater, so that to keep part of the reactor in that section above 600^{o}K which was a reasonable ignition temperature for the CO oxidation reaction. An air flowrate equal to the total flowrate used for the particular experiment was passed through the reactor bed. This was carried out prior to the runs to avoid the extinction of the reaction which would have resulted from the sudden heat removal by the feed due to convection. It usually took about 8 hours to achieve a steady temperature profile in the reactor.

The chromatograph needed approximately 3 hours to stabilize. The temperature profile across the reactor was determined before the start of the run. At zero time the air flowrate was reduced by an equal predetermined amount of carbon monoxide flowrate which was desired by the run. The external heat to the reactor was switched off as soon as CO flow started. A preliminary scan of thermocouples was made to detect any reactor high temperatures so that undesirable conditions could be avoided. The air to CO ratio was varied in each run, however, in most of the runs this ratio was maintained in about 7:1 which resulted in a maximum temperature of 950^{o}K.

The main objective of the experiment is to measure the average peak temperature and to study the moving reaction zones and methods of controlling the reaction zone velocity. The dependence of rate of propagation and peak temperature are investigated by three of system parameters which are most open to manipulation in a series of experi-

mental runs. These variables are inlet velocity, inlet concentration and the initially imposed temperature profile. The initial runs are conducted for a variety of constant feed conditions. In order to control the rate of propagation of reaction zone perturbation in feed,conditions are made in the subsequent runs.

4.3.2. Catalytic Cracking.

The Alumina-Silica cracking catalyst supplied by the manufacturer was analyzed for its carbon content. The analysis showed that the catalyst contained 0.65% carbon by weight. Since this amount of carbon deposition was very low in order to generate enough heat from the resulting exothermic oxidation, therefore the initial task was to deposit a higher carbon content over the solid catalyst. This was achieved by passing a mixture of hydrocarbon diluted with nitrogen at high temperature and high residence time over the catalyst bed. The residence time used during the cracking was 12.69 seconds.

The reactor was slowly heated up to a temperature of 770^{o}K which was required for the endothermic cracking reaction. A preheated feed flowrate of 100 cc/min. containing a mixture of propylene (30%), and nitrogen were then introduced to the reactor. It took about 24 hours to obtain a reasonably uniform and reproducible carbon deposition along the reactor bed. The percentage of carbon deposition which was measured by means of CO and CO_2 analysis was approximately 12% by weight.

4.3.4. Regeneration of Alumina-Silica.

On the completion of the cracking reaction the catalyst bed was at the high temperature used to encourage the endothermic cracking reaction. This was achieved by the imposition of the external heaters. The heaters were then readjusted for the preheated section ($\sim 600^{o}K$), with a region of higher temperature near the exit ($\sim 800^{o}K$). Prior to each run a nitrogen flowrate equal to that of air flowrate used for the regeneration was passed through the reactor. (This is to sustain the same initial temperature profile).

The temperature profile across the reactor was determined before the start of the run. At zero time the nitrogen flowrate was turned off, and immediately a preheated feed stream of air was then introduced to the reactor. The external heat to the exit section was switched off as soon as air flowrate started. The introduction of air to the reactor, generated a reaction zone near the exit that propagated along the reactor axis in a direction counter-current to the feed stream.

4.3.5. System Data Measurement.

The temperature profile were recorded automatically at intervals of 1 minute, and the concentration of the exit gas was performed at intervals of 5-10 minutes. At the start of each run the room temperature and initial temperature profile were recorded. During each run the observations included in addition to temperature profile, the time, the exit concentration of the gases, the air and CO flowrate readings, and the system pressure.

CHAPTER FIVE

5. DISCUSSION OF RESULTS.

5.1 Introduction.

To compare the theory with experimental results, one must take those data which are needed for the model. Most essential are the kinetic constants which are discussed first. Other needed data are the experimentally obtained temperature and concentrations. With these, comparison of experimental with model prediction is possible. The kinetic constants determination were only limited to CO oxidation over cupric oxide. No attempt was made to extend these studies for the carbon oxidation on regeneration of Alumina-Silica catalyst. The kinetic constants for this system was obtained from literature (31).

5.2 Determination of kinetics of CO oxidation.

Literature data on the kinetics of CO oxidation over cupric oxide catalyst (Bone and Andrew (35); Titani, Nakata, Kanome (36); Winter (37)Draper (38); Campbell(39); Venkatachalam et. al. (5)) indicated that the rate for the oxidation can be represented by a power law expression.

$$r = K_o \exp(-E/RT)\, C_A\, C_B$$

The kinetic constants to be determined are the frequency factor K_o and the activation energy E. In a plug flow

reactor (40), the two constants can be determined by finding the extent of CO conversion under known flow conditions at various temperatures.

5.2.1 Experimental Scheme.

The following constrains were placed on the experiments for determining the kinetic constants:

a) The reactor length was limited to 5 cm. to facilitate the maintenance of isothermal conditions at any instant, and to exercise greater control over CO conversion. The remainder of the reactor was packed with inerts (Silica glass).

b) The runs utilized a high air to CO ratio (approximately 1% to 2% CO) to minimize thermal effects and keep runs near isothermal.

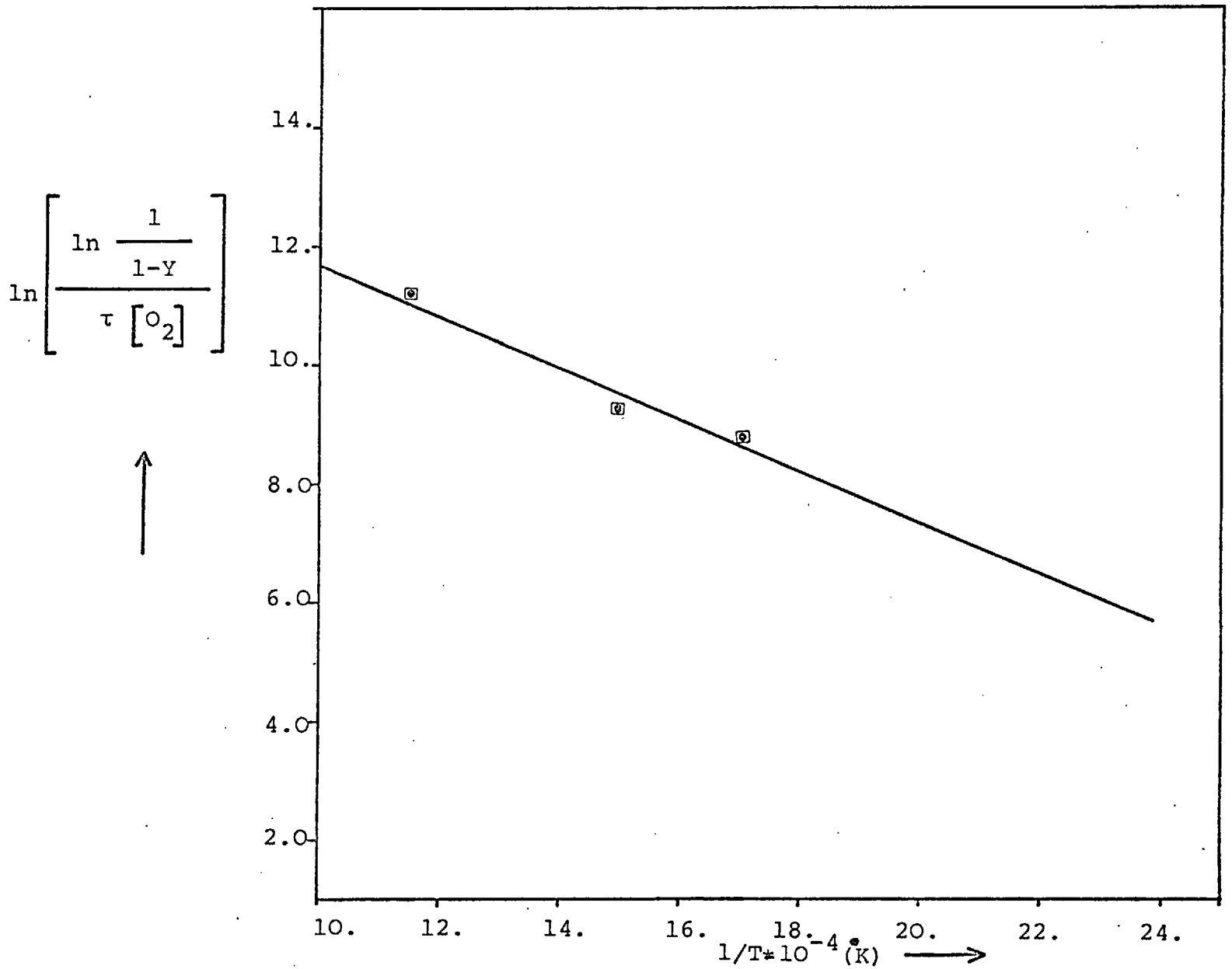
c) The reactor was assumed to be under plug flow conditions.

5.2.2 Analysis of kinetics data.

Since the runs utilized a high air to CO ratio, pseudo first order kinetics with respect to CO was assumed. This was supported by the work of Bone and Andrew (35) who reported the presence of a multilayer of adsorbed oxygen on the cupric oxide surface. Thus homogeneous kinetics could be justified.

FIG.(5.1)FIRST ORDER FIT FOR KINETIC DATA.

(CO OXIDATION OVER CuO)



The oxidation of CO over cupric oxide can be represented by the form :

$$r = K_o \exp (- E/RT) C_A C_B$$

If the concentration of oxygen can be considered to remain constant (= $[O_2]$) due to an excess air in the feed, the rate reduces to a pseudo first order form

$$r = K_o^* \exp (-E/RT) C_A$$

where $K_o^* = K_o [O_2]$.

Figure (5.1) shows the pseudo first order fit for the kinetics data. The analysis of data is presented in appendix A. The order of residence time was between 0.255×10^{-3} to 0.396×10^{-3} min.

The frequency factor and activation energy were found to be 3.165×10^6 m^3/K mol s and 3.6×10^4 KJ/K mol respectively. These results were used in the theoretical predictions. The activation energy of CO oxidation over cupric oxide catalyst reported by Winter (37) is in the range of 3.76×10^4 to 4.18×10^4 KJ/K mol . Venkatachalam et. al. in their kinetics studies found the frequency factor and activation energy to be 2.25×10^6 m^3/K mol s and 3.9×10^4 KJ/Kmol respectively.

5.3 Carbon Monoxide Oxidation Results.

Data on reverse operation for this system are presented for 14 runs (Run Nos. 30, 31, 32, 37, 43, 44, 45,

46, 47, 49, 50, 52, 53 and 55). The observations for each run include :

a) The room temperature ^{o}K.

b) Flowrate of air and CO.

c) Feed concentration of CO and oxygen.

d) Feed temperature.

e) Pressure gauge readings.

f) The initial temperature profile along the reactor.

g) The peak temperature.

h) The temperature profile along the reactor as f(t).

i) The concentration analysis of the exit gases with time.

j) Power input to the heating tapes.

Tables (5.1 - 5.3) summarize the operating conditions of the reactor for the runs. Tables (C1-C9, appendix C) present the data on runs (44,45,46,47,49,50,52,53 and 55) respectively. Temperature profiles were recorded at intervals of one minute, however these are tabulated here at five minutes intervals. Although 24 thermocouples were placed along the reactor axis to measure the temperature profile at any instant, 3 of them failed to record and eventually broke during the runs. Therefore these readings have been omitted in the tables (C1-C9). The positions of these thermocouples along the normalized distance of the reactor were at 0.208, 0.750 and 0.958 respectively. As a large number of thermocouples were used, the remaining 21 thermocouples readings adequately described the temperature profiles.

In the graphical presentation, only selected data points are illustrated to avoid confusion. To indicate the accuracy of the profiles, some of these graphs are drawn with various symbols corresponding to the temperature and the position along the reactor.

By imposition of an initial temperature profile in the exit section the CO flow was introduced to the reactor at zero time and the external heater was switched off immediately. Having ignited the reactor it took about 4 to 5 minutes to establish a uniformly moving reaction zone. The establishment of a zone that moved against the flow depends on the chosen velocity which must be reasonably low to prevent blow-out. The sustained reaction zone traverses the bed upstream to the inlet of the reactor with a constant velocity of propagation. If during a run no alteration has been made in feed conditions the reactor is at pseudo-steady-state operating conditions. However if any disturbance is made in feed conditions by perturbing the feed velocity or the feed concentration the behaviour of the system is totally altered. To investigate such behaviour, and ability to control the movement of the zone perturbations are made with different feed velocities and feed concentrations at any desired time. In order to isolate the effect of the individual variable u_o and C_{Ao} it is important that perturbation must be carried out on one variable while the other conditions is maintained constant.

All the runs were made with excess air. The initial runs were carried out for a variety of constant feed conditions. For the purpose of control, however, the

subsequent runs were made with alteration in feed conditions.

Perturbations were made either in feed velocity keeping concentration constant, or vice versa. The alteration in concentration varied from 3.45×10^{-3} to 6.5×10^{-3} K mol/m^3; and from 0.179 to 1.45 m/s for the feed velocity. Higher concentration were not used so as to maintain excess air to utilize the pseudo first order kinetics data in the theoretical model, and also to avoid damaging the equipment due to the excessive rise in temperature. The gas flow (CO + air) varied from 0.35 to 2.83 1/min. The residence time τ through the packed bed reactor was varied from 0.4 to 3.4 secs.

The initial temperature profile along the reactor was imposed by electrical heaters and controlled by auto-transformers (section 4.2.1). The initial ignition temperature profile was of order of 650^{o}K.

The first concentration analysis was performed 10 minutes after the start of the run, after the flowrates of the gases and the pressure gauge readings had stabilized. The exit analysis in all the runs showed complete conversion of carbon monoxide.

During the initial period of operation low inlet velocity must be used, so that the zone can be well established. For this reason the maximum feed velocity that could be used at the start up did not exceed 0.652 m/s. Utilizing higher feed velocity at the start of operation caused blow-out. This situation occurred with a feed velocity of 0.7 m/s. The increased thermal load caused by the proximity of the reactor boundary makes it more

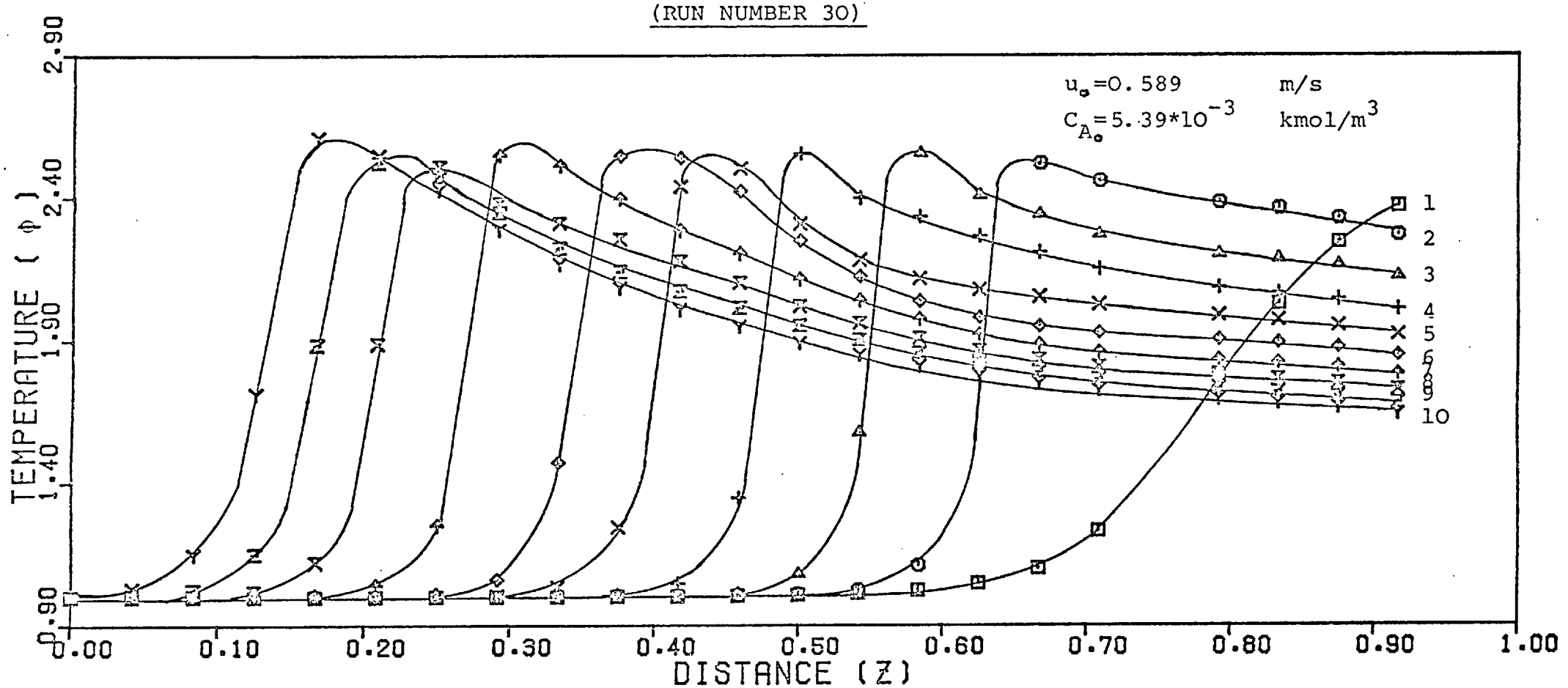
difficult to initiate propagation. Hence, if a high feed rate is used, blow-out will result. To achieve a moving reaction zone with a 0.7 m/s or higher feed velocity the operation must be conducted with a lower feed velocity than that which has already caused the blow-out. Once the propagation has been sustained, and the reaction zone has moved away from the reactor boundary higher feed rates can be used without any difficulty. While a feed velocity of 0.7 m/s resulted in blow-out, by manipulating the above procedure and perturbing the feed flow a sustained moving reaction zone was achieved with a feed velocity of 1.305 m/s (Run 52).

Figures 5.2, 5.3 and 5.4 show the temperature profiles at various times along the reactor with constant feed conditions. It should be noted that these runs differ from one another in feed concentration and feed velocity, however, in each particular run the feed conditions have not been disturbed. The runs indicate an effective reverse propagation of the reaction zone along the reactor bed. The figures show that the rate of propragation of the zone is constant, except when the reaction zone starts to encounter the reactor inlet. The rate of propagation falls when this position is approached. For this reason the perturbation in feed conditions for the following runs are carried out before the reaction zone has reached near the entrance.

For the purpose of control the effects upon transient behaviour of the reaction zone have been examined, when several of the system parameters are perturbed. The propagation of quasi-steady-state profiles are investigated

FIG.(5.2) TEMPERATURE PROFILES WITH CONSTANT FEED CONDITIONS.

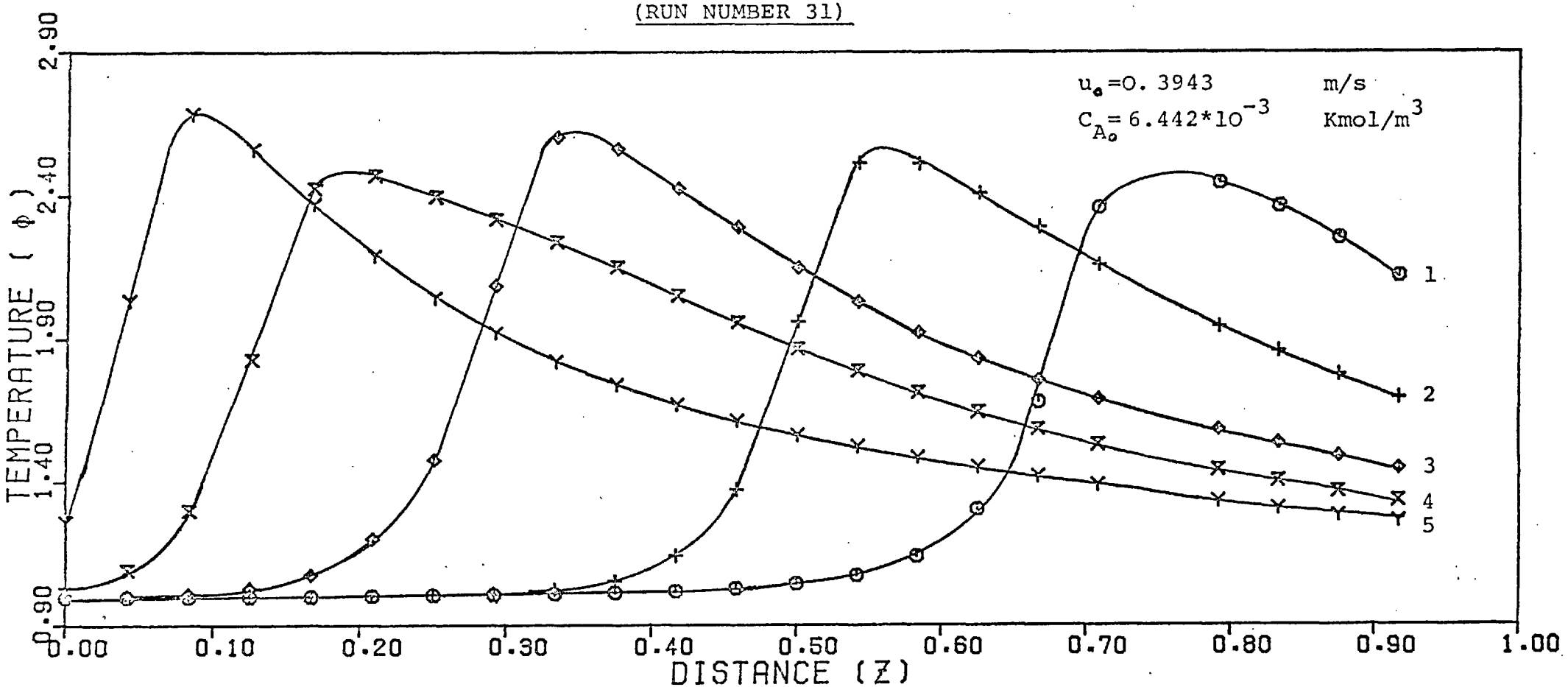
(RUN NUMBER 30)



Time:(1) 0; (2) 10min; (3) 20min; (4) 30min; (5) 40min; (6) 50min; (7) 60min; (8) 70min; (9) 80min; (10) 90min.

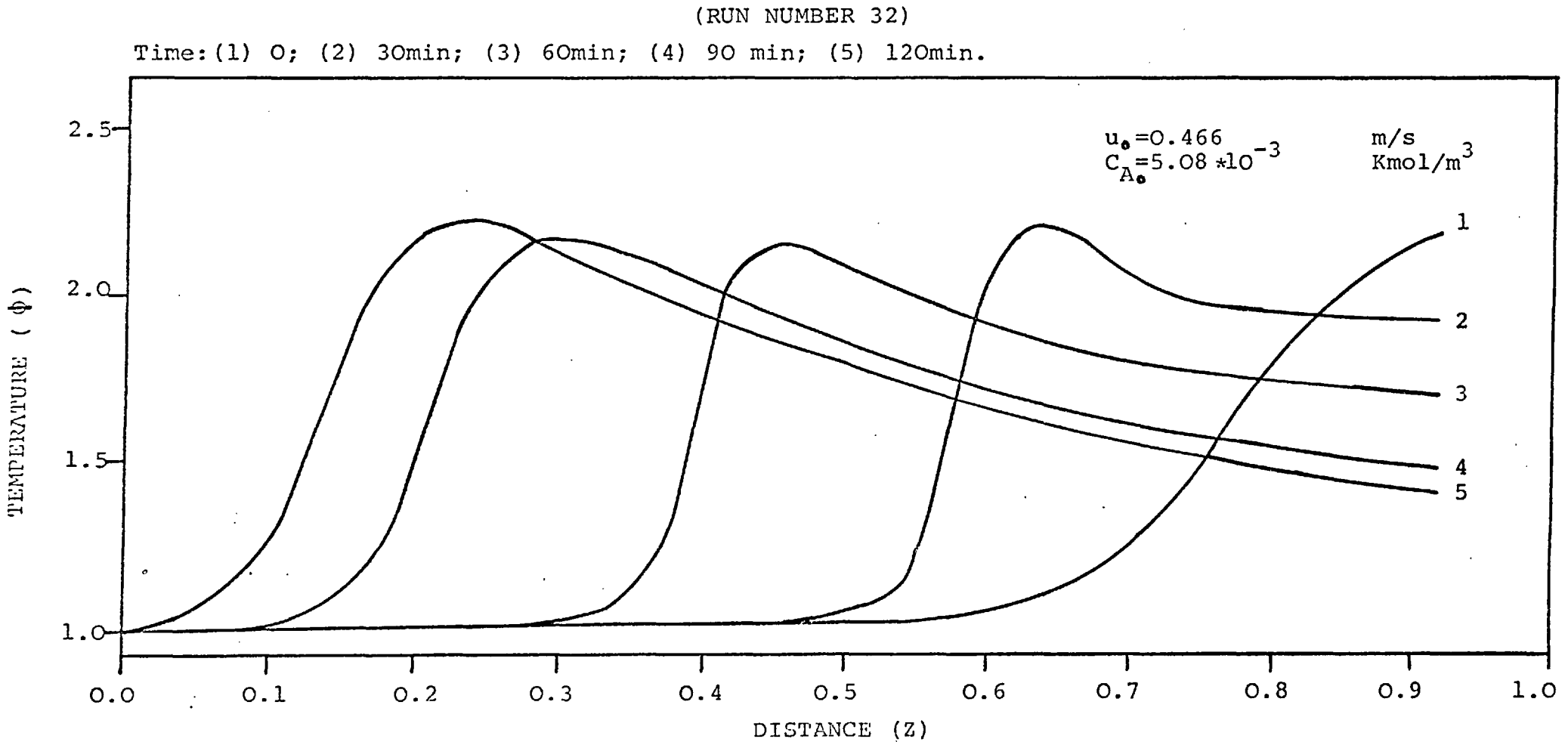
FIG. (5.3) TEMPERATURE PROFILES WITH CONSTANT FEED CONDITIONS.

(RUN NUMBER 31)



Time: (1) 10min; (2) 40min; (3) 70min; (4) 100min; (5) 130min.

FIG. (5.4) TEMPERATURE PROFILES WITH CONSTANT FEED CONDITIONS.



with different values of feed velocity and feed concentration. Variation of the initial temperature profiles upon propagation velocity has also been examined.

There is an alternative scheme in which the diluent flowrate is used as the control variable for a constant reactant flowrate. Since both the feed velocity and concentration would be varied simultaneously it would be difficult to isolate the effect of the individual variables u_o and C_{Ao}. Therefore these studies were restricted to the use of feed velocity and feed concentration as control variables.

It is assumed that complete conversion occurs within a short ignition zone where backward conduction of heat takes place. This conduction depends on the feed velocity and feed concentration.

The transient behaviour of the moving reaction zone was studied with different initial temperature profile. When the imposed temperature profile was too low, the bed had to be heated up by the resulting exothermic reaction in order to obtain a steady moving reaction zone. However, on the imposition of a high temperature profile the zone was established in a shorter time. Both initial conditions approached the same quasi-steady state profile which indicated that a perturbation in the initial temperature profile has only a temporary effects on the propagation rate. The hotter zone with its higher temperature gradients initially has a higher velocity of propagation, but later reverts to the standard velocity, as might be expected.

5.3.1 Feed Concentration (C_{Ao}).

The experimental results indicate that perturbation in feed concentration will quickly lead to a change in peak temperature and velocity of propagation. Increase in feed concentration results to an increase in peak temperature and the zone velocity. However the situation is reversed upon the reduction in feed concentration. If the feed concentration is reduced further below a distinct value, the zone separates and continuously moves out causing blow-out which has been provoked by this reduction. Hence in order to avoid blow-out of the reaction zone, the feed concentration must be kept above the permitted value for a given system.

At higher feed concentration the rate of energy formation is increased; however, the resistance to conduction within the reactor bed allows only a fraction of this extra heat to be dissipated by an increase in the velocity of propagation. The remainder is stored, raising the peak temperature of the reaction zone. Figure (5.5) illustrate the rise of peak temperature and increase in the velocity of propagation as the feed concentration is increased. An increase of 18 per cent in feed concentration increases the velocity of propagation by 29 per cent, while upon a further increase of 8 per cent in feed concentration the velocity of propagation increases by 2 per cent.

Figure (5.6) shows the drop in peak temperature and decrease in the velocity of propagation when the feed

FIG.(5.5) TEMPERATURE PROFILES WITH VARIATION OF CONCENTRATION KEEPING VELOVITY CONSTANT.

(RUN NUMBER 43)

Time:(1) 15min; (2) 50min; (3) 80min.

First increase of concentration after 15 min.,second increase of concentration after 50min.

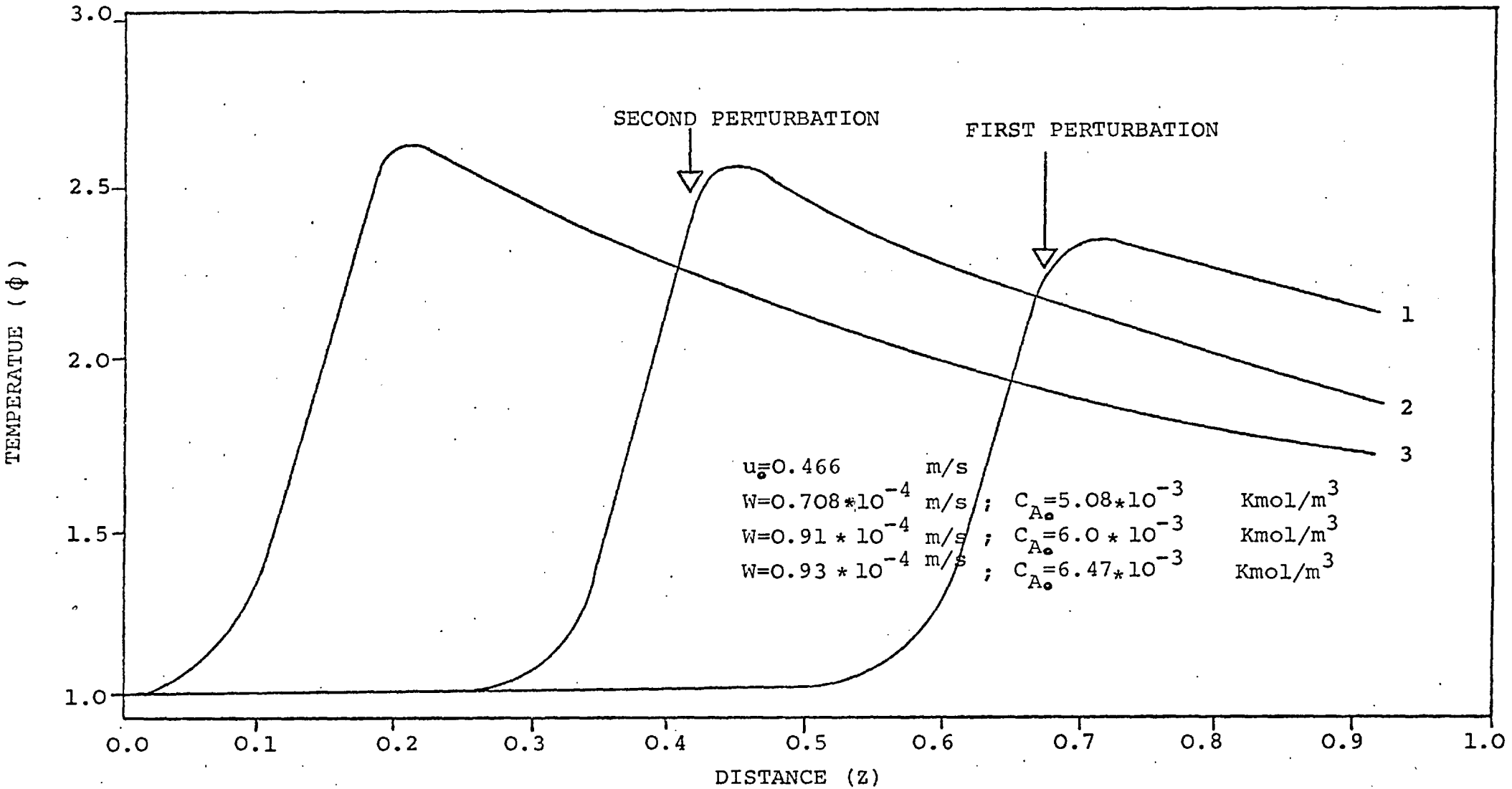
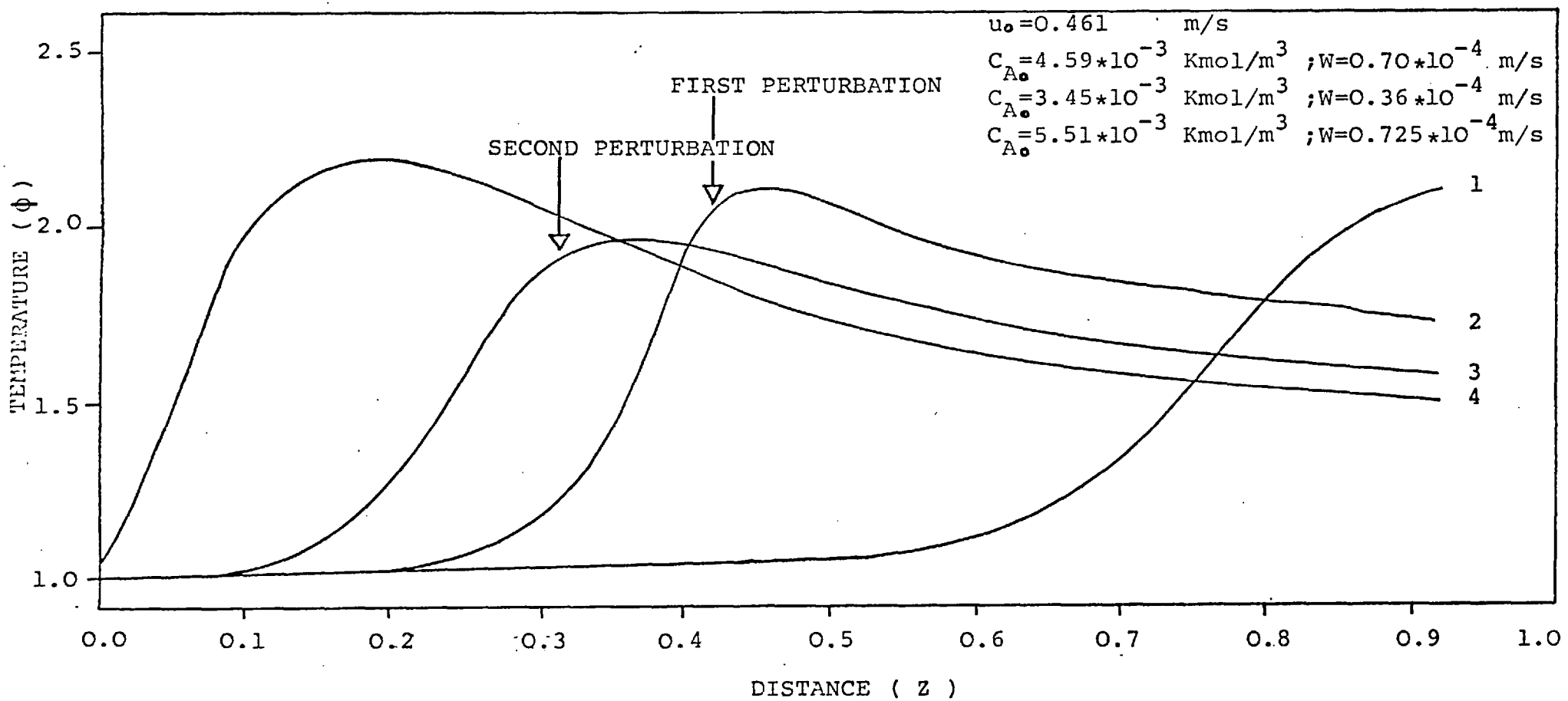


FIG.(5.6) TEMPERATURE PROFILES WITH VARIATION OF CONCENTRATION KEEPING VELOCITY CONSTANT.

(RUN NUMBER 53)

DECREASE OF CONCENTRATION AFTER 65 min.,INCREASE OF CONCENTRATION AFTER 105 min.



Time:(1) 0; (2) 65min; (3) 105min; (4) 125min.

concentration is reduced. By a reduction of 33 per cent in feed concentration, the resulting velocity of propagation is decreased by as much as 94%. However the situation is once again altered upon the perturbation when the concentration is increased. The effect of an increase of 60 per cent in the feed concentration is to increase the velocity of propagation by 101 per cent.

The above result suggest the existence of an exponential relationship between the velocity of propagation and the feed concentration, such a relationship with a given correlation has been discussed in detail in section 5.3.4. Figure (5.17) illustrates the increase in the velocity of propagation with increased feed concentration.

5.3.2 Feed Velocity (u_o).

As mentioned earlier, a low inlet velocity must be used during the initial period of operation, so that the zone can be well established. Once propagation is obtained higher feed velocities can be used. At high inlet velocities the initial temperature profile is unable to readjust quickly enough and the complete blow-out of the reaction ensues. Proper inlet velocity leads to a sustained propagation with constant geometry which can travel upstream fee from the influence of the boundary conditions on the catalyst bed. It is then that increase in the inlet velocity will not cause blow-out.

An increase in inlet velocity has a threefold effect upon the behaviour of the reactor. Firstly the cooling by convection in the front part of the reactor will be

increased because more feed must be heated up to reaction temperature. Thus the reaction zone moves deeper into the reactor.Secondly the heat transfer between fluid and catalyst is increased, with the result that the excess temperatures of the catalyst phase are lowered and the reaction zone moves further back into the reactor. On the assumption that the main resistance lies within the pores of the catalyst therefore a change of feed velocity is almost insignificant to the mass transfer. Thirdly the effective heat conductivity is increased (41). This effect acts against the preceeding two but it cannot prevent the reaction zone from being blown out of the reactor with increasing feed velocity.

Figures (5.7 - 5.15) represent the temperature profiles with perturbation in feed velocity maintaining constant feed concentration. Since the runs conducted with constant feed conditions had shown that the propagation velocity decreases when the reaction zone approaches the entrance of the reactor, therefore perturbations in feed velocity were made long before the reaction zone had reached this position. The results of perturbation runs indicate that the system responds to change in feed velocity within 100 residence times of the perturbation.

High inlet velocity increase the rate at which fuel is fed to the reaction zone, raising the rate of heat output, and the peak temperature, but also raising the sensible heat load on the system.

In order to avoid blow-out of the reaction zone and the excessive rise of the peak temperature, the alteration of

the inlet velocities were initially conducted by 10-20 per cent. These perturbations in feed velocity were increased by 50 - 100 per cent in the later runs, so that the effect upon the reaction zone due to the sudden variation and very high inlet velocities could be studied. Where such high perturbations were made, the feed concentration used was low enough to avoid the excessive temperature rise in the reaction zone. The results indicate that high inlet velocity increase the peak temperature which is due to the higher fuel fed into the reaction zone. The increase in peak temperature is higher when as a result of increased feed velocity the propagation velocity has decreased. This is because of the resistance to conduction within the catalyst bed which allows only a fraction of the extra heat to be dissipated by an increase in the feed velocity , hence the rise in the peak temperature. These effects can be observed from Figures (5.7 - 5.15).

Depending on the inlet velocity used during the operation , the effect of higher velocity is either to increase or decrease the rate of propagation velocity. With increasing feed velocity the reaction zone will inevitably separate, moving downstream and leaves the reactor, Figure (5.17) shows the effects upon the velocity of propagation when the feed velocity is perturbed. In summary, high inlet velocity increases the rate of propagation. As the inlet velocity is increased further, the velocity of propagation starts to decrease; for even higher inlet velocities the reaction zone changes its direction from

FIG. (5.7) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 20min. KEEPING CONCENTRATION CONSTANT.

(RUN NUMBER 37)

Time : (1) 0; (2) 20min; (3) 30min; (4) 40min; (5) 50min.

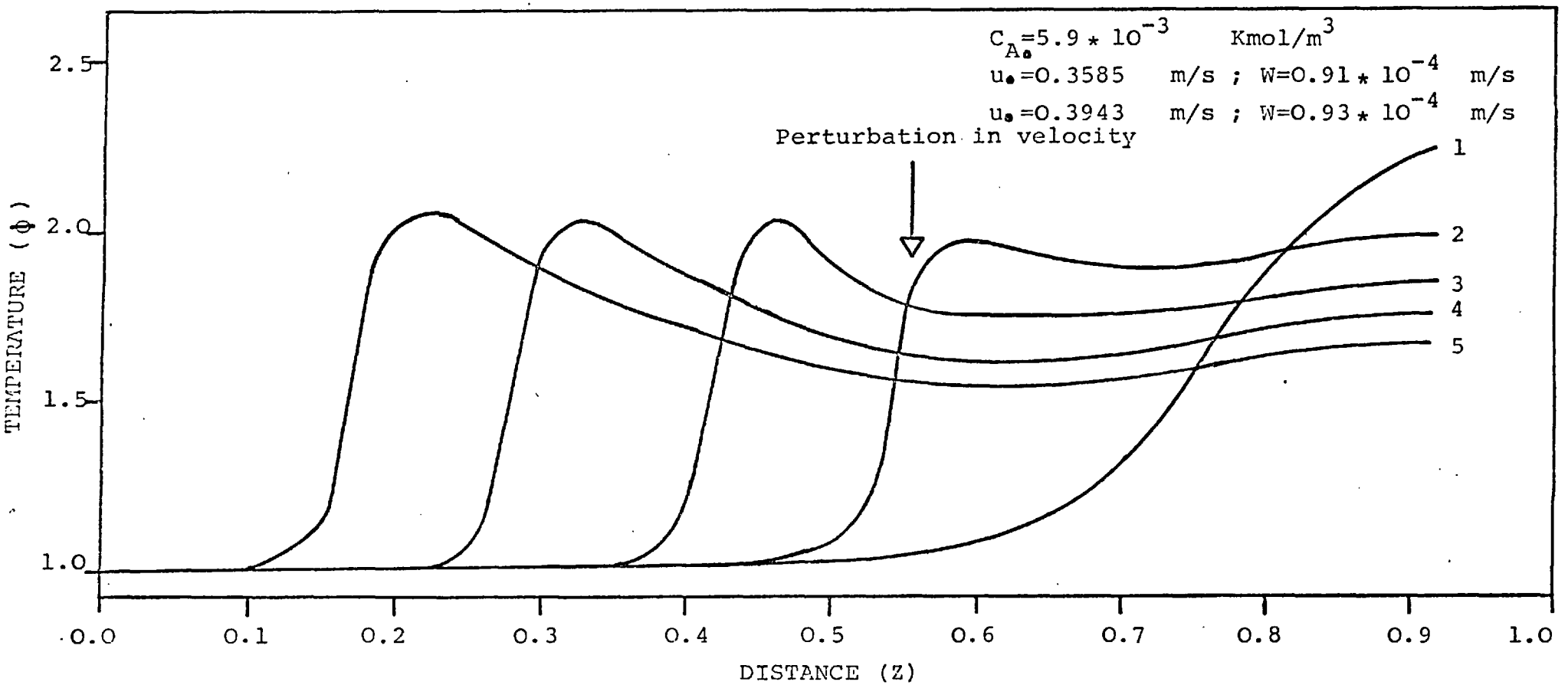


FIG. (5.8) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 20 min. KEEPING CONCENTRATION CONSTANT.

(RUN NUMBER 44)

Time : (1) 0; (2) 10min; (3) 20min; (4) 30min; (5) 50min; (6) 70min; (7) 90min.

$u_* = 0.466$ m/s ; $W = 0.879 * 10^{-4}$ m/s.

$u_* = 0.513$ m/s ; $W = 0.577 * 10^{-4}$ m/s.

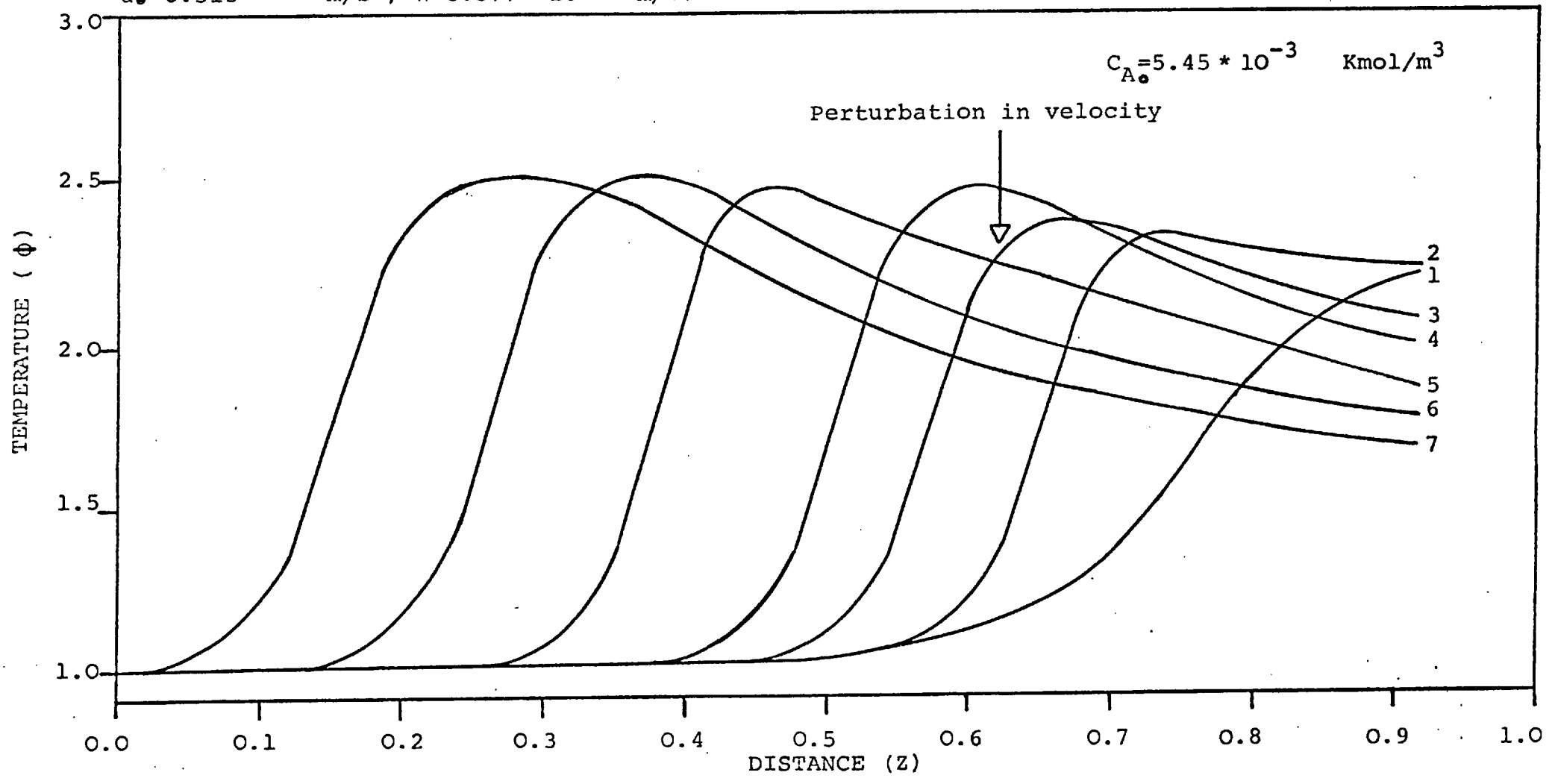


FIG. (5.9) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 20 min. KEEPING CONCENTRATION CONSTANT.

(RUN NUMBER 45)

Time : (1) 0; (2) 20min; (3) 30min; (4) 50min; (5) 70min; (6) 90min.

u_s=0.5377 m/s ; W=0.833 * 10^{-4} m/s.

u_s=0.5915 m/s ; W=0.717 * 10^{-4} m/s.

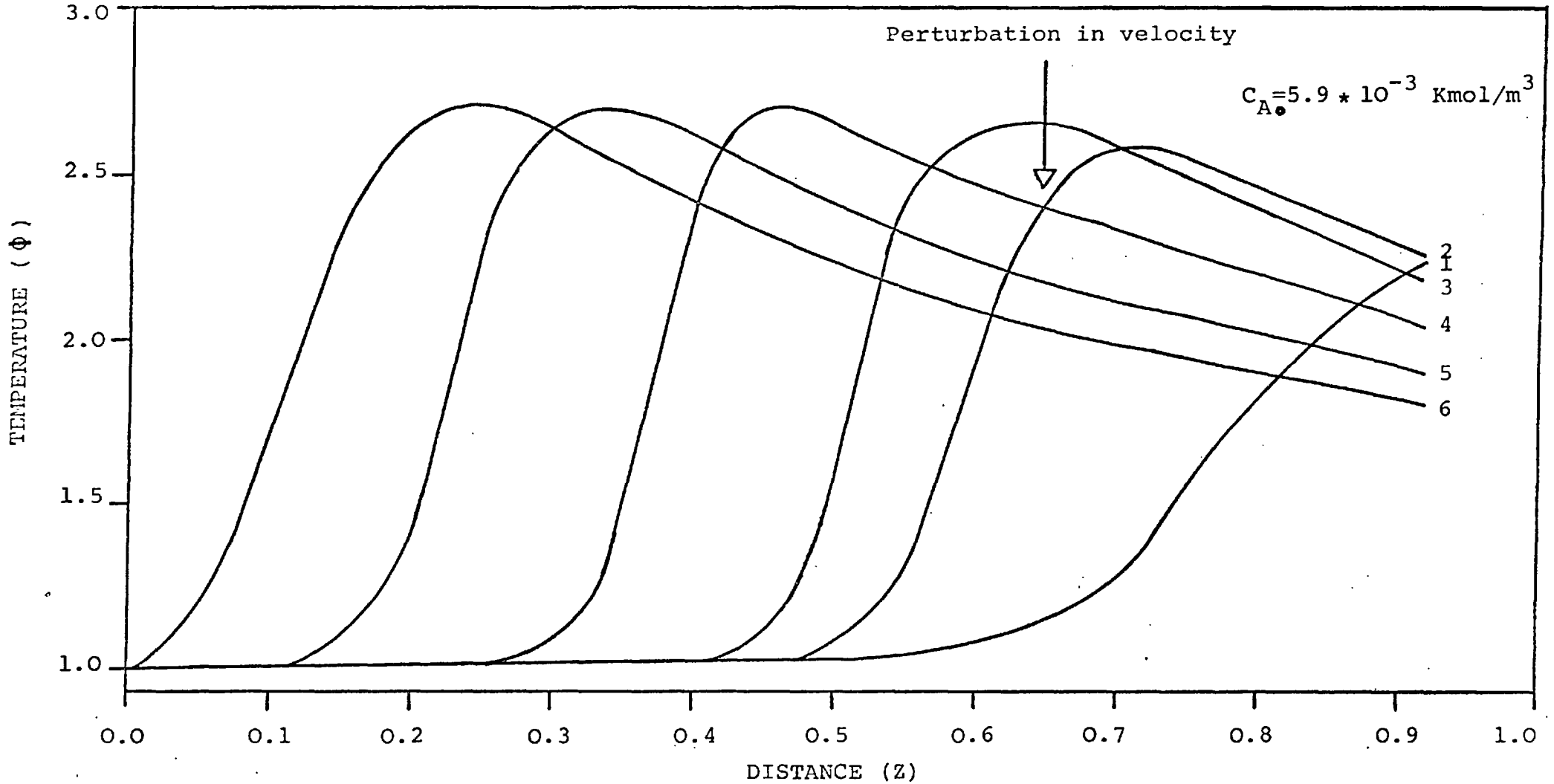


FIG. (5.10) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 10, 30, and 70min. RESPECTIVELY KEEPING CONCENTRATION CONSTANT. (RUN NUMBER 46)

u_o=0.215 m/s ; W=0.58 * 10^{-4} m/s.

u_o=0.233 m/s ; W=0.593*10^{-4} m/s.

u_o=0.269 m/s ; W=0.611*10^{-4} m/s.

