THERMAL BEHAVIOUR OF A FIXED BED REACTOR

A THESIS

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BY

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CERTIFICATION OF THESIS WORK

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The author would like to dedicate this thesis work to the departed soul of his beloved wife, **SHABINA KAMRUN NAHAR FOARA**, who expired at 5.40 pm on July 11, 1992.

SUMMARY

Knowledge of the thermal behaviour of a fixed bed reactor is important to predict responses to changes in feed conditions, for control purposes, for planning start-ups and shut downs and to evaluate changes in operating conditions in case of the necessity to vary product quality and so forth.

An extensive literature survey on experimental systems was done for fixed bed reactor and for the mechanisms and kinetics of methanation reaction. A fixed bed reactor system with adequate provisions was erected so that the system could be used for any solid catalyzed gas phase reaction. The equipment worked satisfactorily and a large amount of data were taken at various conditions of operation.

The thermal behaviour was studied at steady state at different operating conditions of temperatures, carbon oxides concentrations and nitrogen flow rates. The reactor showed generally acceptable pattern of temperature profiles. At lower inlet temperature and higher inlet concentration the reactor showed the profile with down ward trend. But at higher inlet temperature the reactor overcame this peculiarity. At low inlet temperature, conversion of carbon oxides varies inversely with inlet concentration. At higher inlet temperature, there was no effect of inlet concentration on theconversion. At lower space velocity the reactor showed the higher temperature profile.

For kinetic studies of the methanation reaction, an isothermal fixed bed reactor was designed by immersing the reactor in a fluidized sand bath. However, the data were not analyzed to obtain a rate equation for the reaction because isothermal condition could not be achieved in the experiments. However, all data have been presented in the appendices.

The dynamic experiments were carried out by introducing step disturbances in concentrations and flowrates. The dynamic behaviour was followed by taking measurements of the transient temperature profiles in a non-isothermal fixed bed reactor. The results showed general agreement with information available in the literature.

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At last but not the least, his recently departed wife, FOARA, for her constant encouragement and great patience during the thesis work and his little daughter, NOYON, for making a pleasant atmosphere at home.

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CHAPTER 1

INTRODUCTION

The interest in the research on the fixed bed reactor stems from its industrial importance. The objective of the present work was to carry out experimental work at different conditions of operation both at steady and unsteady states and evaluate the thermal behaviour of the fixed bed reactor. Experiments were also conducted to establish the kinetics of the test reaction. The literature review includes a study on the significant features in modeling the reactor.

Fixed bed reactors are ubiquitous in the chemical industry. This reactor consists of a cylindrical tube filled with catalyst pellets. They are regarded as the work horse of the chemical industry with respect to the number of reactors employed and the economic value of the materials produced. The types of processes carried out in such reactors include primary and secondary reforming, methanation, synthesis of ammonia, sulphuric acid or methanol, and the production of ethylene oxide, ethylene dichloride, vinylacetate, butadiene, malic anhydride, phthalic anhydride, cyclohexane and styrene. It is self evident why the focus of so much reaction engineering research and development is in this immediate area. Fixed bed reactors are extensively used in laboratory studies because of ease of operation and relative simplicity of design and construction. For kinetic studies, differential reactors have been preferred because of its advantage of ensuring isothermal operation and easy interpretation of data. Isothermal operation of this reactor is ensured by putting the reactor in a high heat transfer environment such as fluidized sand bath, molten salt, forced air circulated oven, etc. Integral reactors have not been favoured as it is difficult to keep these reactors isothermal.

In laboratories most of the reactors are operated at atmospheric pressure while much higher pressures are used in industries. Operation at low pressures is often sufficient to characterize the fixed bed reactor behaviour. Adiabatic condition of operation in the laboratory is maintained by enclosing the reactor in a vacuum environment or by putting compensating heaters around the reactor to take care of the heat loss to the surroundings. The reactor axial temperatures are measured by placing thermocouple or by using a travelling thermocouple in a thermowell. Temperatures are often measured in the transverse direction to find