Time : (1) 0; (2) 10min; (3) 15min; (4) 30min; (5) 35min; (6) 70min; (7) 75min; (8) 100min.

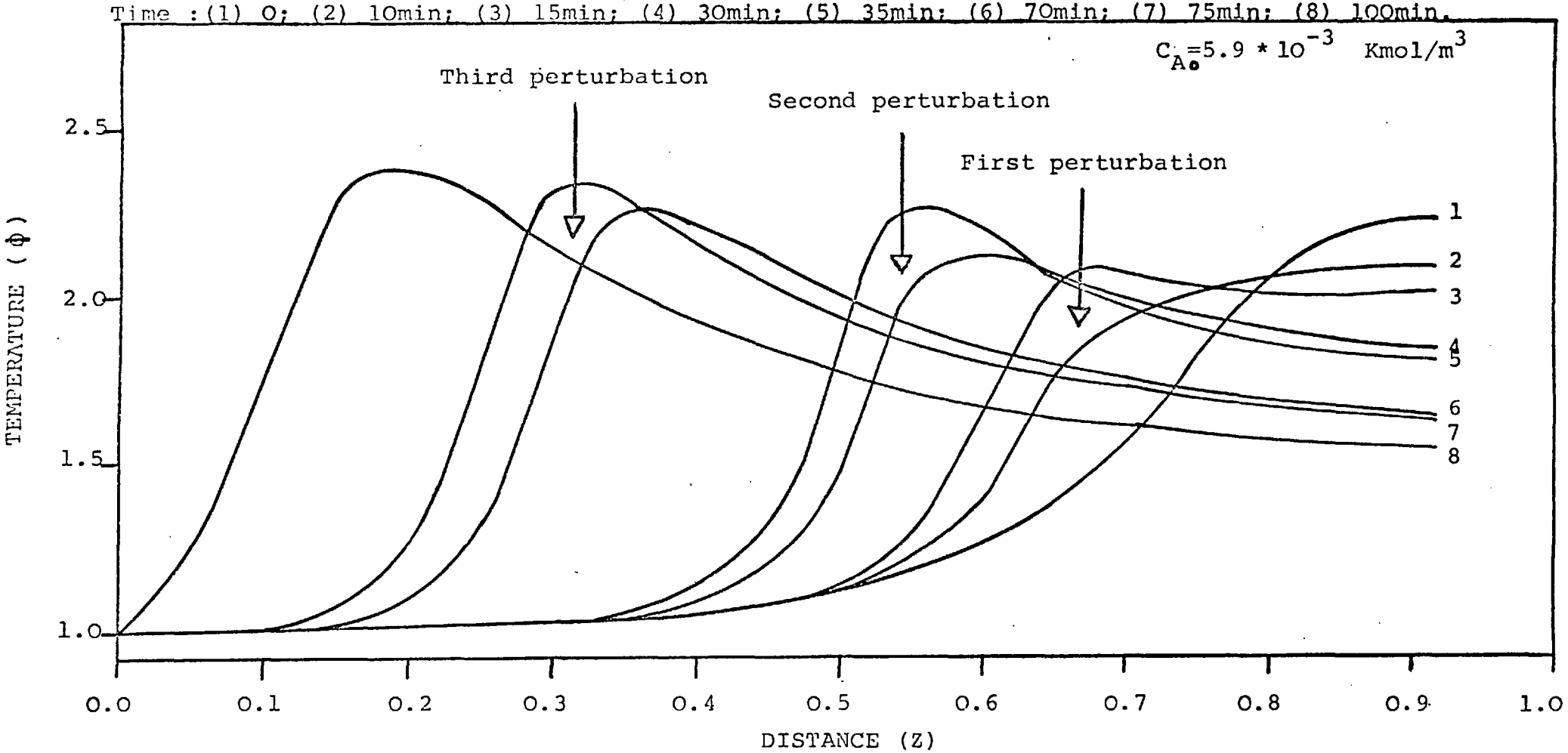


FIG. (5.11) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 20 min. KEEPING CONCENTRATION CONSTANT.

(RUN NUMBER 47)

u_o=0.385 m/s ; W=0.384 $*10^{-4}$ m/s.

u_s=0.437 m/s ; W=0.500 $*10^{-4}$ m/s.

Time : (1) 0; (2) 20min; (3) 30 min; (4) 90 min; (5) 150min.

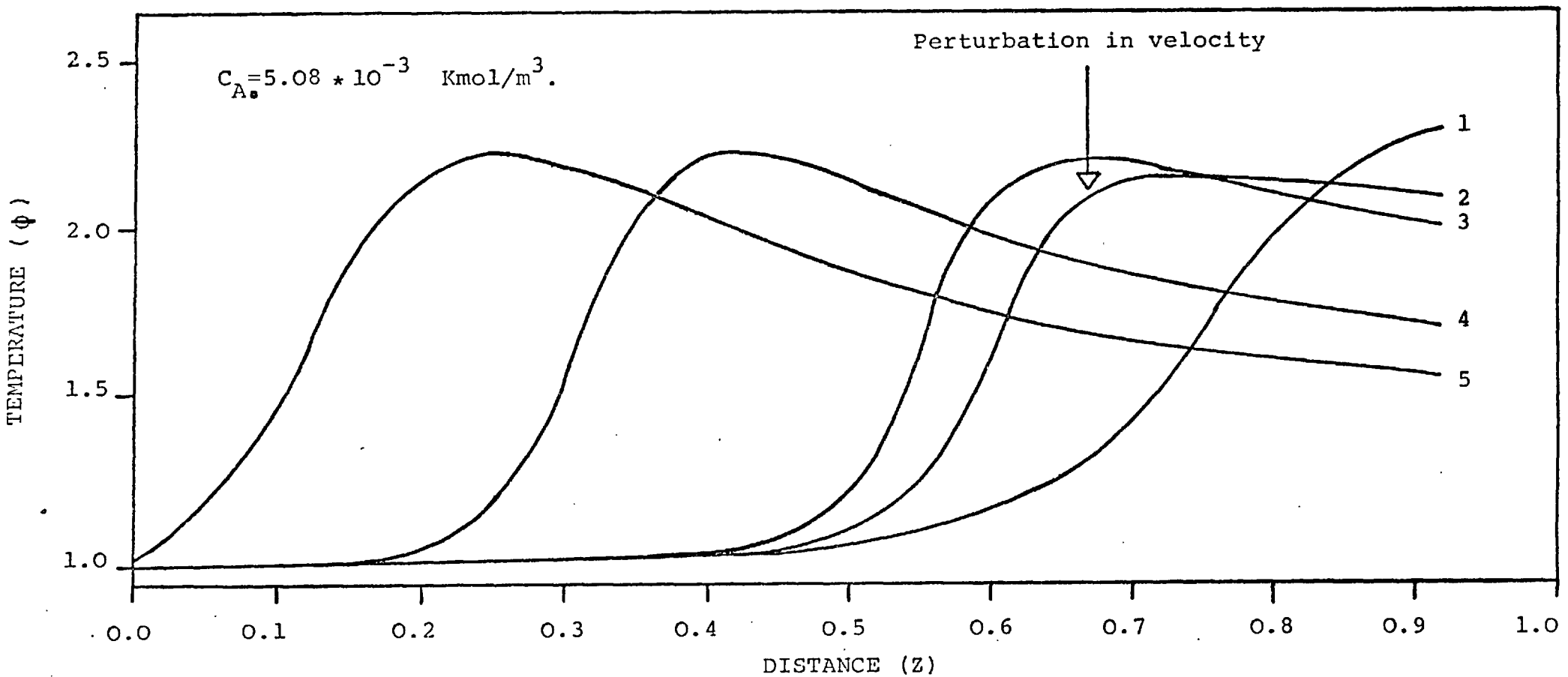
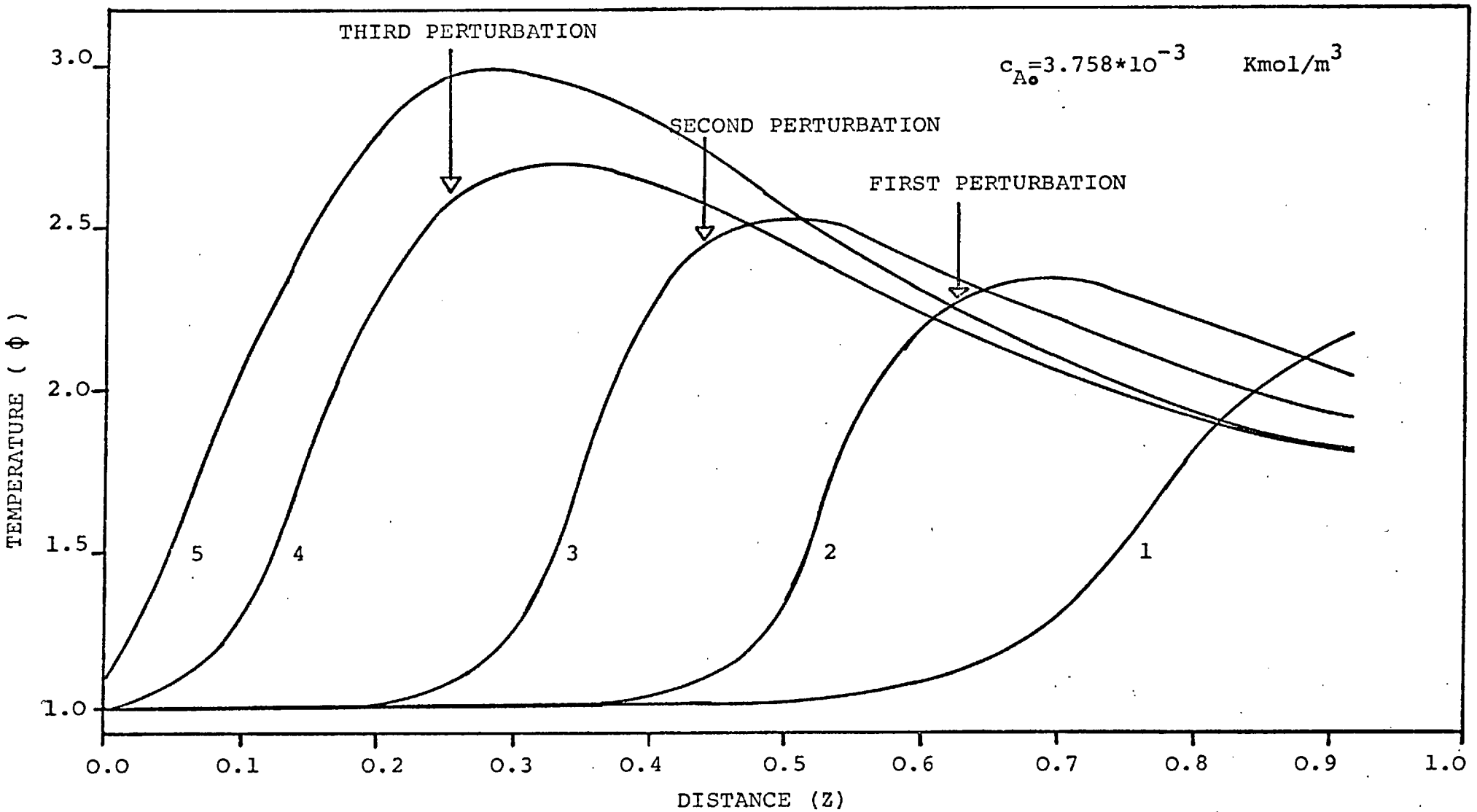


FIG.(5.12) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY 60,120 and 180 min. RESPECTIVELY KEEPING CONCENTRATION CONSTANT.

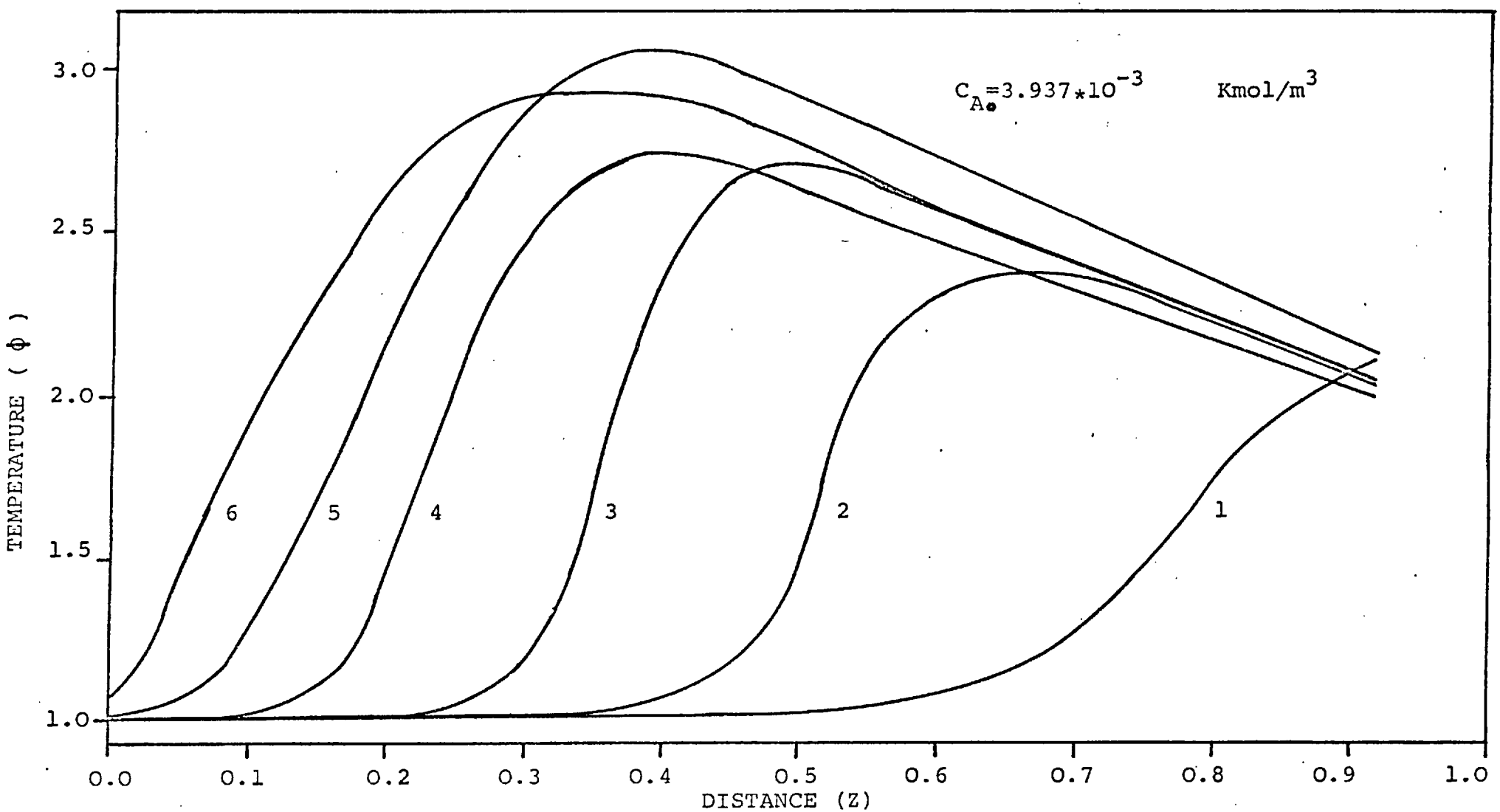
(RUN NUMBER 49)



Time:(1) 0; (2) 60min; (3) 120min; (4) 180min; (5) 240min.

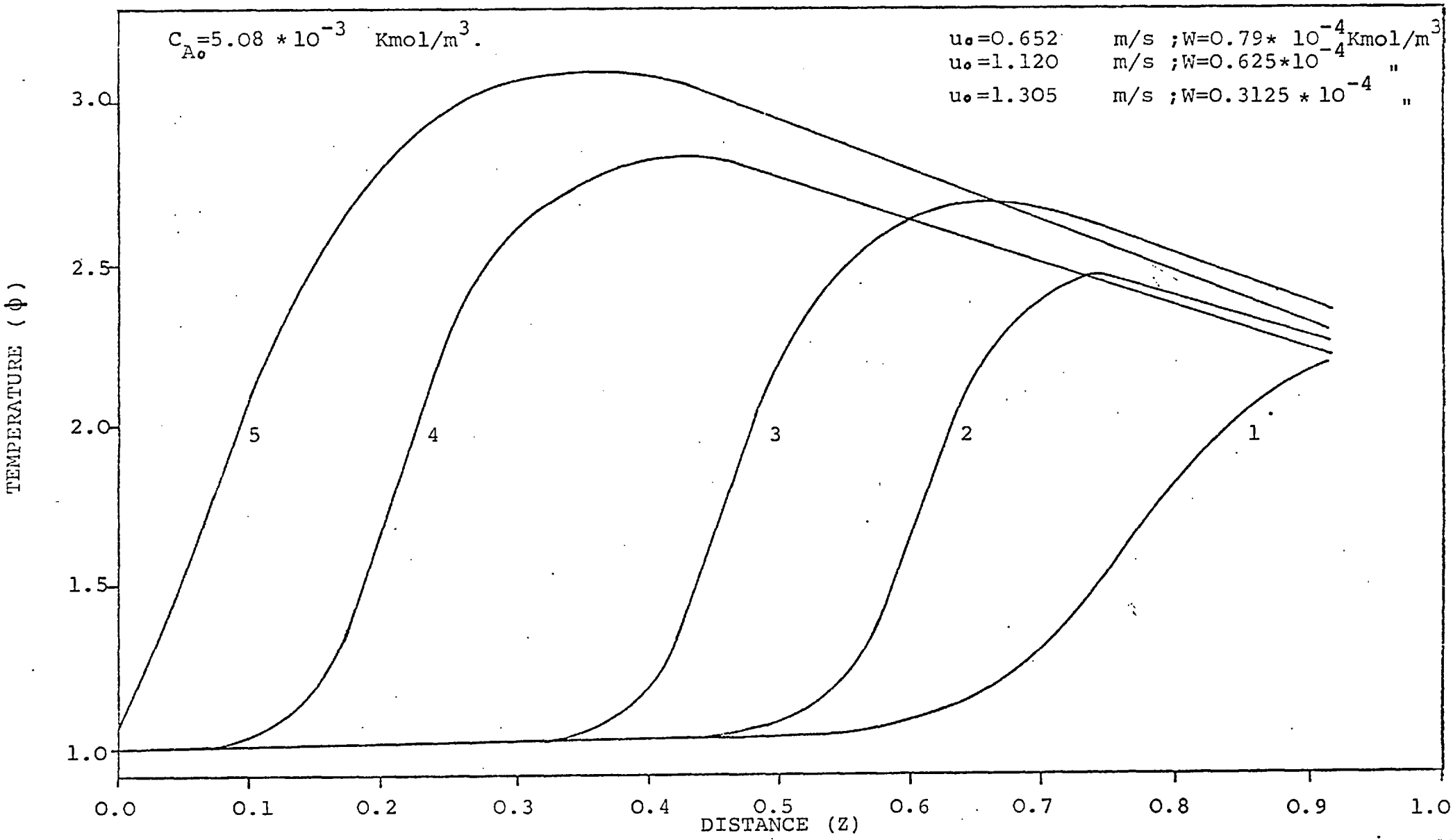
FIG.(5.13) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 60,100,130 and 180 min. RESPECTIVELY KEEPING CONCENTRATION CONSTANT.

(RUN NUMBER 50)



Time:(1) 0; (2) 60min; (3) 100min; (4) 130min; (5) 180min;(6)270min.
Increase in feed velocity after 60,100 and 130min.Decrease in feed velocity after 180min.

FIG.(5.14) TEMPERATURE PROFILES WITH PERTURBATION IN VELOCITY AFTER 20,40,and80min.RESPECTIVELY KEEPING CONCENTRATION CONSTANT. (RUN NUMBER 52)



Time:(1) 0; (2) 20min; (3) 40min; (4) 80min; (5) 120min.

FIG. (5.15) TEMPERATURE PROFILES OF BLOW-OUT OF REACTION.
(RUN NUMBER 55)

(1) Time = 30 min.
(2) Time = 60 "
(3) Time = 80 "
(4) Time =100 "
(5) Time =120 "
(6) Time =140 "
(7) Time =160 "
(8) Time =180 "

$C_{A_o}=3.82 * 10^{-3}$ Kmol/m^3

$u_o=0.5633$ m/s; $W=0.33 * 10^{-4}$ Kmol/m^3
$u_o=1.1267$ m/s; $W=-0.182 * 10^{-4}$ "

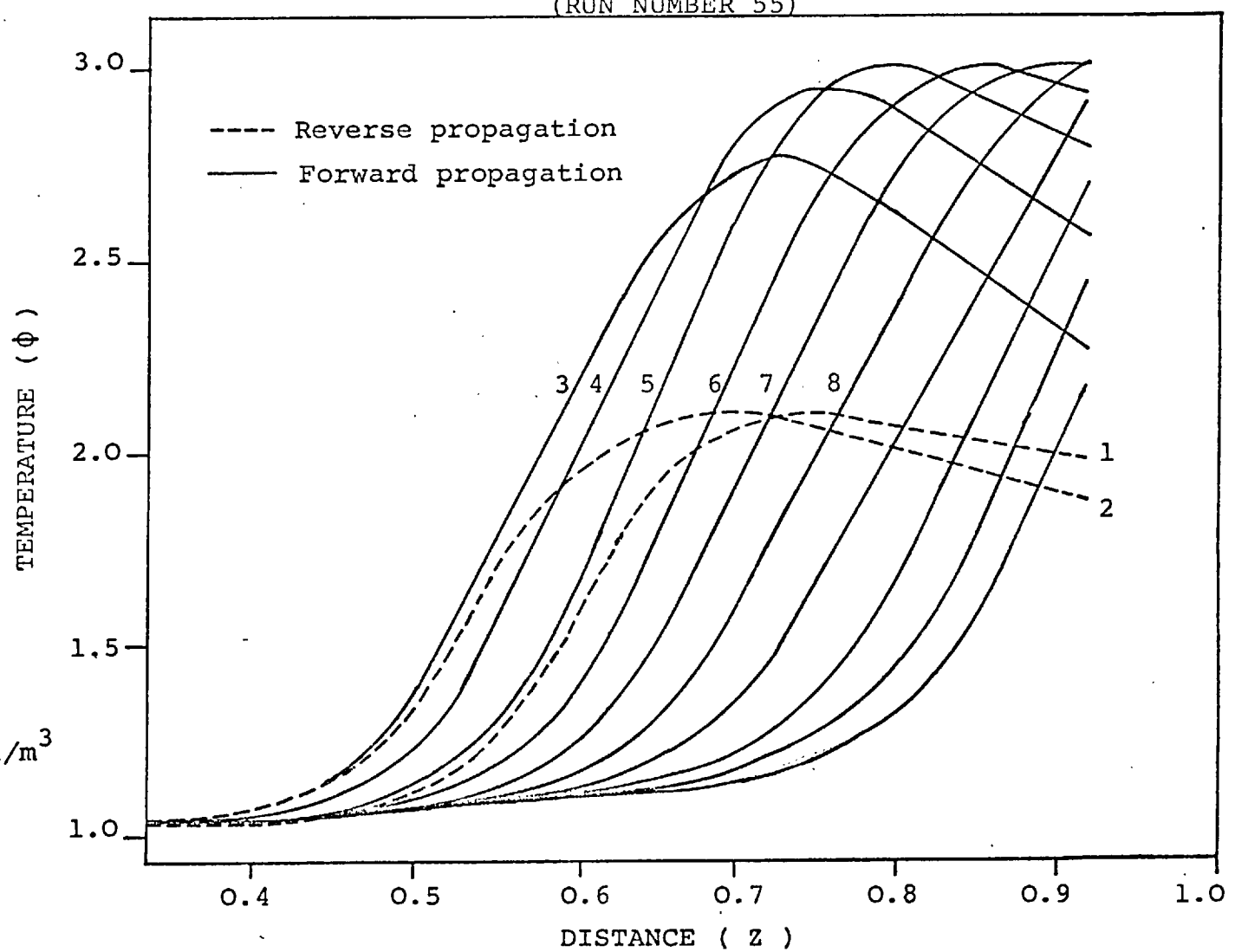
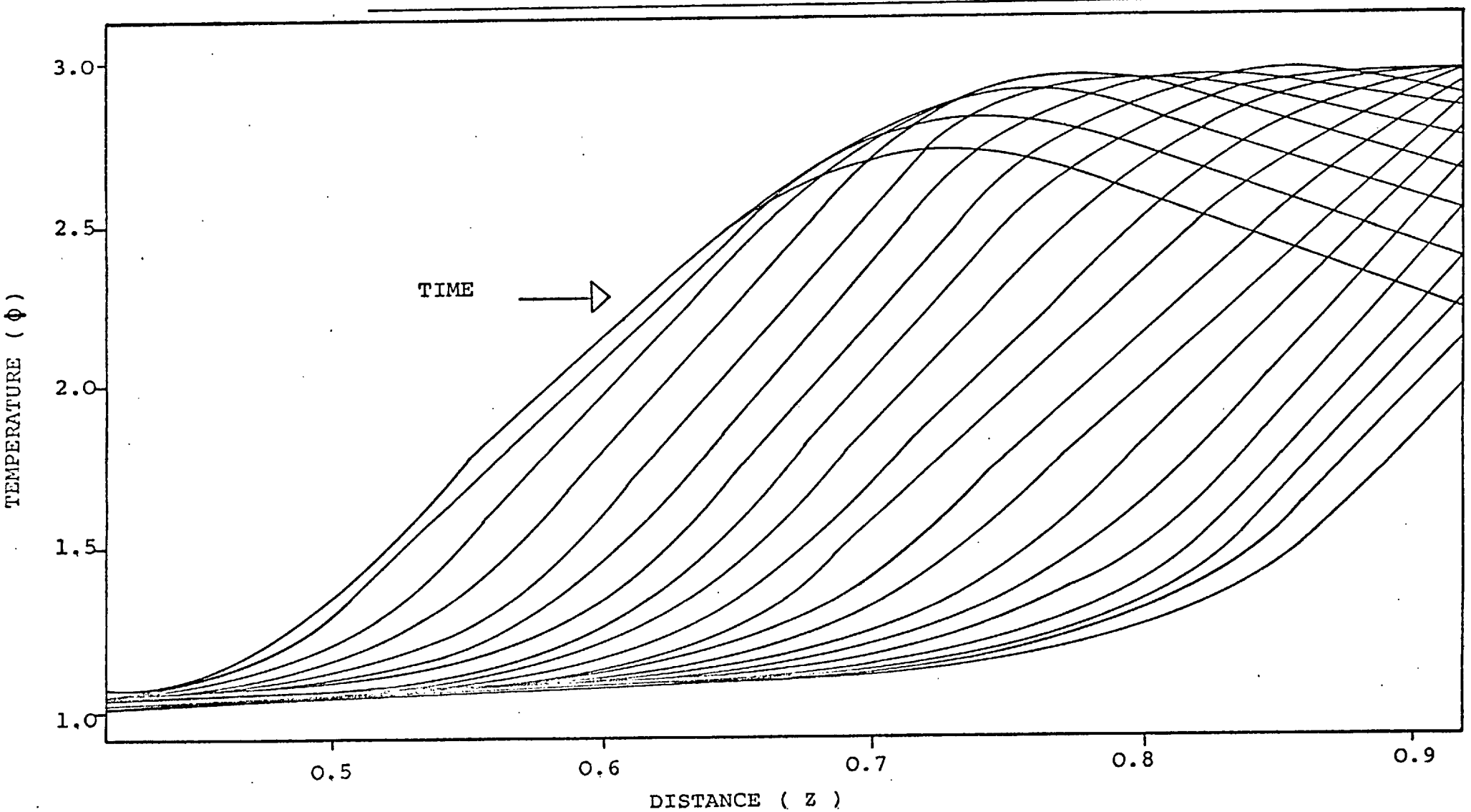


FIG.(5.15a)TEMPERATURE PROFILES OF BLOW-OUT OF REACTION.



the reverse to forward propagation, and eventually breaks down completely causing blow-out. Figure (5.15) illustrates the change in the direction of the reaction zone when the inlet velocity is increased by 100 per cent. Correlation of velocity of propagation with feed velocity and feed concentration is discussed in section 5.3.4.

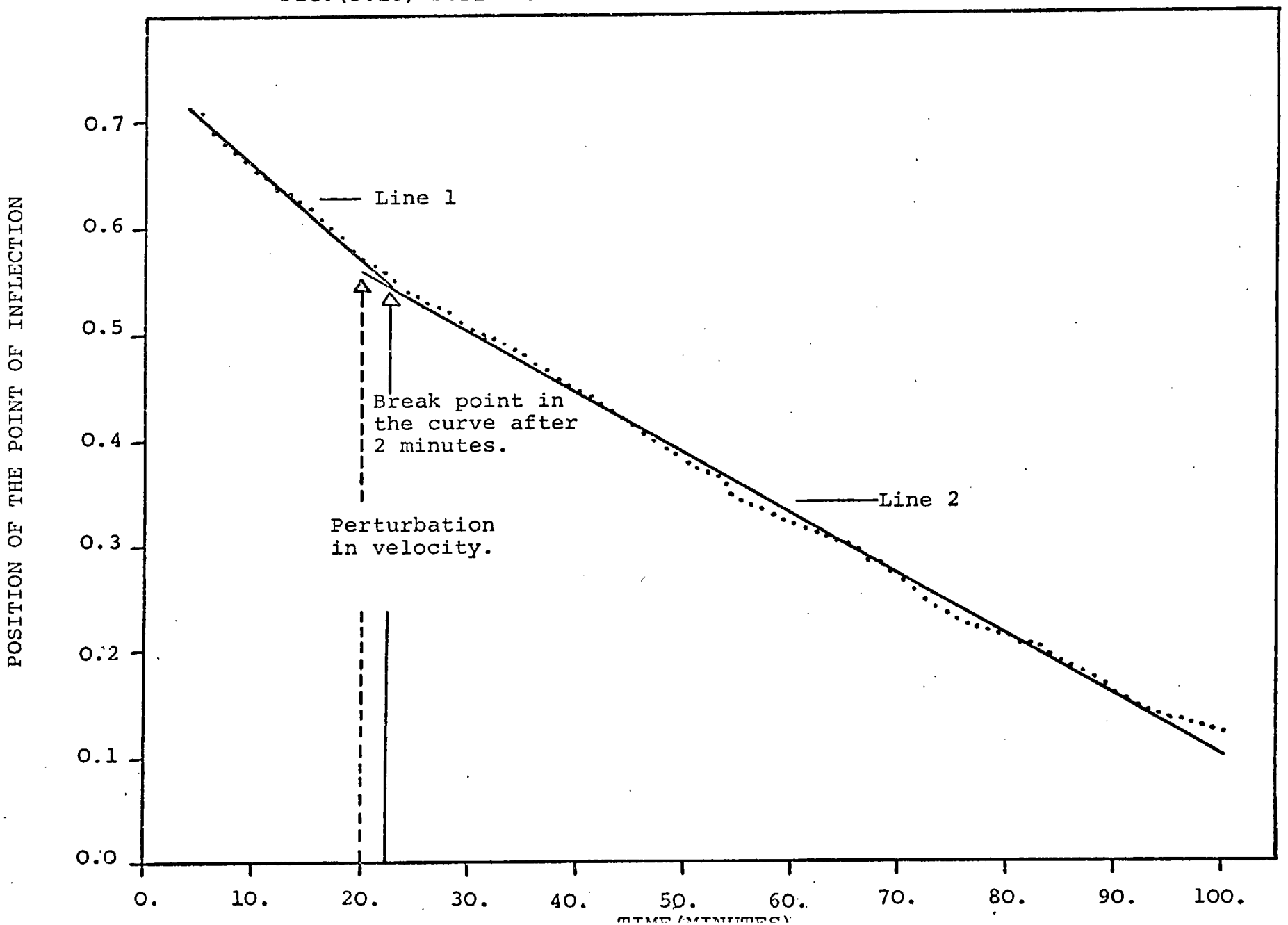
5.3.3 Determination of the velocity of propagation, W.

Since the geometry of the profile varies very slowly with time, it is assumed that the velocity of the point of inflection characterizes the velocity of the profile as a whole.

In order to find the point of inflection, a third order polynomial fit was made for the region in question on each profile, and the inflection point found from the resulting constants.

The average velocity of propagation is measured directly from the slope of the plot of the position at the point of inflection against time. The slope of the plot in turn is determined from a linear fit. Since perturbation in feed condition was made either in feed velocity or feed concentration during the runs and these alterations lead to a change in velocity of propagation, therefore the slope of the plot changes accordingly once such a perturbation has been carried out. The new slope is obtained by another linear fit from the time that perturbation in feed condition is made. A typical plot of the position of the point of inflection against time is shown in Figure (5.16). Line 1 and line 2 represent the linear fits before and after perturbation in feed velocity respectively.

FIG.(5.16) POSITION OF THE POINT OF INFLECTION AGAINST TIME



Intersection of the two lines is resulted by extending line 1.

It was found that this method of determining the velocity of propagation was much more accurate and reproducible than a simple differencing technique. The propagation velocities are indicated on the graphs of variable feed runs, shown in Figures (5.2 - 5.15).

5.3.4 Correlation of velocity of propagation.

The data were then tested against the semi-emperical correlations proposed by Wicke and Vortmeyer (1). This correlation was confirmed by Vortmeyer and Jahnel (7). In the later work it was found that, over a wide range of conditions, the direction and velocity of propagation W, the reaction zone depend heavily on the feed velocity and feed concentration, hence W could be correlated in the form

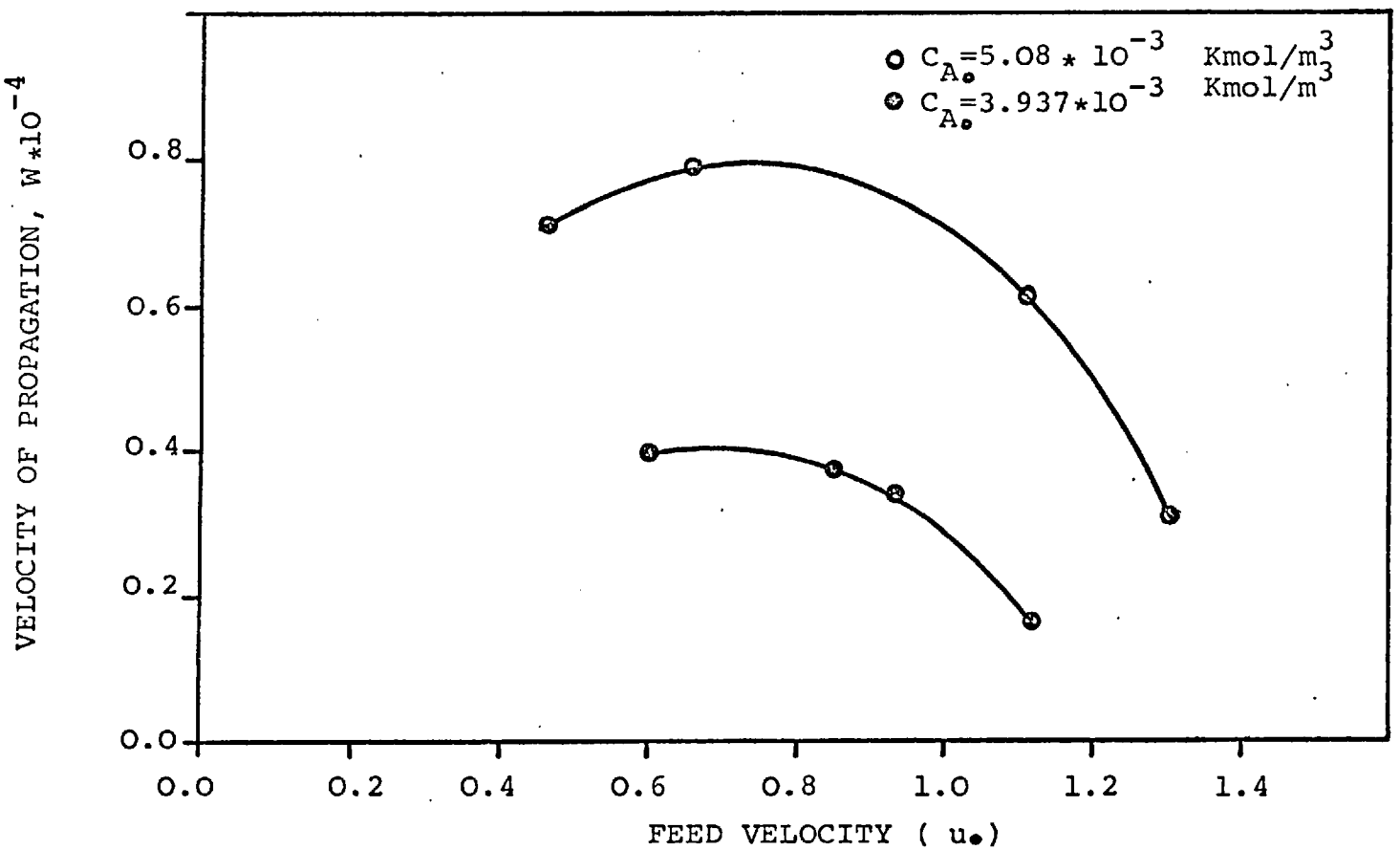
$$W = \alpha\, u_o^{0.77}\, C_{Ao}^{0.5} - \beta u_o$$

where u_o is the feed velocity (m/s), C_{Ao} is the feed concentration (k mol/m^3) , β is the ratio of gas to solid thermal conductivity, and α is essentially an empirical constant. For the oxidation of CO over CuO, $\beta = 3.07 \times 10^{-4}$.

They further demonstrated that different reaction kinetics do not change the exponents for feed velocity and feed concentration.

Positive values of W denote movement of the propagation of the reaction zone against the gas flow, while negative

FIG. (5.17) VELOCITY OF PROPAGATION FOR SELECTED VALUES OF FEED VELOCITY.



values indicate that the reaction zone is being blown out of the reactor.

All the previous work has been done at pseudo-steady-state operating conditions in which the feed conditions were kept constant for long periods of time. For purposes of control, however, it is important to know whether alterations in the feed velocity will quickly lead to a corresponding change in the velocity of propagation according to the above correlation. It is quite conceivable, that a rapid change in feed conditions could alter the behaviour of the system so that it obeyed the above correlation only after a long period of time, if at all. A prime example of such a perturbation is at start up where blow-out is very possible under conditions which would normally lead to propagation.

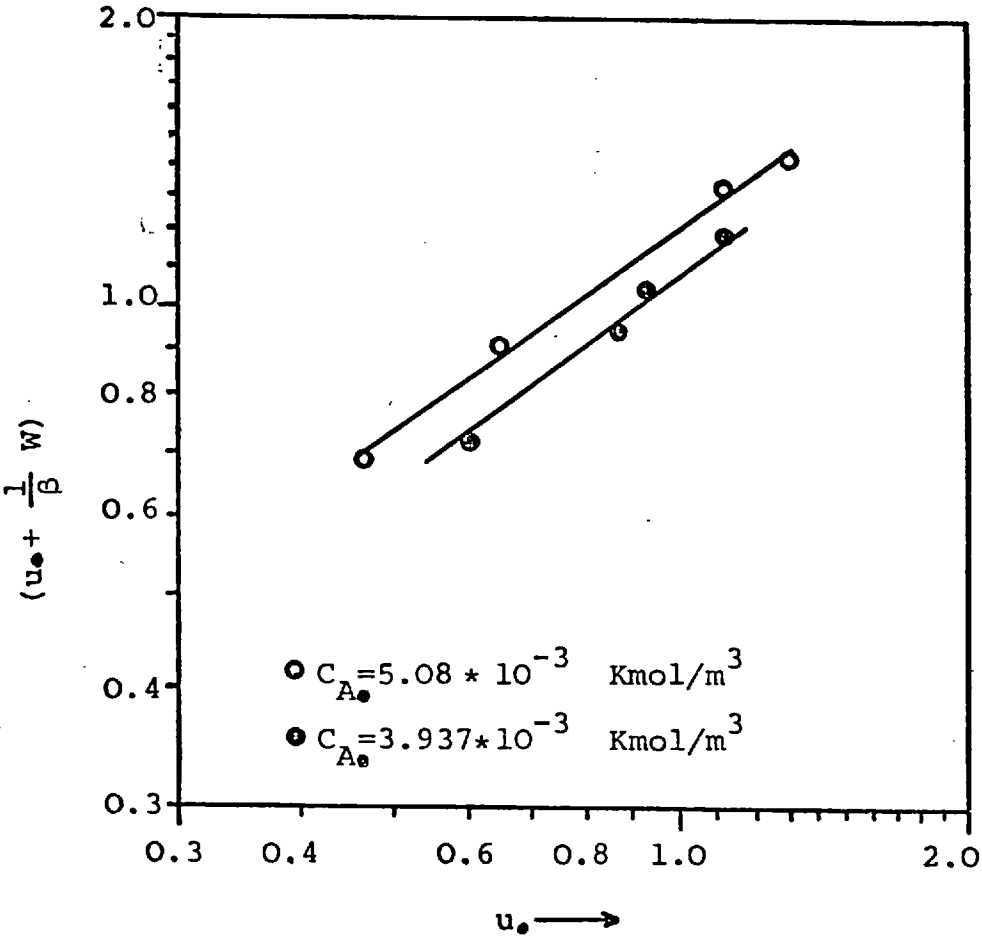
For other than start-up conditions it was found that the system responds to change in feed conditions within several thermal time constants of the perturbation. This is shown typically in Figure (5.16) where the break point in the curve occurs approximately 2 minutes after the disturbance. The new velocity of propagation then satisfies the correlation quoted above. A typical plot of velocity of propagation as a function of feed velocity is shown in Figure (5.17).

When the values of velocity of propagation, feed velocity, and feed concentration are plotted in double logarithmic form of Figure (5.17a)

$$\ln\left(u_o + \frac{1}{\beta} W\right) = f\left(\ln u_o, \ln C_{Ao}\right)$$

the resulting gradients of the straight lines lead to

FIG.(5.17a) DOUBLE LOGARITHMIC PLOT.



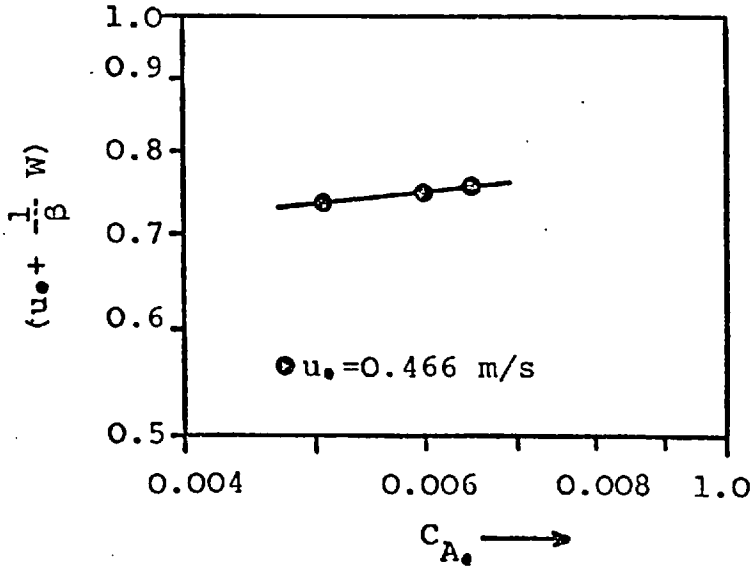


TABLE (5.1)
VALUES OF THE PHYSICAL PARAMETERS FOR THE EXPERIMENTAL RUNS
(CARBON MONOXIDE OXIDATION)

PHYSICAL PARAMETER	RUN NO.30	RUN NO. 31	RUN NO.32	RUN NO.37	RUN NO.43
C_{Ao} K mol/m^3	5.39×10^{-3}	6.442×10^{-3}	5.08×10^{-3}	5.9×10^{-3}	5.08×10^{-3} 6.0×10^{-3} 6.47×10^{-3}
u_o m/s	0.589	0.3943	0.466	0.3585 0.3943	0.466
τ s	1.019	1.5217	1.2875	1.674 1.522	1.2875
W m/s	0.75×10^{-4}	0.725×10^{-4}	0.71×10^{-4}	0.916×10^{-4} 0.93×10^{-4}	0.708×10^{-4} 0.91×10^{-4} 0.93×10^{-4}
C_{Bo} K mol/m^3	7.549×10^{-3}	7.328×10^{-3}	7.632×10^{-3}	7.441×10^{-3}	7.632×10^{-3} 7.441×10^{-3} 7.346×10^{-3}

TABLE (5.2)

VALUES OF THE PHYSICAL PARAMETERS FOR THE EXPERIMENTAL RUNS
(CARBON MONOXIDE OXIDATION)

PHYSICAL PARAMETER	RUN NO.44	RUN NO.45	RUN NO.46	RUN NO.46	RUN NO.49
C_{Ao} Kmol/m^3	5.45×10^{-3}	5.9×10^{-3}	5.9×10^{-3}	5.08×10^{-3}	3.758×10^{-3}
u_o m/s	0.466 0.513	0.5377 0.5915	0.1792 0.215 0.233 0.2688	0.385 0.437	0.5126 0.6084 0.6535 0.7492 0.6535
τ s	1.2875 1.171	1.116 1.014	3.347 2.789 2.575 2.232	1.5606 1.3733	1.17 0.9862 0.9182 0.8008 0.9182
W m/s	0.879×10^{-4} 0.577×10^{-4}	0.833×10^{-4} 0.717×10^{-4}	— 0.58×10^{-4} 0.593×10^{-4} 0.611×10^{-4}	0.384×10^{-4} 0.50×10^{-4}	0.347×10^{-4} 0.278×10^{-4} 0.250×10^{-4} —
C_{Bo} Kmol/m^3	7.537×10^{-3}	7.441×10^{-3}	7.411×10^{-3}	7.632×10^{-3}	7.892×10^{-3}

TABLE (5.3)
VALUES OF THE PHYSICAL PARAMETERS FOR THE EXPERIMENTAL RUNS
(CARBON MONOXIDE OXIDATION)

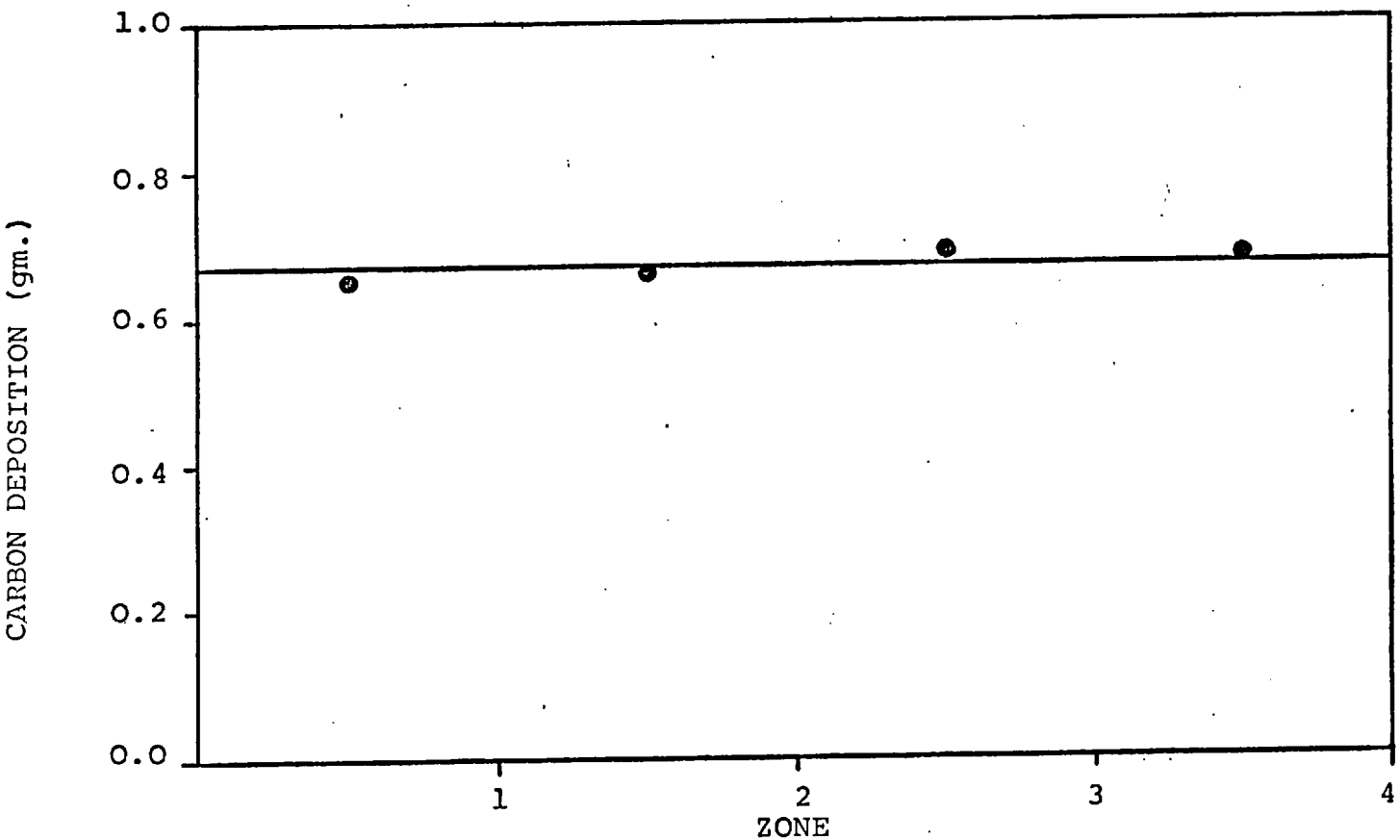
PHYSICAL PARAMETER	RUN NO. 50	RUN NO.52	RUN NO.53	RUN NO.55
C_{Ao} Kmol/m^3	3.937×10^{-3}	5.08×10^{-3}	4.59×10^{-3} 3.45×10^{-3} 5.51×10^{-3}	3.82×10^{-3}
u_o m/s	0.6079 0.8496 0.9356 1.1195 0.9356	0.652 1.12 1.305 1.45	0.461	0.5633 1.1267
τ s	0.9870 0.7062 0.6413 0.5364 0.6413	0.9196 0.5364 0.4598 0.4153	1.3015	1.065 0.5325
W m/s	0.39×10^{-4} 0.37×10^{-4} 0.35×10^{-4} 0.166×10^{-4} —	0.79×10^{-4} 0.625×10^{-4} 0.3125×10^{-4} —	0.70×10^{-4} 0.36×10^{-4} 0.725×10^{-4}	0.33×10^{-4} -0.182×10^{-4}
C_{Bo} Kmol/m^3	7.855×10^{-3}	7.632×10^{-3}	7.717×10^{-3} 7.958×10^{-3} 7.524×10^{-3}	7.892×10^{-3}

exponents for u_o and C_{Ao}. The exponents for the corresponding feed velocity and feed concentration found to be 0.72 and 0.45 respectively which compares reasonably well with the exponents of 0.77 and 0.5 by Vortmeyer and Jahnel (7)

5.4 Method of Carbon Deposition.

Carbon deposition was carried out by passing a mixture of preheated propylene and nitrogen over alumina-silica catalyst through the reactor bed at a temperature of 770°K. A propylene flow of 30 cc/min and nitrogen flow of 70 cc/min was used. Preliminary experimentation indicated reverse propagation was effective with the bed containing a carbon deposition of at least 7% by weight. A period of 15 hours was needed for this amount of deposition. However every attempt to obtain a uniform carbon deposition of the order of 7-8% proved unsuccessful, since after this period of the hydrocarbon cracking the catalyst in the bed was still active especially where less carbon was deposited. When the preheated mixture was allowed to pass through the bed for a period of 24 hours, the resulting carbon deposition was approximately 12% by weight. This deposition was found to be reasonably uniform along the reactor. The procedure to find out this uniformity throughout the bed was achieved by means of burning the carbon on each of the available four zones separately (section 4.2.1). The deposition on each zone was measured from the CO and CO_2 analysis. The resulting analysis showed that each zone contained approximately 0.67 gm of carbon. A typical plot of carbon depostion in each zone is shown in Figure (5.18a).

FIGURE (5.18a) CARBON DEPOSITION IN EACH ZONE ALONG THE REACTOR.



5.5 Carbon Oxidation Results.

Data on regeration of cracking catalyst are presented for 10 runs (Run Nos. 71,72,73,74,75,76,77,78, 79 and 80). The observations for each run include :

a) The room temperature.
b) Air flowrate.
c) Feed concentration of oxygen.
d) Feed temperature.
e) Pressure gauge readings.
f) The initial temperature profile along the reactor.
g) The peak temperature.
h) The temperature profile along the reactor as f(t).
i) The concentration analysis of the exit gases with time.
j) Power input to the heating tapes.

Tables (5.4 and 5.5) summarize the operating conditions of the reactor for the runs. Tables (C10 - C19, appendix C) present the data on runs (71,72,73,74,75,76,77,78,79 and 80) respectively. Temperature profiles were recorded at intervals of one minute, however in the interest of brevity these are tabulated at five minute intervals (appendix C). During the preliminary runs 7 thermocouples broke due to the excessive rise in temperature in the reaction zone. Therefore 17 thermocouples were available for the measurement of the temperature profiles. The positions of broken thermocouples along the normalized distance of the reactor were at 0.125, 0.250, 0.667, 0.708, 0.792, 0.833 and 0.875

respectively. Since the temperature varied uniformly along the reactor the temperature at positions of faulty thermocouples were interpolated from the adjoining thermocouple readings.

The regeneration operation is highly exothermic and must be conducted carefully to prevent the permanent deactivation of the catalyst. Alumina-Silica catalysts are quite stable up to temperatures of 900^{o}K. Sintering brings about essentially complete loss of surface area of Alumina-Silica catalyst with a short time at 1273^{o}K (42). Therefore the amount of air flow was limited to a maximum of 300 cc/min. Higher air flow rates increase the rate at which fuel is fed to the reaction zone, raising the rate of heat liberated, and the peak temperature. Hence by operating above 300 cc/min air flow the reaction zone would experience a severe temperature rise in the reaction zone which inevitably cause the deactivation of the catalyst and also damage the equipment.

The regeneration was conducted by burning the carbon using air. Except in the preliminary investigation where the air was diluted with nitrogen, no attempt was made to use this diluent as a control variable for velocity of propagation, since this method did not indicate an effective control upon the system for the range of air flow used.

The air flow varied from 0.23 to 0.3 l/min. This corresponds to a variation in residence time τ through the packed bed from 4.23 to 5.52 secs. The initial ignition temperature imposed was of order of 800^{o}K.

The first concentration analysis was performed 10 minutes after the start of the run. Thereafter the analysis

were conducted at five minute intervals. The exit analysis in all the runs showed approximately 98% conversion of oxygen.

Using air at room temperature with the imposed temperature profile near the exit section, the reaction zone proceeded upstream only for a short distance. As the thermal load of preheating the air was too great, the reaction zone changed its direction causing the blow-out of the reaction zone. The initial movement of reaction zone upstream was due to the effect of the imposed temperature profile. This suggested that reverse propagation is possible with a preheated feed. It was found that the feed had to be preheated to at least 570^{o}K in order to lead to a stable reverse propagation and prevent the blow-out of the reaction zone.

The control variables used for this system, therefore were the feed velocity u_o, and the feed temperature To. All the runs were carried out for a variety of constant feed conditions. As opposed to the previous system no perturbation was made during the steady-state operating conditions.

The variation in feed velocity during all the runs with constant feed conditions in each particular run, including those with variable preheated feed temperature was limited from 0.1087 to 0.148 m/s. Since the air flow used was not diluted , further increase in the inlet velocity result in an increase in the amount of heat evolved from the highly exothermic oxidation reaction. Utilizing higher feed velocity would have caused deactivation of the catalyst as a direct result of excessive temperature rise

in the reaction zone. This limitation of inlet velocity was too low for any attempt to perturb the operating condition during the steady-state runs to achieve some objective.Also because of using low inlet velocity, on the introduction of the feed flow to the reactor at the start up with the proper feed temperature the reaction zone was quickly established and led to propagation upstream without any difficulties.

Perturbation in feed temperature during the steady-state operation is not possible, since this mode of operation to alter the preheated feed temperature to the desired value while conducting an experimental run would require a long time to get readjusted.

With the preheated feed, all the runs indicate an effective reverse propagation of the reaction zone. Figures (5.18 - 5.29) illustrate the temperature profiles along the reactor with constant feed conditions during the regeneration of the fouled cracking catalyst.

The reaction zone propagates counter to the flow of reactant with a constant velocity. When the zone reaches the reactor entrance the zone changes its direction from reverse to foward propagation. This movement continues advancing forward with a slower propagation rate compared to that of reverse propagation, and the zone travels to the exit section. The amount of carbon burnt during the reverse propagation was 20 to 33% depending on the feed velocity and feed temperature used for the operation.

Since most of the carbon remains unburnt during reverse operation, the mode of propagation is severely altered when the zone reaches the reactor inlet. Hence forward

FIG. (5.18) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST. (RUN NUMBER 74)

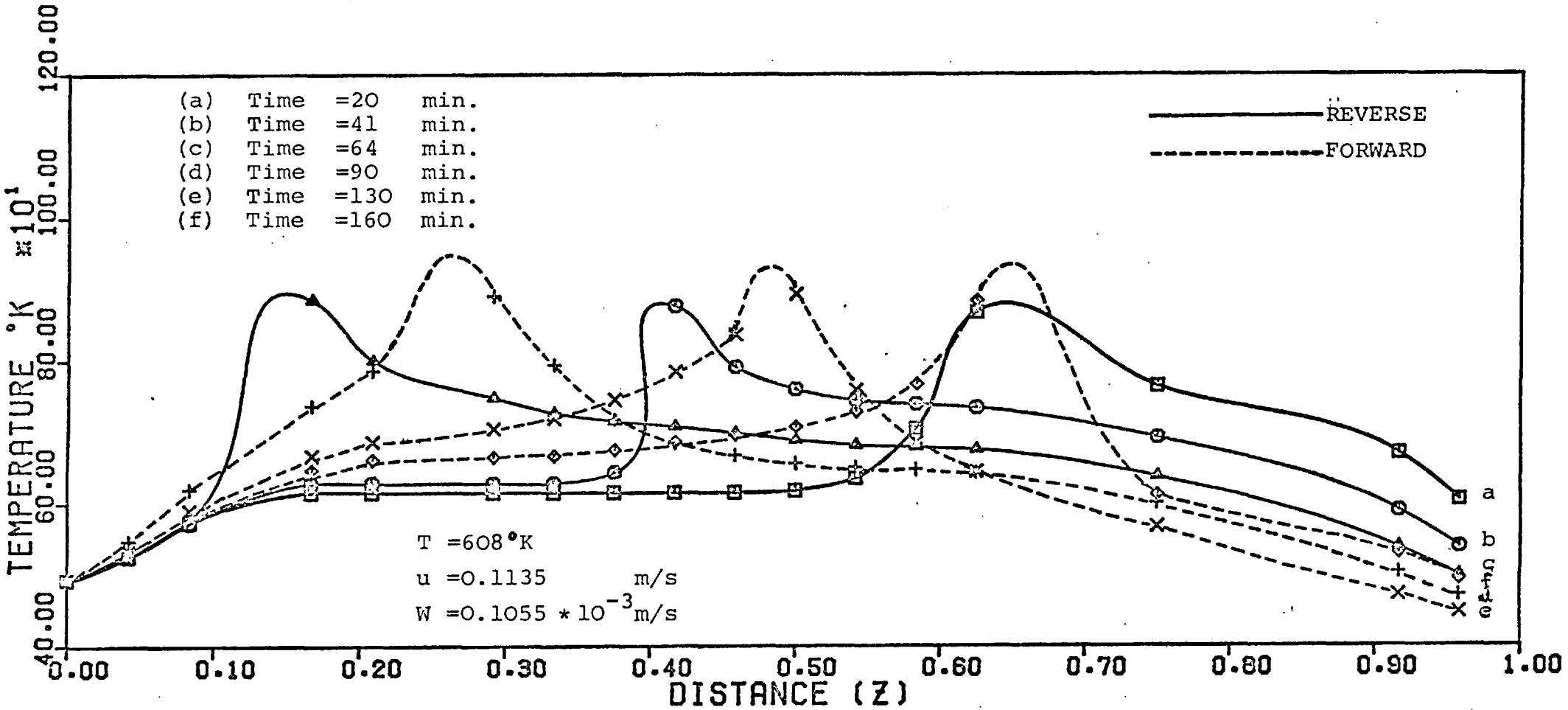


FIG. (5.19) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST. (RUN NUMBER 77)

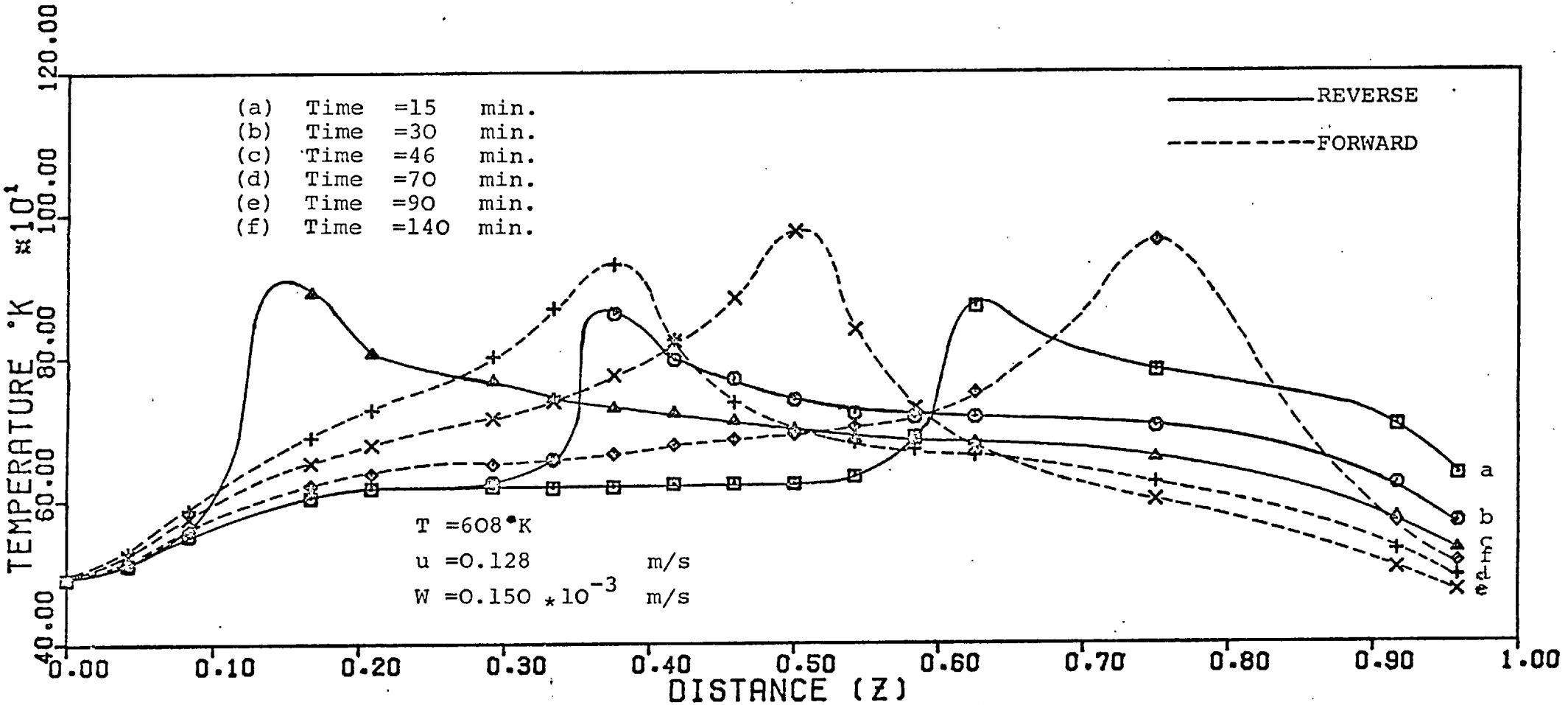


FIG.(5.20) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 71)

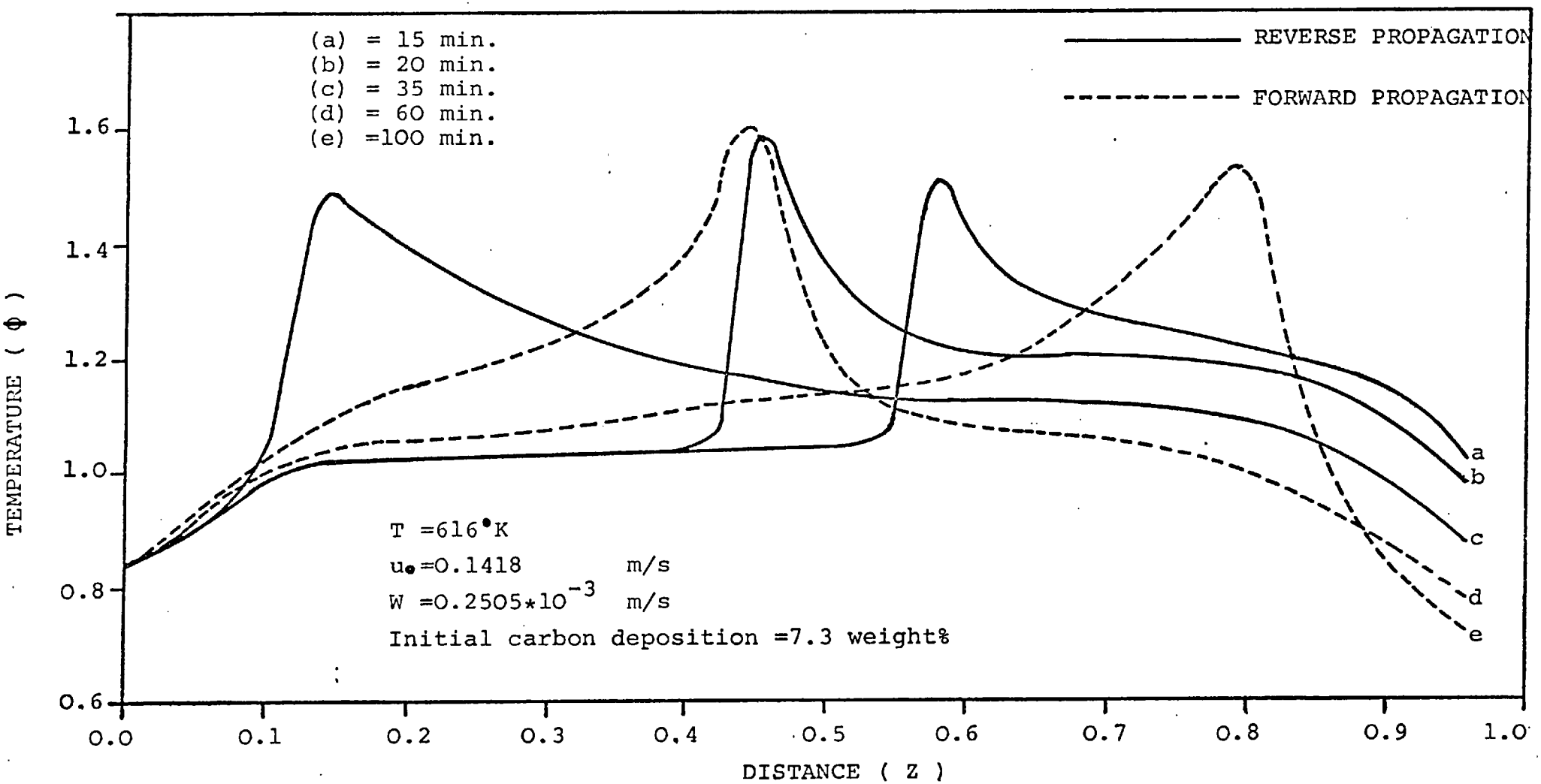


FIG. (5.21) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

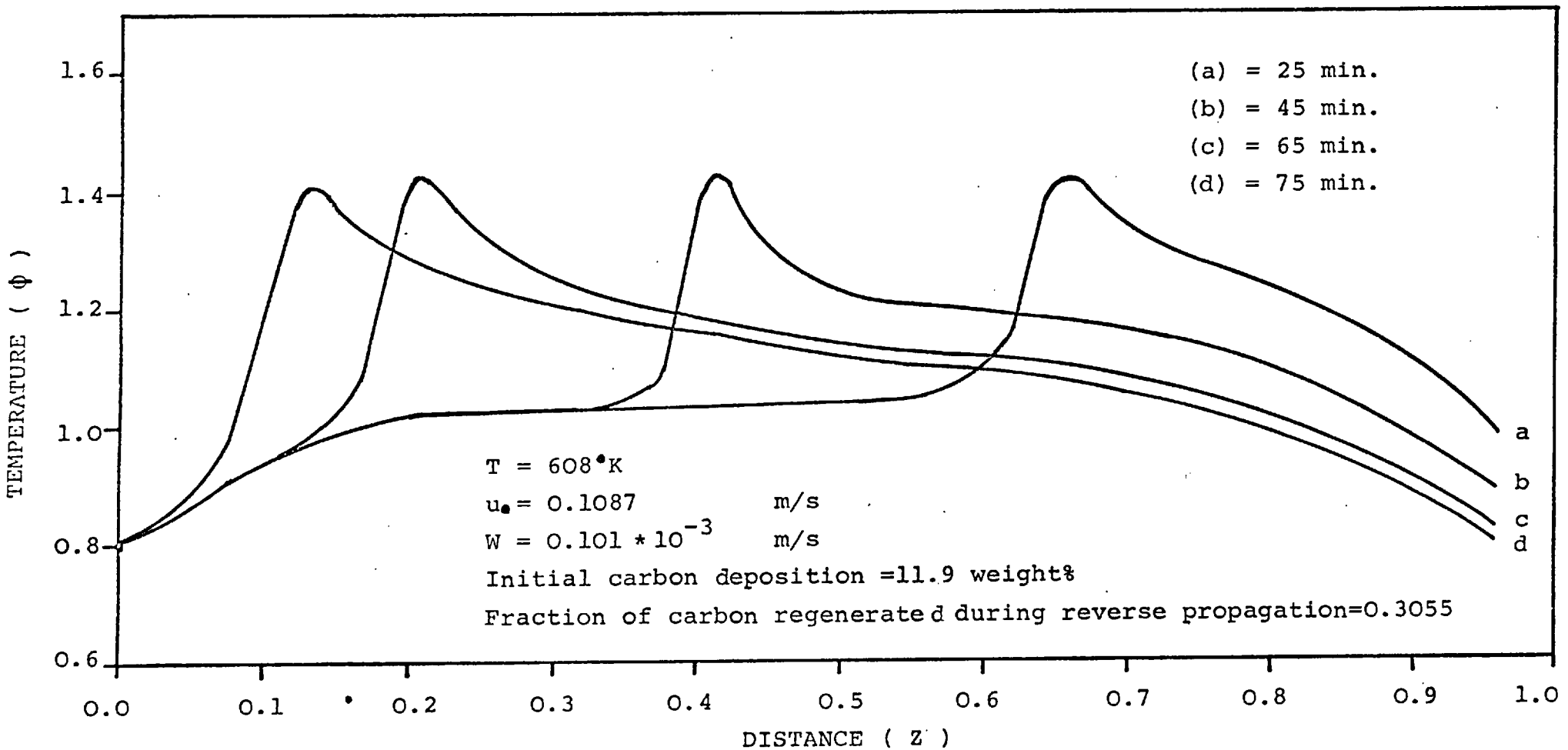


FIG. (5.22) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 74)

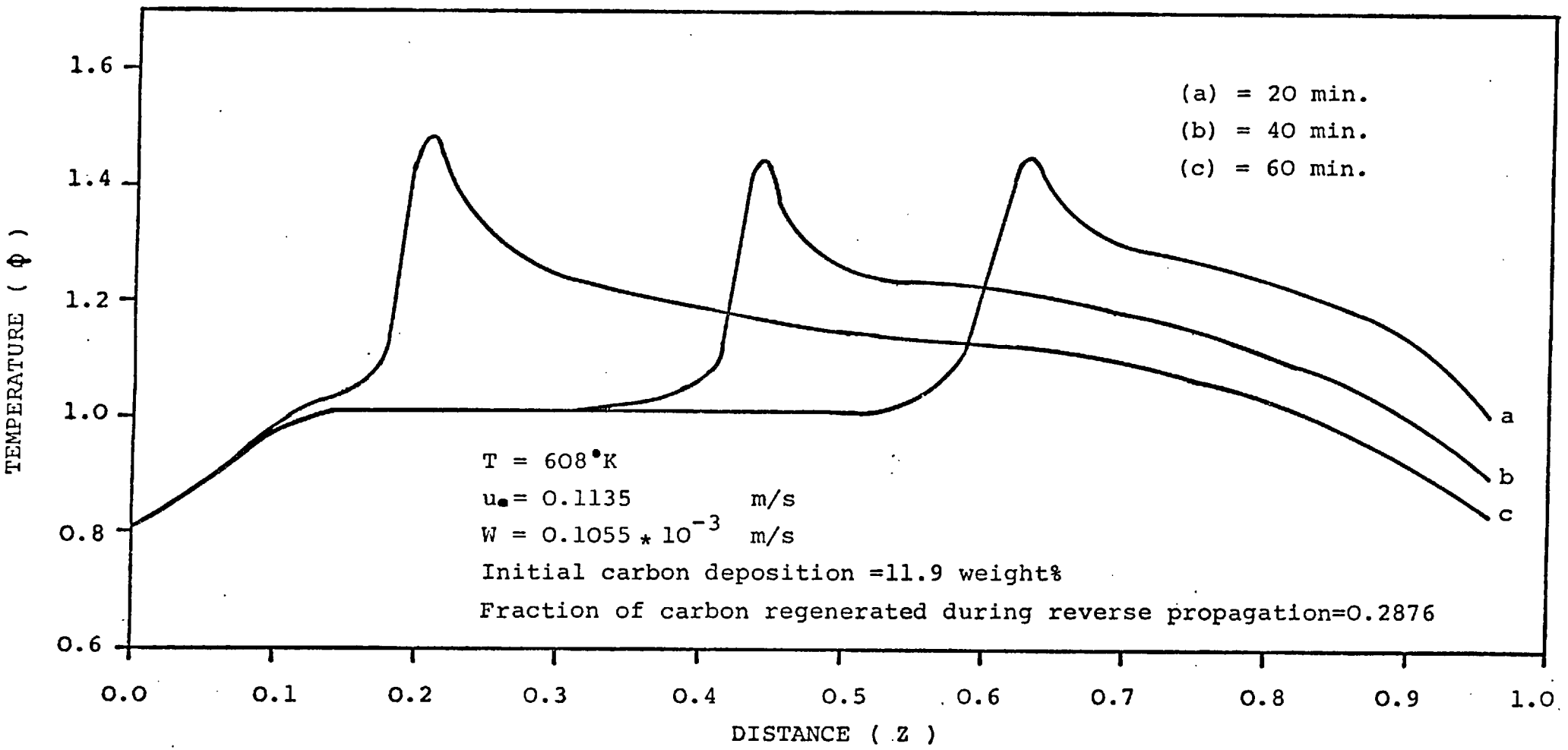


FIG. (5.23) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 75)

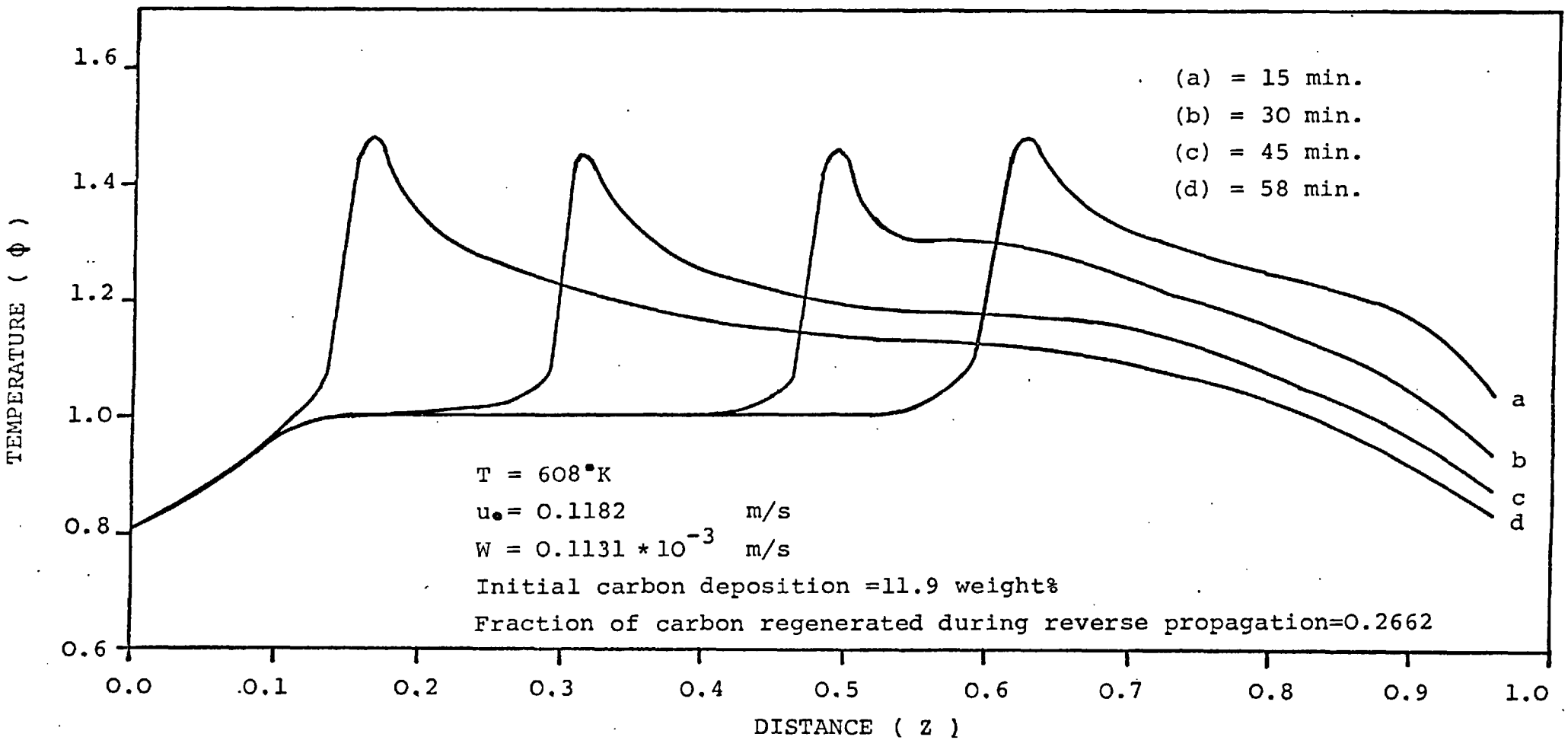


FIG. (5.24) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 76)

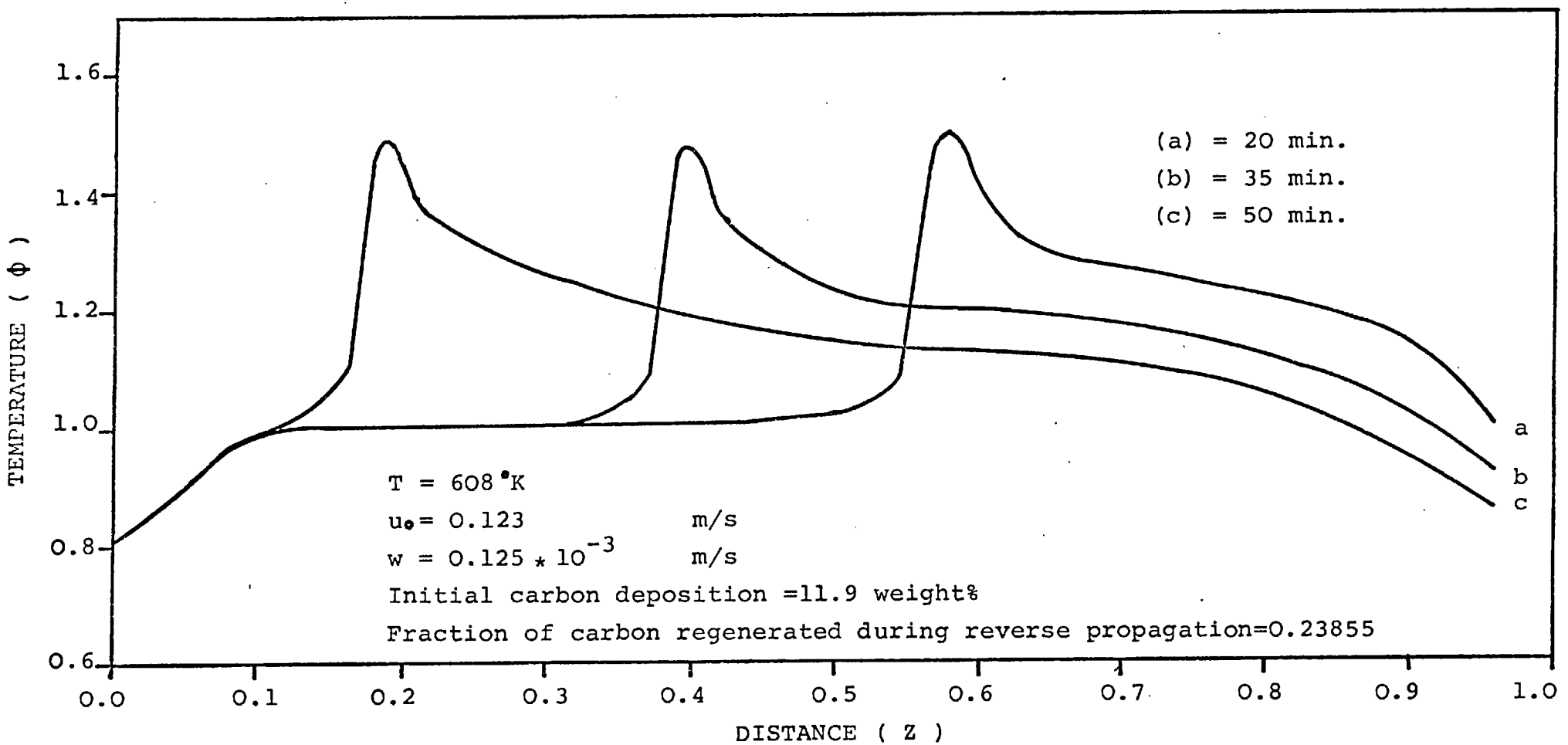


FIG. (5.25) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 77)

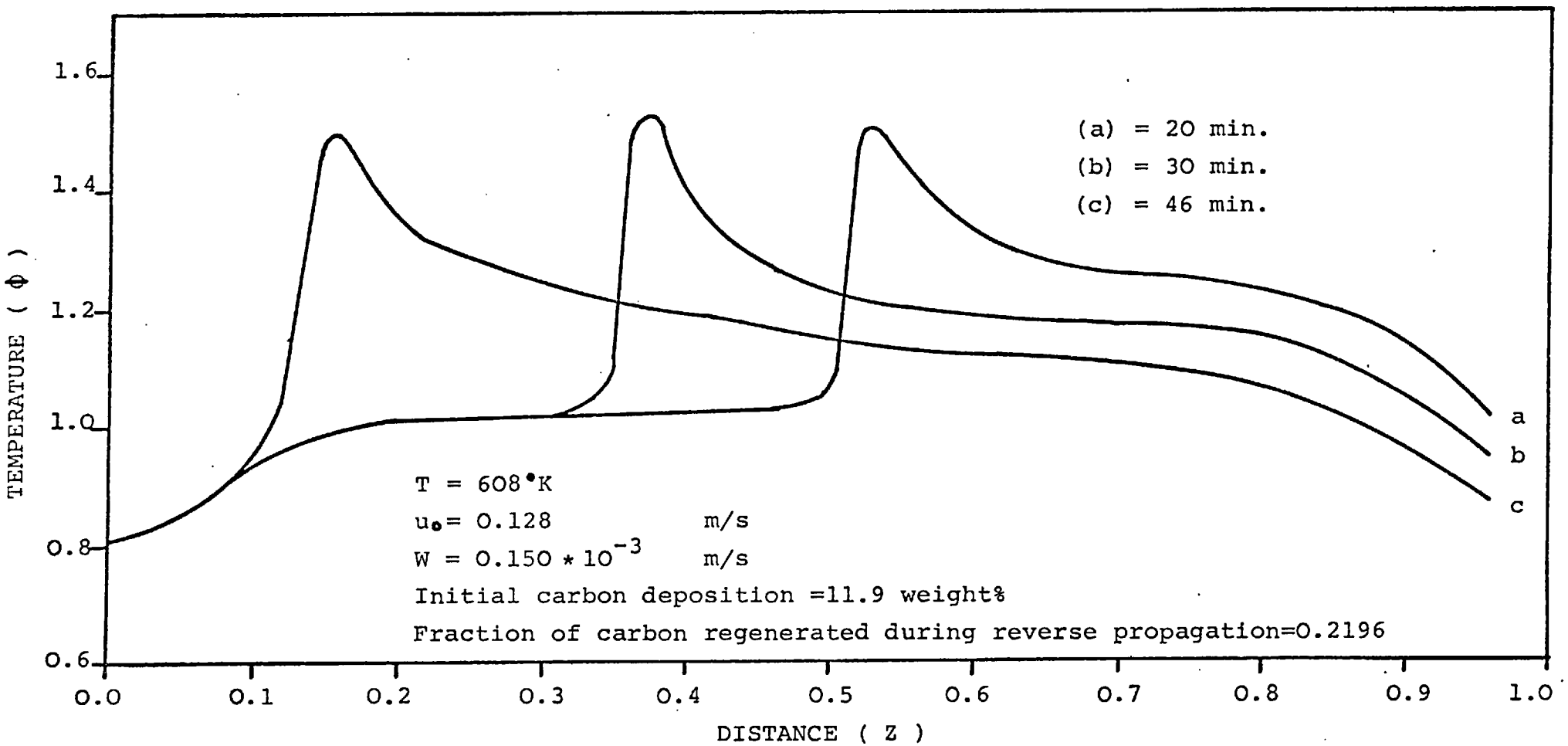


FIG. (5.26) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 78)

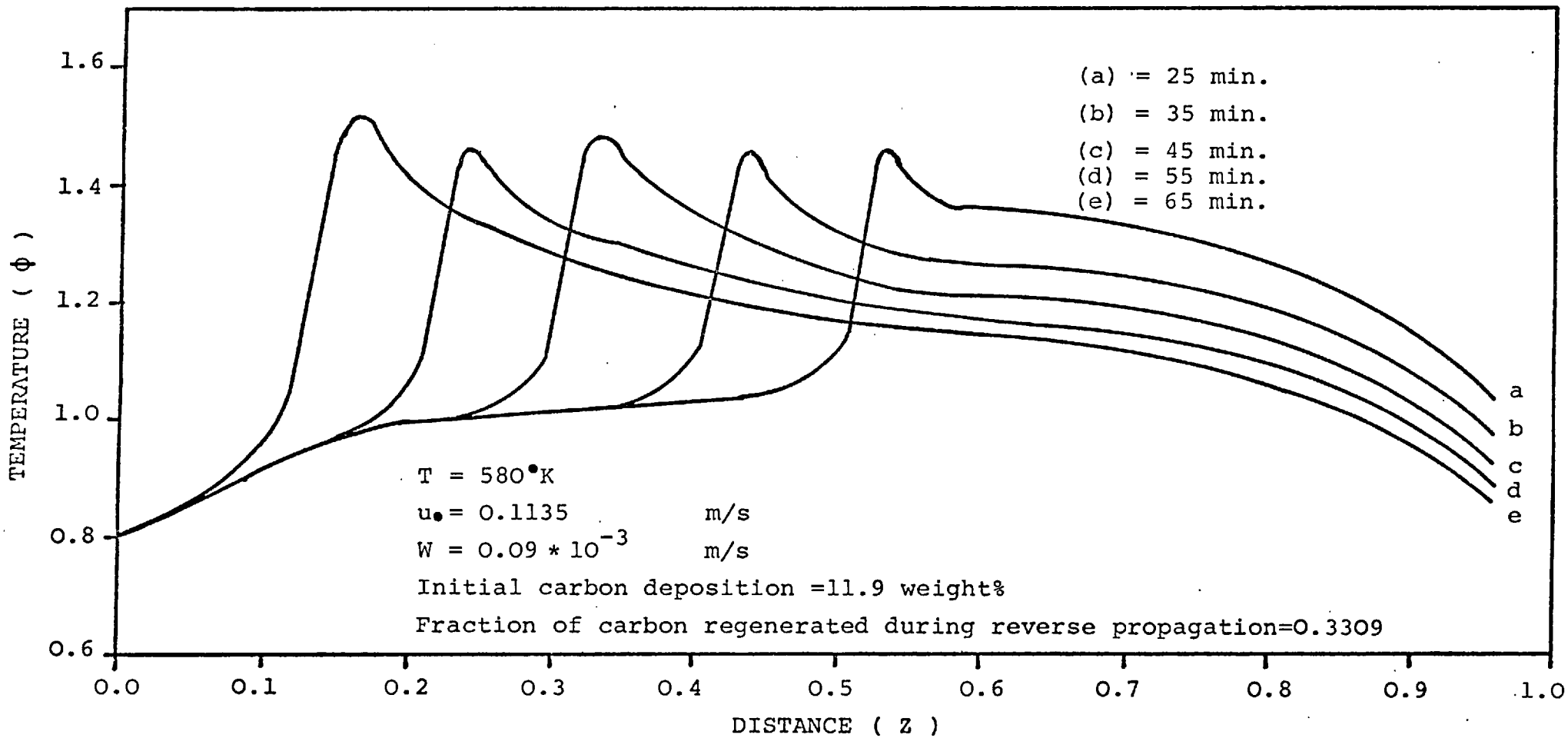


FIG. (5.27) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 79)

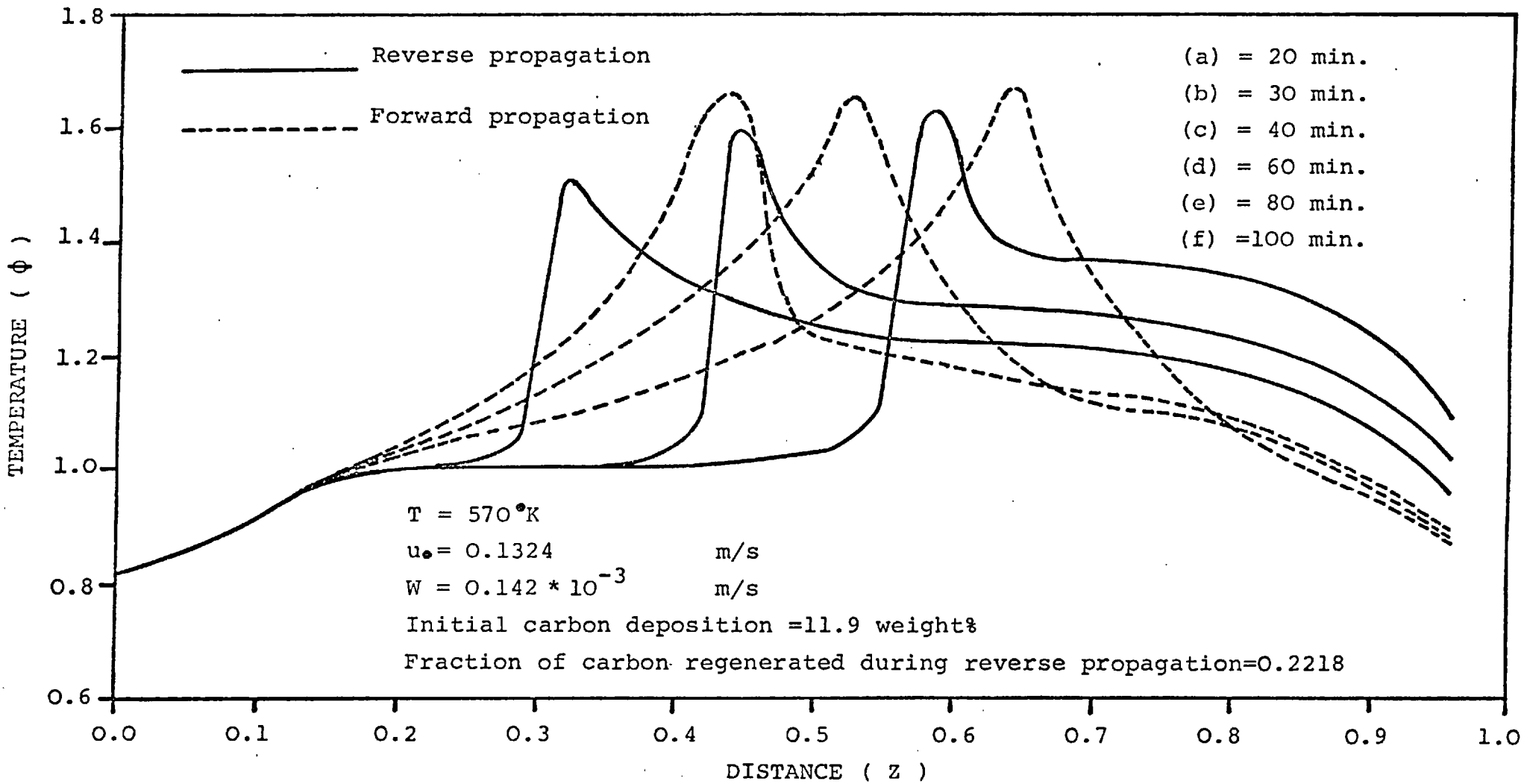


FIG. (5.28) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 80)

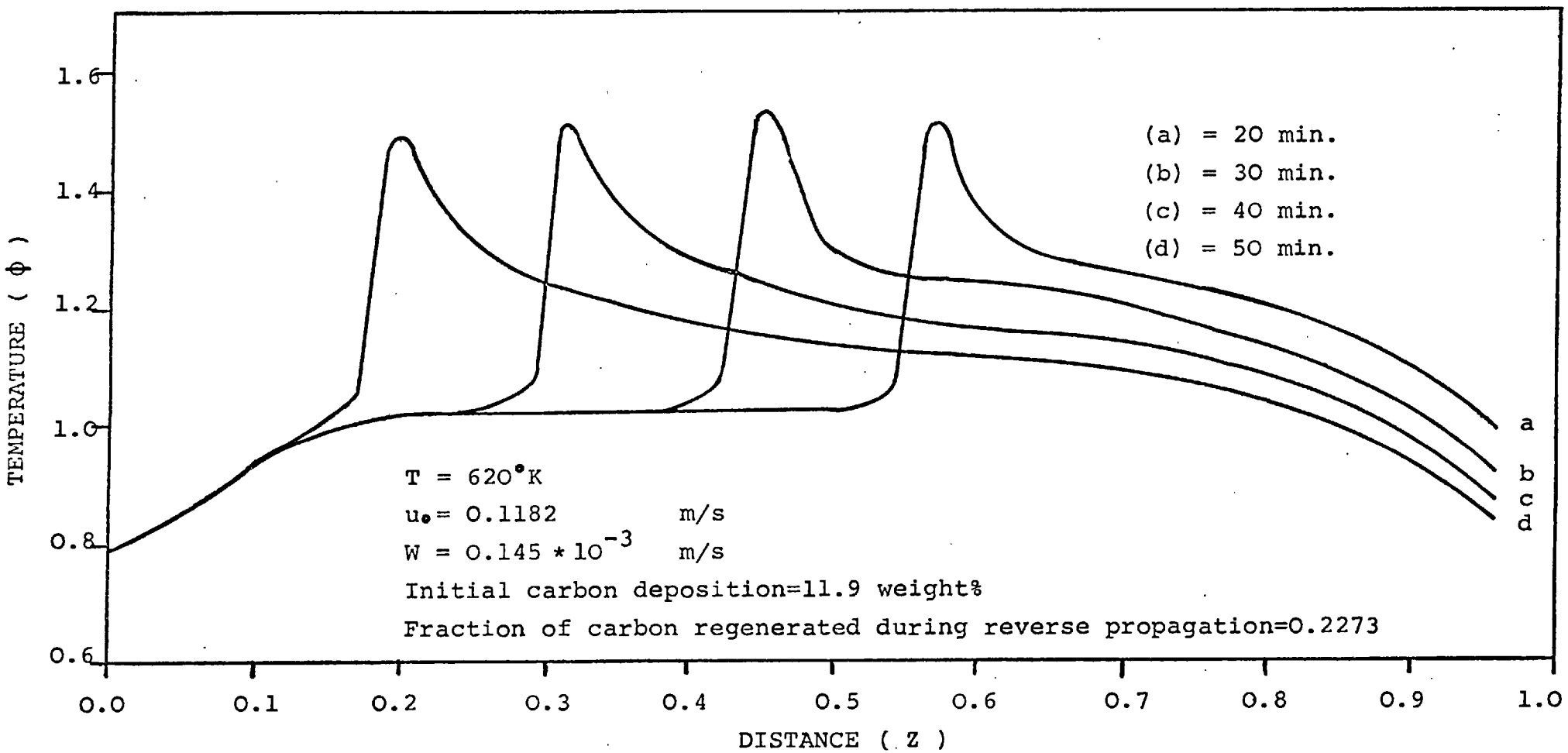
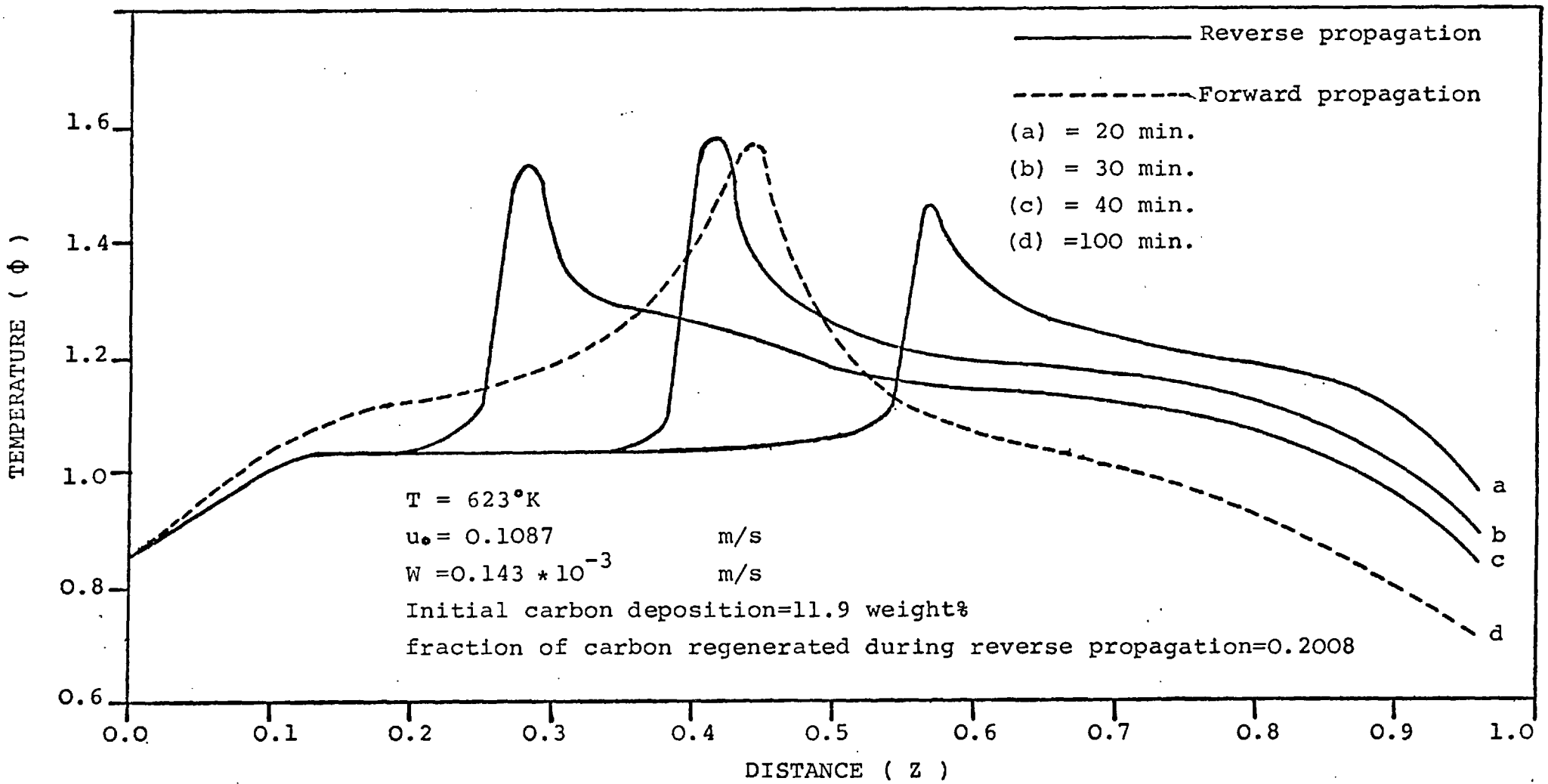


FIG. (5.29) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

(RUN NUMBER 72)



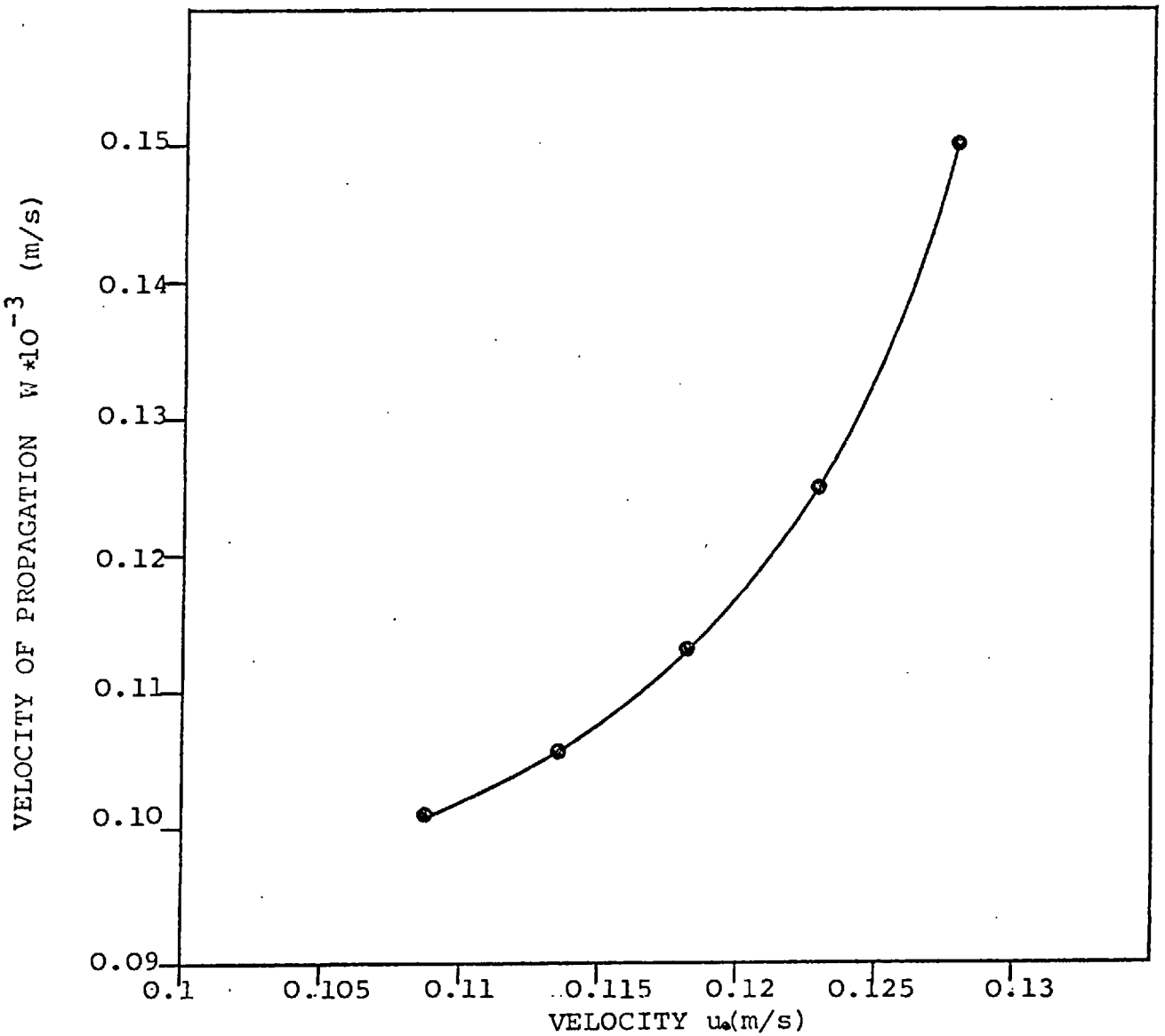
propagation ensues. The remaining 67-80% of the carbon deposition burn during the forward operation. This would result to a slower propagation rate, and higher peak temperature. The change in direction of velocity of propagation can be seen in Figures (5.18 and 5.19).

Run No. 71, Figure (5.20) is the only experiment presented here with the bed containing 7.3% by weight of carbon deposition. As mentioned in section 5.3, this deposition was not uniform through the reactor, therefore no possible conclusion can be drawn from this particular run. All the other runs were conducted with a carbon deposition of 11.9% by weight.

5.5.1 Feed velocity (u_o).

In order to study the effect of feed velocity upon the velocity of propagation and carbon regeneration a series of five runs were carried out with a preheated feed temperature of $608^{o}K$, and feed concentration of 4.2×10^{-3} K mol/m^3. These runs differ from one another only in feed velocity. With all other conditions maintained the same, the feed velocity was varied from 0.1087 m/s (Run No: 73) to 0.128 m/s (Run No: 77). Figure (5.30) indicates that with the increase in feed velocity the velocity of propagation increases exponentially from 0.101×10^{-3} to 0.150 m/s. The shape of this curve is different from that of CO oxidation results (section 5.3.4). For that system the velocity of propagation increased with feed velocity and reached a maximum with increasing feed velocity. With feed velocities slightly above the one that allows the

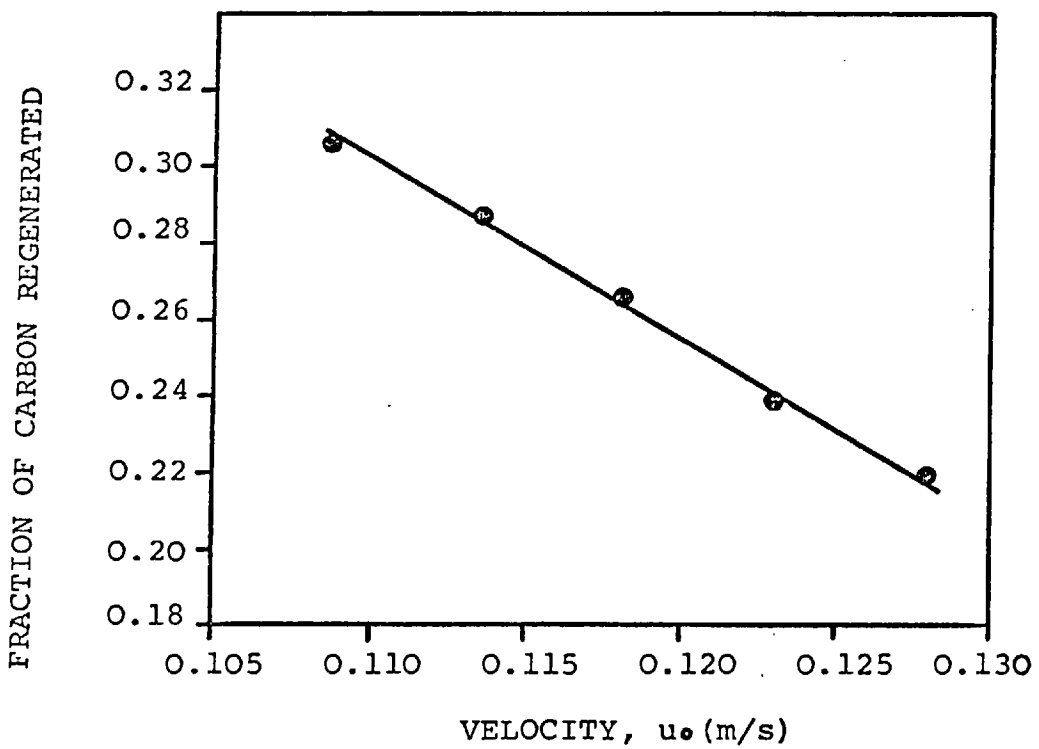
FIG. (5.30) VELOCITY OF PROPAGATION FOR SELECTED VALUES OF FEED VELOCITY.



maximum velocity of propagation, the propagation velocity started to decrease. In that system the reverse propagation of the reaction zone was effective without preheating the feed flow. This enabled utilization of a much higher feed velocity during the operation. The maximum feed velocity used was 1.45 m/s and with a feed velocity below 0.165 m/s the reaction zone was quickly extinguished. From Figure (5.17) (section 5.3.4) it can be seen that the maximum propagation velocity was achieved with a feed velocity of 0.7 to 0.79 m/s depending on inlet concentration. However in the regeneration process of the fouled Alumina-Silica the operating condition for an effective reverse propagation was dictated by preheating the feed to a high temperature and as a result of preheating this imposed a further constraint on the inlet velocity. Whereas an inlet velocity of 0.16 m/s was too low to sustain the reaction zone for CO oxidation system, the same inlet velocity was found to be beyond the maximum allowable operating condition for the regeneration operation. Because of these variations in operating conditions between the two systems and inability to investigate the higher inlet velocities the difference in the shape of the two curves is not surprising. High feed velocity increases the rate of heat liberated, thereby increases the velocity of propagation and peak temperature. These effects can be observed from Figures (5.21 - 5.25) for a constant preheated feed temperature of $608^{o}K$.

Figure (5.31) represent the fraction of carbon regenerated during the reverse propagation against the feed velocity. The amount of carbon regenerated decreases with increase in feed

FIG.(5.31) CARBON REGENERATION DURING REVERSE PROPAGATION AGAINST FEED VELOCITY.



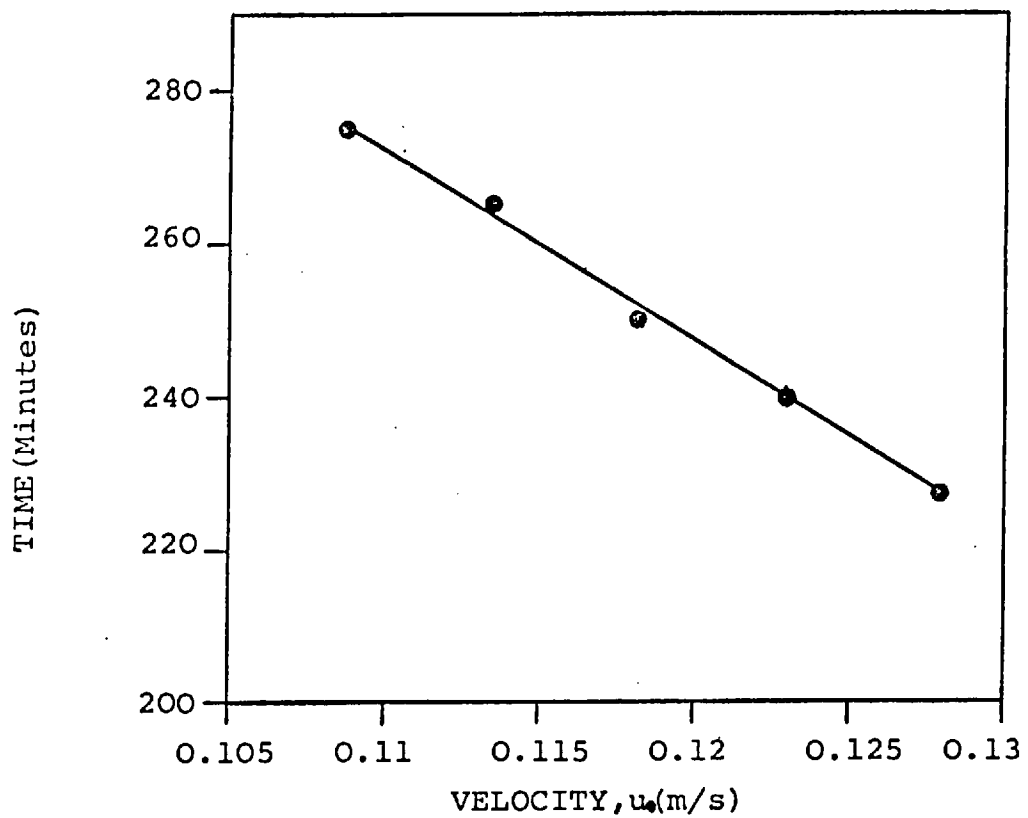
velocity. Evidently this is to be expected since the rate of propagation increases 50% by an increase of 18% in feed velocity. Obviously the total time required for the complete regeneration is decreased with increase in feed velocity. Figure (5.32) shows this decrease from 275 to 227 minutes. The total time required for the regeneration is measured by the time taken during reverse and forward propagation of the operation.

5.5.2. Feed Temperature (T_o).

In order to sustain propagation the feed had to be preheated to a temperature of at least 570^{o}K. With a preheated feed below this temperature blow-out of the reaction zone will result. Even at 570^{o}K the reaction zone does not propagate upstream more than 2/3 of the reactor. This is evident from Figure (5.27). The peak temperature is lowered from 930^{o}K at time 20 minutes to 855^{o}K at time 40 minutes. Immediately after this time the direction of reaction zone is switched to that of forward propagation. Therefore the catalyst in the entire initial portion of the reactor remains fouled. However this problem does not arise when the feed temperature is increased to 580^{o}K. With the increase in feed temperature from 570 - 580^{o}K the temperature profile moves to the inlet of the reactor under influence of backward conduction.

A series of four runs were carried out with different preheated feed temperature. By comparing Figures (5.22 and 5.26) , (5.23 and 5.28) and (5.21 and 5.29) where the difference between each set of two runs is only in the

FIG.(5.32) TOTAL TIME REQUIRED FOR REGENERATION AGAINST FEED VELOCITY.



feed temperature, the following conclusions can be drawn.

Higher feed temperature increase the velocity of propagation. However as a result of this increase in the propagation velocity which is of the order of 40% the amount of carbon regenerated during the reverse operation is decreased. Hence regeneration during reverse propagation is maximum with a preheated feed temperature of $580^{o}K$. With a feed velocity of 0.1135 m/s the amount of carbon burnt increases approximately 11% by lowering the feed temperature from $623^{o}K$ to $608^{o}K$.

TABLE (5.4)

VALUES OF THE PHYSICAL PARAMETERS FOR THE EXPERIMENTAL RUNS
(CARBON OXIDATION)

PHYSICAL PARAMETER	RUN NO. 71	RUN NO. 72	RUN NO. 78	RUN NO. 79	RUN NO. 80
u_o m/s	0.1418	0.1087	0.1135	0.1324	0.1182
τ s	4.23	5.52	5.289	4.53	5.08
T_o ^oK	616	623	580	570	620
W m/s	0.2505×10^{-3}	0.143×10^{-3}	0.09×10^{-3}	0.142×10^{-3}	0.145×10^{-3}
FRACTION OF CARBON REGENERATED DURING REVERSE PROPAGATION	—	0.2008	0.3309	0.2218	0.2273
DURATION OF REVERSE PROPAGATION min.	35	51	73	—	53
TOTAL REGENERATION PERIOD min.	145	265	275	210	230

TABLE (5.5)

VALUES OF THE PHYSICAL PARAMETERS FOR THE EXPERIMENTAL RUNS.

(CARBON OXIDATION)

PHYSICAL PARAMETER	RUN NO.73	RUN NO.74	RUN NO.75	RUN NO.76	RUN NO.77
u_o m/s	0.1087	0.1135	0.1182	0.123	0.128
τ s	5.52	5.289	5.08	4.882	4.701
W m/s	0.101×10^{-3}	0.1055×10^{-3}	0.1131×10^{-3}	0.125×10^{-3}	0.150×10^{-3}
FRACTION OF CARBON REGENERATED DURING REVERSE PROPAGATION.	0.3055	0.2876	0.2662	0.23855	0.2196
DURATION OF REVERSE PROPAGATION min	75	65	58	50	46
TOTAL REGENERATION PERIOD min	275	265	250	240	227

$T_o = 608^oK$

CHAPTER SIX

6. COMPARISON OF THEORY WITH EXPERIMENTAL DATA.

The non-adiabatic homogeneous one dimensional model described in Chapter Three was simulated for comparison with the experimental studies.

6.1 Theoretical and Experimental comparison of CO Oxidation.

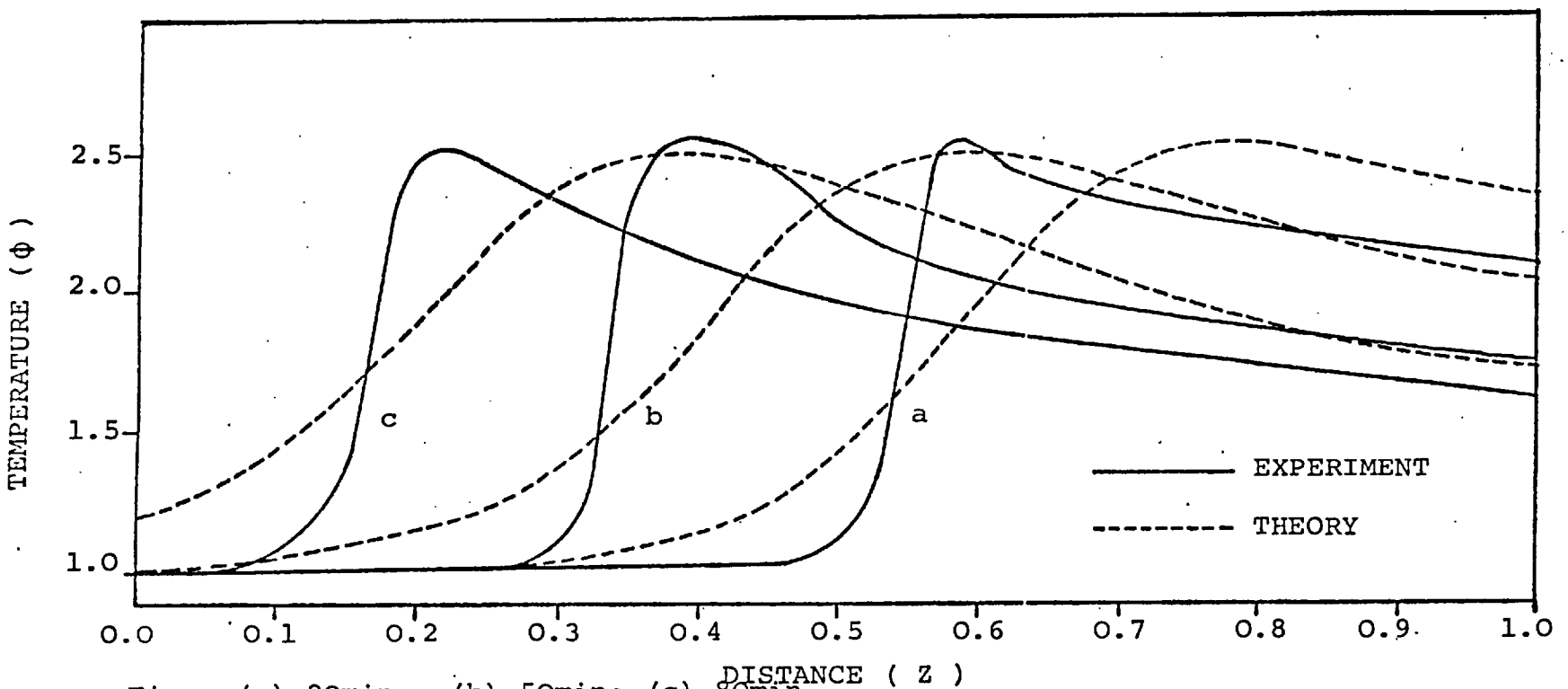
Figures 6.1, 6.2, 6.3 and 6.4 show the temperature profiles at various times along the reactor obtained from experiment and theory for run numbers 30, 32, 44 and 45 respectively. Figures 6.5 and 6.6 show the theoretically predicted conversion profiles along the reactor for run numbers 30 and 44 respectively.

In using the theoretical model, the dimensionless groups J, B, Q_1, G_1, A and U_1 (section 3.1.4) had to be computed. These dimensionless group contain physical constants that can be experimentally measured. Table B.1(Appendix B) presents the values of the physical parameters and the corresponding dimensionless groups. In using the computation scheme, the initial temperature profiles along the reactor are required. Therefore the temperature profile measured experimentally was used as input data.

Since the external heat to the reactor was switched off as soon as CO flow started while conducting the experiment (section 4.3.1), and the feed flow was not preheated, the dimensionless group A in energy balance equation 3.16 (section 3.1.4.2) is set equal to zero.

In evaluating the Peclet number P for the axial energy transport the value of the effective thermal conductivity K_e of the bed was required. The data in this field are limited (Hlavacek (43); Bischoff (44); Yagi ,Kunii

FIG. (6.1) TEMPERATURE PROFILES ALONG THE REACTOR. (RUN NUMBER 30)

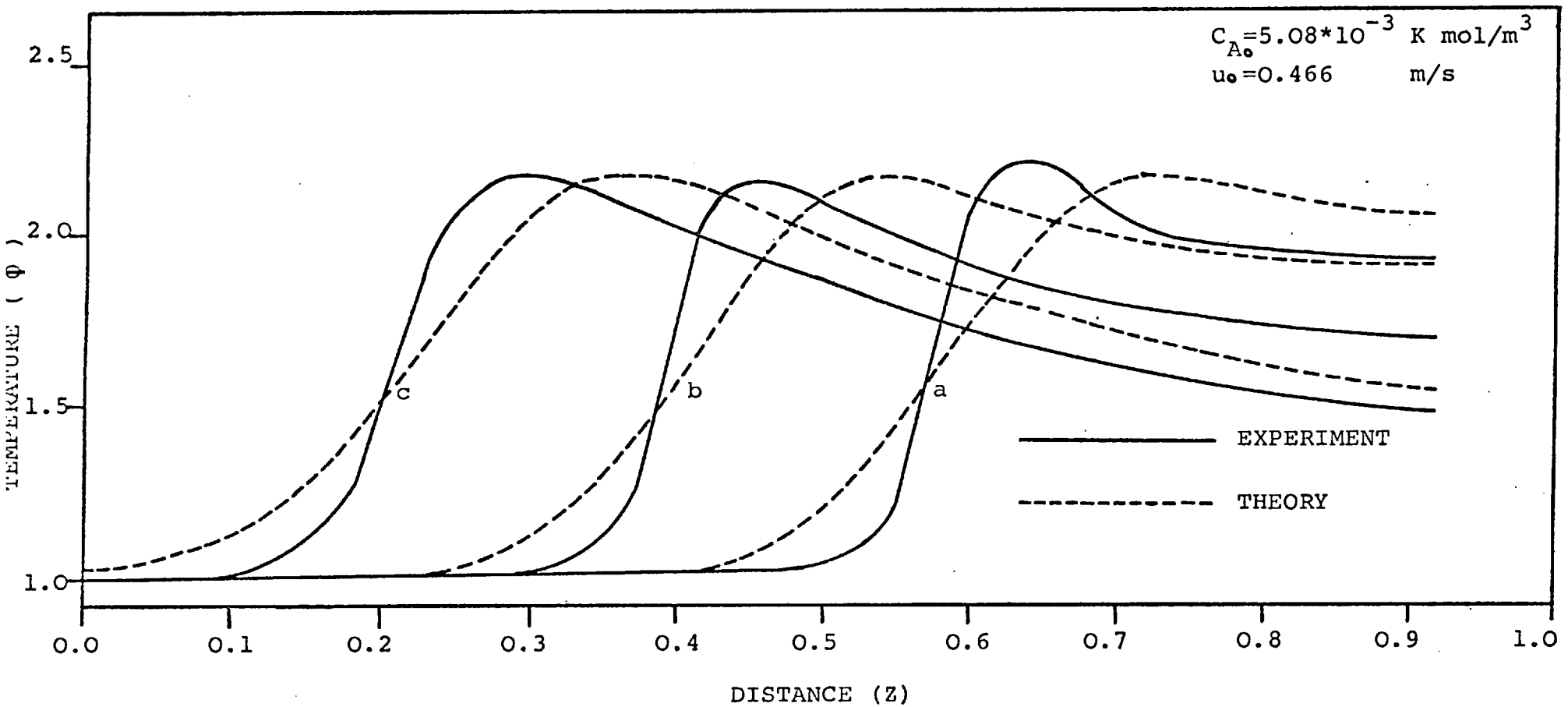


Time: (a) 20min ; (b) 50min; (c) 80min.

$C_{A_o} = 5.39 * 10^{-3}$ Kmol/m^3

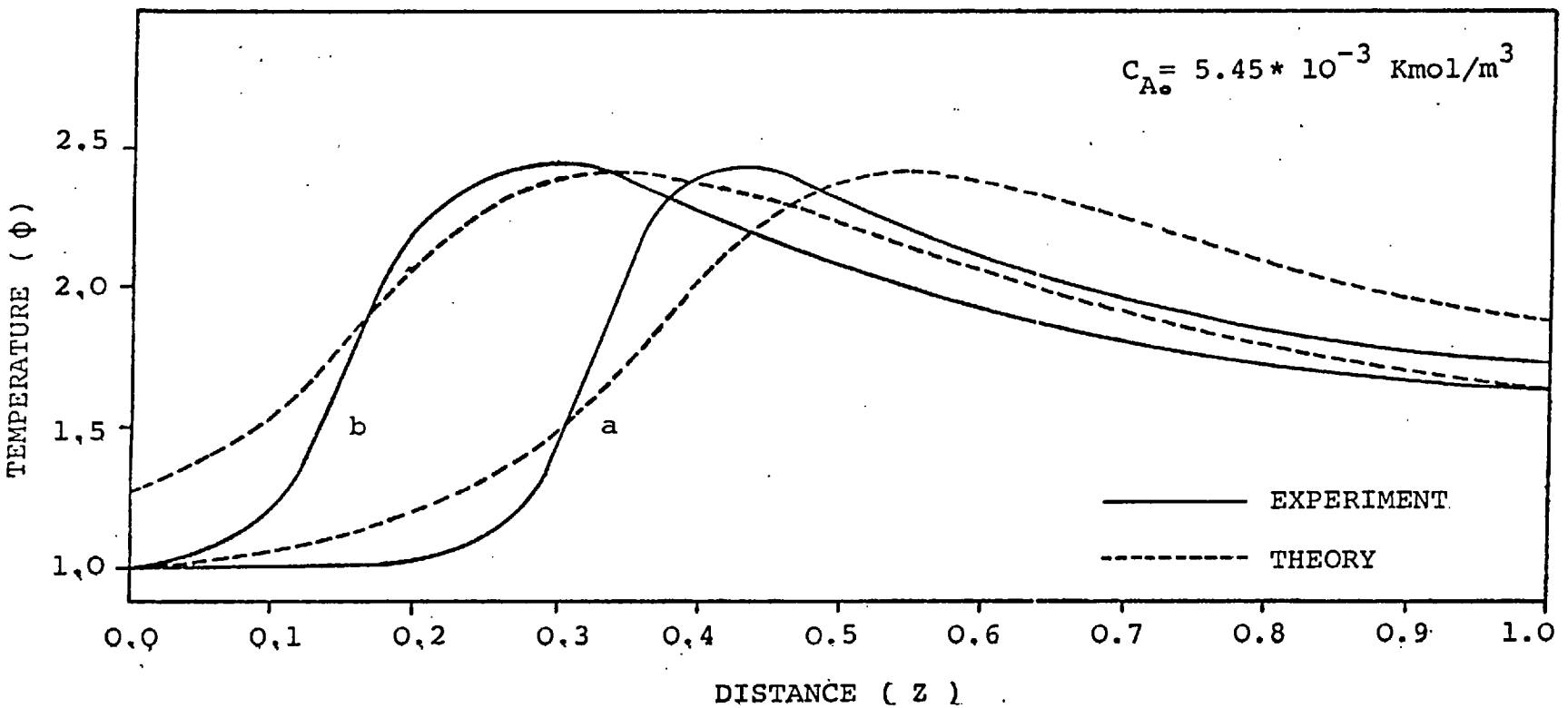
$u_o = 0.589$ m/s

FIG.(6.2) TEMPERATURE PROFILES ALONG THE REACTOR (RUN NO.32)



Time: (a)30 min; (b)60 min; (c)90 min.

FIG. (6.3) TEMPERATURE PROFILES ALONG THE REACTOR (RUN NUMBER 44)



Time: (a) 50min; (b) 90min.

FIG.(6.4) TEMPERATURE PROFILES ALONG THE REACTOR (RUN NO.45)

Time : (a) 50min; (b) 90min.

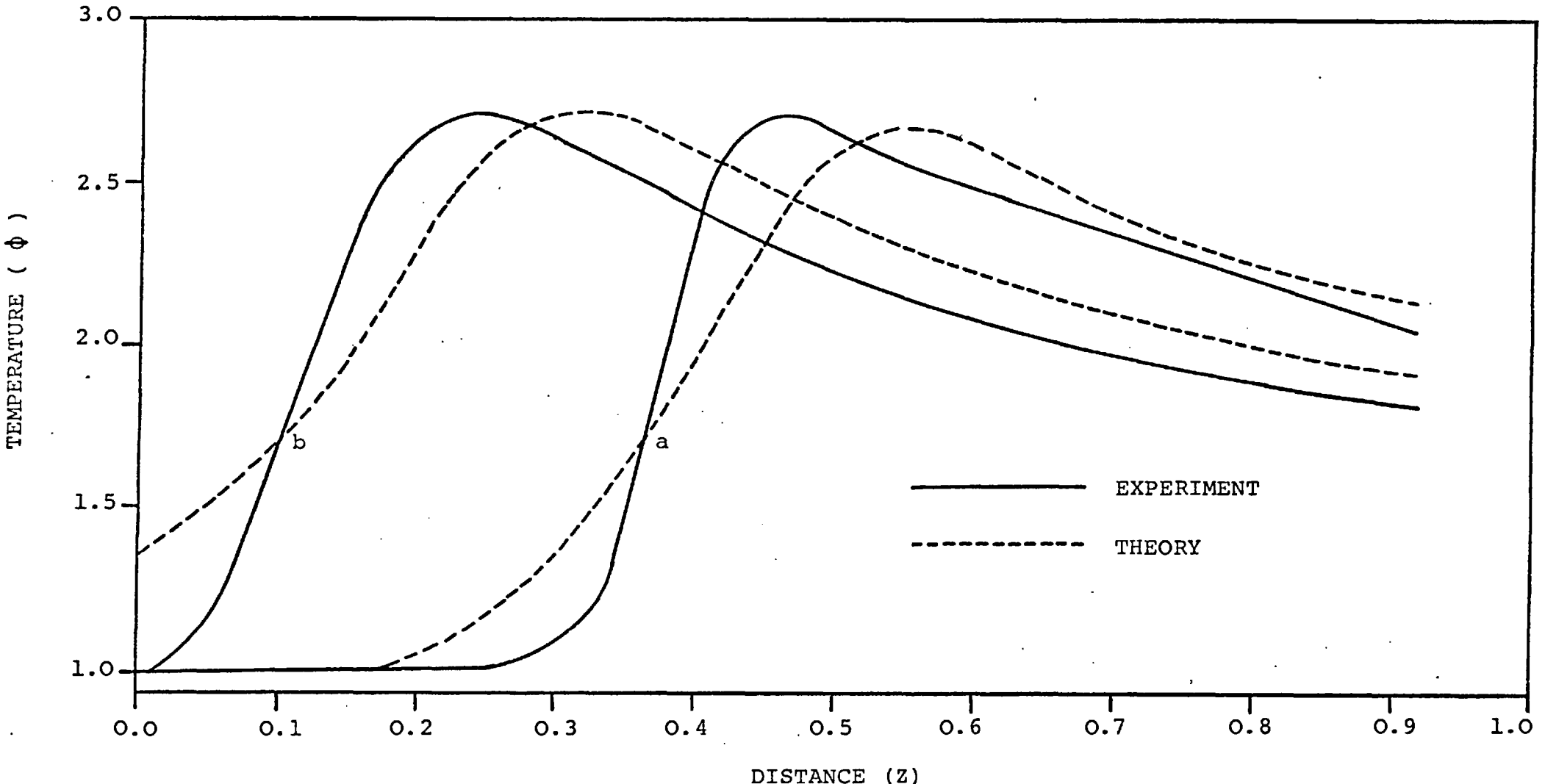


FIG. (6.5) CONVERSION PROFILES ALONG THE REACTOR FROM THEORY(RUN NUMBER 30)

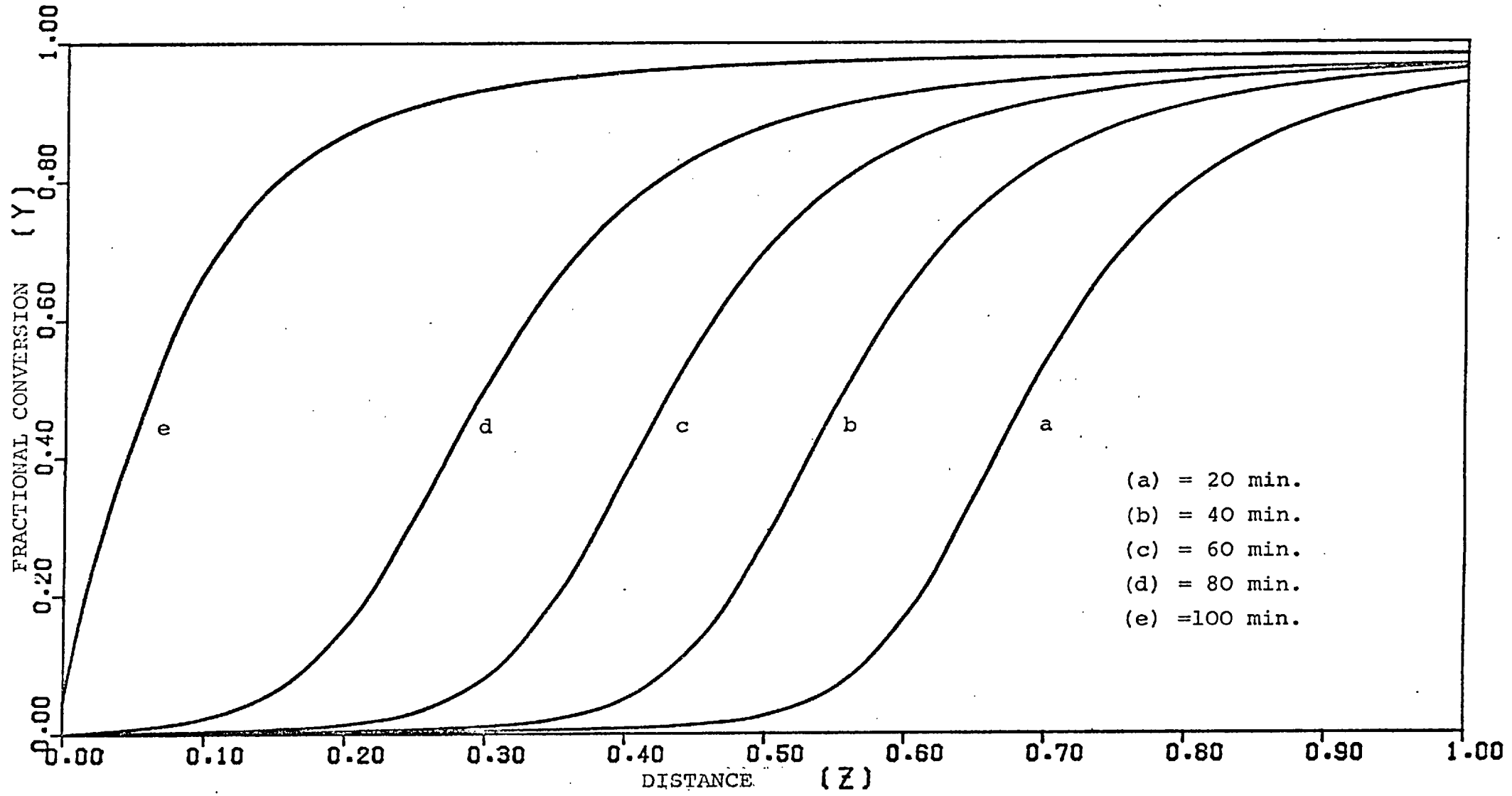
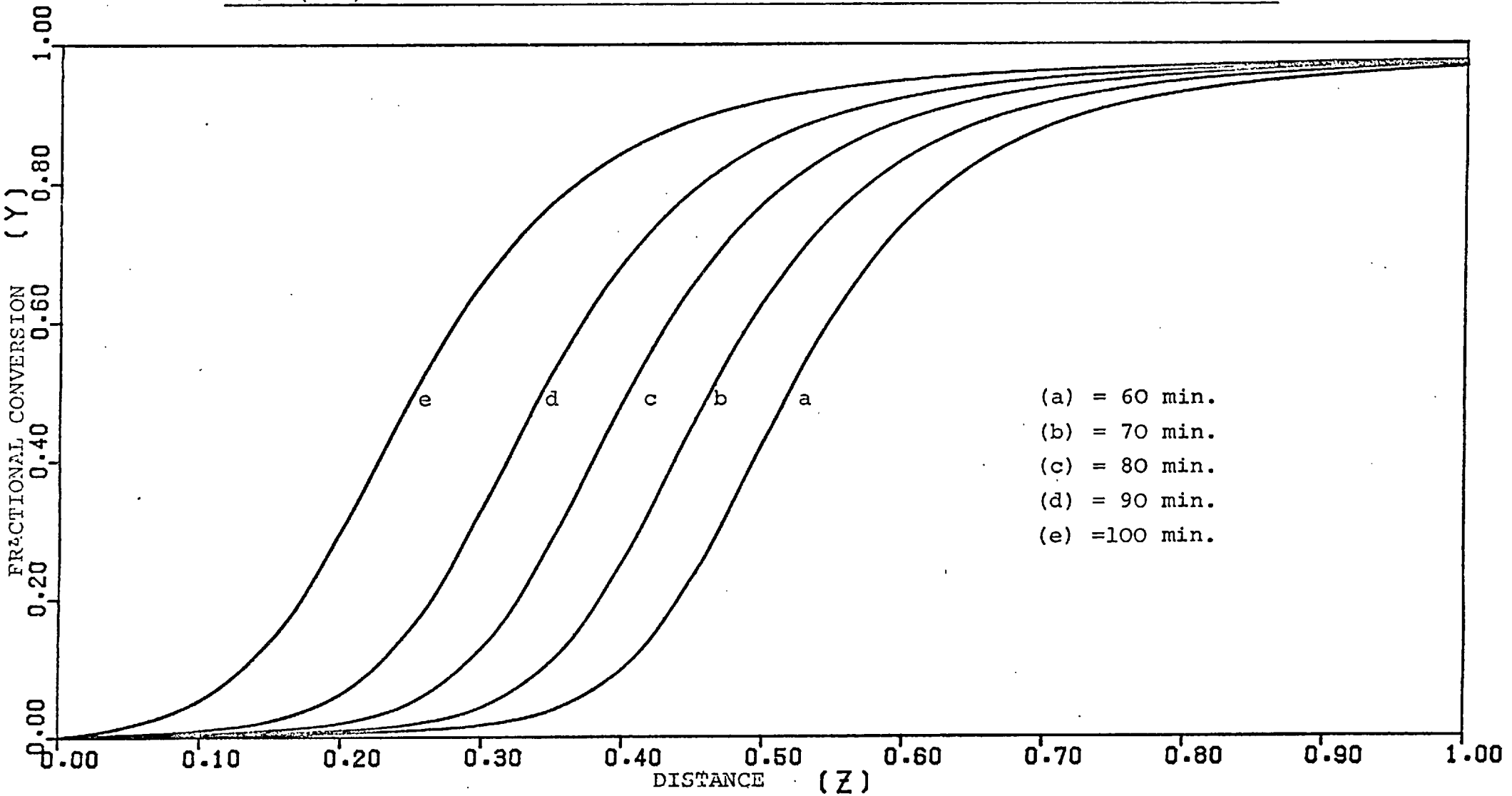


FIG. (6.6) CONVERSION PROFILES ALONG THE REACTOR FROM THEORY(RUN NUMBER 44)



and Wakao (41)). The work of Yagi et. al. (41) involved experimental measurement of K_e for various packings at low gas flow rates. Bischoff (44), from an entirely theoretical standpoint, has correlated the Reynold's number of flow through a packed bed to the conductivity ratio K_e/K_g. Hlavacek(42), in reviewing various correlations for mass and heat transfer data, has summarized the correlations available in literature for the estimation of effective heat conductivities (in radial and axial directions).

Bischoff (44) used the data of Yagi, Kunii and Wakao (41) to develop his model. Basically, the correlation he obtained relates the Reynold's number of flow (superficial) to the effective gas conductivity ratio K_e/K_g. Using Bischoff's correlation for the particle Reynold's number used in the present work for Re ≈ 12. (750°K) and Re ≈ 5 (298°K) predicts a K_e of 4.73×10^{-3} KJ/m sec °K. When this value is used in the theoretical model, the reaction zone propagation rate is grossly under-predicted (by about 60%).

While attempting to use other correlations, the conventional approach of using a value of 1 for the particle Peclet number (Lee (34); Liu and Amundson (22-24)) was tried. It should be noted that a value of particle Peclet number of 1 corresponds to a value of Ke of 0.733 KJ/m sec °K. This value of K_e overpredicted the reaction zone propagation rate by 120% .

Venkatachalam (25) working between Re ≈ 14 (298°K) and Re ≈ 7 (690°K) experienced the same difficulty in evaluating the value of K_e. In that work in order to find a value of K_e suitable for the system the value obtained from Bischoff's

correlation was multiplied by a factor of 10. This resulted to a value of Peclet number P of 2×10^4 based on the reactor length.

This wide discrepancy in the value of K_e predicted by different correlations is an indication of the uncertainty in its value. Bischoff (44) in his work mentions that the values of K_e are highly specific to the system employed and that his correlation only serves to obtain an approximate value for a system.

Votruba, Hlavacek and Marek (48) have shown that for a particle Reynolds number ($Re = \frac{\rho_{go} u_o d_p}{\mu}$) within the range 10-20 the Peclet number for axial heat transport becomes constant, while below this range the Peclet number varies directly with the Reynold's number.

To get a value of K_e that would give nearly the same propagation rate as that observed experimentally, the value obtained from Bischoff's correlation was increased in steps. A value of K_e that predicted the propagation rate well for all the runs was 3.31×10^{-2} KJ/m sec ^oK, that is 7 times that of Bischoff's correlation. This value of K_e corresponds to a particle Peclet number of about 22. Using this value of K_e results in a Peclet number P of 2×10^4 based on the reactor length. In view of the fact that this value of K_e predicts the reaction zone propagation rate reasonably well in all the runs, it is believed that this value is in the right order of magnitude.

In incorporating the heat loss effects, the dimensionless heat loss group U_1 contains the average heat transfer coefficient term U between the reactor and its environ (section 3.1.4.2). The value of heat transfer coefficient

was estimated for the system to be 4.09 J/m^2 sec ^oK.

In spite of the uncertainties in the evaluation of the effective thermal conductivity K_e and the average heat transfer between the system and its surroundings the model predicts the peak temperatures and the propagation rates of the reaction zone. Figures 6.1, 6.2, 6.3 and 6.4 all indicate reasonable agreement in temperature profiles between theory and experiment. The discrepancy between the two may be attributed to the use of such a simple model which neglects the radiative energy transport and differences between catalyst and bulk gas temperature. However the point of inflection of the profiles obtained both by the model and the experiment coincide, and yield the same velocity of propagation.

6.2 Theoretical and Experimental Comparison of Carbon Oxidation.

Figures 6.7, 6.8, 6.9, 6.10 and 6.11 show the temperature profiles at various times along the reactor obtained from experiment and theory for run numbers 73, 74, 75, 76 and 77 respectively. Figures 6.12, 6.13, 6.14, 6.15 and 6.16 illustrate the theoretically predicted concentration profiles of carbon along the reactor for the above runs during the regeneration of the fouled cracking catalyst. Table B.2 (Appendix B) present the values of the physical parameters and the corresponding dimensioness groups J, B, G_2, Q_2 and U_1' (section 3.1.5). In using the computation scheme the temperature profile measured experimentally was used as input data for the initial temperature profile.

Since the electrical heat input to the exit section

a) Temperature profile at 35 minutes.
b) " " " 50 "
c) " " " 65 "

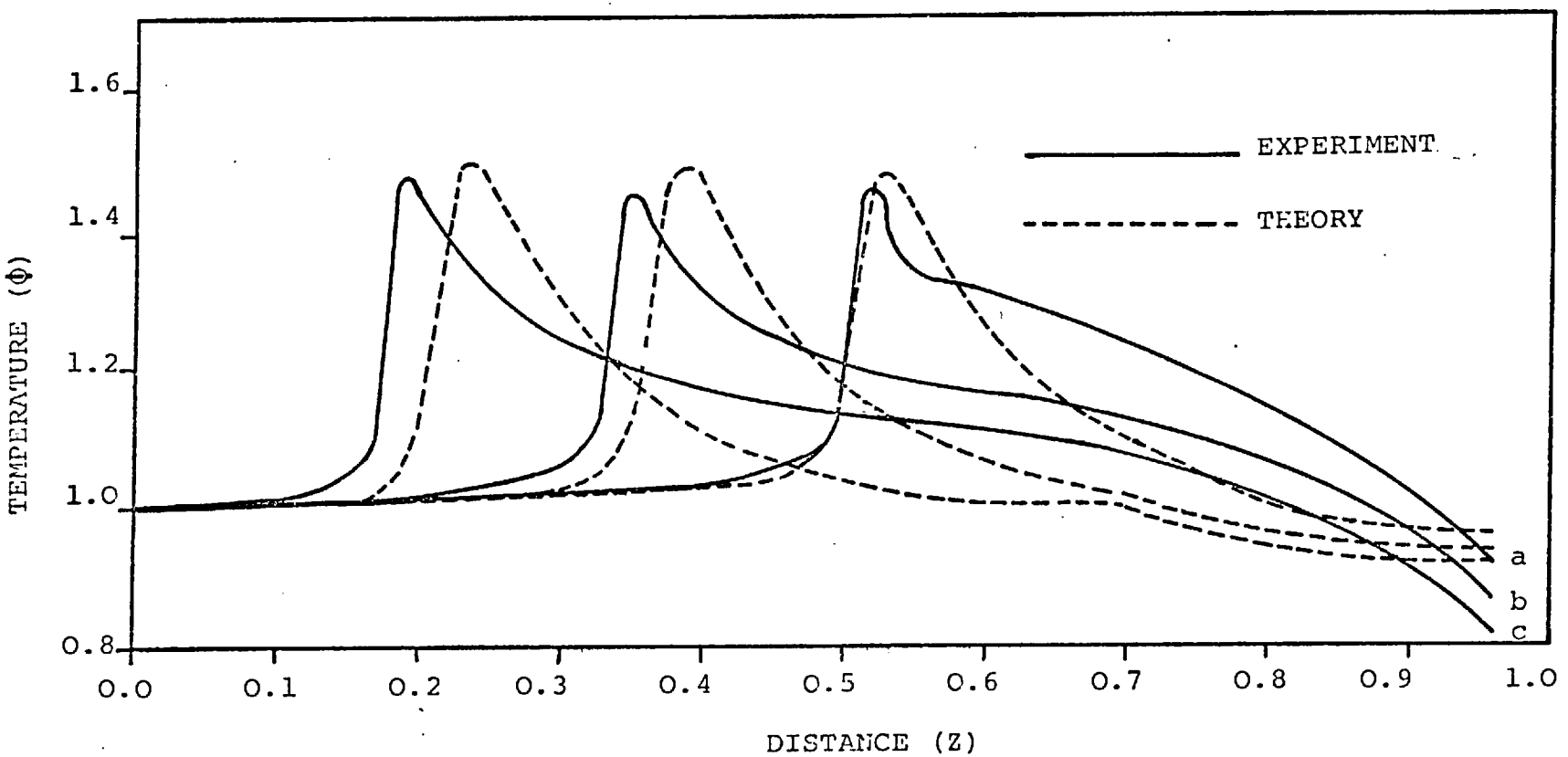


FIG.(6.7) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

a) Temperature profile at 33 minutes.
b) " " " 46 "
c) " " " 60 "

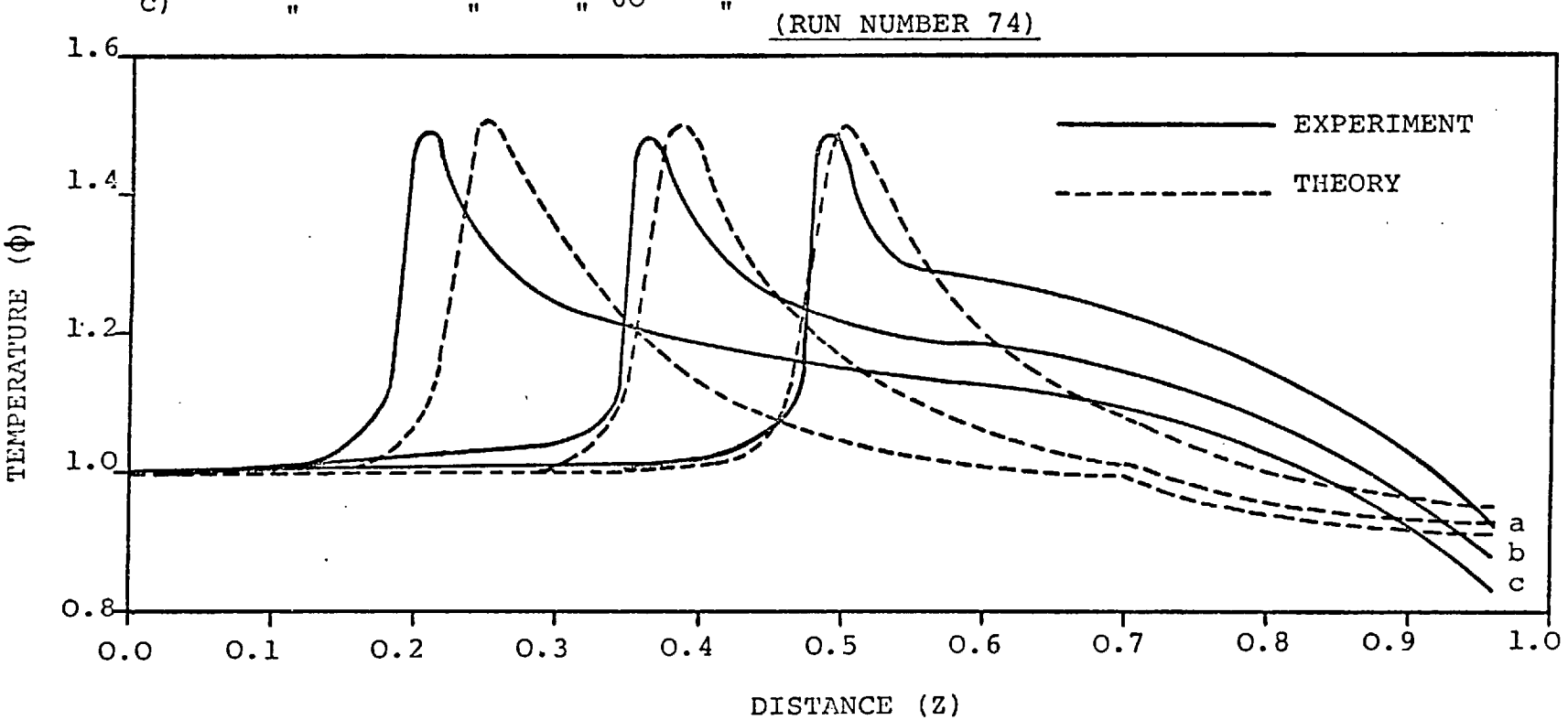


FIG. (6.8) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

a) Temperature profile at 35 minutes.
b) " " " 45 "
c) " " " 55 "

(RUN NUMBER 75)

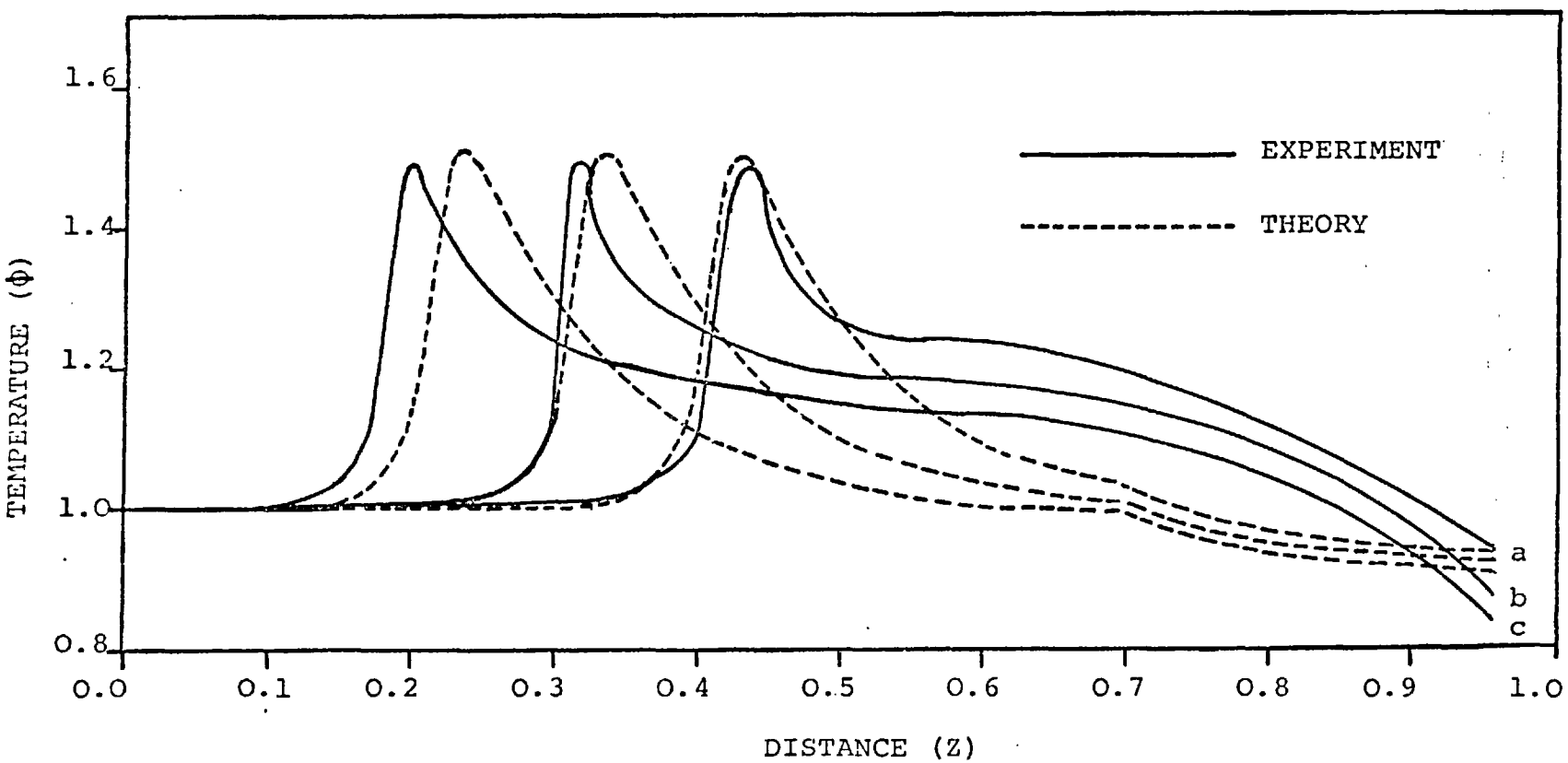


FIG. (6.9) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

a) Temperature profile at 30 minutes.
b) " " " 40 "
c) " " " 50 "

(RUN NUMBER 76)

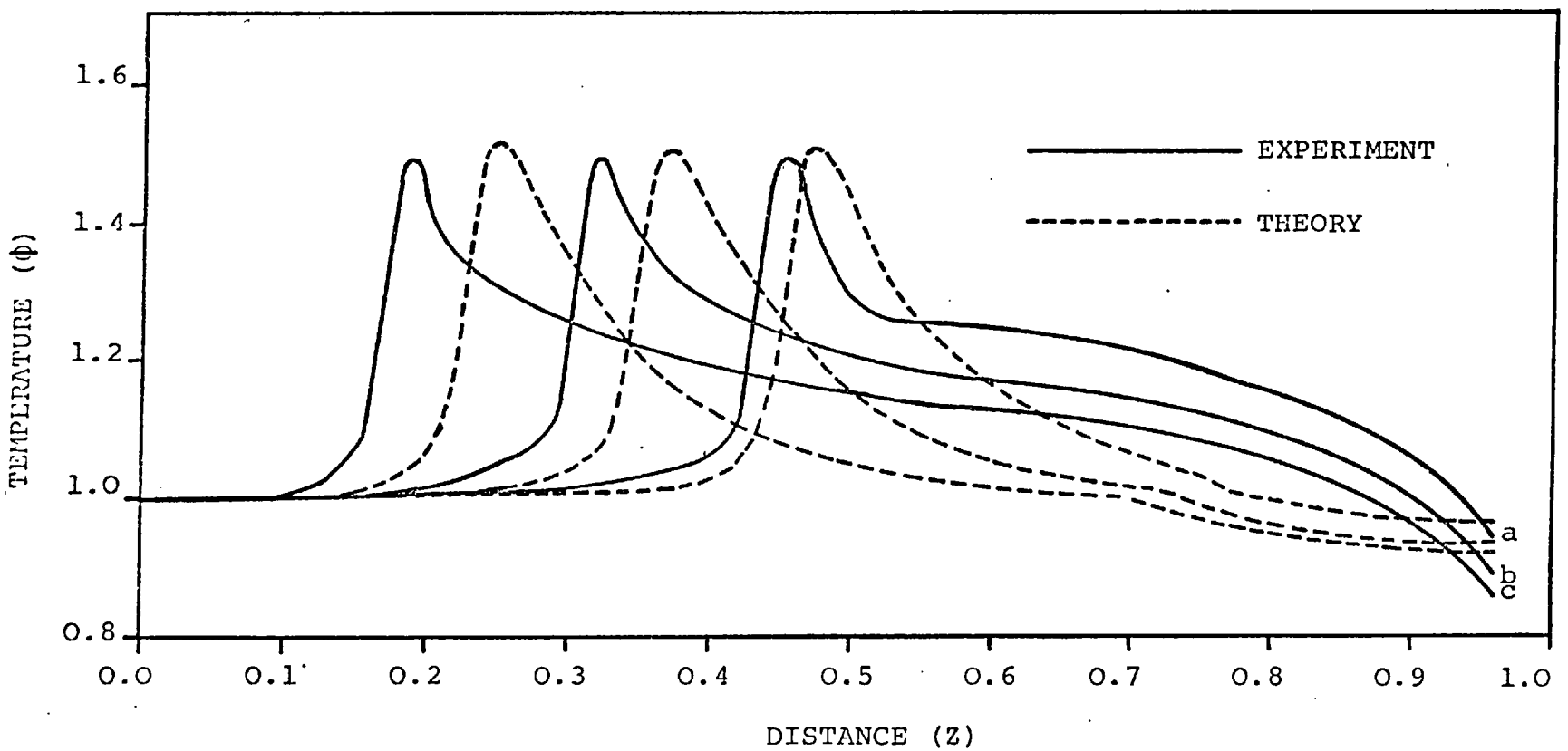


FIG. (6.10) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

a) Temperature Profile at 26 minutes.

b) " " " 33 "

c) " " " 46 "

(RUN NUMBER 77)

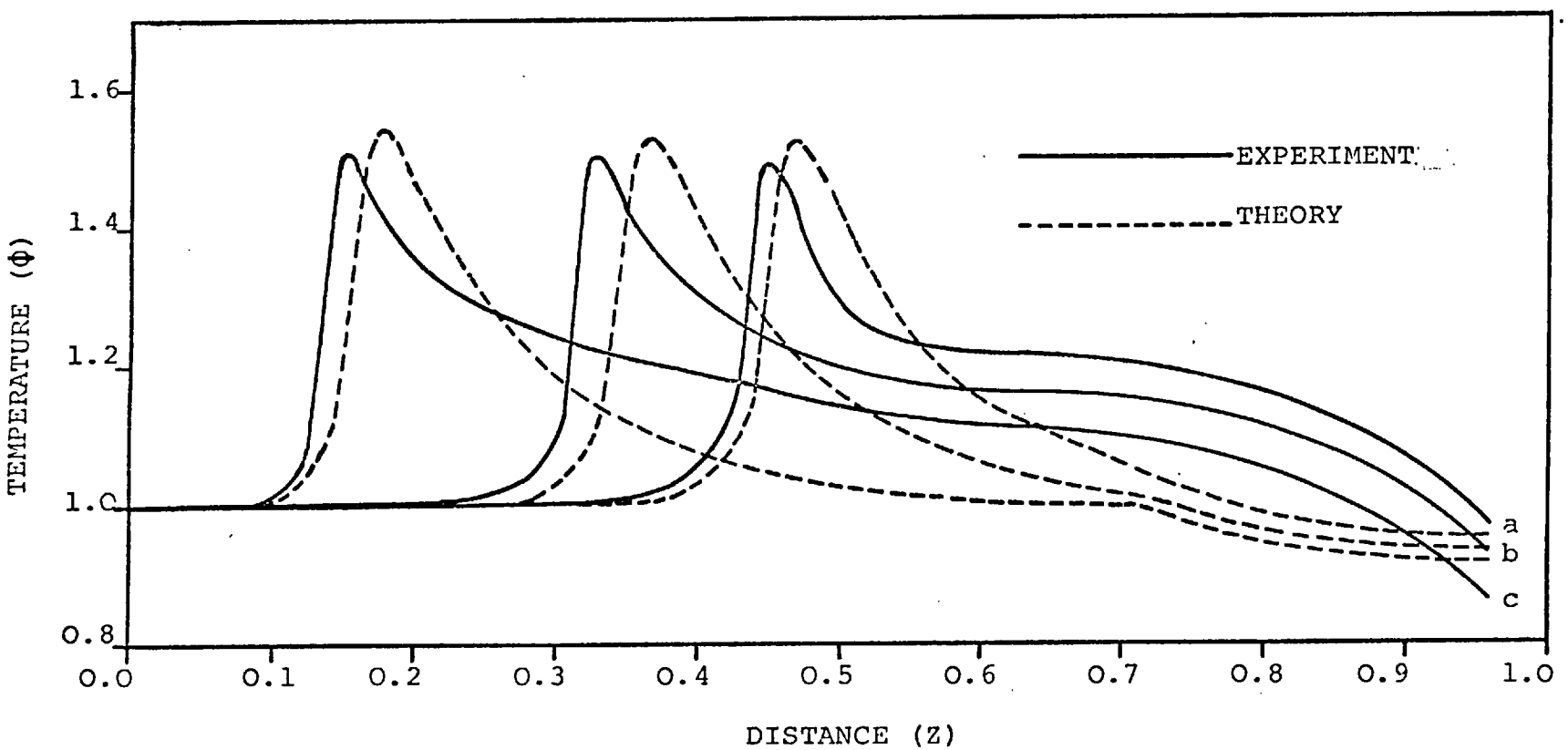


FIG. (6.11) TEMPERATURE PROFILES ALONG THE REACTOR DURING THE REGENERATION OF THE FOULED CRACKING CATALYST.

FIG.(6.12) CONCENTRATION PROFILES OF CARBON ALONG THE REACTOR FROM THEORY

(RUN NO. 73)

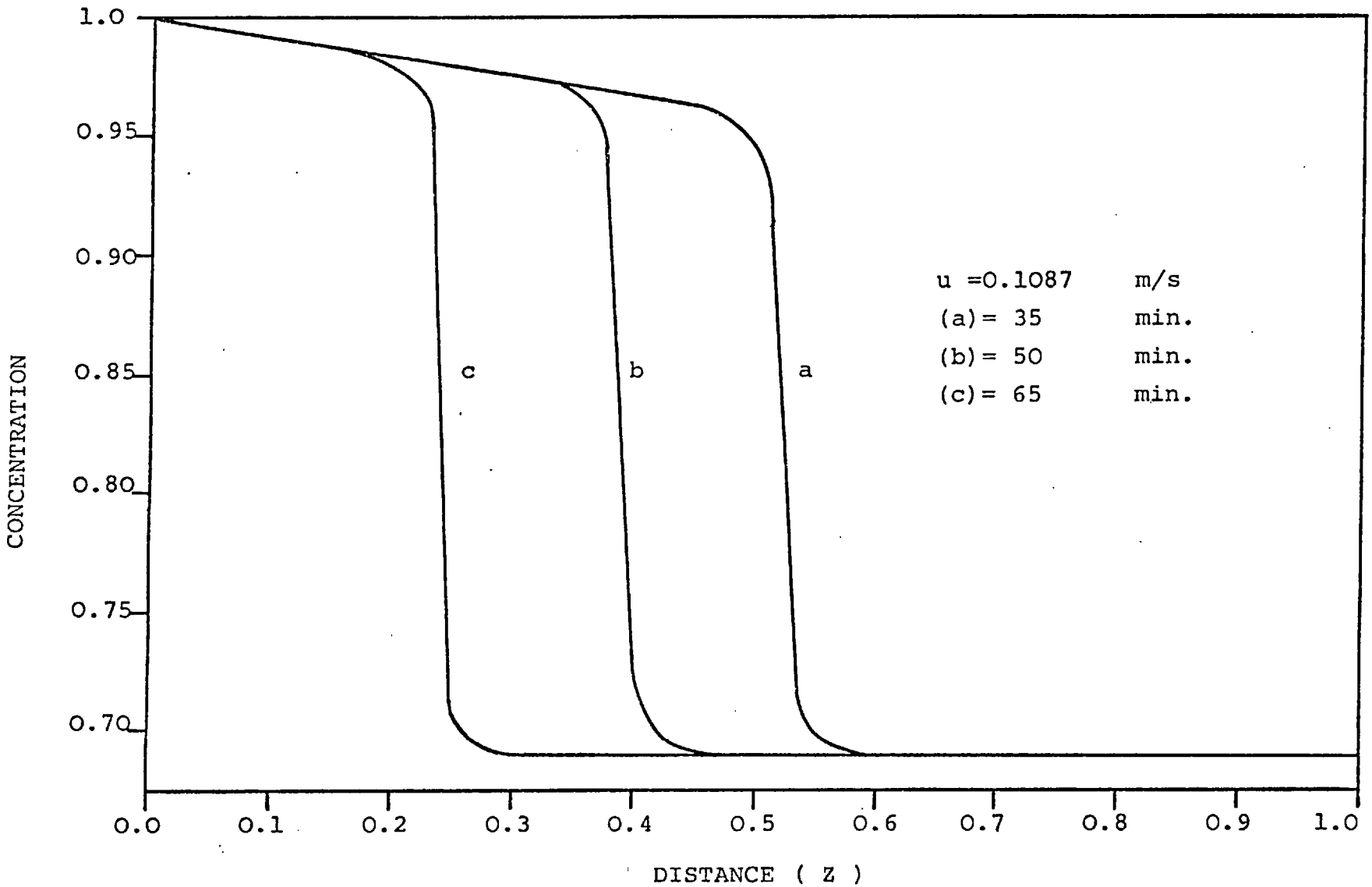


FIG. (6.13) CONCENTRATION PROFILES OF CARBON ALONG THE REACTOR FROM THEORY

(RUN NO. 74)

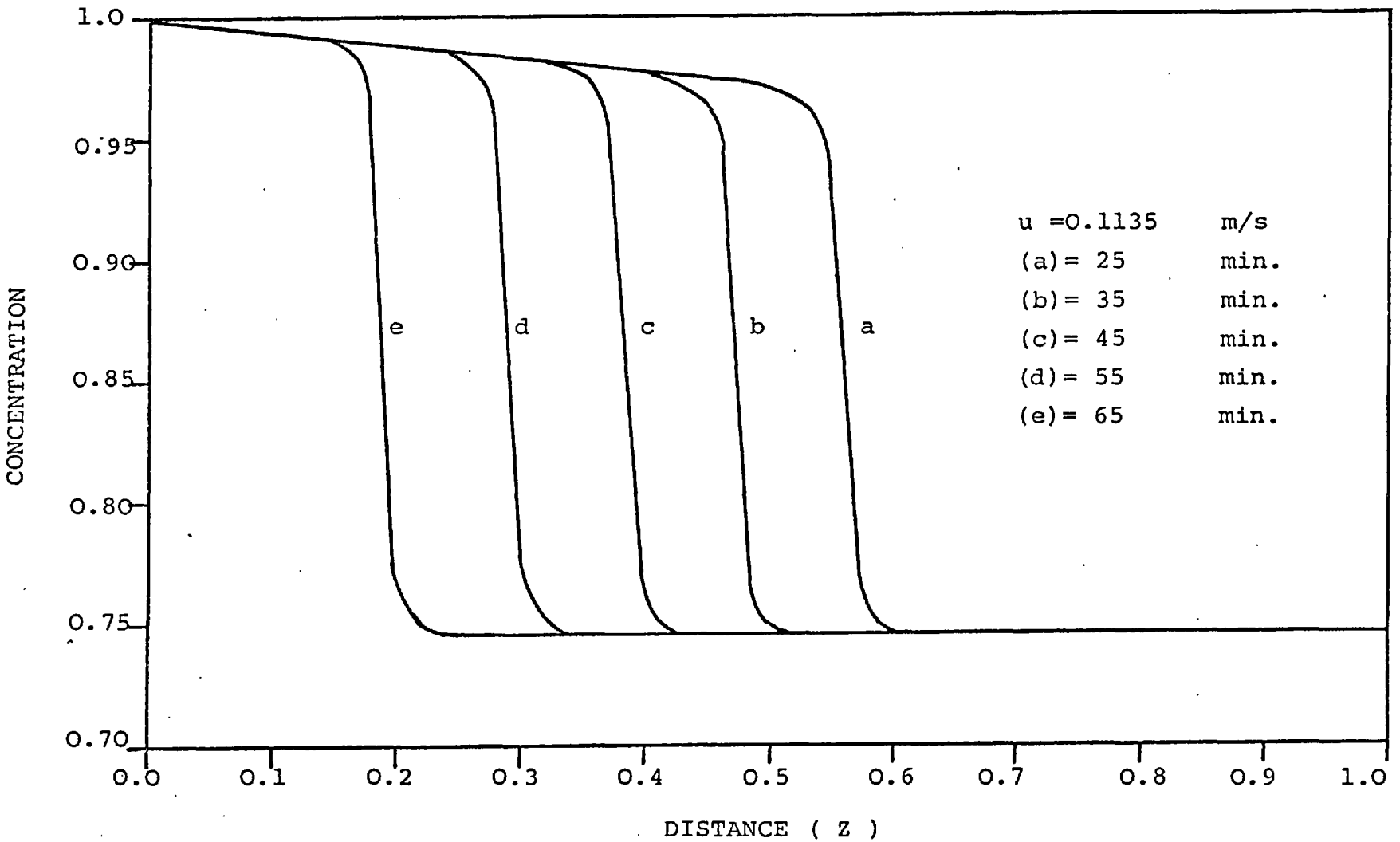


FIG.(6.14) CONCENTRATION PROFILES OF CARBON ALONG THE REACTOR FROM THEORY

(RUN NO. 75)

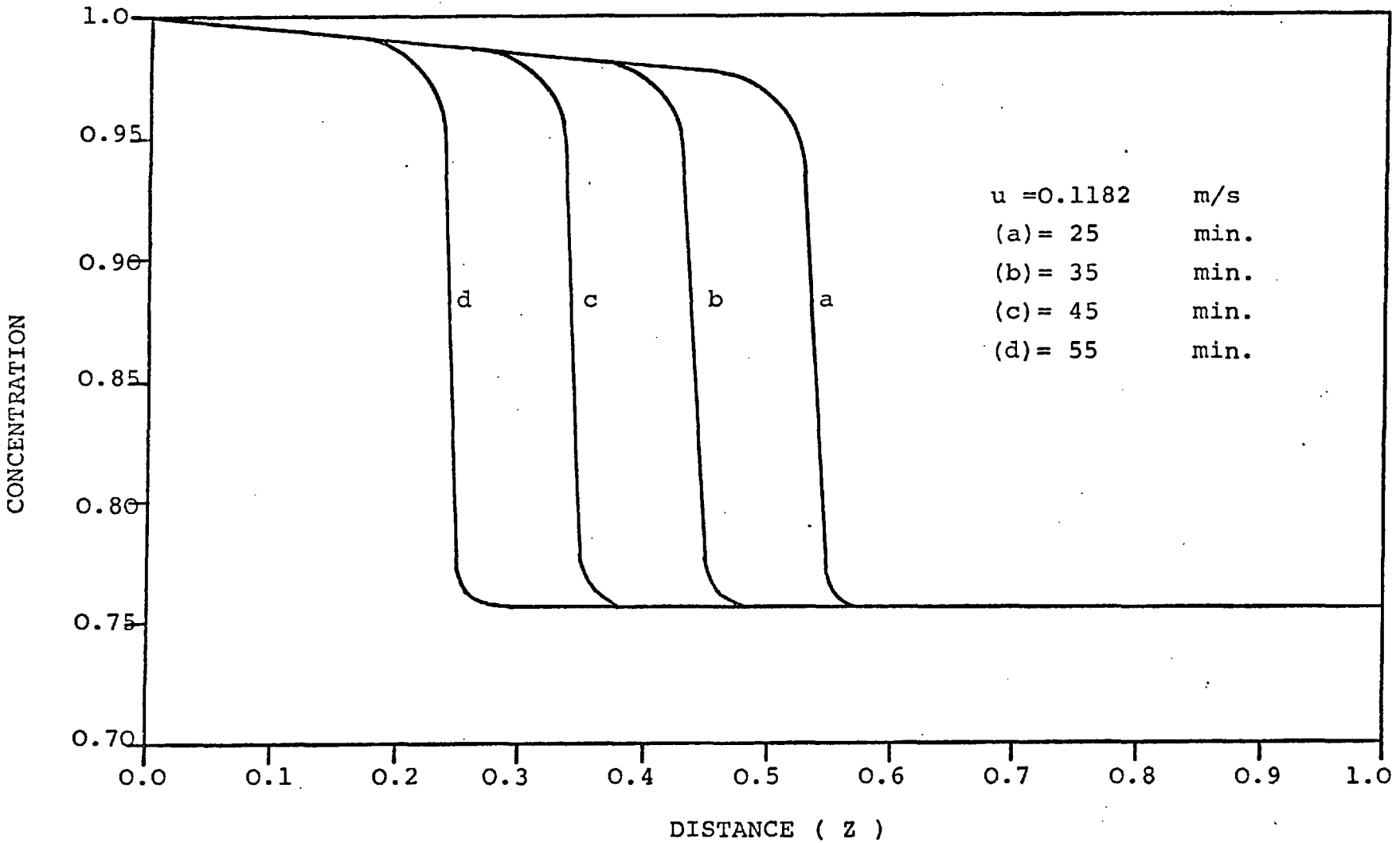


FIG.(6.15) CONCENTRATON PROFILES OF CARBON ALONG THE REACTOR FROM THEORY

(RUN NO. 76)

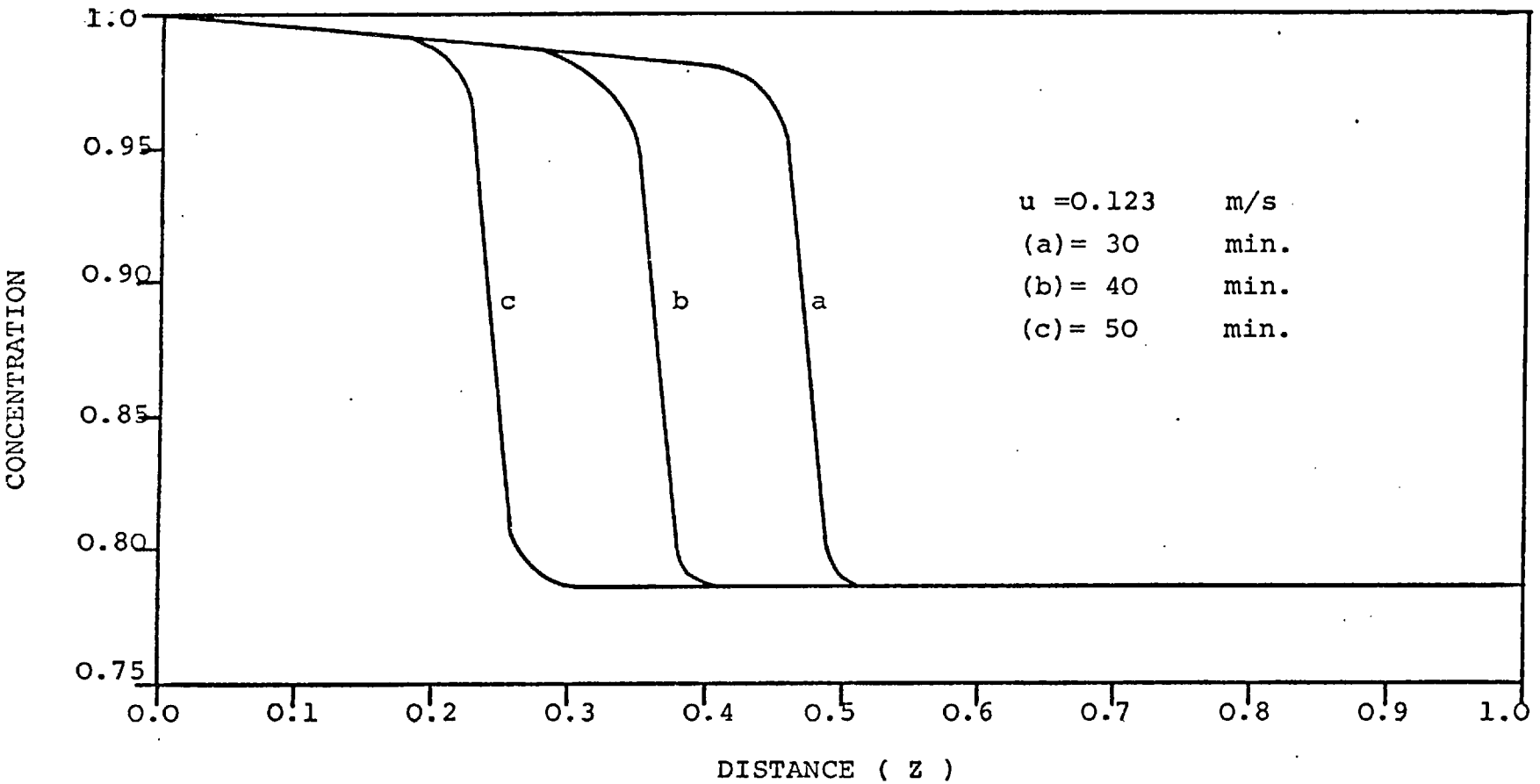
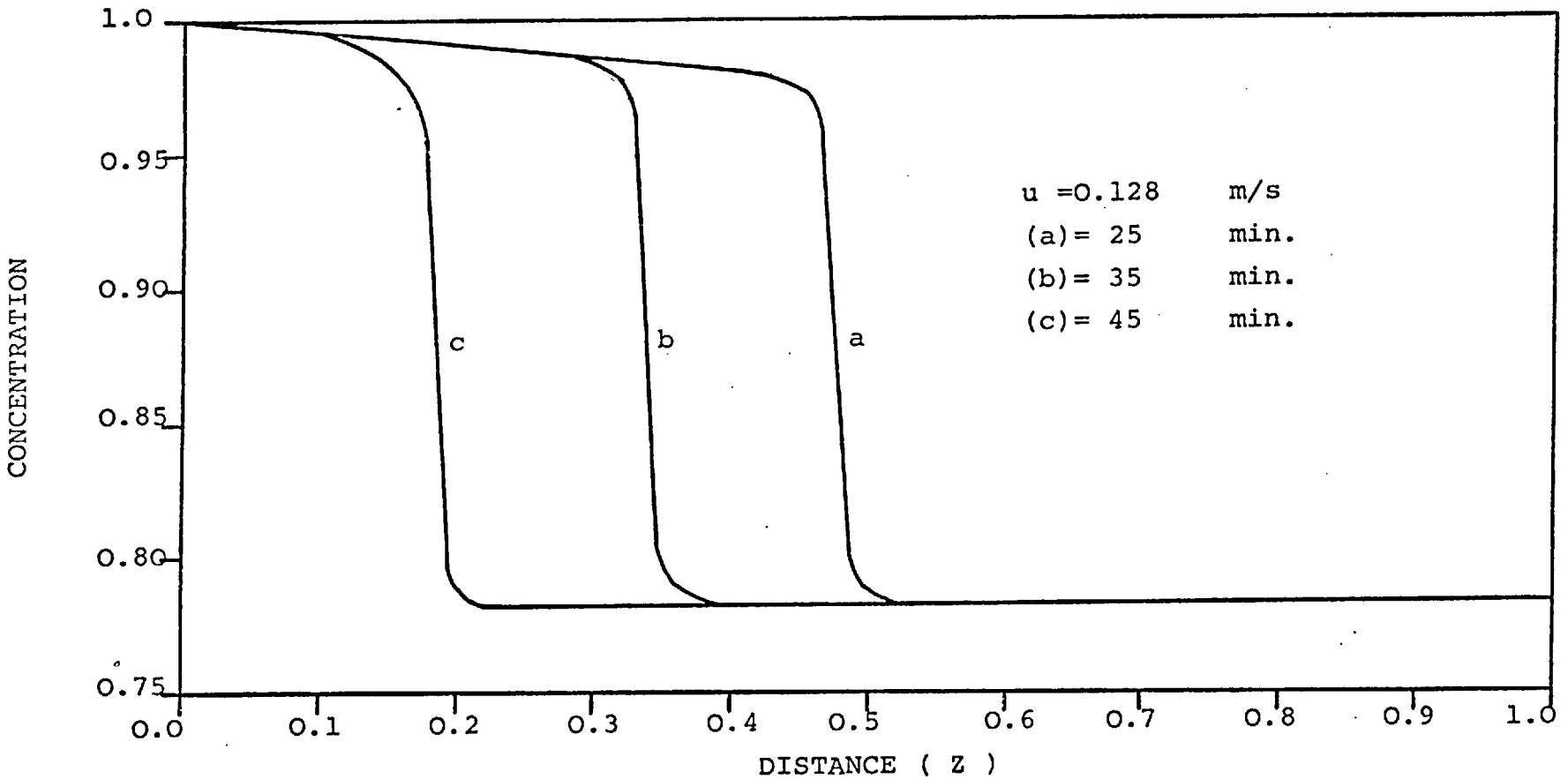


FIG.(6.16) CONCENTRATION PROFILES OF CARBON ALONG THE REACTOR FROM THEORY

(RUN NO. 77)



was turned off as soon as air flow was introduced to the reactor while conducting the experiment (section 4.3.3), therefore, the dimensionless rate of electrical heat input A' in energy balance equation 3.20 (section 3.1.5.1) is set equal to zero for any position of $Z > 0.75$.

To compare the theory with experimental results, one must take those data which are needed for the model. Most essential are the frequency factor k'_o and the activation energy E. Due to the lack of time no attempt was made to measure these kinetic constants. Therefore those values were obtained from the literature (31). It was found that the reported frequency factor had to be reduced by a factor of 2 in order to produce the same propagation rate as that observed experimentally.

In evaluating the Peclet number P for axial energy transport in the theoretical computation the value of thermal conductivity of the bed K_e was required. To obtain the value of K_e, the same difficulty as that of the previous system was experienced by using the available correlations (section 6.1). To get a value of K_e that would give nearly the same propagation rate as that observed experimentally, the value obtained from Bischoff's correlation has to be decreased by approximately 2.5 times. A value of K_e that predicted the propagation rate for all the runs was 1.95×10^{-3} KJ/m sec ^{o}K. Using this value of K_e results in a Peclet number P of 6×10^{4} based on the reactor length .

In incorporating the heat loss effects, the value of the average heat transfer coefficient term U' between the reactor and its surroundings was measured experimentally (appendix B4). This value was found to be 8 J/m^2 sec ^{o}K.

In spite of the uncertainties in the evaluation of the effective thermal conductivity K_e, and the kinetics constants, the model predicts the peak temperatures and the propagation rates of the reaction zone. Figures 6.7, 6.8, 6.9, 6.10 and 6.11 all indicate reasonable agreement in temperature profiles between the theory and the experiment.

In the above Figures the theoretical prediction of the temperature profiles are drawn in dashed lines. From the observation of these graphs it is clear that there is a discontinuity in the curves along the reactor axis for the normalized distance $Z > 0.7$. This is because the dimensionless rate of electrical heat input A' in energy balance 3.20 (section 3.1.5.1) was set equal to zero for any position of $Z > 0.75$ in the model, since while conducting the experiments the external heat input to the exit section was switched off on the introduction of the air flow to the reactor at time zero.

By comparing the experimental and theoretical temperature profiles a noticeable difference between the two can be observed in the exit section. The explanation for this is that during the experimentation in order to minimize the heat losses from the end flange a heating tape was wrapped round the outlet tubing of the reactor (section 4.2.1). This external heat input which contribute heat to the reactor by conduction was not included in the theoretical model.

Similarly as in the case of the previous system, the discrepancy in temperature profiles between the theory and experiment may be attributed to the use of such a simple model which neglects the radiative energy transport and differences between the catalyst and bulk gas temperature.

CHAPTER SEVEN

CONCLUSIONS

7.1 Conclusions reached in this work.

To provide an alternative and a more efficient method of reactor operation, studies have been presented on the dynamics and the effects upon transient behaviour of the moving reaction zones when several of the system parameters are perturbed. On the investigation of transient behaviour of reverse operation two chemical reactions have been studied experimentally and both systems demonstrated an effective reverse propagation of the reaction zone. A quasi-homogeneous one dimensional model in which the propagation of high temperature zone was assumed to occur by conduction though the solid phase was simulated for comparison with the experimental studies. The experimental results compared quite well with the model which was described by two coupled non-linear parabolic partial differential equations. These were solved by quasi-linearization and application of a Crank Nicholson finite difference algorithm. The agreement obtained by the comparison of the theoretical and experimental results are a further indication that the homogeneous mathematical model for a fixed-bed catalytic reactor gives satisfactory results. On the other hand the use of a two phase model will induce more sophistication in the theoretical analysis. However this is achieved on the inclusion of more experimentally uncertain parameters.

The results revealed that while maintaining constant feed conditions the reaction zone traversed the bed upstream to the inlet of the reactor with a constant velocity of propagation. However the propagation velocity decreased when the reaction zone approached the beginning of the reactor. For the CO oxidation system it was found that upon perturbation in feed conditions the velocity of propagation increased with increase in either feed concentration or feed velocity. The increased velocity of propagation reached a maximum with increasing feed velocity. For feed velocities slightly above the one that allows the maximum velocity of propagation, the propagation velocity started to decrease. As the feed velocity was raised still further this affect became more dominant, consequently the reaction zone separated and moved downstream causing blow-out.

The direction and velocity of propagation of the zone W was shown to depend heavily on the inlet velocity u_o and inlet concentration C_{Ao} . When the data was tested against the semi-empirical correlation proposed by Vortmeyer and Jahnel (7) it was found that

$$W = \alpha u_o^{0.72} \quad C_{Ao}^{0.45} - \beta u_o$$

which compares reasonably well with the exponents of 0.77 for inlet velocity and 0.5 for inlet concentration reported by Vortmeyer and Jahnel.

For the carbon oxidation during the regeneration of the fouled cracking catalyst it was demonstrated that feed velocity and feed temperature were capable of influencing

the propagation velocity of the reaction zone. The propagation velocity increased exponentially with increased feed velocity. Only above a distinct value of feed temperature reverse propagation of the reaction zone was possible for the conditions of carbon content and air composition tested. Operating with a feed temperature below that specified value caused the reaction zone to be blown out of the reactor. Increase in feed temperature resulted in an increase in the velocity of propagation.

As variation in feed velocity and feed concentration in CO oxidation systems were shown capable of influencing the propagation of the reaction zone, either of these variables could be used as the control. The choice between the two control variables is a choice between two distinct operating conditions. Using a variable inlet velocity and a constant inlet concentration a limited potential from heat generation is combined with an unlimited ability for convective heat loss, while the opposite is true for an operating policy with a variable inlet concentration and constant inlet velocity. While no absolute conclusion could be presented as to which is the better mode of control, the experimental results suggest that a control scheme based upon the inlet velocity would have a greater ability to manipulate the propagation properties of the reaction zone over a wider range of operating conditions . The variation in these control variables and their effects upon the propagation velocity with a correlation were then discussed in detail.

For the regeneration of the fouled Alumina-Silica it

was found that the amount of carbon that could be burnt during the reverse propagation was only 20 to 33% depending on the feed velocity and the feed temperature used for the operation. The remaining 67-80% of the carbon deposition burnt during forward propagation . The forward propagation occured from the change of direction of the reaction zone when it reached the reactor entrance. For the given reactor geometry, the system investigated in the present study indicates that fouled Alumina-Silica catalysts can be partially regenerated by the application of the reverse propagation provided that:

a) The carbon deposition over the bed must be at least of the order of 7% by weight

b) The feed must be preheated to a temperature of about $570^{o}K$, otherwise blow-out will result.

c) The feed velocity utilized must evolve the necessary heat in the reaction zone from the resulting exothermic reactions, so that enough heat can be dissipated by conduction through the solid phase of the fixed bed reactor.

NOMENCLATURE

a' = catalyst activity.

a_o = initial catalyst activity.

a = a'/a_o = normalized catalyst activity.

$A = \dfrac{P''}{\pi/4\ D_i^2 L_2} \cdot \dfrac{L}{u_o (\rho C_p)_e T_o}$ dimensionless rate of electrical heat input for CO oxidation system.

$A' = \dfrac{P''}{\pi/4 D_i^2 L_2} \cdot \dfrac{L}{u_o (\rho C_p)_e T_o}$ dimensionless rate of electrical heat input for carbon oxidation system.

$B = \rho_{go}\ C_{pg}\ \varepsilon/(\rho C_p)_e$ = dimensionless convection group.

C = total gaseous concentration in the reactor (Kmol m^{-3})

C_o = total gaseous concentration in the reactor feed (Kmol m^{-3})

C_{Ao} = concentration of A(CO) in the reactor feed (Kmol m^{-3})

C_A' = concentration of A(CO) in the reactor (Kmol m^{-3})

C_{Bo} = concentration of B(O_2) in the reactor feed (Kmol m^{-3})

C_B' = concentration of B(O_2) in the reactor (Kmol m^{-3})

C_{Eo} = concentration of E(O_2) in the reactor feed (Kmol m^{-3})

C_E' = concentration of E(O_2) in the reactor (Kmol m^{-3})

C_{pg} = mean heat capacity of the gaseous stream (J $Kmol^{-1} K^{-1}$)

C_{ps} = mean heat capacity of the solid phase (J $Kg^{-1} K^{-1}$)

D_{AB} = mass diffusivity. ($m^2\ s^{-1}$)

D_o = mass diffusivity at inlet conditions ($m^2\ s^{-1}$)

D_i = inside diameter of the reactor (m)

E = activation energy for the main reaction (KJ K mol^{-1})

$G_1 = \dfrac{a_o K_o L C_{Ao}}{2\ u_o}$ = dimensionless reaction rate group for CO oxidation.

$G_2 = \dfrac{K_2 L}{u_o}$ = dimensionless reaction rate group for carbon oxidation.

$J = \dfrac{E}{RT_o}$ = dimensionless activation energy group.

K_e = effective thermal conductivity of the bed ($J\ K^{-1}m^{-1}s^{-1}$)

K_o = pre-exponential frequency factor ($m^3\ Kmol^{-1}s^{-1}$)

K'_o = pre-exponential frequency factor ($k\ mol\ m^{-3}\ sec^{-1}atmos^{-1}$)

K_2 = pre-exponential frequency factor (sec^{-1})

$K_3 = \dfrac{K_2 L}{u_o}$, dimensionless

L = total length of the reactor (m)
L_2 = length of reactor heated by external heaters. (m)
ℓ = distance along the reactor axis (m)

$M = 2\ M_{Bo}/M_{Ao}$, dimensionless

M_A = molar flowrate of CO ($K\ mol\ s^{-1}$)

M_{Ao} = molar flowrate of CO in the feed ($K\ mol\ s^{-1}$)

M_{Bo} = molar flowrate of O_2 in the feed ($K\ mol\ s^{-1}$)

m = denotes the m^{th} grid interval along time axis.

n = denotes the n^{th} iteration.

$P' = \dfrac{u_o L}{D_o}$ = Peclet number for axial mass transport.

$P = \dfrac{u_o L (\rho C_p)_e}{K_e}$ = Peclet number for axial energy transport.

P'' = Electrical power input. (KJ)

$Q_1 = G_1 \cdot \dfrac{(-\Delta H)\ C_{Ao}\ \varepsilon}{(\rho C_p)_e T_o}$, dimensionless.

$Q_2 = G_2 \cdot \dfrac{(-\Delta H)\ C_{Eo}\ \varepsilon}{(\rho C_p)_e\ T_o}$, dimensionless.

Q' = Electrical heat input/volume of the reactor ($KJ\ m^{-3}$)

R = gas constant ($J\ K\ mol^{-1}K^{-1}$

r = denotes the r^{th} grid interval along the spatial axis.

s = $\Delta\Theta$ time axis mesh point, dimensionless

T = Temperature in the reactor (^oK)

T_o = Temperature of the feed (^oK)

t = time from start up (s)

U = average heat transfer coefficient between the system and its environ for CO oxidation ($J\ s^{-1}m^{-2}K^{-1}$)

U' = average heat transfer coefficient between the system and its environ for carbon oxidation ($J\ s^{-1}m^{-2}K^{-1}$)

$U_1 = \frac{4U}{D_i} \cdot \frac{L}{u_o(\rho C_p)_e}$ = dimensionless heat loss group for CO oxidation.

$U_1' = \frac{4U}{D_i} \cdot \frac{L}{u_o(\rho C_p)_e}$ = dimensioness heat loss group for carbon oxidation.

u_o = interstitial feed velocity (m/s)

u' = interstitial velocity. (m/s)

W = velocity of propagation. (m/s)

X_A = mole fraction of CO.

X_{Ao} = mole fraction of CO at the feed

X_B = mole fraction of O_2

X_{Bo} = mole fraction of O_2 at the feed

x = denotes a state variable

Y = fractional conversion, dimensionless.

z = ℓ/L = normalized dimensionless distance.

SUBSCRIPTS

e = effective property, a combination of the gas and catalyst physical properties.

g = gas

s = solid (catalyst).

GREEK SYMBOLS

ΔH = heat of reaction (J $Kmol^{-1}$)

ε = voidage of the bed

Θ = dimensionless time

ρ_g = molar density of the gas (K mol m^{-3})

ρ_{go} = molar density of the gas at the feed (K mol m^{-3})

ρ_s = density of the solid (Kg m^{-3})

$(\rho C_p)_e$ = effective value of the product of density and heat capacity. (J $K^{-1}m^{-3}$)

$\tau = \frac{L}{u_o}$ = residence time

$\phi = \frac{T}{T_o}$ = dimensionless temperature.

ϕ_a = dimensionless temperature of the ambient or cooling medium.

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APPENDICES

APPENDIX A

EXPERIMENTAL DATA FOR DETERMINING THE KINETICS OF REACTION

Experimental data as well as calculated results for the kinetics of CO oxidation are summarized in this appendix.

A.1 Raw Data for the Kinetic Runs.

The raw data for the kinetic runs is presented in Table A.2. The data contain the temperature of operation of the reactor, residence time and corresponding conversion of carbon monoxide. The operating conditions of the reactor for the kinetics data are presented in Table A.1.

A.2 Analysis of Kinetic Data.

The oxidation of CO over cupric oxide can be represented by the form:

$$r = K_o \exp(-E/RT)\, C_A C_B \qquad (A.1)$$

If the concentration of oxygen can be considered to remain constant (= $[O_2]$) due to an excess air in the feed, the rate reduces to a pseudo first order form

$$r = K_o^* \exp(-E/RT)\, C_A \qquad (A.2)$$

where $K_o^* = K_o\,[O_2]$.

If τ is the residence time in a plug flow reactor based on porosity, then the fractional conversion of A can be related to the residence time for a pseudo first order reaction as (Levenspiel (40)):

$$\tau = C_{Ao} \cdot \int_{o}^{Y} \frac{dY}{r} = C_{Ao} \int_{o}^{Y} \frac{dY}{K_o [O_2] \exp(-E/RT)\ C_{Ao}(1-Y)} \qquad (A.3)$$

$$\ln \frac{1}{1-Y} = K_o\ [O_2]\ \tau \exp\ (-E/RT)$$

$$\ln \left(\frac{\ln \frac{1}{1-Y}}{\tau\ [O_2]} \right) = \ln K_o - E/R(\tfrac{1}{T}) \qquad (A.4)$$

Equation (A. 4) offers a convenient form for the determination of kinetic constants knowing the values of and conversion Y at various temperatures. From Figure 5.1 (section 5.2.2)

slope = -E/RT

intercept = ln K_o

$E = 3.6 \times 10^4$ KJ/K mol.

$K_o = 3.165 \times 10^6$ m^3/K mol s.

The kinetics of CO oxidation over cupric oxide for a pseudo first order reaction with respect to CO can be

APPENDIX A (continued)

TABLE A.1

REACTOR OPERATING CONDITIONS FOR KINETICS DATA.

REACTOR LENGTH - 0.05 m

AMOUNT OF CATALYST (CUPRIC OXIDE) IN THE REACTOR - 10.1×10^{-3} Kg.

VOIDAGE OF THE PACKED BED - 0.48 (SEE APPENDIX B).

REACTOR INSIDE DIAMETER - 0.93×10^{-2} m.

AREA OF CROSS SECTION - 0.678×10^{-4} m^2.

VOLUME OF REACTOR (BASED ON VOIDAGE) - 1.6272×10^{-6} m^3.

NUMBER OF THERMOCOUPLES 3 (EQUALLY SPACED 0.025m APART).

REACTOR SET-UP - A 0.3 m PRE-HEATER PACKED WITH INERTS (SILICA-GLASS).
A 0.05 m ACTIVE SECTION WITH CATALYST , AND THE EXIT
SECTION OF 0.25 m PACKED WITH INERTS.

APPENDIX A (continued)

TABLE A.2

ANLAYSIS FOR PSEUDO FIRST ORDER KINETIC CONSTANTS

RUN NO.	$\frac{1}{T}$ $(^{o}K)^{-1}$	τ s	Y	$\ln\left(\frac{\ln\frac{1}{1-Y}}{\tau[O_2]}\right)$
20	$17.x10^{-4}$	7.795	0.1463	7.795
23	$14.9x10^{-4}$	8.27	0.292	8.27
25	11.5×10^{-4}	10.166	0.83	10.166

represented as:

$$r = 3.165 \times 10^{6} \; [O_2] \; \exp\left(-\frac{3.6 \times 10^{4}}{RT}\right) C_A \qquad (A.5)$$

A.3 Operation of column switching system of chromatograph.

The system employed is illustrated in Figure (A.1). With Tap 1 open and Tap 2 closed the sample is eluted through the columns in the normal manner. By opening Tap 2 and closing Tap 1 the flow through column 1 is reversed, carrier gas now being supplied via the secondary supply from PR2. The provision of a small bleed round Tap 1 through the fixed restrictor X merely ensures that the material being back-flushed from Column 1 does not collect in the line IJ. A suitable backflush flowrate is obtained by appropriate adjustment of needle valve NV1.

Essential features of the column switching system are the use of the same secondary carrier gas supply from PR2 to switch flow directions and the use of a three way tap (Tap 4) to route gas from this source either via A to C or via B to D.

Proper operation is achieved by the correct adjustment of the secondary pressure PR2. Suppose for a moment that one of the secondary column is removed and that PR2 is isolated. For sake of discussion it is supposed that the pressure on the inlet of the primary column is 30 psig and the pressure between the columns is 20 psig. If now, without altering the pressure settings, the other secondary column is placed in the system as illustrated in Figure (A.1)

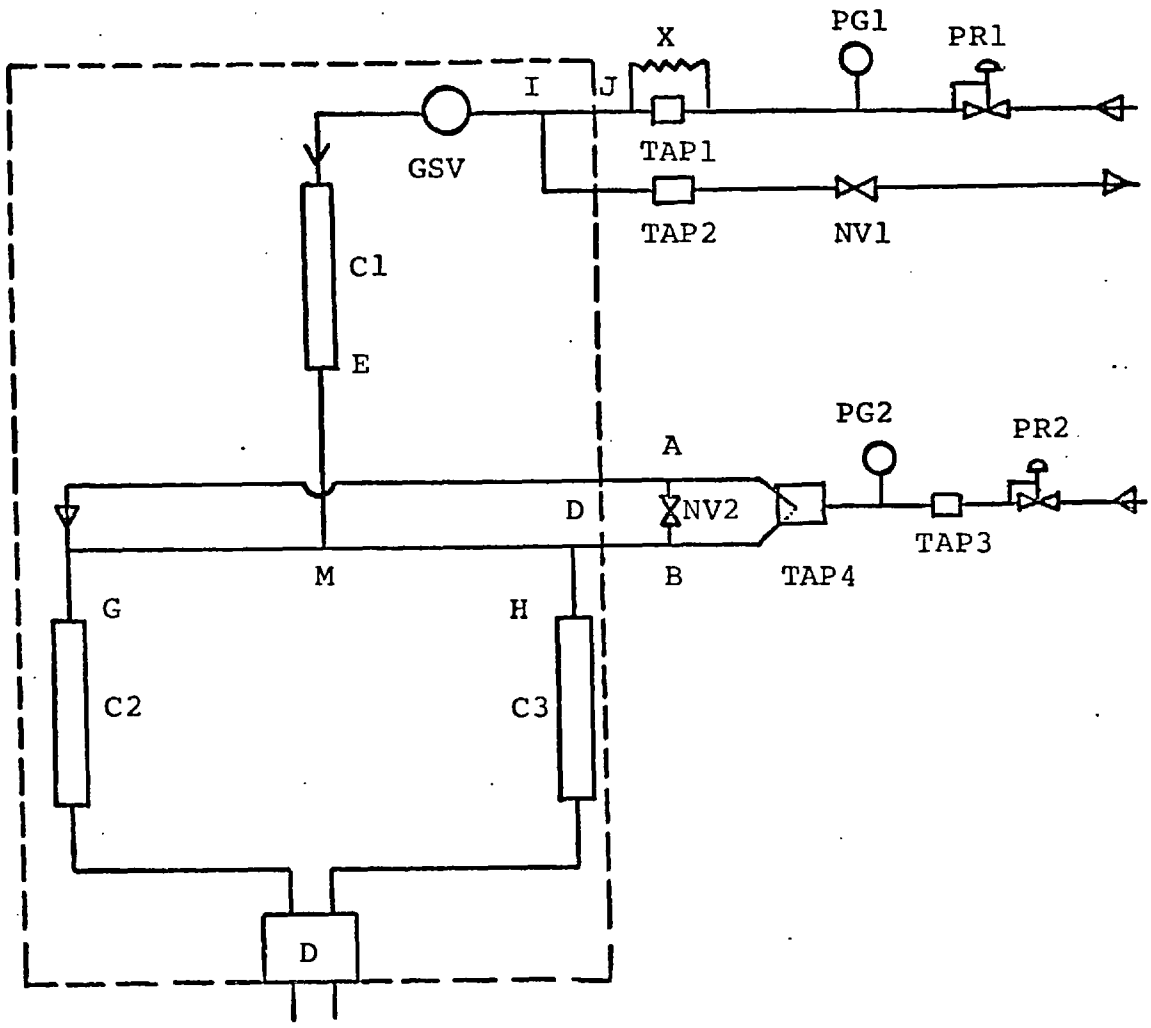


FIG. (A.1)

PR1 , PR2	Pressure regulators
PG1 , PG2	Pressure gauges
TAP1, TAP2	On / off taps or solenoid valve
TAP4	Three way tap or solenoid valve
TAP3	On / off tap
NV1 , NV2	Needle valves
C1,C2,C3	Columns
X	Fixed restrictor
G.S.V	Gas sample valve
A,B,D...J,M	See text

then with PR2 still isolated the pressure at the 'mid point' M will drop to, say, 15 psig as a consequence of increased total flow and the full effluent from the primary column will be split between the two secondary columns. If, however, PR2 is switched in and used to supply gas at pressure slightly in excess of 20 psig via A to C the second secondary column will be 'pneumatically isolated' from the first with carrier gas supplied from PR2. Some gas from the source will also pass along the route ACM and the total effluent of the primary column will pass to the first secondary column under conditions very similar to those described in the hypothetical case where the other secondary column was missing. By reversing Tap 4 the flow is switched in the opposite direction. The secondary carrier gas pressure must be set slightly higher than the pressure which would exist if the secondary column with the highest pneumatic resistance were in the system on its own. In the hypothetical case it was assumed that this higher figure is 20 psig. The needle value NV2 is necessary to ensure that whichever of the two legs BD and AC is not directly connected to the secondary carrier gas supply is purged with a small flow of gas to prevent part of the sample diffusing up what would otherwise be a dead space.

Thus with Tap 4 in the position shown in Figure (A.1) the gas flows are as follows. Carrier gas and sample emerging from E pass to MDH. Secondary gas passes along ACG to Column 2 and also along ACM to ensure a total switching of the sample to Column 3. A small purge of gas along

ABD through NV2 ensures that no sample is trapped in DB where it would be subsequently eluted onto Column 2 when Tap 4 was reversed. In purely practical terms successful operation of this column switching system depends on the correct adjustment of the secondary pressure at PR2 and the correct setting of the needle valve NV2.

APPENDIX B

EXPERIMENTAL DATA

This appendix contains all the experimental observations made to check the validity of the model. Preliminary objectives included determining the equivalent diameter of the catalyst particles, the voidage and the bulk density of the catalyst.

B.1 Equivalent diameter of the cupric oxide catalyst particles (d_{eq}.)

The catalyst particles were cylindrical in shape of length ($\ell_{p\ell}$) 2mm and diameter ($d_{p\ell}$) 0.5 mm . The equivalent diameter d_{eq} is the diameter of a sphere which has the same volume to surface area ratio as the particle itself. The equivalent diameter helps in calculating the Reynold's number and other parameters such as Peclet number, etc.

$$d_{eq} = \frac{6 \times \text{volume of the particle}}{\text{particle surface area}}$$

The particles were cylindrical in shape of length (ℓ_{p_ℓ}) 2mm and diameter ($d_{p\ell}$) 0.5 mm.

$$d_{eq} = \frac{6\ [\pi/4\ d_{p_\ell}^2\ \ell_{p\ell}\ ]}{\left[\pi d_{p\ell}\ \ell_{p\ell} + 2\ \pi/4\ \ d^2_{p\ell}\right]}$$

$$= \frac{6\left[\frac{\pi}{4} \times (0.5)^2 \times 2\right]}{\left[\pi \times 0.5 \times 2 + 2\frac{\pi}{4} \times (0.5)^2\right]}$$

$$= 0.666 \text{ mm}$$

$$= 0.666 \times 10^{-3} \text{ m.}$$

B.2 Measurement of Bed voidage and Bulk density. (CuO Catalyst).

The voidage of the reactor was determined by packing the catalyst in the reactor. This was achieved by filling a known quantity of the catalyst in the reactor one by one piece at a time followed by tapping the sides and ends of the reactor so that the particles settled to a tightly packed and uniform condition. Since it was not possible to observe the uniformity of the bed, it was decided to duplicate this method using a glass tube of the same size. The packing in the glass tube showed the desired uniformity of the catalyst packing with a 4% drop in voidage compared to that of the reactor. The higher voidage in the stainless steel reactor is expected since 23 thermocouples were placed in the central axis, causing a decreased of 8% in the amount of catalyst packed. This method of packing was repeated several times and results were consistent.

The bulk density of the catalyst was measured by displacement of the catalyst particles in a density bottle with alcohol. A 25 cc density bottle was weighed with and without the alcohol content. A known amount of catalyst was then placed into the density bottle containing the alcohol and was weighed.

volume of bottle = 25 cc

weight of empty bottle = 16.62 gms

weight of bottle + alcohol = 36.26 gms

weight of alcohol = 19.64 gms

Therefore, density of alcohol = $\frac{19.64}{25}$ = 0.7856 gm/cc

weight of catalyst placed in the bottle = 18.64 gms

weight of bottle + alcohol left = 52.36 gms

Therefore, weight of alcohol displaced = (36.26 + 18.64) - 52.36

= 2.54 gms

Consequently,

volume of alcohol displaced = $\frac{2.54}{0.7856}$

= 3.233 cc

Therefore,

$$\text{density of catalyst} = \frac{\text{mass of catalyst}}{\text{volume displaced}}$$

$$= \frac{18.64}{3.233} = 5.76 \text{ gm/cc}$$

BED VOIDAGE (ε))

Weight of catalyst in the reactor = 121.14 gms

number of thermocouples = 23

$$\varepsilon = \frac{\text{void volume}}{\text{(volume of reactor-volume of thermocouples)}} = \frac{V}{V1}$$

$$Vl = \left(\frac{\pi D_i^2}{4} L - 23 \frac{\pi d^2}{4} \ell_1 \right)$$

where

D_i = internal diameter of the reactor = 0.92837 cm

L = Total length of the reactor = 60 cm

ℓ_1 = length of thermocouple inserted in the reactor = 0.5 cm

d = diameter of the thermocouple = 0.1 cm

$$Vl = 40.5 \text{ c.c}$$

$$V = Vl - V_{cat} = Vl - \frac{\text{mass of the catalyst}}{\text{density of the catalyst}}$$

V_{cat} = volume of catalyst

$$V = \left(40.5 - \frac{121.14}{5.76}\right)$$

$$= 19.47 \text{ c.c.}$$

Therefore

$$\varepsilon = \frac{19.47}{40.5}$$

$$= 0.48$$

B.3 Measurement of Bed voidage and Bulk density (Alumina-Slica Catalyst).

The procedure adopted for the determination of the voidage of the reactor was the same as that already discussed in Section B2.

However the bulk density of Alumina-Silica catalyst was measured by using a mercury balance. The catalyst pellet was weighed and in turn was immersed in the mercury. The weight of displacement of mercury excluding the weight of the pellet was noted.

weight of the pellet	=	0.7877	gm
displaced weight of Hg excluding weight of the pellet.	=	9.42	gm
Displaced weight.		10.2077	gm
volume of the pellet	=	$\frac{10.2077}{13.6}$	
	=	0.7506	c.c

Therefore

bulk density of the catalyst = $\frac{0.7877}{0.7506}$

= 1.05 gm/c.c

Bed voidage (ε)

$$\varepsilon = \frac{\text{void volume}}{\text{(volume of reactor - volume of thermocouples)}} = \frac{V}{Vl}$$

Weight of the catalyst in the reactor = 20.32 gms

$Vl = 40.5$ c.c.

$$Vl = Vl - V_{cat} = Vl - \frac{\text{mass of the catalyst}}{\text{density of the catalyst}}$$

$$V = (40.5 - \frac{20.32}{1.05})$$

$V = 21.147$

Therefore $= \frac{21.147}{40.5}$

$= 0.52$

B.4 Estimation of the average heat transfer coefficient between the system and its surroundings.

The reactor was heated up by means of the external heaters. A nitrogen flow of 240 cc/min was passed through the reactor bed and the electrical heat input was measured by a digital wattmeter. A period of approximately 8 hours was required to establish a steady state condition. By controlling the heat input through the variacs several runs were made at different temperatures. A typical calculation of heat balance at the steady state is outlined below. At steady state,

Heat lost to the ambient = Electrical heat input - heat lost by forced convection to gas.

Heat lost by forced convection = $\rho_g C_{pg} F_g (T-T_o)$

F_g = feed flowrate = 240 cc/min = $4. \times 10^{-6}$ m^3/s.

T = bed temperature = 878^oK

T_o = feed temperature = 290^oK

Heat lost by forced convection = $\frac{1}{22.4} \times \frac{273}{878} \times 7. \times 4. \times 10^{-6} \times (878-290)$

$= 0.22853 \times 10^{-3}$ K cal/s

$= 0.95681$ J/S

Therefore,

Heat lost to the ambient = 86 - 0.95681

$= 85.04319$ J/S

Convective heat loss from the reactor to the ambient = $U'A\Delta T$

where U' = heat transfer coefficient based on the inside diameter of the reactor, $J/m^2\ 5^oK$

$$A = \pi D_i L = 0.01753 \quad m^2.$$

Equating the heat loss :

$$U'\ A\ \Delta T = 85.04319$$

$$U' = \frac{85.04319}{0.01753 \times 588}$$

$$= 8.25 \qquad J/m^2\ s\ ^oK.$$

The average value of U' used in the theoretical model to compute the temperature profile was 8. $J/m^2\ s\ ^oK$.

TABLE (B.1)

VALUES OF THE DIMENSIONLESS GROUP FOR THE THEORETICAL COMPUTATION.

PHYSICAL SYSTEM	RUN NO. 30	RUN NO. 32	RUN NO. 44	RUN NO. 45
DIMENSIONLESS GROUP:				
B	3.07×10^{-4}	3.07×10^{-4}	3.07×10^{-4}	3.07×10^{-4}
M	2.8	3.0	2.766	2.522
J	14.54	14.53	14.54	14.53
G_1	8688.97	10350.8	10087.28	9470.92
P	2.0×10^{4}	2.0×10^{4}	2.0×10^{4}	2.0×10^{4}
Q_1	11.557	12.975	13.566	13.789
U_1	0.0010	0.001266	0.00115	0.0010

TABLE (B.2)

VALUES OF THE DIMENSIONLESS GROUP FOR THE THEORETICAL COMPUTATION.

PHYSICAL SYSTEM	RUN NO. 73	RUN NO. 74	RUN NO. 75	RUN NO.76	RUN No. 77
DIMENSIONLESS GROUP.					
B	1.88×10^{-4}	1.88×10^{-4}	1.88×10^{-4}	1.88×10^{-4}	1.88×10^{-4}
J	21.546	21.546	21.546	21.546	21.546
G_2	$.50782\times10^{9}$	$.48634\times10^{9}$	$.4600\times10^{9}$	$.44878\times10^{9}$	$.43125\times10^{9}$
P	$6.\times10^{4}$	$6.\times10^{4}$	$6.\times10^{4}$	$6.\times10^{4}$	$6.\times10^{4}$
Q_2	0.43655×10^{6}	0.41809×10^{6}	0.39544×10^{6}	0.38579×10^{6}	0.39773×10^{6}
U_1'	0.0112	0.0112	0.0112	0.0112	0.0112

APPENDIX C

TABLE (C.1)

DATA ON CARBON MONOXIDE OXIDATION
(RUN NO. 44)

Air flow	=	790	cc/min.
after 20 min.	=	869	cc/min.
CO flow	=	120	cc/min.
after 20 min.	=	132	cc/min.
Total flow	=	910	cc/min.
after 20 min.	=	1001	cc/min.
Feed velocity (u_o)	=	0.466	m/s.
after 20 min.	=	0.513	
Residence time (τ)	=	1.2875	s.
after 20 min.	=	1.171	s.
Feed concentration (C_{A_o})	=	5.45×10^{-3}	$Kmol/m^3$
Oxygen concentration (C_{B_o})	=	7.537×10^{-3}	$Kmol/m^3$

Pressure gauge readings during run (p.s.i.g)

= P.G1-3. : P.G2 -2.

(RUN NUMBER 44)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.001658	1.001658	1.001658	1.001658	1.001658
.083	1.002492	1.002492	1.002492	1.002492	1.002492
.125	1.003327	1.003327	1.004161	1.003327	1.003327
.167	1.004996	1.004996	1.004996	1.004996	1.004996
.250	1.008324	1.009168	1.009168	1.009168	1.009168
.292	1.011672	1.011672	1.011672	1.011672	1.011672
.333	1.015010	1.015010	1.015010	1.015010	1.015010
.375	1.019182	1.020016	1.019182	1.019182	1.020851
.417	1.025858	1.025858	1.025858	1.026692	1.030030
.458	1.033368	1.033368	1.034203	1.036706	1.050058
.500	1.046720	1.047555	1.048389	1.062576	1.113480
.542	1.067583	1.068417	1.076762	1.137680	1.331283
.583	1.099293	1.100128	1.146025	1.366332	1.892670
.625	1.150198	1.155205	1.371339	1.895971	2.227706
.667	1.236151	1.284551	1.935507	2.238191	2.313855
.708	1.375511	1.645611	2.230126	2.309033	2.286517
.792	1.814835	2.150905	2.235772	2.210756	2.163863
.833	1.983113	2.193791	2.201064	2.161434	2.114408
.875	2.111160	2.254312	2.187324	2.128205	2.075387
.917	2.165482	2.263173	2.165482	2.091657	2.033815

DISTANCE Z	time= 25 Φ	time= 30 Φ	time=35 Φ	time= 40 Φ	time= 45 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.001658	1.001658	1.001658	1.001658	1.001658
.083	1.002492	1.002492	1.002492	1.002492	1.002492
.125	1.003327	1.003327	1.003327	1.003327	1.003327
.167	1.004996	1.004996	1.004161	1.004996	1.004996
.250	1.009168	1.009168	1.010003	1.010837	1.014175
.292	1.011672	1.011672	1.014175	1.018347	1.030865
.333	1.015010	1.017513	1.023354	1.039210	1.083438
.375	1.022520	1.031690	1.055065	1.111811	1.282048
.417	1.040879	1.075928	1.159377	1.366332	1.877806
.458	1.087611	1.199433	1.445609	1.997034	2.268005
.500	1.258682	1.607507	2.098161	2.374054	2.368441
.542	1.822311	2.208333	2.321087	2.438126	2.369243
.582	2.272836	2.386078	2.381269	2.397295	2.326710
.625	2.385276	2.384475	2.350794	2.323497	2.259951
.667	2.365233	2.327513	2.287322	2.247059	2.191366
.708	2.285713	2.244641	2.205103	2.167101	2.120091
.792	2.134694	2.098161	2.063172	2.032183	1.997034
.833	2.080270	2.043608	2.010123	1.979836	1.947836
.875	2.036264	1.998671	1.963435	1.933039	1.902569
.917	1.989666	1.952764	1.917402	1.886892	1.857131

(RUN NUMBER 44)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.000000	1.000000	1.000000	1.000823	1.000823
.042	1.001658	1.001658	1.001658	1.002492	1.003327
.083	1.002492	1.002492	1.003327	1.004161	1.007499
.125	1.004161	1.004161	1.005830	1.010003	1.018347
.167	1.005830	1.008334	1.013341	1.025023	1.052562
.250	1.025023	1.049224	1.104300	1.226971	1.541576
.292	1.065914	1.145191	1.319600	1.670927	2.205103
.333	1.206943	1.452285	1.872021	2.221250	2.385276
.375	1.657434	2.107911	2.315463	2.406907	2.435726
.417	2.274446	2.402903	2.451725	2.434125	2.396494
.458	2.398096	2.438926	2.421320	2.372450	2.317070
.500	2.350794	2.347584	2.313052	2.266395	2.214793
.542	2.288126	2.252701	2.213986	2.171956	2.128205
.582	2.234965	2.178429	2.133883	2.093283	2.054208
.625	2.180855	2.119279	2.071316	2.030550	1.993760
.667	2.126583	2.068059	2.020749	1.979836	1.945371
.708	2.068059	2.018298	1.974098	1.936329	1.902569
.792	1.962615	1.927280	1.893495	1.861269	1.832270
.833	1.916578	1.886066	1.855475	1.826462	1.799036
.875	1.873674	1.845536	1.818158	1.790712	1.765699
.917	1.829781	1.803196	1.778213	1.754006	1.730579

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.000823	1.001658	1.001658	1.003327	1.006665
.042	1.004996	1.010003	1.019182	1.040044	1.078431
.083	1.014175	1.031699	1.062576	1.134342	1.249503
.125	1.041713	1.090949	1.183577	1.391367	1.630388
.167	1.132673	1.280379	1.545748	1.956869	2.163863
.250	2.099786	2.285713	2.377261	2.414915	2.468518
.292	2.406106	2.482905	2.481307	2.435726	2.435726
.333	2.457324	2.486102	2.460522	2.397295	2.364431
.375	2.425322	2.419719	2.394886	2.334740	2.290540
.417	2.347584	2.320283	2.289735	2.245447	2.204295
.458	2.260757	2.222864	2.192983	2.157385	2.121714
.500	2.164672	2.125771	2.095722	2.066430	2.037080
.542	2.085151	2.048501	2.018298	1.992123	1.966717
.582	2.015846	1.981475	1.952764	1.927280	1.905042
.625	1.959332	1.927280	1.899270	1.875327	1.853819
.667	1.912459	1.882763	1.856303	1.833100	1.812342
.708	1.872021	1.844707	1.818989	1.796540	1.776545
.792	1.804860	1.779880	1.756512	1.735604	1.716329
.833	1.773209	1.749826	1.728066	1.707098	1.688609
.875	1.742299	1.719684	1.698698	1.679351	1.661653
.917	1.708777	1.687768	1.668399	1.650680	1.633773

APPENDIX C

TABLE (C.2)

DATA ON CARBON MONOXIDE OXIDATION
(RUN NO. 45)

Air flow	=	900	cc/min.
after 20 min.	=	990	cc/min.
CO flow	=	150	cc/min.
after 20 min.	=	165	cc/min.
Total flow	=	1050	cc/min.
after 20 min.	=	1155	cc/min.
Feed velocity (u_o)	=	0.5337	m/s.
after 20 min.	=	0.5915	m/s.
Residence time (τ)	=	1.116	s.
after 20 min.	=	1.014	s.
Feed concentration (C_{Ao})	=	5.9×10^{-3}	K mol/m^3
Oxygen concentration (C_{Bo})	=	7.441×10^{-3}	K mol/m^3

Pressure gauge readings during run (psig)

= P.G1-3 : P.G2 - 2.

(RUN NUMBER 45)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.000000	1.000000
.167	1.000000	1.000000	1.000000	1.000000	1.000000
.250	1.000000	1.000000	1.000000	1.000000	1.000000
.292	1.000000	1.000000	1.000000	1.000000	1.000000
.333	1.000000	1.000000	1.000000	1.000000	1.000000
.375	1.002492	1.002492	1.002492	1.002492	1.002492
.417	1.005830	1.006665	1.005830	1.006665	1.007499
.458	1.010837	1.011672	1.010837	1.012506	1.018347
.500	1.019182	1.019182	1.020016	1.025858	1.051727
.542	1.032534	1.032534	1.036706	1.069252	1.180239
.582	1.054231	1.055065	1.077597	1.211116	1.583300
.625	1.092618	1.095121	1.217792	1.652369	2.154955
.667	1.162715	1.192757	1.688609	2.235772	2.419719
.708	1.292896	1.512368	2.237385	2.453325	2.497288
.792	1.746482	2.264784	2.442126	2.444526	2.418117
.833	1.931394	2.247059	2.389283	2.373252	2.342768
.875	2.084338	2.308230	2.344373	2.311445	2.275251
.917	2.163863	2.355608	2.306622	2.255118	2.210756

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.000000	1.000000
.167	1.000000	1.000000	1.000000	1.000000	1.000000
.250	1.000000	1.000000	1.000000	1.000000	1.000000
.292	1.000000	1.000000	1.000000	1.000823	1.009168
.333	1.000000	1.000000	1.003327	1.015010	1.050893
.375	1.003327	1.007499	1.022520	1.070921	1.231144
.417	1.012506	1.030865	1.099293	1.290393	1.891845
.458	1.035872	1.107638	1.357152	1.952764	2.390084
.500	1.129335	1.434760	2.169529	2.423721	2.537216
.542	1.506527	2.245447	2.480508	2.609815	2.572329
.582	2.234159	2.502880	2.593068	2.617789	2.546794
.625	2.469317	2.573924	2.592271	2.562755	2.492494
.667	2.550785	2.573924	2.546794	2.496489	2.430924
.708	2.526838	2.510867	2.466919	2.414915	2.357212
.792	2.391687	2.349991	2.304210	2.260757	2.215600
.833	2.314659	2.275251	2.233352	2.192983	2.153335
.875	2.244641	2.207526	2.168719	2.131450	2.094909
.917	2.178429	2.142801	2.105474	2.070502	2.037080

(RUN NUMBER 45)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.000000	1.025023
.167	1.000000	1.000000	1.001658	1.025858	1.125163
.250	1.006665	1.036706	1.138515	1.562438	2.247059
.292	1.044217	1.164384	1.542410	2.319480	2.532426
.333	1.195260	1.624461	2.276056	2.517256	2.601043
.375	1.765699	2.354003	2.556371	2.596258	2.581901
.417	2.456524	2.609018	2.629748	2.574722	2.515659
.458	2.613005	2.640112	2.598651	2.515659	2.441326
.500	2.562755	2.553977	2.506075	2.427723	2.356410
.542	2.493293	2.458123	2.411712	2.346781	2.283299
.582	2.438126	2.376459	2.327513	2.272031	2.215600
.625	2.388482	2.313855	2.259146	2.208333	2.158195
.667	2.340360	2.263173	2.205910	2.156575	2.110348
.708	2.282494	2.212371	2.156575	2.109536	2.066430
.792	2.167101	2.116032	2.069688	2.027284	1.989666
.833	2.111972	2.068059	2.026467	1.988028	1.952764
.875	2.057468	2.020749	1.983113	1.947836	1.915755
.917	2.003580	1.969998	1.937151	1.905867	1.875327

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.010837
.042	1.000000	1.012506	1.053396	1.116818	1.300407
.083	1.018347	1.078431	1.224468	1.429753	1.948657
.125	1.089280	1.317097	1.677667	1.973278	2.276861
.167	1.354649	1.974918	2.268005	2.379666	2.425322
.250	2.410911	2.486901	2.587485	2.642503	2.563552
.292	2.583497	2.525241	2.541207	2.585092	2.544400
.333	2.606625	2.516457	2.473314	2.486102	2.471715
.375	2.569935	2.489298	2.421320	2.406106	2.394892
.417	2.489298	2.426923	2.359619	2.325906	2.309033
.458	2.403704	2.352398	2.293757	2.254312	2.231739
.500	2.312248	2.267200	2.219636	2.180855	2.154145
.542	2.237385	2.196216	2.155765	2.119279	2.091657
.582	2.170338	2.130639	2.094909	2.061543	2.033815
.625	2.114408	2.077014	2.043608	2.012576	1.985571
.667	2.069688	2.032999	2.000308	1.971638	1.945371
.708	2.028100	1.992941	1.961794	1.934684	1.909988
.792	1.956048	1.924811	1.895971	1.870367	1.846365
.833	1.920695	1.891019	1.863751	1.838905	1.815666
.875	1.885241	1.857131	1.831441	1.807354	1.785714
.917	1.848022	1.822311	1.798204	1.775711	1.754841

APPENDIX C

TABLE (C.3)

DATA ON CARBON MONOXIDE OXIDATION

(RUN NO. 46)

Air flow	=	300	cc/min.
after 10 min.	=	360	cc/min.
after 30 min.	=	390	cc/min.
after 70 min.	=	450	cc/min.
CO flow			
after 10 min.	=	50	cc/min.
after 30 min.	=	60	cc/min.
after 70 min.	=	75	cc/min.
Total flow	=	350	cc/min.
after 10 min.	=	420	cc/min.
after 30 min.	=	455	cc/min.
after 70 min.	=	525	cc/min.
Feed velocity (u_o)	=	0.1792	m/s; Residence time (τ) = 3.347 s
after 10 min.	=	0.215	m/s; = 2.789 s
after 30 min.	=	0.233	m/s; = 2.575 s
after 70 min.	=	0.2688	m/s; = 2.232 s

Feed concentration (C_{Ao}) = 5.9×10^{-3} K mol/m^3

Feed concentration (C_{Bo}) = 7.441×10^{-3} K mol/m^3

Pressure gauge readings during run (psig)

= P.G1-3 : P.G2 - 2.

(RUN NUMBER 46)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.001658
.125	1.002492	1.002492	1.002492	1.002492	1.002492
.167	1.005830	1.005830	1.005830	1.005830	1.005830
.250	1.015844	1.015844	1.015844	1.015844	1.015844
.292	1.022520	1.023354	1.023354	1.023354	1.023354
.333	1.031699	1.031699	1.033368	1.033368	1.033368
.375	1.044217	1.045051	1.045886	1.046720	1.046720
.417	1.061741	1.062576	1.063410	1.065914	1.065914
.458	1.080935	1.083438	1.085107	1.090114	1.094287
.500	1.111811	1.113480	1.118487	1.136846	1.170226
.542	1.157708	1.161046	1.179405	1.231144	1.350476
.583	1.218626	1.226971	1.285386	1.422243	1.692814
.625	1.300407	1.323773	1.497347	1.780714	1.985571
.667	1.416401	1.513203	1.796540	2.009306	2.061543
.708	1.568280	1.773209	1.909163	2.029733	2.020749
.792	1.982294	2.075387	2.006852	1.974918	1.929749
.833	2.103849	2.153335	2.050132	1.985571	1.937151
.875	2.175193	2.190558	2.071316	1.992123	1.919049
.917	2.176002	2.177620	2.059098	1.978197	1.907515

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.002942	1.002942	1.002942	1.002942	1.002942
.167	1.006665	1.006665	1.006665	1.006665	1.006665
.250	1.015844	1.015844	1.015844	1.018347	1.022520
.292	1.023354	1.023354	1.026692	1.031699	1.041713
.333	1.032534	1.035872	1.026692	1.055900	1.082604
.375	1.050058	1.058403	1.076762	1.115983	1.186081
.417	1.080935	1.106804	1.158543	1.258682	1.439767
.458	1.134342	1.196095	1.323773	1.532396	1.871194
.500	1.266192	1.418905	1.727228	2.023200	2.263173
.542	1.580797	1.861269	2.184899	2.267200	2.218022
.583	1.992123	2.081083	2.180855	2.183281	2.119279
.625	2.075387	2.067245	2.085151	2.071316	2.024833
.667	2.046055	2.012576	1.997034	1.974098	1.940440
.708	1.988847	1.952764	1.927280	1.900095	1.872848
.792	1.911636	1.821480	1.828952	1.815666	1.789046
.833	1.895971	1.832270	1.826462	1.793210	1.764864
.875	1.884415	1.818158	1.789879	1.774877	1.745645
.917	1.866233	1.790712	1.787380	1.756512	1.728066

(RUN NUMBER 46)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000823	1.002492	1.004996
.125	1.002492	1.004161	1.004996	1.008334	1.015010
.167	1.008334	1.010003	1.014175	1.023354	1.041713
.250	1.030865	1.046720	1.077597	1.142687	1.276206
.292	1.061741	1.103466	1.185246	1.356318	1.669242
.333	1.136011	1.246999	1.456457	1.818158	2.129016
.375	1.333786	1.605832	2.007670	2.184899	2.192175
.417	1.769872	2.170338	2.242223	2.203487	2.137937
.458	2.178429	2.243835	2.191366	2.127394	2.059098
.500	2.230126	2.143612	2.081083	2.024833	1.968358
.542	2.141991	2.051763	1.989666	1.941262	1.895145
.583	2.050947	1.977377	1.919872	1.875327	1.835588
.625	1.970818	1.913283	1.865405	1.824802	1.789879
.667	1.900095	1.856303	1.818158	1.783214	1.751498
.708	1.840563	1.807354	1.776545	1.747318	1.719684
.792	1.763194	1.738115	1.715490	1.692814	1.670927
.833	1.738115	1.713812	1.691973	1.670927	1.650680
.875	1.718845	1.694495	1.673455	1.653213	1.633773
.917	1.701219	1.677667	1.657434	1.638003	1.619378

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.002492
.042	1.001658	1.005830	1.015844	1.036706	1.083438
.083	1.010837	1.025023	1.055065	1.120990	1.260351
.125	1.030030	1.068417	1.146860	1.316262	1.615140
.167	1.085107	1.193591	1.403050	1.770706	2.168719
.250	1.611748	2.098974	2.309837	2.309033	2.265589
.292	2.183281	2.276056	2.305014	2.243029	2.166291
.333	2.255118	2.210756	2.192175	2.142801	2.073758
.375	2.184090	2.120902	2.082711	2.041976	1.988028
.417	2.084338	2.024833	1.982294	1.945371	1.904218
.458	1.999489	1.946192	1.905042	1.871194	1.837247
.500	1.917402	1.872021	1.835588	1.804028	1.774877
.542	1.852991	1.813173	1.780714	1.751498	1.725552
.583	1.799868	1.764864	1.735604	1.708777	1.684402
.625	1.758183	1.727228	1.700379	1.675982	1.654057
.667	1.723038	1.696177	1.671770	1.648990	1.627849
.708	1.693655	1.669242	1.647301	1.627002	1.605832
.792	1.649835	1.629542	1.610052	1.591645	1.574121
.833	1.630388	1.611748	1.593314	1.575790	1.559935
.875	1.615140	1.595818	1.579962	1.564107	1.549086
.917	1.601659	1.584969	1.569949	1.555762	1.541576

APPENDIX C

TABLE (C.4)

DATA ON CARBON MONOXIDE OXIDATION
(RUN NO. 47)

Air flow	=	660	cc/min.
after 20 min.	=	750	cc/min.
CO flow	=	90.75	cc/min.
after 20 min.	=	103.1	cc/min.
Total flow	=	750.75	cc/min.
after 20 min.	=	853.1	cc/min.
Feed velocity (u_o)	=	0.385	m/s.
after 20 min.	=	0.437	m/s.
Residence time (τ)	=	1.5606	s.
after 20 min.	=	1.3733	s.

Feed concentration (C_{Ao}) = 5.08×10^{-3} K mol/m^3

Oxygen concentration (C_{Bo}) = 7.632×10^{-3} K mol/m^3

Pressure gauge readings during run (psig)

= P.G1-3 : P.G2 - 2.

(RUN NUMBER 47)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.000000	1.000000
.167	1.000000	1.000000	1.000000	1.000000	1.000000
.250	1.000000	1.000000	1.000000	1.000000	1.000000
.292	1.001658	1.001658	1.001658	1.001658	1.001658
.333	1.005830	1.006665	1.006665	1.006665	1.006665
.375	1.013341	1.013341	1.013341	1.013341	1.014175
.417	1.023354	1.023354	1.023354	1.023354	1.025858
.458	1.034203	1.034203	1.034203	1.036706	1.043382
.500	1.051727	1.051727	1.053396	1.061741	1.080935
.542	1.081769	1.080935	1.087611	1.118487	1.177736
.582	1.123494	1.124328	1.151032	1.246999	1.399712
.625	1.186915	1.193591	1.306248	1.540741	1.780714
.667	1.289558	1.331283	1.665026	1.936329	2.032183
.708	1.442271	1.610900	1.972458	2.068059	2.098974
.792	1.900920	2.142801	2.138748	2.111972	2.088405
.833	2.067245	2.252701	2.184899	2.124960	2.080270
.875	2.184090	2.315463	2.217215	2.135505	2.076200
.917	2.226899	2.309837	2.208333	2.123337	2.059913

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.000000	1.000000
.167	1.000000	1.000000	1.000000	1.000000	1.000000
.250	1.000000	1.000000	1.000000	1.000000	1.000000
.292	1.001658	1.001658	1.002492	1.003327	1.004996
.333	1.006665	1.007499	1.009168	1.011672	1.017513
.375	1.015010	1.017513	1.022520	1.032534	1.048389
.417	1.029196	1.037541	1.052562	1.080935	1.125163
.458	1.053396	1.075093	1.115149	1.187750	1.288724
.500	1.112645	1.177736	1.290393	1.476485	1.691973
.542	1.278710	1.464802	1.733092	1.974918	2.066430
.582	1.645611	1.935507	2.059913	2.135505	2.175193
.625	1.987209	2.100599	2.150095	2.161434	2.175193
.667	2.113596	2.149285	2.162243	2.146043	2.138748
.708	2.128205	2.130639	2.124148	2.100599	2.082711
.792	2.073758	2.051763	2.028100	2.001126	1.976557
.833	2.050947	2.021566	1.992123	1.963435	1.937151
.875	2.037080	1.999489	1.965076	1.933862	1.905042
.917	2.016663	1.974918	1.938795	1.905042	1.875327

(RUN NUMBER 47)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.000000	1.000000
.167	1.000000	1.000000	1.000000	1.000000	1.000000
.250	1.000000	1.002492	1.005830	1.010837	1.020016
.292	1.008334	1.014175	1.022520	1.036706	1.060907
.333	1.026692	1.040879	1.063410	1.100128	1.169391
.375	1.073424	1.113480	1.173564	1.278710	1.465637
.417	1.195260	1.297903	1.452285	1.700379	1.978197
.458	1.448947	1.653213	1.886892	2.030550	2.119279
.500	1.945371	2.049317	2.103849	2.124148	2.122525
.542	2.124960	2.159005	2.158195	2.136316	2.096535
.582	2.168719	2.167101	2.147664	2.113596	2.063987
.625	2.153335	2.133883	2.108723	2.074573	2.026467
.667	2.114408	2.087591	2.060728	2.028100	1.986390
.708	2.057468	2.031366	2.005216	1.976557	1.941262
.792	1.951943	1.928103	1.905042	1.881111	1.855475
.833	1.910812	1.887718	1.863751	1.841392	1.818158
.875	1.877806	1.853819	1.830611	1.808186	1.786547
.917	1.848022	1.823141	1.800700	1.779046	1.758183

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.000000	1.000000	1.000000	1.000000	1.000000
.042	1.000000	1.000000	1.000000	1.000000	1.000000
.083	1.000000	1.000000	1.000000	1.000000	1.000000
.125	1.000000	1.000000	1.000000	1.001658	1.007499
.167	1.000000	1.003327	1.009168	1.017513	1.030865
.250	1.035872	1.059238	1.095956	1.151032	1.237820
.292	1.101797	1.161046	1.253675	1.386360	1.580797
.333	1.271199	1.413898	1.609204	1.829781	1.995397
.375	1.681035	1.898445	2.026467	2.100599	2.140370
.417	2.085151	2.137937	2.167101	2.177620	2.168719
.458	2.171956	2.184090	2.178429	2.163863	2.137127
.500	2.139559	2.137937	2.121714	2.100599	2.072130
.542	2.083524	2.072130	2.052578	2.030550	2.004398
.582	2.032183	2.010123	1.988028	1.965076	1.941262
.625	1.988847	1.960153	1.935507	1.912459	1.889369
.667	1.948657	1.918225	1.891845	1.867887	1.845536
.708	1.907515	1.877806	1.851335	1.828122	1.806523
.792	1.830611	1.805691	1.781547	1.760689	1.739789
.833	1.795707	1.773209	1.751498	1.730579	1.711295
.875	1.764864	1.744809	1.723876	1.705418	1.686926
.917	1.738952	1.719684	1.701219	1.683560	1.666713

APPENDIX C

TABLE (C.5)

DATA ON CARBON MONOXIDE OXIDATION
(RUN NO. 49)

Air flow	=	910	cc/min.
after 60 min.	=	1080	cc/min.
after 120 min.	=	1160	cc/min.
after 180 min.	=	1330	cc/min.
after 240 min.	=	1160	cc/min.
CO flow	=	91	cc/min.
after 60 min.	=	108	cc/min.
after 120 min.	=	116	cc/min.
after 180 min.	=	133	cc/min.
after 240 min.	=	116	cc/min.
Total flow	=	1001	cc/min.
after 60 min.	=	1188	cc/min.
after 120 min.	=	1276	cc/min.
after 180 min.	=	1463	cc/min.
after 240 min.	=	1276	cc/min.

Feed velocity (u_o) = 0.5126 m/s; Residence time (τ) = 1.17 s

after 60 min. = 0.6084 m/s; = 0.9862s

after 120 min. = 0.6535 m/s; = 0.9182s

after 180 min. = 0.7492 m/s; = 0.8008s

after 240 min. = 0.6535 m/s; = 0.9182s

Feed concentration (C_{Ao}) = 3.758×10^{-3} K mol/m^3

Oxygen concentration (C_{Bo}) = 7.892×10^{-3} K mol/m^3

Pressure gauge readings during run (psig)

= P.G1 - 3 : P.G2 - 2.

(RUN NUMBER 49)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.006665	1.006665	1.006665	1.007499	1.007499
.042	1.006665	1.006665	1.007499	1.007499	1.007499
.083	1.007499	1.007499	1.007499	1.007499	1.007499
.125	1.008334	1.008334	1.008334	1.008334	1.008334
.167	1.009168	1.009168	1.009168	1.009168	1.009168
.250	1.011672	1.011672	1.011672	1.011672	1.011672
.292	1.013341	1.013341	1.013341	1.013341	1.013341
.333	1.015844	1.015010	1.015844	1.015010	1.015010
.375	1.018347	1.018347	1.018347	1.018347	1.018347
.417	1.022520	1.022520	1.022520	1.022520	1.023354
.458	1.028361	1.028361	1.028361	1.028361	1.029196
.500	1.037541	1.037541	1.037541	1.039210	1.043382
.542	1.053396	1.053396	1.054231	1.060907	1.075928
.583	1.078431	1.078431	1.085107	1.109307	1.152701
.625	1.120156	1.121825	1.153536	1.231144	1.351311
.667	1.194426	1.206109	1.335455	1.537403	1.762359
.708	1.322104	1.393870	1.711295	1.957690	2.073758
.792	1.738115	2.003580	2.187324	2.238191	2.262368
.833	1.903393	2.107099	2.213178	2.235772	2.240610
.875	2.037080	2.199448	2.226092	2.221250	2.208333
.917	2.106287	2.253506	2.231739	2.201064	2.172766

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.007499	1.007499	1.007499	1.008334	1.008334
.042	1.007499	1.007499	1.008334	1.008334	1.008334
.083	1.008334	1.008334	1.008334	1.008334	1.008334
.125	1.008334	1.008334	1.009168	1.009168	1.009168
.167	1.009168	1.010003	1.009168	1.010003	1.010003
.250	1.011672	1.011672	1.011672	1.011672	1.011672
.292	1.013341	1.013341	1.013341	1.013341	1.013341
.333	1.015010	1.015844	1.015844	1.015844	1.016679
.375	1.018347	1.019182	1.020016	1.021685	1.023354
.417	1.024189	1.025858	1.027527	1.030865	1.035872
.458	1.032534	1.035872	1.041713	1.050058	1.062576
.500	1.050893	1.061741	1.077597	1.101797	1.136011
.542	1.099293	1.132673	1.179405	1.248668	1.344635
.583	1.218626	1.303745	1.422243	1.577459	1.768203
.625	1.504023	1.660809	1.823971	1.955227	2.054208
.667	1.939618	2.038712	2.110348	2.167101	2.209141
.708	2.158195	2.214793	2.246253	2.262368	2.271226
.792	2.267200	2.272836	2.267200	2.252701	2.234159
.833	2.232546	2.224478	2.212371	2.194599	2.174384
.875	2.190558	2.173575	2.156575	2.137127	2.116032
.917	2.146854	2.124148	2.102224	2.081083	2.059098

(RUN NUMBER 49)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.008334	1.008334	1.008334	1.008334	1.008334
.042	1.008334	1.008334	1.008334	1.008334	1.008334
.083	1.008334	1.009168	1.008334	1.009168	1.009168
.125	1.009168	1.009168	1.009168	1.009168	1.009168
.167	1.010003	1.010003	1.010003	1.010003	1.010003
.250	1.011672	1.011672	1.012506	1.012506	1.012506
.292	1.014175	1.014175	1.015010	1.015844	1.016679
.333	1.017513	1.019182	1.020851	1.022520	1.025023
.375	1.025858	1.029196	1.034203	1.038375	1.045886
.417	1.043382	1.053396	1.066748	1.080935	1.105135
.458	1.080100	1.103466	1.136011	1.177736	1.245330
.500	1.183577	1.244496	1.332118	1.462299	1.632927
.542	1.466471	1.602494	1.790712	1.978197	2.079456
.583	1.919049	2.006034	2.078642	2.189750	2.289735
.625	2.129828	2.181664	2.210756	2.280080	2.269243
.667	2.243029	2.272031	2.278470	2.318677	2.379666
.708	2.275251	2.283299	2.276056	2.300190	2.334740
.792	2.213178	2.197024	2.179238	2.588133	2.194599
.833	2.152525	2.133072	2.113596	2.116844	2.120091
.875	2.093283	2.072944	2.052578	2.052578	2.051763
.917	2.037080	2.015846	1.996216	1.994579	1.991304

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.008334	1.009168	1.009168	1.009168	1.009168
.042	1.008334	1.009168	1.009168	1.009168	1.009168
.083	1.009168	1.009168	1.009168	1.010003	1.010003
.125	1.010003	1.010003	1.010003	1.010003	1.010837
.167	1.010003	1.010837	1.010837	1.011672	1.011672
.250	1.013341	1.014175	1.015844	1.017513	1.020851
.292	1.017513	1.020016	1.024189	1.029196	1.037541
.333	1.028361	1.035872	1.045886	1.060072	1.085942
.375	1.059238	1.081769	1.110976	1.157708	1.240323
.417	1.146860	1.217792	1.300407	1.437264	1.663340
.458	1.362994	1.524051	1.704579	1.917402	2.071316
.500	1.906691	2.037896	2.116032	2.192983	2.257535
.542	2.180855	2.271226	2.328316	2.359619	2.374054
.583	2.335543	2.384475	2.424521	2.430924	2.416516
.625	2.397295	2.412513	2.433325	2.429324	2.404505
.667	2.396494	2.394091	2.398898	2.388482	2.362827
.708	2.341965	2.333937	2.329119	2.317070	2.295366
.792	2.190558	2.180046	2.170338	2.157385	2.141991
.833	2.113596	2.103849	2.094097	2.081897	2.068873
.875	2.044423	2.034632	2.024833	2.013394	2.001126
.917	1.983113	1.973278	1.962615	1.951943	1.941262

(RUN NUMBER 49)

DISTANCE Z	time=100 Φ	time=105 Φ	time=110 Φ	time=115 Φ	time=120 Φ
.000	1.010003	1.010003	1.010003	1.010003	1.010003
.042	1.010003	1.010003	1.010003	1.010003	1.010837
.083	1.010003	1.010837	1.010837	1.010837	1.011672
.125	1.010837	1.011672	1.011672	1.013341	1.014175
.167	1.012506	1.014175	1.015844	1.017513	1.020851
.250	1.025858	1.035037	1.046720	1.062576	1.085942
.292	1.052562	1.076762	1.108473	1.152701	1.219461
.333	1.131839	1.202771	1.285386	1.405553	1.559100
.375	1.388029	1.559935	1.740626	1.914931	2.035448
.417	1.951943	2.079456	2.165482	2.238191	2.305818
.458	2.197832	2.294561	2.360421	2.403704	2.437326
.500	2.308230	2.374856	2.426923	2.451725	2.461322
.542	2.369243	2.389283	2.414915	2.424521	2.422120
.583	2.382872	2.366837	2.367639	2.363629	2.353201
.625	2.362827	2.330725	2.313855	2.299386	2.284908
.667	2.322693	2.285713	2.259951	2.238998	2.220443
.708	2.261562	2.226899	2.198640	2.175193	2.154955
.792	2.120902	2.096535	2.073758	2.051763	2.031366
.833	2.050947	2.032183	2.011758	1.992123	1.973278
.875	1.986390	1.970818	1.953585	1.936329	1.919049
.917	1.928103	1.914931	1.900095	1.884415	1.869541

DISTANCE Z	time=125 Φ	time=130 Φ	time=135 Φ	time=140 Φ	time=145 Φ
.000	1.010003	1.010837	1.010837	1.010837	1.011672
.042	1.010837	1.010837	1.011672	1.012506	1.014175
.083	1.012506	1.013341	1.014175	1.016679	1.020851
.125	1.015844	1.017513	1.020851	1.027527	1.040044
.167	1.024189	1.030030	1.040879	1.060907	1.100962
.250	1.115149	1.173564	1.273703	1.485665	1.779880
.292	1.308752	1.478989	1.727228	2.036264	2.200256
.333	1.769037	1.998671	2.165482	2.296974	2.406907
.375	2.169750	2.330725	2.444526	2.498087	2.541207
.417	2.431725	2.535620	2.599448	2.599448	2.589080
.458	2.530031	2.591473	2.615397	2.595461	2.565148
.500	2.520450	2.545996	2.549987	2.527636	2.496489
.542	2.455724	2.466119	2.461322	2.442926	2.416516
.583	2.370045	2.373252	2.366035	2.350794	2.329119
.625	2.290540	2.288931	2.279275	2.265589	2.248671
.667	2.219636	2.214793	2.204295	2.190558	2.176002
.708	2.150095	2.142801	2.132261	2.118467	2.105474
.792	2.023200	2.013394	2.001944	1.990485	1.978197
.833	1.964256	1.954406	1.943727	1.932217	1.922342
.875	1.909988	1.900920	1.891019	1.880285	1.870367
.917	1.861269	1.852991	1.843050	1.833929	1.824802

(RUN NUMBER 49)

DISTANCE Z	time=150 Φ	time=155 Φ	time=160 Φ	time=165 Φ	time=170 Φ
.000	1.011672	1.012506	1.012506	1.013341	1.014175
.042	1.015844	1.019182	1.023354	1.029196	1.040044
.083	1.027527	1.036706	1.049224	1.070086	1.104300
.125	1.059238	1.084273	1.120156	1.182743	1.282882
.167	1.156039	1.228640	1.331283	1.501520	1.728904
.250	1.971638	2.077828	2.180855	2.278470	2.350794
.292	2.294561	2.367639	2.422921	2.470116	2.498886
.333	2.483704	2.539611	2.565148	2.570733	2.567542
.375	2.587485	2.620181	2.628154	2.612207	2.590675
.417	2.599448	2.611410	2.610613	2.587485	2.558765
.458	2.555573	2.553977	2.547592	2.525241	2.497288
.500	2.476511	2.465320	2.454924	2.435726	2.411712
.542	2.393290	2.378864	2.366035	2.349189	2.329119
.583	2.307426	2.290540	2.276861	2.262368	2.245447
.625	2.229319	2.213118	2.198640	2.184899	2.171147
.667	2.159005	2.143612	2.129828	2.116844	2.103849
.708	2.091657	2.077014	2.063987	2.051763	2.039528
.792	1.967537	1.956048	1.944549	1.933862	1.923165
.833	1.911636	1.900920	1.891019	1.880285	1.871194
.875	1.860441	1.851335	1.841392	1.832270	1.823141
.917	1.815666	1.806523	1.798204	1.789879	1.781547

DISTANCE Z	time=175 Φ	time=180 Φ	time=185 Φ	time=190 Φ	time=195 Φ
.000	1.015844	1.018347	1.020851	1.024189	1.027527
.042	1.055065	1.072590	1.083438	1.103466	1.136846
.083	1.151032	1.200267	1.238654	1.300407	1.414732
.125	1.396374	1.501520	1.598321	1.708777	1.835588
.167	1.885241	1.969998	2.032999	2.096535	2.150905
.250	2.432525	2.496489	2.573924	2.629748	2.647286
.292	2.545996	2.599448	2.685544	2.735750	2.746110
.333	2.577913	2.605828	2.680762	2.730171	2.746110
.375	2.576317	2.582699	2.645692	2.694310	2.716624
.417	2.534023	2.523644	2.571531	2.615397	2.640112
.458	2.470116	2.453325	2.489298	2.525241	2.549987
.500	2.386879	2.368441	2.394892	2.421320	2.442926
.542	2.308230	2.289735	2.307426	2.327513	2.345176
.583	2.227706	2.210756	2.222057	2.237385	2.251895
.625	2.155765	2.140370	2.148474	2.159005	2.170338
.667	2.090031	2.077014	2.083524	2.091657	2.099786
.708	2.028100	2.015846	2.020749	2.027284	2.032999
.792	1.913283	1.903393	1.907515	1.911636	1.914107
.833	1.861269	1.852163	1.856303	1.858786	1.860441
.875	1.814835	1.805691	1.809017	1.811511	1.812342
.917	1.773209	1.765699	1.768203	1.769872	1.771541

(RUN NUMBER 49)

DISTANCE Z	time=200 Φ	time=205 Φ	time=210 Φ	time=215 Φ	time=220 Φ
.000	1.034203	1.047555	1.063410	1.078431	1.090114
.042	1.252006	1.362159	1.415567	1.451450	1.467306
.083	1.760689	1.909163	1.935507	1.943727	1.943727
.125	2.090844	2.198640	2.249477	2.272836	2.284104
.167	2.255118	2.371649	2.460522	2.519652	2.553179
.250	2.583497	2.605828	2.669604	2.732562	2.781177
.292	2.672792	2.650475	2.676777	2.718218	2.762049
.333	2.691919	2.648880	2.648083	2.668807	2.702280
.375	2.681559	2.636923	2.619383	2.623370	2.644895
.417	2.624167	2.589080	2.565148	2.558765	2.569137
.458	2.545198	2.521249	2.498886	2.487700	2.490097
.500	2.445326	2.432525	2.415716	2.404505	2.402903
.542	2.351596	2.346781	2.336346	2.325906	2.321890
.583	2.259951	2.259951	2.254312	2.246253	2.242223
.625	2.177620	2.180855	2.177620	2.173575	2.168719
.667	2.106287	2.109536	2.109536	2.107099	2.103849
.708	2.037896	2.041160	2.042792	2.041160	2.039528
.792	1.916578	1.918225	1.919872	1.920695	1.919872
.833	1.862096	1.863751	1.865405	1.865405	1.865405
.875	1.813173	1.814004	1.815666	1.816497	1.815666
.917	1.771541	1.771541	1.772375	1.773209	1.773209

DISTANCE Z	time=225 Φ	time=230 Φ	time=235 Φ	time=240 Φ	time=245 Φ
.000	1.098459	1.103466	1.105969	1.106804	1.109307
.042	1.468975	1.463968	1.454788	1.441436	1.445609
.083	1.933039	1.914931	1.892670	1.866233	1.850786
.125	2.283299	2.269616	2.247865	2.220443	2.194599
.167	2.568340	2.566744	2.553179	2.532426	2.498087
.250	2.818643	2.845754	2.864896	2.877660	2.837779
.292	2.802699	2.836982	2.866492	2.890427	2.855325
.333	2.739734	2.777989	2.813062	2.844159	2.816251
.375	2.676777	2.713436	2.751688	2.787554	2.763643
.417	2.592271	2.624167	2.660040	2.695904	2.675980
.458	2.506075	2.531628	2.563552	2.597853	2.580306
.500	2.412513	2.430924	2.456524	2.485303	2.469317
.542	2.326710	2.339557	2.358817	2.382070	2.368441
.583	2.243835	2.251089	2.265589	2.284104	2.273641
.625	2.169529	2.173575	2.183281	2.197832	2.188941
.667	2.103037	2.105474	2.111972	2.122525	2.112784
.708	2.037896	2.039528	2.044423	2.051763	2.041160
.792	1.919049	1.919872	1.921519	1.924811	1.913283
.833	1.865405	1.865405	1.866233	1.868714	1.857131
.875	1.815666	1.815666	1.816497	1.817328	1.807354
.917	1.773209	1.773209	1.773209	1.774043	1.764029

APPENDIX C

TABLE (C.6)

DATA ON CARBON MONOXIDE OXIDATION

(RUN NO. 50)

Air flow	=	1074	cc/min.
after 60 min.	=	1501	cc/min.
after 100 min.	=	1653	cc/min.
after 130 min.	=	1976	cc/min.
after 180 min.	=	1653	cc/min.
CO flow	=	113	cc/min.
after 60 min.	=	158	cc/min.
after 100 min.	=	174	cc/min.
after 130 min.	=	208	cc/min.
after 180 min.	=	174	cc/min.
Total flow	=	1187	cc/min.
after 60 min.	=	1659	cc/min.
after 100 min.	=	1827	cc/min.
after 130 min.	=	2184	cc/min.
after 180 min.	=	1827	cc/min.

Feed velocity (u_o) = 0.6079 m/s; Residence time (τ) = 0.9870

after 60 min. = 0.8496 m/s: = 0.7062

after 100 min. = 0.9356 m/s; = 0.6413

after 130 min. = 1.1195 m/s; = 0.5364

after 180 min. = 0.9356 m/s; = 0.6413

Feed Concentration (C_{Ao}) = 3.937×10^{-3} K mol/m^3

Oxygen concentration (C_{Ao}) = 7.855×10^{-3} K mol/m^3

Pressure gauge readings during runs (psig)

= P.G1 - 3 : P.G2 -2.

(RUN NUMBER 50)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.010837	1.010837	1.010837	1.010837	1.010837
.042	1.011672	1.011672	1.011672	1.011672	1.011672
.083	1.011672	1.011672	1.011672	1.012506	1.012506
.125	1.012506	1.012506	1.013341	1.013341	1.013341
.167	1.013341	1.013341	1.014175	1.014175	1.014175
.250	1.015010	1.015010	1.015010	1.015010	1.015844
.292	1.016679	1.016679	1.016679	1.016679	1.016679
.333	1.019182	1.019182	1.019182	1.019182	1.019182
.375	1.021685	1.022520	1.022520	1.022520	1.022520
.417	1.025858	1.026692	1.026692	1.027527	1.027527
.458	1.031699	1.032534	1.032534	1.033368	1.034203
.500	1.040879	1.040879	1.041713	1.043382	1.047555
.542	1.055065	1.055900	1.057569	1.064245	1.079266
.583	1.076431	1.080100	1.085942	1.109307	1.153536
.625	1.116818	1.120156	1.147694	1.222799	1.347973
.667	1.185246	1.199433	1.308752	1.516541	1.766534
.708	1.303745	1.373008	1.667556	1.951121	2.101412
.792	1.697017	2.025650	2.223671	2.272836	2.303406
.833	1.857958	2.135505	2.261562	2.283299	2.285713
.875	1.991304	2.229319	2.277666	2.273641	2.255118
.917	2.063172	2.289735	2.284104	2.253506	2.220443

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.011672	1.011672	1.011672	1.011672	1.011672
.042	1.011672	1.011672	1.011672	1.011672	1.011672
.083	1.012506	1.012506	1.012506	1.012506	1.012506
.125	1.013341	1.013341	1.013341	1.013341	1.013341
.167	1.014175	1.014175	1.014175	1.014175	1.014175
.250	1.015844	1.015844	1.015844	1.015844	1.015844
.292	1.017513	1.017513	1.017513	1.017513	1.018347
.333	1.020016	1.020016	1.020851	1.020851	1.021685
.375	1.023354	1.024189	1.025023	1.026692	1.028361
.417	1.029196	1.030865	1.033368	1.037541	1.044217
.458	1.036706	1.041713	1.048389	1.058403	1.075928
.500	1.055065	1.067583	1.085942	1.116818	1.165219
.542	1.103466	1.139349	1.196095	1.286220	1.420574
.583	1.222799	1.317931	1.461464	1.666713	1.906691
.625	1.510699	1.690291	1.886892	2.041976	2.154955
.667	1.962615	2.077828	2.164672	2.231739	2.279275
.708	2.197832	2.261562	2.294561	2.311445	2.317873
.792	2.313855	2.320283	2.309837	2.288126	2.260757
.833	2.278470	2.269616	2.253506	2.229319	2.201064
.875	2.234965	2.216408	2.195407	2.170338	2.141991
.917	2.190558	2.164672	2.139559	2.113596	2.085151

(RUN NUMBER 50)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.011672	1.011672	1.011672	1.012506	1.012506
.042	1.011672	1.012506	1.012506	1.012506	1.012506
.083	1.012506	1.012506	1.013341	1.013341	1.013341
.125	1.013341	1.013341	1.013341	1.013341	1.014175
.167	1.014175	1.014175	1.015010	1.015010	1.015010
.250	1.016679	1.016679	1.016679	1.016679	1.017513
.292	1.018347	1.019182	1.020851	1.020851	1.021685
.333	1.023354	1.025023	1.027527	1.029196	1.030865
.375	1.031699	1.037541	1.045886	1.049224	1.059238
.417	1.054231	1.068417	1.092618	1.106804	1.149363
.458	1.100962	1.136011	1.198598	1.246165	1.390532
.500	1.232813	1.328780	1.494009	1.663340	2.013394
.542	1.581631	1.803196	2.021566	2.162243	2.315463
.583	2.040344	2.133072	2.218829	2.370847	2.482905
.625	2.231739	2.274446	2.296974	2.442926	2.539611
.667	2.319480	2.336346	2.322693	2.444526	2.526039
.708	2.325906	2.325103	2.299386	2.392488	2.456524
.792	2.238191	2.218022	2.189750	2.240610	2.273641
.833	2.175193	2.152525	2.125771	2.159814	2.184090
.875	2.116032	2.091657	2.065616	2.089218	2.106287
.917	2.059098	2.034632	2.010123	2.028917	2.039528

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.012506	1.012506	1.012506	1.012506	1.012506
.042	1.012506	1.012506	1.013341	1.013341	1.013341
.083	1.013341	1.013341	1.013341	1.014175	1.014175
.125	1.014175	1.014175	1.014175	1.014175	1.015010
.167	1.015010	1.015010	1.015844	1.015844	1.017513
.250	1.018347	1.019182	1.021685	1.026692	1.038375
.292	1.023354	1.027527	1.034203	1.051727	1.088445
.333	1.038375	1.050058	1.075093	1.136848	1.251172
.375	1.085107	1.125997	1.218626	1.444774	1.742299
.417	1.241158	1.376346	1.675982	2.136316	2.313052
.458	1.618531	1.923988	2.178429	2.383673	2.528435
.500	2.180046	2.292148	2.396494	2.474913	2.577115
.542	2.446126	2.518853	2.539611	2.522846	2.555573
.583	2.566744	2.609018	2.588283	2.529233	2.508471
.625	2.585092	2.606625	2.577913	2.510867	2.462921
.667	2.553179	2.565148	2.539611	2.478110	2.422921
.708	2.476511	2.484503	2.467718	2.419719	2.368441
.792	2.286517	2.292953	2.288126	2.266395	2.234965
.833	2.195407	2.201064	2.199448	2.188516	2.164672
.875	2.114408	2.119279	2.118467	2.110348	2.094909
.917	2.045239	2.047686	2.047686	2.041160	2.029733

(RUN NUMBER 50)

DISTANCE Z	time=100 Φ	time=105 Φ	time=110 Φ	time=115 Φ	time=120 Φ
.000	1.012506	1.013341	1.013341	1.013341	1.013341
.042	1.013341	1.013341	1.014175	1.014175	1.014175
.083	1.014175	1.014175	1.015010	1.015844	1.017513
.125	1.015844	1.016679	1.017513	1.020851	1.025858
.167	1.019182	1.021685	1.026692	1.035872	1.056734
.250	1.057569	1.090114	1.146860	1.257847	1.532396
.292	1.151032	1.262020	1.432257	1.745645	2.137127
.333	1.440602	1.732254	2.004398	2.214793	2.375657
.375	2.064801	2.274446	2.385276	2.477311	2.531628
.417	2.426122	2.559563	2.593068	2.606625	2.598651
.458	2.595461	2.658445	2.652069	2.635329	2.603436
.500	2.619383	2.657648	2.648880	2.618586	2.573924
.542	2.577115	2.611410	2.616194	2.588283	2.539611
.583	2.506874	2.530830	2.543602	2.526039	2.483704
.625	2.441326	2.451725	2.464520	2.454924	2.422921
.667	2.386879	2.386078	2.394091	2.388482	2.363629
.708	2.327513	2.319480	2.321087	2.317873	2.298582
.792	2.202679	2.189750	2.184090	2.178429	2.166291
.833	2.137937	2.125771	2.118467	2.112784	2.103037
.875	2.074573	2.064801	2.057468	2.050947	2.042792
.917	2.014211	2.006852	2.000308	1.993760	1.986390

DISTANCE Z	time=125 Φ	time=130 Φ	time=135 Φ	time=140 Φ	time=145 Φ
.000	1.013341	1.014175	1.014175	1.014175	1.015010
.042	1.015844	1.017513	1.018347	1.020851	1.025023
.083	1.020851	1.026692	1.030865	1.040044	1.057569
.125	1.038375	1.057569	1.072590	1.110976	1.177736
.167	1.100128	1.162715	1.229475	1.374677	1.571617
.250	1.877806	2.055838	2.186516	2.299386	2.386879
.292	2.291344	2.370847	2.469317	2.535620	2.595461
.333	2.493293	2.551583	2.632140	2.663228	2.699889
.375	2.599448	2.641706	2.725390	2.750095	2.770816
.417	2.616991	2.648083	2.748501	2.777192	2.782771
.458	2.591473	2.607423	2.710249	2.753282	2.756470
.500	2.542804	2.541207	2.633734	2.684747	2.695904
.542	2.498087	2.482106	2.555573	2.609815	2.628951
.583	2.442126	2.416516	2.468518	2.520450	2.545996
.625	2.384475	2.355608	2.390886	2.434925	2.462921
.667	2.330725	2.301798	2.326710	2.362827	2.390084
.708	2.271226	2.244641	2.263979	2.292148	2.315463
.792	2.149285	2.130639	2.142801	2.160624	2.176811
.833	2.089218	2.073758	2.085151	2.098161	2.111972
.875	2.031366	2.018298	2.028917	2.040344	2.050947
.917	1.977377	1.965897	1.977377	1.987209	1.996216

(RUN NUMBER 50)

DISTANCE Z	time=150 Φ	time=155 Φ	time=160 Φ	time=165 Φ	time=170 Φ
.000	1.015844	1.016679	1.017513	1.019182	1.020016
.042	1.032534	1.040044	1.045886	1.050893	1.056734
.083	1.083438	1.107638	1.125163	1.141853	1.156874
.125	1.266192	1.327945	1.369670	1.405553	1.438098
.167	1.751498	1.810680	1.828952	1.840563	1.849678
.250	2.466919	2.514062	2.526039	2.524443	2.518055
.292	2.656054	2.719015	2.751688	2.762846	2.765237
.333	2.739734	2.799510	2.837779	2.852134	2.861706
.375	2.793133	2.840172	2.875267	2.892023	2.909582
.417	2.788351	2.819440	2.855325	2.873671	2.889629
.458	2.755673	2.775598	2.808279	2.828211	2.840969
.500	2.695904	2.709452	2.740531	2.765237	2.777192
.542	2.633734	2.644098	2.672792	2.703076	2.719015
.583	2.554775	2.565148	2.590675	2.624167	2.647286
.625	2.475712	2.486901	2.509270	2.542005	2.570733
.667	2.404505	2.416516	2.436526	2.467718	2.498087
.708	2.330725	2.343571	2.361223	2.389283	2.418918
.792	2.189750	2.201064	2.215600	2.236578	2.261562
.833	2.123337	2.134694	2.146854	2.164672	2.185707
.875	2.061543	2.071316	2.082711	2.097348	2.116032
.917	2.006034	2.015028	2.024833	2.037896	2.053393

DISTANCE Z	time=175 Φ	time=180 Φ	time=185 Φ	time=190 Φ	time=195 Φ
.000	1.021685	1.022520	1.023354	1.024189	1.026692
.042	1.061741	1.066748	1.070086	1.072590	1.085107
.083	1.171060	1.182743	1.190253	1.193591	1.222799
.125	1.464802	1.483996	1.493175	1.493175	1.524886
.167	1.856303	1.857958	1.854647	1.846365	1.874501
.250	2.511666	2.503679	2.494092	2.482905	2.496489
.292	2.764440	2.762846	2.761252	2.758064	2.757267
.333	2.870480	2.879256	2.888831	2.896811	2.884841
.375	2.928743	2.947911	2.967887	2.986272	2.958297
.417	2.907985	2.928743	2.951107	2.975080	2.938326
.458	2.853729	2.869682	2.888033	2.908784	2.870480
.500	2.786757	2.797916	2.809873	2.825021	2.784365
.542	2.729375	2.738938	2.748501	2.758861	2.718218
.583	2.661634	2.671995	2.681559	2.691122	2.652866
.625	2.589080	2.602638	2.613802	2.623370	2.587485
.667	2.520450	2.538014	2.550785	2.561957	2.526039
.708	2.443726	2.463720	2.479708	2.491695	2.458923
.792	2.285713	2.307426	2.327513	2.343571	2.317070
.833	2.208333	2.229319	2.249477	2.266395	2.244641
.875	2.135505	2.155765	2.174384	2.191366	2.172766
.917	2.071316	2.089218	2.106287	2.123337	2.105474

(RUN NUMBER 50)

DISTANCE Z	time=200 Φ	time=205 Φ	time=210 Φ	time=215 Φ	time=220 Φ
.000	1.028361	1.030030	1.031699	1.033368	1.034203
.042	1.093452	1.100128	1.105135	1.110142	1.115149
.083	1.240323	1.254510	1.267027	1.278710	1.288724
.125	1.553259	1.575790	1.594149	1.611748	1.626155
.167	1.895971	1.913283	1.928103	1.940440	1.951121
.250	2.511666	2.526838	2.542005	2.556371	2.570733
.292	2.764440	2.774004	2.785959	2.798713	2.810671
.333	2.881650	2.884841	2.891225	2.899205	2.907187
.375	2.946314	2.944716	2.947113	2.951906	2.957498
.417	2.920758	2.915170	2.915968	2.919162	2.923154
.458	2.848147	2.840172	2.838577	2.840969	2.845754
.500	2.758861	2.747704	2.742922	2.743719	2.746110
.542	2.689529	2.673589	2.665619	2.662431	2.662431
.583	2.621775	2.602638	2.591473	2.584294	2.581901
.625	2.555573	2.534821	2.520450	2.511666	2.506075
.667	2.495690	2.473314	2.457324	2.446126	2.438126
.708	2.430124	2.408509	2.391687	2.378864	2.370045
.792	2.293757	2.275251	2.259951	2.247059	2.235772
.833	2.223671	2.207526	2.192983	2.180855	2.170338
.875	2.154955	2.140370	2.127394	2.116032	2.107099
.917	2.090031	2.077014	2.065616	2.055838	2.046055

DISTANCE Z	time=225 Φ	time=230 Φ	time=235 Φ	time=240 Φ	time=245 Φ
.000	1.035872	1.036706	1.038375	1.039210	1.040044
.042	1.120156	1.124328	1.128501	1.135177	1.145191
.083	1.298738	1.309586	1.320435	1.337124	1.373008
.125	1.638848	1.650680	1.665026	1.684402	1.721361
.167	1.960153	1.967537	1.975738	1.984752	1.998671
.250	2.582699	2.593068	2.601043	2.605031	2.601043
.292	2.821832	2.830603	2.837779	2.840172	2.833792
.333	2.915170	2.921557	2.927944	2.930340	2.925549
.375	2.963092	2.968686	2.974281	2.977478	2.975080
.417	2.928743	2.934333	2.939125	2.943119	2.943119
.458	2.850539	2.856122	2.861706	2.867289	2.868885
.500	2.750095	2.755673	2.761252	2.766831	2.770816
.542	2.664025	2.668010	2.671995	2.676777	2.679965
.583	2.581104	2.582699	2.585092	2.588283	2.592271
.625	2.502880	2.502880	2.502880	2.505276	2.507672
.667	2.433325	2.430924	2.430124	2.430924	2.431725
.708	2.363629	2.359619	2.357212	2.356410	2.356410
.792	2.228512	2.222057	2.217215	2.214793	2.212371
.833	2.162243	2.155765	2.150095	2.146854	2.143612
.875	2.098161	2.091657	2.085965	2.081897	2.078642
.917	2.038712	2.031366	2.026467	2.021566	2.017480

APPENDIX C

TABLE (C.7)

DATA ON CARBON MONOXIDE OXIDATION (RUN NO. 52)

Air flow	=	1120	cc/min.
after 20 min.	=	1920	cc/min.
after 40 min.	=	2240	cc/min.
after 80 min.	=	2480	cc/min.
CO flow	=	154	cc/min.
after 20 min.	=	264	cc/min.
after 40 min.	=	308	cc/min.
after 80 min.	=	341	cc/min.
Total flow	=	1274	cc/min.
after 20 min.	=	2184	cc/min.
after 40 min.	=	2548	cc/min.
after 80 min.	=	2821	cc/min.

Feed velocity (u_o) = 0.65245 m/s: Residence time (τ) = 0.9196s
= 1.1185 m/s: = 0.5364s
= 1.3049 m/s: = 0.4598s
= 1.4447 m/s: = 0.4153s

Feed concentration (C_{Ao}) = 5.08×10^{-3} K mol/m^3

Oxygen concentration (C_{Bo}) = 7.632×10^{-3} K mol/m^3

Pressure gauge reading during run
= P.G1 - 3 : P.G2 - 2.

(RUN NUMBER 52)

DISTANCE z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.010837	1.011672	1.011672	1.011672	1.011672
.042	1.012506	1.012506	1.012506	1.012506	1.012506
.083	1.014175	1.014175	1.014175	1.014175	1.014175
.125	1.016679	1.015844	1.015844	1.015844	1.015844
.167	1.018347	1.018347	1.018347	1.018347	1.018347
.250	1.021685	1.021685	1.021685	1.021685	1.021685
.292	1.025023	1.025023	1.025023	1.024189	1.024189
.333	1.028361	1.028361	1.028361	1.028361	1.028361
.375	1.033368	1.033368	1.032534	1.032534	1.032534
.417	1.039210	1.039210	1.039210	1.039210	1.039210
.458	1.045051	1.045051	1.045051	1.045886	1.049224
.500	1.055065	1.055065	1.055065	1.059238	1.075093
.542	1.070921	1.070921	1.073424	1.092618	1.155205
.583	1.095956	1.095956	1.110142	1.185246	1.394705
.625	1.136011	1.138515	1.210281	1.463968	1.872848
.667	1.206943	1.226971	1.515706	1.988847	2.223671
.708	1.332118	1.453119	2.015846	2.278470	2.380467
.792	1.766534	2.190558	2.402102	2.415716	2.391687
.833	1.947836	2.299386	2.394091	2.375657	2.340360
.875	2.100599	2.369243	2.373252	2.332331	2.288931
.917	2.181664	2.402102	2.348386	2.289735	2.239804

DISTANCE z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.011672	1.011672	1.011672	1.011672	1.011672
.042	1.012506	1.012506	1.012506	1.012506	1.012506
.083	1.013341	1.013341	1.012506	1.012506	1.012506
.125	1.015010	1.014175	1.014175	1.013341	1.013341
.167	1.016679	1.015844	1.015844	1.015010	1.015010
.250	1.019182	1.018347	1.018347	1.018347	1.019182
.292	1.021685	1.020851	1.020851	1.021685	1.025858
.333	1.025858	1.024189	1.025023	1.031699	1.050893
.375	1.030030	1.029196	1.035037	1.065914	1.158543
.417	1.036706	1.040044	1.073424	1.209447	1.604997
.458	1.049224	1.071755	1.207778	1.648990	2.126583
.500	1.090114	1.224468	1.821480	2.147664	2.398096
.542	1.269530	1.862924	2.179238	2.408509	2.577913
.583	1.829781	2.194599	2.425322	2.561957	2.653663
.625	2.162243	2.418117	2.567542	2.617789	2.670401
.667	2.426122	2.583497	2.640112	2.637720	2.667213
.708	2.564350	2.645692	2.645692	2.616991	2.632937
.792	2.545198	2.586687	2.559563	2.520450	2.521249
.833	2.454924	2.503679	2.488499	2.455724	2.452525
.875	2.368441	2.418117	2.413314	2.388482	2.383673
.917	2.300190	2.341965	2.341965	2.323497	2.320283

(RUN NUMBER 52)

DISTANCE z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.011672	1.011672	1.011672	1.011672	1.011672
.042	1.011672	1.011672	1.011672	1.011672	1.011672
.083	1.012506	1.012506	1.012506	1.012506	1.013341
.125	1.013341	1.013341	1.014175	1.015844	1.020016
.167	1.015010	1.015844	1.018347	1.024189	1.048389
.250	1.023354	1.042548	1.088445	1.196095	1.720522
.292	1.048389	1.126832	1.294565	1.658278	2.253506
.333	1.149363	1.443940	1.833100	2.158195	2.433325
.375	1.574121	2.099786	2.321890	2.482905	2.593866
.417	2.280885	2.503679	2.616194	2.664025	2.676777
.458	2.499684	2.679965	2.750892	2.733359	2.699889
.500	2.586687	2.735750	2.789945	2.759658	2.695904
.542	2.630545	2.728578	2.786757	2.772410	2.695107
.583	2.638517	2.675980	2.730968	2.741328	2.670401
.625	2.630545	2.624167	2.661634	2.685544	2.630545
.667	2.616991	2.582699	2.600246	2.627356	2.587485
.708	2.583497	2.536418	2.536418	2.558765	2.532426
.792	2.485303	2.440526	2.419719	2.424521	2.410111
.833	2.426122	2.384475	2.362827	2.360421	2.349189
.875	2.364431	2.413314	2.308230	2.300190	2.288931
.917	2.305014	2.278470	2.255118	2.244641	2.233352

DISTANCE z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.010837	1.010837	1.010837	1.010837	1.012506
.042	1.012506	1.014175	1.016679	1.027527	1.050058
.083	1.017513	1.025023	1.038375	1.095121	1.196095
.125	1.037541	1.070086	1.156039	1.398043	1.684402
.167	1.128501	1.255344	1.661653	2.002762	2.141991
.250	2.124960	2.264784	2.488499	2.669604	2.707061
.292	2.439726	2.530830	2.659243	2.773207	2.822630
.333	2.606625	2.663228	2.722999	2.800307	2.858515
.375	2.708655	2.745313	2.797916	2.853729	2.907985
.417	2.738938	2.784365	2.835387	2.865694	2.907187
.458	2.721405	2.766831	2.825819	2.847349	2.880054
.500	2.680762	2.715030	2.780380	2.802699	2.832995
.542	2.651272	2.668010	2.734156	2.761252	2.791539
.583	2.610613	2.609018	2.666416	2.698295	2.730171
.625	2.568340	2.551583	2.596258	2.630545	2.662431
.667	2.530031	2.504477	2.538813	2.570733	2.601841
.708	2.482905	2.454125	2.478110	2.506874	2.535620
.792	2.378864	2.352398	2.363629	2.381269	2.402903
.833	2.324300	2.300190	2.306622	2.319480	2.337952
.875	2.268810	2.247059	2.251089	2.260757	2.276056
.917	2.215600	2.205103	2.201064	2.207526	2.219636

APPENDIX C

TABLE (C.8)

DATA ON CARBON MONOXIDE OXIDATION.

(RUN NO. 53)

Air flow	=	800	cc/min.
after 65 min.		825	cc/min.
after 105 min.	=	780	cc/min.
CO flow	=	100	cc/min.
after 65 min.	=	75	cc/min.
after 105 min.	=	120	cc/min.
Total flow	=	900	cc/min.
Feed velocity (u_o)	=	0.461	m/s.
Residence time (τ)	=	1.3015	s.
Feed concentration (C_{Ao})	=	4.59×10^{-3}	$Kmol/m^3$.
after 65 min.	=	3.45×10^{-3}	$Kmol/m^3$.
after 105 min.	=	5.51×10^{-3}	$Kmol/m^3$.
Oxygen concentration (C_{Bo})	=	7.717×10^{-3}	$Kmol/m^3$.
after 65 min.	=	7.958×10^{-3}	$Kmol/m^3$.
after 105 min.	=	7.524×10^{-3}	$Kmol/m^3$.

Pressure gauge readings during run (psig)

= P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 53)

DISTANCE z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.016679	1.016679	1.016679	1.016679	1.016679
.042	1.018347	1.018347	1.018347	1.018347	1.018347
.083	1.019182	1.019182	1.019182	1.019182	1.019182
.125	1.020851	1.020851	1.020851	1.020851	1.020851
.167	1.022520	1.022520	1.022520	1.022520	1.022520
.250	1.027527	1.027527	1.027527	1.027527	1.027527
.292	1.030865	1.030865	1.030865	1.030865	1.030865
.333	1.034203	1.034203	1.034203	1.034203	1.035037
.375	1.039210	1.040044	1.040044	1.040044	1.040044
.417	1.045886	1.046720	1.046720	1.047555	1.049224
.458	1.054231	1.055065	1.055065	1.056734	1.061741
.500	1.066748	1.067583	1.069252	1.074259	1.089280
.542	1.086776	1.088445	1.092618	1.110976	1.155205
.583	1.116818	1.119321	1.132673	1.187750	1.306248
.625	1.163550	1.170226	1.220295	1.381353	1.627002
.667	1.243661	1.264523	1.443105	1.764029	1.973278
.708	1.365835	1.447278	1.808186	2.015028	2.083524
.792	1.759854	2.017480	2.124148	2.119279	2.092470
.833	1.912459	2.134694	2.162243	2.123337	2.079456
.875	2.032183	2.207526	2.180855	2.120902	2.066430
.917	2.089218	2.229319	2.176811	2.106287	2.046870

DISTANCE z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.016679	1.016679	1.016679	1.016679	1.016679
.042	1.018347	1.018347	1.018347	1.017513	1.017513
.083	1.019182	1.019182	1.019182	1.019182	1.019182
.125	1.020851	1.020851	1.020851	1.020851	1.020851
.167	1.023354	1.023354	1.023354	1.023345	1.023354
.250	1.027527	1.028361	1.028361	1.029196	1.030865
.292	1.030865	1.031699	1.032534	1.035037	1.039210
.333	1.035037	1.036706	1.039210	1.045051	1.055900
.375	1.042548	1.045051	1.052562	1.068417	1.095956
.417	1.054231	1.064245	1.084273	1.125997	1.196095
.458	1.073424	1.097624	1.146860	1.244496	1.397208
.500	1.120990	1.185246	1.317097	1.547417	1.844707
.542	1.245330	1.422243	1.728066	1.981475	2.052578
.583	1.519044	1.831441	2.005216	2.071316	2.076200
.625	1.878633	2.017480	2.063987	2.062357	2.049317
.667	2.050947	2.072130	2.063172	2.033815	2.009306
.708	2.089218	2.066430	2.034632	1.997034	1.965897
.792	2.059913	2.018298	1.975738	1.934684	1.898445
.833	2.038712	1.994579	1.951943	1.910812	1.875327
.875	2.019115	1.973278	1.930571	1.890194	1.854647
.917	1.996216	1.951121	1.909163	1.869541	1.834759

(RUN NUMBER 53)

DISTANCE z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.015844	1.015844	1.015844	1.016679	1.016679
.042	1.017513	1.017513	1.018347	1.018347	1.018347
.083	1.019182	1.019182	1.020016	1.020016	1.020851
.125	1.020851	1.021685	1.022520	1.023354	1.025023
.167	1.024189	1.025023	1.025858	1.029196	1.034203
.250	1.034203	1.039210	1.049224	1.070086	1.100962
.292	1.046720	1.060072	1.084273	1.136846	1.204440
.333	1.075093	1.106804	1.166888	1.294565	1.419739
.375	1.143522	1.223633	1.381353	1.652369	1.773209
.417	1.314593	1.502354	1.814835	2.036264	2.004398
.458	1.624461	1.873674	2.019932	2.086778	2.044423
.500	2.013394	2.062357	2.055023	2.041976	2.010941
.542	2.085151	2.076200	2.033815	1.986390	1.956048
.583	2.062357	2.040344	1.995397	1.942084	1.905867
.625	2.019932	1.993760	1.953585	1.904218	1.866233
.667	1.976557	1.947014	1.911636	1.869541	1.833100
.708	1.933039	1.903393	1.872021	1.836418	1.803196
.792	1.866233	1.837247	1.809017	1.780714	1.754006
.833	1.842221	1.812342	1.784881	1.758183	1.733092
.875	1.821480	1.792377	1.765699	1.739789	1.716329
.917	1.803196	1.774877	1.748990	1.724714	1.702899

DISTANCE z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.016679	1.016679	1.017513	1.017513	1.017513
.042	1.019182	1.020016	1.020851	1.021685	1.022520
.083	1.022520	1.023354	1.025023	1.027527	1.030030
.125	1.027527	1.030865	1.035037	1.040044	1.046720
.167	1.040879	1.048389	1.057569	1.069252	1.084273
.250	1.131004	1.164384	1.209447	1.267027	1.344635
.292	1.262854	1.331283	1.419739	1.528224	1.651524
.333	1.513203	1.616836	1.727228	1.821480	1.885241
.375	1.829781	1.879459	1.919049	1.948657	1.966717
.417	1.989666	1.983933	1.977377	1.970818	1.963435
.458	2.013394	1.990485	1.969178	1.948657	1.931394
.500	1.981475	1.956048	1.930571	1.905867	1.883589
.542	1.930571	1.907515	1.883589	1.859614	1.837247
.583	1.881111	1.859614	1.837247	1.814835	1.793210
.625	1.840563	1.818989	1.798204	1.777379	1.757348
.667	1.806523	1.784881	1.764864	1.745645	1.726390
.708	1.777379	1.755677	1.735604	1.717168	1.698698
.792	1.730579	1.709616	1.690291	1.671770	1.654901
.833	1.711295	1.690291	1.670927	1.653213	1.637157
.875	1.694495	1.675140	1.656590	1.638848	1.623615
.917	1.682719	1.663340	1.646456	1.630388	1.615140

(RUN NUMBER 53)

DISTANCE Z	time=100 Φ	time=105 Φ	time=110 Φ	time=115 Φ	time=120. Φ
.000	1.017513	1.018347	1.018347	1.019182	1.020851
.042	1.024189	1.025858	1.028361	1.035037	1.046720
.083	1.033368	1.039210	1.047555	1.066748	1.100962
.125	1.055065	1.067583	1.089280	1.143522	1.231978
.167	1.105969	1.136011	1.201936	1.347973	1.556597
.250	1.454788	1.584969	1.956869	2.118467	2.159005
.292	1.769872	1.858786	2.103037	2.180855	2.171147
.333	1.922342	1.947014	2.059098	2.119279	2.113596
.375	1.965897	1.960153	1.996216	2.033815	2.036264
.417	1.948657	1.930571	1.928103	1.938795	1.941262
.458	1.910812	1.889369	1.874501	1.868714	1.867060
.500	1.861269	1.839734	1.819819	1.804028	1.796540
.542	1.815666	1.794875	1.774877	1.754841	1.741462
.583	1.773209	1.753170	1.733929	1.712973	1.697017
.625	1.738115	1.719684	1.701219	1.681035	1.664183
.667	1.707937	1.690291	1.672613	1.653213	1.636311
.708	1.681035	1.664183	1.647301	1.629542	1.613445
.792	1.638003	1.622767	1.605832	1.589976	1.574955
.833	1.620226	1.604997	1.589976	1.574955	1.560769
.875	1.607507	1.592480	1.578293	1.564107	1.550755
.917	1.599990	1.585804	1.572452	1.559935	1.548252

DISTANCE Z	time=125 Φ	time=130 Φ	time=135 Φ	time=140 Φ	time=145 Φ
.000	1.022520	1.026692	1.034203	1.044217	1.060072
.042	1.067583	1.108473	1.169391	1.246999	1.376346
.083	1.166888	1.283717	1.436429	1.615988	1.870367
.125	1.408891	1.635465	1.821480	1.945371	2.080270
.167	1.895971	2.060728	2.131450	2.157385	2.155765
.250	2.148474	2.164672	2.171147	2.171956	2.126583
.292	2.114408	2.095722	2.092470	2.090844	2.059913
.333	2.061543	2.025650	2.011758	2.006034	1.984752
.375	1.999489	1.962615	1.942905	1.931394	1.914931
.417	1.920695	1.891845	1.870367	1.856303	1.842221
.458	1.852991	1.831441	1.812342	1.798204	1.784881
.500	1.784881	1.769037	1.752334	1.738952	1.726390
.542	1.729741	1.716329	1.702899	1.690291	1.678509
.583	1.684402	1.671770	1.659121	1.647301	1.636311
.625	1.649635	1.638003	1.625308	1.614292	1.602494
.667	1.621920	1.608355	1.596652	1.584969	1.574955
.708	1.597487	1.584969	1.572452	1.561604	1.551590
.792	1.561604	1.548252	1.536569	1.525720	1.515706
.833	1.547417	1.534900	1.523217	1.512368	1.502354
.875	1.538238	1.526555	1.515706	1.505692	1.495678
.917	1.536569	1.525720	1.516541	1.506527	1.497347

APPENDIX C

TABLE (C.9)

DATA ON CARBON MONOXIDE OXIDATION
(RUN NO. 55)

Air flow	=	1000	cc/min.
after 60 min.	=	2000	cc/min.
CO flow	=	100	cc/min.
after 60 min.	=	200	cc/min.
Total flow	=	1100	cc/min.
after 60 min.	=	2200	cc/min.
Feed velocity (u_o)	=	0.5633	m/s.
after 60 min.	=	1.1267	m/s.
Residence time (τ)	=	1.065	s.
	=	0.5325	s.
Feed concentration (C_{Ao})	=	3.758×10^{-3} K mol/m^3	
Oxygen concentration (C_{Bo})	=	7.892×10^{-3} K mol/m^3	

Pressure gauge readings during run (psig)

= P.G1 - 3 : P.G2 - 2.

(RUN NUMBER 55)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	1.010003	1.010003	1.010003	1.010003	1.010837
.042	1.011672	1.011672	1.011672	1.011672	1.011672
.083	1.012506	1.012506	1.012506	1.012506	1.013341
.125	1.013341	1.013341	1.014175	1.014175	1.014175
.167	1.015844	1.015844	1.015844	1.015844	1.015844
.250	1.020851	1.020851	1.020851	1.020851	1.020851
.292	1.023354	1.023354	1.023354	1.023354	1.023354
.333	1.026692	1.026692	1.026692	1.026692	1.026692
.375	1.031699	1.031699	1.031699	1.031699	1.031699
.417	1.037541	1.037541	1.037541	1.037541	1.038375
.458	1.045051	1.045051	1.044217	1.045051	1.047555
.500	1.056734	1.056734	1.056734	1.059238	1.065914
.542	1.074259	1.074259	1.075928	1.085942	1.107638
.583	1.100128	1.100128	1.108473	1.141018	1.200267
.625	1.141853	1.143522	1.181074	1.281213	1.427250
.667	1.215288	1.228640	1.372173	1.599156	1.791544
.708	1.337124	1.410560	1.726390	1.894320	1.971638
.792	1.737278	1.972458	2.051763	2.056653	2.042792
.833	1.899270	2.103849	2.111972	2.077828	2.045239
.875	2.033815	2.197832	2.154955	2.094097	2.046870
.917	2.104662	2.242223	2.172766	2.099786	2.044423

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	1.010837	1.010837	1.010837	1.010837	1.010837
.042	1.011672	1.011672	1.012506	1.012506	1.012506
.083	1.013341	1.013341	1.013341	1.013341	1.013341
.125	1.014175	1.014175	1.015010	1.015010	1.015010
.167	1.015844	1.015844	1.016679	1.016679	1.016679
.250	1.020016	1.020016	1.020016	1.020851	1.020851
.292	1.023354	1.024189	1.024189	1.024189	1.025023
.333	1.026692	1.027527	1.028361	1.029196	1.030865
.375	1.031699	1.033368	1.035037	1.037541	1.040044
.417	1.040044	1.043382	1.047555	1.053396	1.060907
.458	1.052562	1.058403	1.067583	1.080935	1.097624
.500	1.078431	1.095121	1.118487	1.150198	1.189419
.542	1.140184	1.186081	1.246165	1.325442	1.408891
.583	1.281213	1.388029	1.508196	1.640539	1.742299
.625	1.574121	1.709616	1.803196	1.867887	1.916578
.667	1.885241	1.941262	1.979016	1.999489	2.019115
.708	2.012576	2.031366	2.041976	2.042792	2.045239
.792	2.032999	2.022383	2.010941	1.999489	1.988028
.833	2.020749	1.999489	1.982294	1.965897	1.950300
.875	2.010941	1.981475	1.957690	1.937151	1.918225
.917	2.000308	1.965897	1.937151	1.913283	1.892670

(RUN NUMBER 55)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	1.010837	1.010837	1.011672	1.011672	1.011672
.042	1.012506	1.012506	1.012506	1.012506	1.012506
.083	1.013341	1.013341	1.014175	1.013341	1.013341
.125	1.015010	1.015010	1.015844	1.015010	1.014175
.167	1.016679	1.016679	1.017513	1.015844	1.015844
.250	1.021685	1.021685	1.022520	1.020016	1.019182
.292	1.025858	1.026692	1.027527	1.024189	1.022520
.333	1.032534	1.035037	1.036706	1.031699	1.030030
.375	1.045051	1.049224	1.054231	1.045886	1.042548
.417	1.070086	1.080100	1.090949	1.075928	1.075093
.458	1.115149	1.133508	1.153536	1.132673	1.143522
.500	1.226971	1.263689	1.304579	1.307083	1.349642
.542	1.478989	1.543245	1.608355	1.712134	1.754841
.583	1.793210	1.824802	1.851335	1.966717	2.032999
.625	1.945371	1.964256	1.976557	2.128205	2.246253
.667	2.038712	2.050947	2.056653	2.255924	2.414915
.708	2.055023	2.063172	2.065616	2.296170	2.472515
.792	1.982294	1.980655	1.979016	2.171147	2.329119
.833	1.940440	1.933039	1.928103	2.075387	2.217215
.875	1.904218	1.893495	1.885241	1.993760	2.113596
.917	1.875327	1.862096	1.851335	1.934684	2.033815

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	1.011672	1.011672	1.011672	1.012506	1.012506
.042	1.012506	1.012506	1.012506	1.012506	1.013341
.083	1.013341	1.013341	1.013341	1.013341	1.013341
.125	1.014175	1.014175	1.014175	1.014175	1.014175
.167	1.015010	1.015010	1.015010	1.015010	1.015010
.250	1.018347	1.018347	1.017513	1.018347	1.018347
.292	1.022520	1.021685	1.021685	1.021685	1.021685
.333	1.029196	1.028361	1.028361	1.028361	1.027527
.375	1.042548	1.042548	1.042548	1.041713	1.040879
.417	1.077597	1.077597	1.076762	1.074259	1.070086
.458	1.149363	1.149363	1.145191	1.136846	1.123494
.500	1.359656	1.351311	1.332118	1.300407	1.257847
.542	1.750662	1.730579	1.697017	1.643076	1.557431
.583	2.046055	2.037080	2.014211	1.975738	1.915755
.625	2.299386	2.318677	2.315463	2.296170	2.258340
.667	2.503679	2.549189	2.569137	2.573126	2.565946
.708	2.585092	2.652866	2.693513	2.721405	2.744516
.792	2.448526	2.542804	2.618586	2.680762	2.738141
.833	2.327513	2.420519	2.499684	2.569137	2.632937
.875	2.213178	2.299386	2.377261	2.447726	2.514062
.917	2.121714	2.199448	2.271226	2.339557	2.404505

(RUN NUMBER 55)

DISTANCE Z	time=100 Φ	time=105 Φ	time=110 Φ	time=115 Φ	time=120 Φ
.000	1.012506	1.012506	1.012506	1.012506	1.012506
.042	1.013341	1.013341	1.013341	1.013341	1.013341
.083	1.013341	1.013341	1.014175	1.014175	1.014175
.125	1.014175	1.014175	1.015010	1.015010	1.014175
.167	1.015010	1.015010	1.015010	1.015844	1.015844
.250	1.018347	1.018347	1.018347	1.017513	1.018347
.292	1.021685	1.021685	1.021685	1.020851	1.020851
.333	1.027527	1.026692	1.026692	1.025858	1.025858
.375	1.038375	1.037541	1.035872	1.034203	1.033368
.417	1.065079	1.060072	1.055900	1.052562	1.050058
.458	1.110142	1.098459	1.089280	1.081769	1.075093
.500	1.218626	1.157750	1.163550	1.144356	1.128501
.542	1.466471	1.391367	1.331283	1.282882	1.241992
.583	1.835588	1.749826	1.663340	1.574121	1.489837
.625	2.197832	2.120091	2.036264	1.948657	1.860441
.667	2.537216	2.485303	2.418117	2.340360	2.255118
.708	2.754876	2.745313	2.717421	2.673589	2.614599
.792	2.789945	2.831400	2.860908	2.879256	2.886437
.832	2.693513	2.746907	2.790742	2.826616	2.854527
.875	2.578711	2.638517	2.691919	2.738938	2.780380
.917	2.469317	2.533225	2.590675	2.644098	2.693513

DISTANCE Z	time=125 Φ	time=130 Φ	time=135 Φ	time=140 Φ	time=145 Φ
.000	1.012506	1.012506	1.012506	1.012506	1.012506
.042	1.013341	1.013341	1.013341	1.013341	1.013341
.083	1.014175	1.014175	1.014175	1.013341	1.013341
.125	1.015010	1.015010	1.015010	1.015010	1.015010
.167	1.015844	1.015844	1.015844	1.015844	1.015844
.250	1.017513	1.017513	1.018347	1.018347	1.017513
.292	1.020851	1.020851	1.020016	1.020016	1.020016
.333	1.025023	1.025023	1.024189	1.024189	1.024189
.375	1.032534	1.031699	1.031699	1.030865	1.030030
.417	1.047555	1.045051	1.043382	1.042548	1.040879
.458	1.069252	1.065079	1.061741	1.058403	1.055900
.500	1.115149	1.105135	1.095956	1.089280	1.083438
.542	1.210281	1.184412	1.163550	1.146860	1.133508
.583	1.418905	1.359656	1.310421	1.270365	1.238654
.625	1.774877	1.691973	1.612597	1.537403	1.472313
.667	2.167101	2.079456	1.992941	1.909988	1.830611
.708	2.542804	2.462121	2.376459	2.289735	2.202679
.792	2.880852	2.867289	2.844957	2.816251	2.775598
.833	2.872874	2.882448	2.885639	2.883245	2.876065
.875	2.814657	2.841767	2.862503	2.878458	2.888033
.917	2.738141	2.775598	2.807482	2.836185	2.859313

(RUN NUMBER 55)

DISTANCE Z	time=150 Φ	time=155 Φ	time=160 Φ	time=165 Φ	time=170 Φ
.000	1.012506	1.012506	1.012506	1.012506	1.012506
.042	1.013341	1.013341	1.013341	1.013341	1.013341
.083	1.013341	1.013341	1.013341	1.013341	1.013341
.125	1.014175	1.015010	1.015010	1.015010	1.015010
.167	1.015844	1.015844	1.015844	1.015844	1.015844
.250	1.017513	1.017513	1.017513	1.017513	1.017513
.292	1.019182	1.019182	1.019182	1.019182	1.019182
.333	1.023354	1.023354	1.023354	1.023354	1.023354
.375	1.029196	1.028361	1.028361	1.028361	1.027527
.417	1.040044	1.038375	1.037541	1.036706	1.035872
.458	1.053396	1.051727	1.050058	1.048389	1.046720
.500	1.078431	1.074259	1.070086	1.067583	1.064245
.542	1.122659	1.113480	1.105135	1.098459	1.092618
.583	1.212785	1.190253	1.172729	1.157708	1.144356
.625	1.413898	1.362994	1.320435	1.282048	1.250337
.667	1.755677	1.684402	1.615140	1.544079	1.477320
.708	2.119279	2.039528	1.962615	1.886892	1.810680
.792	2.731765	2.675183	2.609018	2.536418	2.458123
.833	2.860110	2.835387	2.801902	2.758064	2.704670
.875	2.892023	2.889629	2.880054	2.866492	2.845754
.917	2.877660	2.889629	2.896811	2.9L2398	2.906389

DISTANCE Z	time=175 Φ	time=180 Φ	time=185 Φ	time=190 Φ	time=195 Φ
.000	1.012506	1.012506	1.012506	1.012506	1.013341
.042	1.013341	1.013341	1.013341	1.013341	1.014175
.083	1.014175	1.014175	1.014175	1.014175	1.014175
.125	1.015010	1.015010	1.015010	1.015010	1.015844
.167	1.015844	1.015844	1.015844	1.015844	1.016679
.250	1.017513	1.017513	1.017513	1.017513	1.017513
.292	1.019182	1.019182	1.019182	1.019182	1.019182
.333	1.022520	1.022520	1.022520	1.023354	1.023354
.375	1.027527	1.027527	1.027527	1.027527	1.027527
.417	1.035872	1.035037	1.035037	1.035037	1.034203
.458	1.045886	1.045051	1.044217	1.042548	1.042548
.500	1.061741	1.060072	1.057569	1.055900	1.054231
.542	1.087611	1.083438	1.079266	1.075928	1.073424
.583	1.133508	1.123494	1.115983	1.109307	1.102631
.625	1.223633	1.201102	1.182743	1.166888	1.152701
.667	1.417236	1.362159	1.315428	1.275372	1.242827
.708	1.737278	1.663340	1.583300	1.502354	1.428084
.792	2.375657	2.292953	2.209141	2.123337	2.037080
.833	2.639315	2.567542	2.491695	2.412513	2.329922
.875	2.816251	2.778786	2.733359	2.679965	2.618586
.917	2.907187	2.902398	2.892821	2.877660	2.854527

APPENDIX C

TABLE (C.10)

DATA ON CARBON OXIDATION

(RUN NO. 71)

Air flow	=	300 cc/min.
Feed velocity (u_o)	=	0.1418 m/s.
Residence time (τ)	=	4.23 s.
Preheated feed temperature (T_o)	=	616 ^oK.
Velocity of propagation (W)	=	0.2505×10^{-3} m/s.

Fraction of carbon regenerated during reverse propagation of the reaction zone = -

Duration of reverse propagation	=	35 min.
Total regeneration period	=	145 min.
Initial carbon deposition	=	7.3 weight%

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 71)

DISTANCE z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.845656	0.846453	0.846453	0.846453	0.852027
.042	0.890882	0.894042	0.895621	0.895621	0.895621
.083	0.947880	0.952182	0.955309	0.956091	0.956098
.167	1.000066	1.000453	1.011813	1.014523	1.024623
.208	1.000171	1.000426	1.018100	1.024966	1.025740
.292	1.000229	1.011228	1.021458	1.028487	1.030033
.333	1.000286	1.012515	1.024136	1.029166	1.031100
.375	1.000383	1.015228	1.026458	1.031873	1.034966
.417	1.001266	1.021813	1.032260	1.036513	1.056587
.458	1.006699	1.028005	1.038445	1.042308	1.577423
.500	1.008250	1.030713	1.041922	1.048485	1.365173
.542	1.007862	1.030326	1.043466	1.080464	1.260487
.583	1.019102	1.043080	1.059286	1.491225	1.224685
.625	1.041534	1.068148	1.088923	1.341943	1.212870
.750	1.211345	1.239924	1.320625	1.246779	1.199524
.917	1.287132	1.289797	1.217826	1.135718	1.077002
.958	1.155612	1.160199	1.091998	1.019877	0.969752

(RUN NUMBER 71)

DISTANCE z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.846054	0.847648	0.848064	0.848046	0.847648
.042	0.922790	0.923183	0.922005	0.920040	0.917681
.083	1.017166	1.012515	1.006699	1.000878	0.995829
.167	1.184644	1.149876	1.126143	1.108124	1.094303
.208	1.246779	1.194565	1.160581	1.136484	1.118479
.292	1.376222	1.274572	1.220494	1.183499	1.157524
.333	1.478579	1.334709	1.264675	1.219731	1.187697
.375	1.313774	1.440703	1.333948	1.280281	1.235734
.417	1.198761	1.369744	1.453318	1.372792	1.292841
.458	1.151406	1.206770	1.507331	1.478196	1.362506
.500	1.121162	1.136484	1.215920	1.464030	1.495444
.542	1.098528	1.098912	1.119629	1.201813	1.444142
.583	1.090845	1.085464	1.087386	1.114644	1.190750
.625	1.090076	1.081618	1.075847	1.082775	1.109658
.750	1.060056	1.045397	1.032260	1.022200	1.014841
.917	0.891278	0.872284	0.855608	0.840872	0.828092
.958	0.808858	0.793171	0.779855	0.767715	0.756952

DISTANCE z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.846851	0.847250	0.848046	0.848843	0.850037
.042	0.896016	0.896016	0.897594	0.911387	0.918074
.083	0.956872	0.956872	0.965072	1.010965	1.016003
.167	1.024910	1.027232	1.442996	1.321006	1.236115
.208	1.035740	1.061984	1.380413	1.470919	1.342323
.292	1.041149	1.365544	1.275714	1.270765	1.584381
.333	1.105054	1.280281	1.233448	1.217063	1.285610
.375	1.381938	1.243352	1.205626	1.187697	1.196473
.417	1.336993	1.224685	1.186170	1.168606	1.163257
.458	1.283707	1.204864	1.170898	1.156377	1.145668
.500	1.219731	1.177008	1.150259	1.138780	1.126526
.542	1.183499	1.151023	1.128825	1.120012	1.107356
.583	1.172426	1.142225	1.121928	1.113110	1.100447
.625	1.170898	1.142990	1.123078	1.113878	1.099680
.750	1.162875	1.133421	1.108891	1.096607	1.077002
.917	1.029940	0.991943	0.960778	0.937308	0.915322
.958	0.928288	0.896016	0.869111	0.850037	0.830890

DISTANCE z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.847648	0.847250	0.846851	0.851629	0.846453
.042	0.915715	0.914142	0.912174	0.909812	0.909419
.083	0.991554	0.988055	0.984554	0.980662	0.979104
.167	1.083541	1.075078	1.067763	1.061213	1.056587
.208	1.104670	1.093534	1.084310	1.076617	1.070073
.292	1.136866	1.120012	1.106205	1.094687	1.084695
.333	1.161346	1.139929	1.122312	1.108124	1.096223
.375	1.198761	1.170134	1.147964	1.129974	1.115795
.417	1.240305	1.202194	1.174335	1.152171	1.134569
.458	1.288274	1.238400	1.204101	1.176627	1.154847
.500	1.345369	1.276856	1.230544	1.195710	1.167842
.542	1.416262	1.340039	1.265817	1.214014	1.178536
.583	1.415117	1.433826	1.327096	1.246018	1.201050
.625	1.206008	1.407867	1.387078	1.284088	1.229639
.750	1.012903	1.020264	1.049257	1.191895	1.428478
.917	0.816881	0.806448	0.798003	0.793171	0.791559
.958	0.747785	0.739017	0.731844	0.726663	0.722279

APPENDIX C

TABLE (C.11)

DATA ON CARBON OXIDATION.

(RUN NO. 72)

Air flow	=	230 cc/min.
Feed velocity (u_o)	=	0.1087 m/s.
Residence time (τ)	=	5.52 s.
Preheated feed temperature (T_o)	=	623 ^oK.
Velocity of propagation (W)	=	0.143×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.2008
Duration of reverse propagation	=	51 min.
Total regeneration period	=	265 min.
Initial carbon deposition	=	11.9 weight%

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 72)

DISTANCE z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.857385	0.856208	0.856208	0.857777	0.858169
.042	0.903870	0.908536	0.910091	0.910868	0.911256
.083	0.961169	0.968488	0.971952	0.972722	0.973491
.167	1.003011	1.020923	1.022941	1.030849	1.031231
.208	1.004925	1.021360	1.023664	1.032952	1.032334
.292	1.005737	1.022191	1.024888	1.033705	1.034849
.333	1.007821	1.013602	1.025215	1.034033	1.035560
.375	1.008652	1.024044	1.028033	1.038231	1.039757
.417	1.011480	1.027541	1.031283	1.044715	1.045477
.458	1.016837	1.032888	1.037383	1.050051	1.052337
.500	1.017602	1.034796	1.048908	1.051956	1.063379
.542	1.017837	1.035742	1.057002	1.054242	1.125985
.583	1.028687	1.043190	1.062618	1.087703	1.365280
.625	1.053480	1.070606	1.098707	1.265896	1.296002
.750	1.229382	1.240301	1.299765	1.249712	1.209795
.917	1.288852	1.291110	1.217329	1.134309	1.073267
.958	1.151320	1.153587	1.084286	1.012246	0.960784

(RUN NUMBER 72)

DISTANCE z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.857777	0.857777	0.856993	0.857777	0.856993
.042	0.911256	0.910868	0.910868	0.910479	0.910479
.083	0.972491	0.972457	0.972722	0.972337	0.972337
.167	1.031849	1.033086	1.035941	1.036323	1.056527
.208	1.032952	1.033808	1.042046	1.048146	1.163784
.292	1.034849	1.037468	1.053480	1.478641	1.293368
.333	1.035560	1.039757	1.129391	1.299765	1.252723
.375	1.040901	1.070606	1.328370	1.273799	1.231264
.417	1.051956	1.579969	1.292991	1.250841	1.212055
.458	1.100224	1.303905	1.249336	1.218083	1.188309
.500	1.467269	1.267025	1.212055	1.184161	1.160385
.542	1.253476	1.217329	1.178502	1.152831	1.132417
.583	1.234277	1.196981	1.165294	1.141115	1.121443
.625	1.226369	1.187932	1.159252	1.136956	1.117656
.750	1.176993	1.146785	1.121443	1.099466	1.079728
.917	1.026013	0.987712	0.956157	0.929488	0.906204
.958	0.920961	0.888289	0.861699	0.839699	0.819974

DISTANCE z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.857777	0.857777	0.856993	0.857777	0.856993
.042	0.911256	0.910868	0.910868	0.910479	0.910479
.083	0.972491	0.972457	0.972722	0.972337	0.972337
.167	1.031849	1.033086	1.035941	1.036323	1.056527
.208	1.032952	1.033808	1.042046	1.048146	1.163784
.292	1.034849	1.037468	1.053480	1.478641	1.293368
.333	1.035560	1.039757	1.129391	1.299765	1.252723
.375	1.040901	1.070606	1.328370	1.273799	1.231264
.417	1.051956	1.579969	1.292991	1.250841	1.212055
.458	1.100224	1.303905	1.249336	1.218083	1.188309
.500	1.467269	1.267025	1.212055	1.184161	1.160385
.542	1.253476	1.217329	1.178502	1.152831	1.132417
.583	1.234277	1.196981	1.165294	1.141115	1.121443
.625	1.226369	1.187932	1.159252	1.136956	1.117656
.750	1.176993	1.146785	1.121443	1.099466	1.079728
.917	1.026013	0.987712	0.956157	0.929488	0.906204
.958	0.920961	0.888289	0.861699	0.839699	0.819974

DISTANCE z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.863658	0.863267	0.862875	0.862483	0.861699
.042	0.945348	0.942257	0.938390	0.934908	0.931812
.083	1.042808	1.033651	1.024866	1.017220	1.010332
.167	1.196604	1.164916	1.139981	1.121821	1.107428
.208	1.259498	1.210171	1.175107	1.150942	1.132417
.292	1.414316	1.308421	1.251594	1.215069	1.186046
.333	1.279820	1.435854	1.340042	1.277186	1.235030
.375	1.201881	1.290733	1.417337	1.390162	1.316325
.417	1.163028	1.201881	1.313314	1.452121	1.483572
.458	1.136578	1.151698	1.193965	1.280949	1.426782
.500	1.112732	1.117656	1.133552	1.169823	1.247453
.542	1.085045	1.083906	1.087703	1.100224	1.131282
.583	1.071366	1.067564	1.065662	1.068324	1.080108
.625	1.063379	1.057669	1.052718	1.050432	1.052337
.750	1.005737	0.996155	0.986944	0.978491	0.971183
.917	0.816810	0.806514	0.796989	0.788241	0.779875
.958	0.746478	0.738201	0.730714	0.724015	0.717710

APPENDIX C

TABLE (C.12)

DATA ON CARBON OXIDATION.

(RUN NO. 73)

Air flow	=	230 cc/min.
Feed velocity (u_o)	=	0.1087 m/s.
Residence time (τ)	=	5.52 s.
Preheated feed temperature(T_o)	=	608 ^oK.
Velocity of propagation (W)	=	0.101×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.3055
Duration of reverse propagation	=	75 min.
Total regeneration period	=	275 min.
Initial carbon deposition	=	11.9 weight%

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 73)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.803608	0.801974	0.801974	0.801974	0.800749
.042	0.839393	0.840608	0.841418	0.841418	0.841418
.083	0.907006	0.909005	0.912202	0.912202	0.912202
.167	0.987251	0.992776	0.998297	0.999873	1.000268
.208	1.000419	1.000506	1.012193	1.014159	1.019945
.292	1.000601	1.008473	1.013552	1.015695	1.020874
.333	1.000662	1.009325	1.016407	1.019552	1.021124
.375	1.003419	1.012080	1.019552	1.022695	1.024267
.417	1.009325	1.019159	1.026231	1.029764	1.031334
.458	1.009719	1.018372	1.026231	1.029764	1.031727
.500	1.007751	1.016800	1.025445	1.029372	1.032119
.542	1.013260	1.021910	1.032512	1.038003	1.042316
.583	1.030942	1.041532	1.055631	1.063845	1.070489
.625	1.060326	1.073614	1.095460	1.109480	1.118427
.750	1.263184	1.306768	1.321806	1.325662	1.353043
.917	1.311395	1.312937	1.249678	1.191335	1.135137
.958	1.170430	1.173529	1.112204	1.058370	1.014047

(RUN NUMBER 73)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.801566	0.800749	0.800749	0.800749	0.800749
.042	0.840608	0.839798	0.838798	0.839798	0.843847
.083	0.911403	0.911403	0.911403	0.914599	0.932146
.167	0.999994	0.999998	1.010506	1.084933	1.390855
.208	1.019552	1.028194	1.082592	1.418276	1.313323
.292	1.053674	1.371173	1.274758	1.250450	1.239641
.333	1.191458	1.301755	1.250450	1.215307	1.200618
.375	1.311395	1.266271	1.228057	1.196750	1.178563
.417	1.269357	1.239641	1.207964	1.183595	1.128922
.458	1.238097	1.209897	1.184369	1.164618	1.149110
.500	1.203325	1.178563	1.158029	1.141349	1.128922
.542	1.178950	1.157642	1.139020	1.123093	1.111426
.583	1.168106	1.147946	1.129699	1.114149	1.102472
.625	1.161906	1.141349	1.123870	1.107923	1.095460
.750	1.100915	1.079470	1.063454	1.046626	1.031727
.917	0.935330	0.916596	0.900203	0.884966	0.865254
.958	0.860012	0.845466	0.832095	0.819907	0.808911

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.802791	0.802791	0.802791	0.801974	0.802383
.042	0.841823	0.841418	0.841418	0.841013	0.841013
.083	0.912602	0.912602	0.912202	0.911803	0.911403
.167	1.000662	1.000662	1.000673	1.000979	1.001691
.208	1.020731	1.020338	1.020845	1.021552	1.022159
.292	1.021052	1.022445	1.022952	1.023052	1.027409
.333	1.022303	1.023088	1.022695	1.023874	1.037219
.375	1.025838	1.026623	1.027409	1.027979	1.105977
.417	1.033296	1.034473	1.038788	1.072833	1.427938
.458	1.034081	1.037291	1.057196	1.466630	1.284401
.500	1.035258	1.046626	1.137855	1.233850	1.236553
.542	1.047801	1.112593	1.333374	1.250836	1.207964
.583	1.088444	1.415571	1.321420	1.239641	1.197524
.625	1.218399	1.303683	1.295585	1.038396	1.189787
.750	1.276301	1.220331	1.183208	1.121149	0.949641
.917	1.086104	1.045059	1.000662	0.981722	0.956784
.958	0.977770	0.946861	0.919390	0.896998	0.877331

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.801566	0.804016	0.807280	0.808096	0.808911
.042	0.863642	0.891788	0.892991	0.893391	0.890985
.083	1.021910	1.032904	1.030549	1.023481	1.014047
.167	1.275915	1.402824	1.342629	1.279772	1.244660
.208	1.273986	1.311395	1.362300	1.407845	1.358057
.292	1.215694	1.215694	1.222649	1.254309	1.327590
.333	1.184756	1.180498	1.180111	1.187078	1.214921
.375	1.164618	1.158805	1.155315	1.154152	1.161130
.417	1.152989	1.146006	1.142514	1.136690	1.137079
.458	1.136690	1.128922	1.123482	1.118816	1.116872
.500	1.116483	1.109091	1.103251	1.098188	1.095850
.542	1.099746	1.127368	1.086494	1.081422	1.078690
.583	1.091173	1.084543	1.076738	1.071270	1.067754
.625	1.084153	1.077519	1.068926	1.061890	1.056805
.750	1.019159	1.009719	0.998691	0.989620	0.982117
.917	0.858398	0.847489	0.836556	0.827630	0.820314
.958	0.799115	0.790935	0.782741	0.775391	0.769334

APPENDIX C

TABLE (C.13)

DATA ON CARBON OXIDATION.

(RUN NO. 74)

Air flow	=	240 cc/min.
Feed velocity (u_o)	=	0.1135 m/s.
Residence time (τ)	=	5.289 s.
Preheated feed temperature (T_o)	=	608 ^oK.
Velocity of propagation (W)	=	0.1055×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.2876
Duration of reverse propagation	=	65 min.
Total regeneration period	=	265 min.
initial carbon deposition	=	11.9 weight%

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 74)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.810134	0.810542	0.810542	0.810542	0.810542
.042	0.859205	0.860819	0.862835	0.863642	0.864045
.083	0.934534	0.938116	0.942092	0.943682	0.944477
.167	1.000003	1.000023	1.000196	1.002650	1.003827
.208	1.000009	1.000088	1.000234	1.003584	1.004151
.292	1.000076	1.000107	1.004267	1.005623	1.008194
.333	1.000160	1.000219	1.005293	1.006654	1.009834
.375	1.000180	1.000379	1.006964	1.009325	1.010506
.417	1.000276	1.000450	1.008038	1.010900	1.012080
.458	1.000376	1.001662	1.008145	1.010506	1.012473
.500	1.000565	1.001844	1.009719	1.012473	1.016013
.542	1.004238	1.010113	1.019552	1.024267	1.036827
.583	1.021910	1.031334	1.043492	1.052891	1.115705
.625	1.052108	1.064627	1.083763	1.108312	1.434510
.750	1.252766	1.287486	1.346486	1.326048	1.265885
.917	1.304068	1.308310	1.256625	1.173141	1.111036
.958	1.165006	1.169268	1.114927	1.050151	1.002632

(RUN NUMBER 74)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.809319	0.808096	0.808503	0.808503	0.808503
.042	0.862029	0.861222	0.861222	0.863642	0.863642
.083	0.941695	0.941297	0.942092	0.957180	1.045059
.167	1.033689	1.036827	1.073614	1.374260	1.341087
.208	1.049368	1.066191	1.481742	1.313323	1.309852
.292	1.093122	1.355743	1.253537	1.226898	1.210670
.333	1.429871	1.303297	1.223808	1.192495	1.177014
.375	1.297898	1.248134	1.202551	1.173141	1.157254
.417	1.252380	1.219558	1.185917	1.161130	1.145618
.458	1.224194	1.195203	1.167331	1.147170	1.132807
.500	1.195590	1.171979	1.146782	1.130476	1.118039
.542	1.175465	1.156091	1.132419	1.119205	1.107534
.583	1.167331	1.148722	1.126202	1.113371	1.102472
.625	1.160743	1.142125	1.121538	1.107923	1.097019
.750	1.097798	1.079470	1.060717	1.045451	1.032904
.917	0.931747	0.914200	0.897800	0.883359	0.870491
.958	0.856379	0.842228	0.829660	0.818280	0.807688

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.810949	0.810134	0.809727	0.809727	0.809319
.042	0.864045	0.863238	0.862835	0.862835	0.862432
.083	0.944080	0.943285	0.942887	0.942887	0.942092
.167	1.004827	1.006042	1.009258	1.014473	1.034081
.208	1.006151	1.009368	1.010584	1.018193	1.035801
.292	1.008587	1.010194	1.013194	1.020979	1.036435
.333	1.010620	1.011620	1.016407	1.021910	1.057588
.375	1.011293	1.012473	1.017193	1.043492	1.294813
.417	1.013654	1.019159	1.039180	1.170043	1.313323
.458	1.017193	1.040356	1.119205	1.323734	1.265113
.500	1.039964	1.125425	1.364615	1.260483	1.224967
.542	1.166168	1.335688	1.280544	1.230374	1.200618
.583	1.353814	1.329904	1.270515	1.222649	1.192108
.625	1.295585	1.289800	1.255467	1.213762	1.184756
.750	1.223808	1.195590	1.170043	1.142514	1.119205
.917	1.064236	1.030942	1.001450	0.974606	0.952023
.958	0.965107	0.936524	0.912202	0.890985	0.872504

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.812172	0.813802	0.816245	0.822347	0.815838
.042	0.903005	0.906206	0.905406	0.901003	0.899001
.083	1.046626	1.040748	1.032512	1.021517	1.013654
.167	1.365000	1.299441	1.258940	1.219944	1.190948
.208	1.405142	1.491049	1.374646	1.303683	1.258940
.292	1.205644	1.244274	1.341087	1.473603	1.472053
.333	1.165393	1.168106	1.204871	1.290571	1.417503
.375	1.144066	1.135914	1.142902	1.173916	1.233850
.417	1.132807	1.121538	1.116872	1.124648	1.145618
.458	1.120760	1.109091	1.100915	1.098967	1.102862
.500	1.107145	1.096629	1.087274	1.081812	1.078299
.542	1.097798	1.088054	1.079080	1.072052	1.065800
.583	1.093122	1.083373	1.074395	1.066972	1.059935
.625	1.087274	1.077128	1.068535	1.060717	1.053283
.750	1.021517	1.010113	0.999873	0.990409	0.981327
.917	0.859205	0.848298	0.838583	0.830066	0.821127
.958	0.798706	0.790526	0.783151	0.776198	0.768930

APPENDIX C

TABLE (C.14)

DATA ON CARBON OXIDATION.

(RUN NO. 75)

Air flow	=	250 cc/min.
Feed velocity (u_o)	=	0.1182 m/s.
Residence time (τ)	=	5.08 s.
Preheated feed temperature (T_o)	=	608 ^oK.
Velocity of propagation (W)	=	0.1131×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone		0.2662
Duration of reverse propagation	=	58 min.
Total regeneration period	=	250 min.
Initial carbon deposition	=	11.9 weight%.
Pressure gauge readings during run (psig)		P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 75)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.811357	0.811357	0.810949	0.812172	0.812987
.042	0.859606	0.861222	0.862432	0.862835	0.864045
.083	0.934136	0.937718	0.940899	0.941297	0.942887
.167	1.000007	1.000013	1.000064	1.000148	1.000342
.208	1.000012	1.000022	1.000101	1.000235	1.000721
.292	1.000037	1.000056	1.000121	1.000358	1.000955
.333	1.000096	1.000133	1.000316	1.000429	1.001444
.375	1.000132	1.000236	1.000423	1.000653	1.002632
.417	1.000189	1.000312	1.000518	1.000872	1.003813
.458	1.000256	1.000419	1.000920	1.001056	1.005389
.500	1.000310	1.000522	1.000662	1.004207	1.020338
.542	1.000980	1.004995	1.012473	1.019945	1.106755
.583	1.017193	1.027801	1.038396	1.071270	1.365772
.625	1.048193	1.061890	1.082202	1.480967	1.308310
.750	1.250064	1.302912	1.354971	1.287872	1.244660
.917	1.305225	1.307539	1.236939	1.157254	1.098577
.958	1.166556	1.169655	1.106755	1.042708	0.995537

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.812987	0.812987	0.811765	0.810542	0.810949
.042	0.864448	0.864448	0.863642	0.862432	0.862835
.083	0.943682	0.943682	0.943285	0.941695	0.942092
.167	1.000473	1.000866	1.004081	1.022904	1.033296
.208	1.000801	1.001193	1.005409	1.026626	1.048976
.292	1.001874	1.002660	1.005445	1.031727	1.098188
.333	1.002819	1.004293	1.015227	1.051325	1.363072
.375	1.004601	1.008932	1.027801	1.379276	1.285172
.417	1.009325	1.023088	1.119205	1.289414	1.241958
.458	1.024660	1.076738	1.333760	1.253152	1.217240
.500	1.085713	1.436830	1.260869	1.224580	1.196364
.542	1.329518	1.295585	1.240414	1.209124	1.183982
.583	1.375418	1.299827	1.241958	1.207577	1.181660
.625	1.313708	1.292500	1.239641	1.205644	1.178950
.750	1.221103	1.193656	1.165393	1.142125	1.120372
.917	1.057588	1.023481	0.994748	0.970254	0.949244
.958	0.960749	0.932146	0.907805	0.887375	0.870088

(RUN NUMBER 75)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.811357	0.811357	0.810949	0.811765	0.814616
.042	0.862432	0.863238	0.866060	0.891788	0.898200
.083	0.941695	0.943682	0.963126	1.037219	1.027016
.167	1.037219	1.091563	1.320649	1.295970	1.284401
.208	1.069317	1.452692	1.314865	1.321420	1.407073
.292	1.312166	1.251608	1.231146	1.217240	1.233850
.333	1.277072	1.216080	1.193269	1.179724	1.179337
.375	1.237325	1.195203	1.170817	1.157254	1.150662
.417	1.211829	1.180498	1.158805	1.145230	1.135526
.458	1.192108	1.165393	1.146394	1.132030	1.122704
.500	1.173529	1.149498	1.133195	1.119205	1.110258
.542	1.163456	1.139796	1.125425	1.111426	1.103251
.583	1.160743	1.137467	1.123093	1.109091	1.100915
.625	1.158029	1.135137	1.119983	1.107145	1.097798
.750	1.100525	1.078690	1.062672	1.047409	1.034473
.917	0.930154	0.912602	0.897399	0.883359	0.870491
.958	0.854764	0.840608	0.828442	0.817466	0.807280

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.819907	0.817466	0.817466	0.817466	0.817059
.042	0.898601	0.898200	0.895396	0.892590	0.889782
.083	1.020731	1.014440	1.006570	0.998691	0.991987
.167	1.243888	1.205258	1.174691	1.151825	1.134749
.208	1.331832	1.267814	1.225353	1.195590	1.173529
.292	1.353814	1.415571	1.314865	1.262413	1.221103
.333	1.207577	1.307539	1.435670	1.322963	1.260098
.375	1.151049	1.186304	1.274372	1.453466	1.323734
.417	1.128534	1.137079	1.166168	1.252380	1.483681
.458	1.114538	1.112593	1.119983	1.148334	1.230760
.500	1.102862	1.097798	1.096240	1.102472	1.129599
.542	1.098188	1.091173	1.086884	1.086104	1.093122
.583	1.095071	1.089223	1.082983	1.078299	1.077128
.625	1.090003	1.084153	1.076738	1.070098	1.065018
.750	1.027016	1.016013	1.006964	0.999085	0.991593
.917	0.859608	0.849511	0.840203	0.832095	0.824380
.958	0.799115	0.790526	0.783151	0.776602	0.770545

APPENDIX C

TABLE (C.15)

DATA ON CARBON OXIDATION.

(RUN NO. 76)

Air flow	=	260 cc/min.
Feed velocity (u_o)	=	0.123 m/s.
Residence time (τ)	=	4.882 s.
Preheated feed temperature (T_o)	=	608 ^oK.
Velocity of propagation (W)	=	0.125×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.23855
Duration of reverse propagation	=	50 min.
Total regeneration period	=	240 min.
Initial carbon deposition	=	11.9 weight%.

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 -2.

(RUN NUMBER 76)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.819500	0.820721	0.819094	0.818687	0.819500
.042	0.880547	0.881679	0.884564	0.884564	0.884966
.083	0.963126	0.969067	0.973420	0.974211	0.974211
.167	1.000057	1.000057	1.000057	1.000060	1.000060
.208	1.000098	1.000102	1.000110	1.000415	1.000120
.292	1.000342	1.000370	1.000378	1.005340	1.007196
.333	1.000843	1.000895	1.000897	1.009650	1.015083
.375	1.000870	1.000910	1.009346	1.013052	1.020405
.417	1.001450	1.004342	1.013766	1.015695	1.021052
.458	1.002678	1.009325	1.015423	1.019945	1.023481
.500	1.007432	1.009719	1.017193	1.020338	1.030549
.542	1.012563	1.017979	1.027409	1.033296	1.089613
.583	1.029373	1.039572	1.052500	1.069317	1.484844
.625	1.043302	1.072442	1.094681	1.178950	1.324891
.750	1.261255	1.300983	1.378505	1.307924	1.249678
.917	1.316408	1.319878	1.233850	1.174691	1.114538
.958	1.176239	1.180111	1.121149	1.056022	1.008145

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.819094	0.818280	0.818687	0.818280	0.818280
.042	0.884966	0.884564	0.884564	0.884564	0.884564
.083	0.974211	0.973815	0.974211	0.974211	0.974211
.167	1.000060	1.005958	1.021276	1.064395	1.078299
.208	1.000120	1.015613	1.028834	1.089613	1.113760
.292	1.015652	1.020979	1.025890	1.117261	1.328747
.333	1.020788	1.025743	1.063454	1.429871	1.298284
.375	1.029372	1.038788	1.170043	1.317950	1.258168
.417	1.030157	1.082202	1.357671	1.270129	1.228829
.458	1.045451	1.479029	1.284786	1.238869	1.204098
.500	1.146394	1.289414	1.237711	1.206418	1.178176
.542	1.333374	1.253152	1.210283	1.183595	1.160355
.583	1.316408	1.245818	1.202938	1.175465	1.152989
.625	1.285943	1.235394	1.197911	1.171205	1.149498
.750	1.209510	1.175852	1.147170	1.122316	1.100915
.917	1.067363	1.030157	0.998691	0.972233	0.949641
.958	0.970254	0.939706	0.914200	0.892189	0.873711

(RUN NUMBER 76)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.818280	0.818280	0.821941	0.827630	0.830472
.042	0.884163	0.896197	0.956784	0.959559	0.952023
.083	0.975397	1.056022	1.163068	1.136302	1.105587
.167	1.189013	1.334531	1.385451	1.454627	1.354200
.208	1.374646	1.317564	1.330675	1.427165	1.513178
.292	1.269357	1.236939	1.225353	1.228829	1.286715
.333	1.231533	1.202165	1.187852	1.181660	1.191722
.375	1.207964	1.179337	1.164618	1.155315	1.150274
.417	1.190561	1.164231	1.150662	1.140573	1.132030
.458	1.171592	1.148722	1.136690	1.126980	1.118039
.500	1.150274	1.130476	1.121149	1.112982	1.104419
.542	1.135914	1.118039	1.110647	1.103251	1.095850
.583	1.130865	1.113760	1.106366	1.099746	1.092342
.625	1.128534	1.112204	1.103641	1.096240	1.088054
.750	1.081032	1.063845	1.051717	1.041140	1.030157
.917	0.929756	0.912202	0.896998	0.883761	0.872101
.958	0.857187	0.843038	0.830878	0.819907	0.810134

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.831689	0.831284	0.830878	0.829660	0.828442
.042	0.943285	0.935330	0.928162	0.921784	0.916995
.083	1.082592	1.064627	1.049759	1.037611	1.028194
.167	1.297127	1.250450	1.217626	1.193656	1.175465
.208	1.389697	1.315636	1.272058	1.240800	1.216853
.292	1.426005	1.506186	1.385451	1.314865	1.268200
.333	1.255467	1.419049	1.510070	1.392786	1.314480
.375	1.169268	1.228829	1.374260	1.519396	1.400894
.417	1.133195	1.151437	1.202165	1.319107	1.524450
.458	1.113760	1.116483	1.132807	1.176239	1.285558
.500	1.099357	1.097019	1.099357	1.112982	1.149886
.542	1.090393	1.086884	1.084543	1.086494	1.097409
.583	1.086884	1.082592	1.078299	1.075567	1.076347
.625	1.082202	1.076738	1.071270	1.066581	1.063063
.750	1.020731	1.012080	1.003419	1.001450	0.999085
.917	0.861222	0.851128	0.842228	0.847084	0.850319
.958	0.801566	0.793391	0.786430	0.790116	0.792982

APPENDIX C

TABLE (C.16)

DATA ON CARBON OXIDATION.

(RUN NO. 77)

Air flow	=	270 cc/min.
Feed velocity (u_o)	=	0.128 m/s.
Residence time (τ)	=	4.701 s.
Preheated feed temperature (T_o)	=	608 ^oK.
Velocity of propagation (W)	=	0.150×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.2196
Duration of reverse propagation	=	46 min.
Total regeneration period	=	227 min.
Initial carbon deposition	=	11.9 weight%.

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 77)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.806872	0.808096	0.806056	0.806056	0.806056
.042	0.838583	0.839798	0.839798	0.839393	0.838988
.083	0.934205	0.936606	0.937805	0.907405	0.907405
.167	1.000008	1.000030	1.000776	1.000960	1.001354
.208	1.000018	1.000570	1.011473	1.011047	1.014834
.292	1.000042	1.002932	1.011620	1.012979	1.015159
.333	1.000092	1.004601	1.012080	1.014834	1.016013
.375	1.000133	1.006570	1.014047	1.016800	1.018766
.417	1.000176	1.010473	1.019945	1.023088	1.025838
.458	1.000266	1.010867	1.020338	1.023874	1.030157
.500	1.000356	1.011293	1.019159	1.023874	1.060326
.542	1.000995	1.015227	1.025052	1.034081	1.456175
.583	1.021517	1.032904	1.047018	1.086884	1.367701
.625	1.049759	1.063845	1.088054	1.608754	1.292885
.750	1.251608	1.309081	1.381978	1.298284	1.240028
.917	1.312552	1.315636	1.250064	1.170430	1.111815
.958	1.175078	1.178563	1.117261	1.054457	1.006964

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.805648	0.807280	0.807688	0.807280	0.807688
.042	0.838583	0.838988	0.839393	0.839798	0.841418
.083	0.907006	0.906606	0.907405	0.908205	0.914998
.167	1.002960	1.003565	1.004748	1.007357	1.233464
.208	1.014840	1.014940	1.017979	1.114149	1.327590
.292	1.015552	1.023874	1.239255	1.280158	1.264728
.333	1.016300	1.047409	1.335688	1.255467	1.223808
.375	1.023088	1.520562	1.296742	1.235780	1.204098
.417	1.052891	1.338387	1.259712	1.216467	1.191722
.458	1.695789	1.279001	1.226512	1.192882	1.173141
.500	1.303683	1.224967	1.190561	1.165393	1.149498
.542	1.251222	1.192882	1.164618	1.145230	1.130476
.583	1.236167	1.184756	1.156091	1.137467	1.123093
.625	1.229988	1.185143	1.156866	1.137079	1.121149
.750	1.197137	1.162681	1.133584	1.108312	1.086494
.917	1.065018	1.028587	0.997903	0.971046	0.946464
.958	0.969463	0.939706	0.914200	0.892189	0.872906

(RUN NUMBER 77)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.810949	0.810949	0.811357	0.812172	0.812987
.042	0.851128	0.863238	0.867672	0.869686	0.868880
.083	0.958370	0.973024	0.975397	0.973024	0.967879
.167	1.283629	1.247748	1.205644	1.166168	1.137855
.208	1.356900	1.427551	1.313323	1.244660	1.203325
.292	1.261255	1.304840	1.471666	1.435283	1.331832
.333	1.216853	1.221490	1.300598	1.487171	1.462370
.375	1.191335	1.186304	1.210283	1.310624	1.524061
.417	1.178176	1.169268	1.174691	1.206804	1.315636
.458	1.160355	1.152989	1.152989	1.163068	1.198684
.500	1.140573	1.098577	1.133195	1.135914	1.146394
.542	1.123482	1.122704	1.116094	1.116094	1.119205
.583	1.117261	1.035258	1.107534	1.105198	1.104030
.625	1.072052	1.104419	1.100136	1.095460	1.138774
.750	1.073223	1.059935	1.049368	1.039180	1.028587
.917	0.928162	0.905006	0.897399	0.883359	0.872101
.958	0.857590	0.843847	0.831689	0.820314	0.810542

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.813394	0.813394	0.811765	0.808503	0.808096
.042	0.867269	0.865254	0.863238	0.861222	0.858801
.083	0.961541	0.955990	0.951229	0.947655	0.943682
.167	1.116483	1.099746	1.086494	1.076347	1.067363
.208	1.173141	1.150662	1.132807	1.118816	1.107145
.292	1.274372	1.233077	1.204098	1.181273	1.161906
.333	1.366544	1.291343	1.252380	1.221490	1.195203
.375	1.465081	1.388925	1.331446	1.284015	1.245432
.417	1.571204	1.563398	1.453079	1.368473	1.310238
.458	1.354585	1.551700	1.616987	1.474766	1.379276
.500	1.176239	1.267428	1.468179	1.626406	1.485620
.542	1.121927	1.149408	1.219558	1.348800	1.502692
.583	1.098577	1.102083	1.125814	1.182434	1.287872
.625	1.084543	1.078690	1.082592	1.102472	1.148334
.750	1.016407	1.004995	0.994354	0.987251	0.983697
.917	0.861625	0.850724	0.838988	0.829254	0.821534
.958	0.801974	0.793800	0.783151	0.776602	0.770142

APPENDIX C

TABLE (C.17)

DATA ON CARBON OXIDATION.

(RUN NO. 78)

Air flow	=	240 cc/min.
Feed velocity (u_o)	=	0.1135 m/s.
Residence time (τ)	=	5.289 s.
Preheated feed temperature (T_o)	=	580 ^oK.
Velocity of propagation (W)	=	0.09×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.3309
Duration of reverse propagation	=	73 min.
Total regeneration period	=	275 min.
Initial carbon deposition	=	11.9 weight%.

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 78)

DISTANCE z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.812400	0.811977	0.811554	0.811554	0.812400
.042	0.835122	0.835551	0.835979	0.835979	0.835979
.083	0.895182	0.895606	0.897298	0.897298	0.896875
.167	0.972552	0.974641	0.977146	0.977980	0.977563
.208	0.991322	0.995069	0.997566	0.998398	0.998398
.292	1.002973	1.007960	1.011283	1.012529	1.012529
.333	1.003389	1.009207	1.012944	1.014189	1.014604
.375	1.009622	1.015434	1.019168	1.020827	1.020827
.417	1.017924	1.024144	1.028701	1.029944	1.030772
.458	1.019583	1.026216	1.031186	1.032842	1.034912
.500	1.019868	1.026630	1.032428	1.034498	1.045664
.542	1.026216	1.034498	1.041117	1.045664	1.120530
.583	1.040077	1.055163	1.065062	1.081534	1.468928
.625	1.080711	1.092224	1.109464	1.205397	1.370257
.750	1.319312	1.393702	1.524850	1.392489	1.321739
.917	1.398552	1.401382	1.326592	1.240734	1.176904
.958	1.249253	1.252497	1.184237	1.114383	1.063001

DISTANCE z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.811977	0.811554	0.811554	0.811554	0.811554
.042	0.835551	0.835122	0.835122	0.834694	0.834694
.083	0.896452	0.896028	0.895605	0.895605	0.895182
.167	0.977146	0.976728	0.975893	0.975893	0.975893
.208	0.997982	0.997566	0.997150	0.997150	0.999646
.292	1.012529	1.012529	1.013359	1.023729	1.097974
.333	1.014189	1.015019	1.021242	1.074949	1.486339
.375	1.021656	1.025801	1.059702	1.518765	1.382384
.417	1.034498	1.054337	1.265064	1.380767	1.323761
.458	1.054337	1.147528	1.381575	1.328615	1.286937
.500	1.125444	1.451122	1.318098	1.281673	1.250875
.542	1.421597	1.331850	1.278433	1.247631	1.222872
.583	1.353279	1.312435	1.265469	1.235053	1.210276
.625	1.355300	1.306366	1.261011	1.229776	1.204177
.750	1.300700	1.259389	1.218810	1.187901	1.161817
.917	1.129537	1.090580	1.056814	1.027873	1.002973
.958	1.023729	0.990905	0.963774	0.940302	0.919685

(RUN NUMBER 78)

DISTANCE z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.811130	0.811130	0.811977	0.812400	0.813670
.042	0.834694	0.834694	0.835979	0.840262	0.855223
.083	0.895606	0.896452	0.901952	0.918842	0.983821
.167	0.980067	0.996318	1.084002	1.522416	1.336298
.208	1.018753	1.099616	1.512276	1.382384	1.339128
.292	1.463666	1.333872	1.311221	1.307580	1.278838
.333	1.390064	1.306366	1.270331	1.256146	1.239111
.375	1.326188	1.281673	1.248442	1.227340	1.212715
.417	1.299900	1.256957	1.232618	1.211902	1.196856
.458	1.259795	1.230182	1.210683	1.193193	1.179348
.500	1.227746	1.200924	1.185051	1.170790	1.158552
.542	1.202957	1.179756	1.164673	1.152429	1.140989
.583	1.190751	1.169159	1.154470	1.142624	1.131583
.625	1.184644	1.164265	1.148345	1.135674	1.124215
.750	1.139354	1.117662	1.098795	1.083180	1.068771
.917	0.980901	0.961682	0.943661	0.928109	0.914203
.958	0.901952	0.886706	0.872265	0.859915	0.848817

DISTANCE z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.817088	0.820958	0.823536	0.826543	0.828260
.042	0.907025	0.901530	0.901107	0.902798	0.899414
.083	1.086881	1.036981	1.046491	1.034498	1.021656
.167	1.308794	1.442626	1.390872	1.319716	1.280053
.208	1.332254	1.390872	1.401786	1.479049	1.421597
.292	1.267900	1.268711	1.276408	1.315267	1.411489
.333	1.229776	1.227340	1.225715	1.234241	1.271952
.375	1.204177	1.200110	1.195228	1.194414	1.204177
.417	1.188309	1.184644	1.178534	1.172828	1.172420
.458	1.169567	1.163857	1.157328	1.152429	1.149570
.500	1.148345	1.143033	1.136492	1.130765	1.127900
.542	1.131174	1.125034	1.118891	1.113974	1.111514
.583	1.120939	1.114793	1.107823	1.102900	1.099616
.625	1.1144383	1.106593	1.099206	1.093045	1.088525
.750	1.055988	1.046904	1.036153	1.028287	1.020827
.917	0.900261	0.891369	0.879915	0.870564	0.862047
.958	0.838121	0.830834	0.822247	0.814093	0.807321

APPENDIX C

TABLE (C.18)

DATA ON CARBON OXIDATION.

(RUN NO. 79)

Air flow	=	280 cc/min.
Feed velocity (u_o)	=	0.1324 m/s.
Residence time (τ)	=	4.53 s.
Preheated feed temperature (T_o)	=	570 ^oK.
Velocity of propagation (W)	=	0.142×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.2218
Duration of reverse propagation	=	-
Total regeneration period	=	210 min.
initial carbon deposition	=	11.9 weight%.

Pressure gauge readings during run (psig) P.G1 - 3.; P.G2 - 2.

(RUN NUMBER 79)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.830985	0.830985	0.830547	0.831422	0.831422
.042	0.849337	0.849337	0.849337	0.849773	0.849337
.083	0.906145	0.906576	0.907439	0.907870	0.907439
.167	0.977702	0.979831	0.981534	0.981959	0.982385
.208	0.993439	0.996412	0.998110	0.998959	0.999383
.292	0.998110	1.002354	1.004050	1.004898	1.005746
.333	0.996412	1.001081	1.002778	1.004050	1.004474
.375	1.000657	1.005322	1.007442	1.008714	1.009561
.417	1.007866	1.013374	1.015914	1.017184	1.018031
.458	1.010332	1.016338	1.019300	1.020569	1.022684
.500	1.011256	1.017607	1.020992	1.023107	1.031137
.542	1.020569	1.027335	1.031982	1.035782	1.095065
.583	1.042955	1.050962	1.058961	1.071574	1.633548
.625	1.079132	1.089199	1.104275	1.170985	1.407459
.750	1.327637	1.423088	1.578458	1.443245	1.354393
.917	1.413217	1.418975	1.349043	1.264153	1.201282
.958	1.264566	1.270344	1.205013	1.135602	1.084586

(RUN NUMBER 79)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.831860	0.831860	0.832298	0.832736	0.831860
.042	0.849773	0.850210	0.851082	0.851517	0.851953
.083	0.908732	0.910025	0.911317	0.912610	0.913902
.167	0.996412	1.002354	1.006594	1.009137	1.009985
.208	1.042533	1.049277	1.051805	1.052226	1.050962
.292	1.223234	1.194234	1.171400	1.154349	1.139771
.333	1.391418	1.311163	1.263740	1.230268	1.202111
.375	1.498818	1.466701	1.394708	1.337107	1.288082
.417	1.314459	1.584247	1.609498	1.484814	1.397587
.458	1.261676	1.320225	1.538807	1.693873	1.522309
.500	1.231923	1.242673	1.304571	1.483579	1.747405
.542	1.211641	1.210813	1.216197	1.274058	1.412394
.583	1.202111	1.195478	1.185106	1.199624	1.255068
.625	1.197966	1.184690	1.170569	1.167660	1.183030
.750	1.157678	1.139354	1.118490	1.108458	1.103020
.917	0.999808	0.982385	0.964912	0.961497	0.958935
.958	0.920788	0.905282	0.891894	0.889732	0.887135

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.831422	0.831860	0.831860	0.831860	0.831422
.042	0.849337	0.849773	0.849773	0.849773	0.849773
.083	0.907439	0.907439	0.907439	0.907439	0.907870
.167	0.982385	0.982385	0.982385	0.982810	0.987064
.208	0.999383	0.999383	0.999808	1.002778	1.021838
.292	1.006170	1.006594	1.015068	1.092551	1.308279
.333	1.005322	1.007442	1.057278	1.470405	1.400055
.375	1.010409	1.024798	1.575150	1.379900	1.318578
.417	1.023107	1.111385	1.380312	1.321461	1.290969
.458	1.049277	1.524371	1.332167	1.289732	1.264566
.500	1.207499	1.353158	1.285608	1.261263	1.240193
.542	1.389772	1.300038	1.254655	1.238126	1.219923
.583	1.370439	1.291793	1.248046	1.230682	1.213298
.625	1.353570	1.289320	1.248459	1.228200	1.210399
.750	1.303334	1.258785	1.222820	1.199624	1.176386
.917	1.151019	1.109713	1.074934	1.045906	1.020992
.958	1.043798	1.010409	0.981959	0.958935	0.938393

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.832298	0.830547	0.830109	0.829671	0.827945
.042	0.852389	0.851953	0.851953	0.851953	0.851953
.083	0.914763	0.914763	0.914763	0.914763	0.914332
.167	1.010409	1.009561	1.008714	1.007866	1.006170
.208	1.048856	1.046327	1.043798	1.041268	1.038314
.292	1.126424	1.114312	1.103857	1.094646	1.087103
.333	1.177632	1.156846	1.140188	1.126007	1.114312
.375	1.247632	1.215369	1.189670	1.169738	1.153100
.417	1.331343	1.283959	1.248872	1.221993	1.200453
.458	1.418153	1.353570	1.309103	1.274883	1.246806
.500	1.535507	1.442423	1.384014	1.338753	1.302098
.542	1.578044	1.573910	1.511179	1.442011	1.387304
.583	1.371262	1.585902	1.592522	1.565231	1.516537
.625	1.231095	1.321872	1.487697	1.633963	1.631473
.750	1.099671	1.099253	1.104275	1.119743	1.150603
.917	0.954661	0.950385	0.945677	0.940965	0.937107
.958	0.883671	0.879772	0.875869	0.872398	0.868489

APPENDIX C

TABLE (C.19)

DATA ON CARBON OXIDATION.

(RUN NO. 80)

Air flow	=	250 cc/min.
Feed velocity (u_o)	=	0.1182 m/s.
Residence time (τ)	=	5.08 s.
Preheated feed temperature (T_o)	=	620 ^oK.
Velocity of propagation (W)	=	0.145×10^{-3} m/s.
Fraction of carbon regenerated during reverse propagation of the reaction zone	=	0.2273
Duration of reverse propagation	=	53 min.
Total regeneration period	=	230 min.
Initial carbon deposition	=	11.9 weight%.

Pressure gauge readings during run (psig) P.G1 -3.; P.G2 - 2.

(RUN NUMBER 80)

DISTANCE Z	time= 0 Φ	time= 5 Φ	time= 10 Φ	time= 15 Φ	time= 20 Φ
.000	0.789255	0.790455	0.790455	0.790455	0.790455
.042	0.831086	0.831483	0.833069	0.833465	0.833862
.083	0.902769	0.904725	0.907462	0.908244	0.908244
.167	0.987474	0.994806	1.000204	1.000745	1.000745
.208	1.000042	1.000067	1.000220	1.002142	1.012911
.292	1.000213	1.000375	1.003295	1.005600	1.016753
.333	1.000204	1.000603	1.007528	1.007836	1.020989
.375	1.001745	1.001758	1.007528	1.008220	1.021758
.417	1.006753	1.007144	1.013295	1.015600	1.024137
.458	1.004057	1.014067	1.015836	1.018526	1.025216
.500	1.007891	1.017908	1.018682	1.019759	1.026369
.542	1.008047	1.018678	1.019221	1.026220	1.076551
.583	1.012527	1.024063	1.033281	1.048237	1.439763
.625	1.039036	1.053600	1.069671	1.148916	1.310592
.750	1.234195	1.285257	1.382112	1.293576	1.233438
.917	1.287526	1.294332	1.229275	1.148536	1.089151
.958	1.149676	1.152334	1.093729	1.029825	0.983226

(RUN NUMBER 80)

DISTANCE Z	time= 50 Φ	time= 55 Φ	time= 60 Φ	time= 65 Φ	time= 70 Φ
.000	0.791255	0.791255	0.792855	0.798849	0.804836
.042	0.834654	0.837032	0.867444	0.919958	0.942542
.083	0.910198	0.924248	1.095255	1.146637	1.150815
.167	1.046321	1.411296	1.291307	1.334420	1.416227
.208	1.448882	1.333285	1.282232	1.286769	1.324585
.292	1.259541	1.245546	1.217920	1.208075	1.206182
.333	1.225491	1.203909	1.183826	1.173967	1.167897
.375	1.205803	1.181172	1.162585	1.153474	1.146637
.417	1.193301	1.169035	1.151195	1.142837	1.136376
.458	1.173587	1.151575	1.134856	1.127249	1.120781
.500	1.148916	1.128771	1.113928	1.107453	1.102118
.542	1.130292	1.112024	1.097924	1.090677	1.086479
.583	1.122303	1.104405	1.090296	1.082662	1.077697
.625	1.118878	1.101356	1.086098	1.077315	1.069671
.750	1.067377	1.049004	1.032513	1.019067	1.007908
.917	0.909807	0.892195	0.876493	0.862716	0.851273
.958	0.837032	0.823147	0.810815	0.799648	0.790055

DISTANCE Z	time= 25 Φ	time= 30 Φ	time= 35 Φ	time= 40 Φ	time= 45 Φ
.000	0.790455	0.790455	0.790455	0.790455	0.790455
.042	0.833862	0.833862	0.833862	0.833862	0.834258
.083	0.908244	0.908244	0.908244	0.908244	0.908635
.167	1.000745	1.000975	1.000975	1.001360	1.004828
.208	1.020526	1.021758	1.021758	1.023295	1.040954
.292	1.020753	1.022453	1.029057	1.083425	1.345770
.333	1.021373	1.022526	1.040954	1.419262	1.308701
.375	1.022911	1.029057	1.148536	1.318534	1.266349
.417	1.030977	1.063170	1.358636	1.274291	1.240627
.458	1.042871	1.503718	1.276938	1.239492	1.211862
.500	1.105929	1.291307	1.228897	1.203530	1.180414
.542	1.320803	1.251977	1.201636	1.177001	1.156891
.583	1.327989	1.248950	1.195575	1.168277	1.147017
.625	1.295845	1.241384	1.192164	1.164482	1.141317
.750	1.202394	1.168656	1.136756	1.110882	1.089151
.917	1.043638	1.007523	0.977042	0.950699	0.929314
.958	0.946039	0.916837	0.891803	0.870200	0.852853

DISTANCE Z	time= 75 Φ	time= 80 Φ	time= 85 Φ	time= 90 Φ	time= 95 Φ
.000	0.810416	0.812408	0.814000	0.813602	0.811611
.042	0.941765	0.930871	0.919958	0.910198	0.901986
.083	1.123825	1.090296	1.063935	1.044405	1.027137
.167	1.460288	1.389689	1.331394	1.284122	1.239492
.208	1.412434	1.485414	1.502573	1.428371	1.339716
.292	1.223220	1.272400	1.353338	1.431788	1.499903
.333	1.169794	1.185342	1.226248	1.285257	1.380597
.375	1.143217	1.145117	1.159548	1.189512	1.238736
.417	1.130673	1.128010	1.129912	1.143217	1.166379
.458	1.115832	1.110882	1.109358	1.112786	1.122303
.500	1.096780	1.091440	1.089151	1.089151	1.092203
.542	1.081516	1.075022	1.073494	1.071965	1.072347
.583	1.072729	1.065465	1.062787	1.060491	1.058960
.625	1.064317	1.055898	1.051685	1.048621	1.045555
.750	0.997505	0.987088	0.978589	0.972014	0.967756
.917	0.839804	0.829499	0.820762	0.812408	0.810815
.958	0.781644	0.773619	0.765579	0.759195	0.757612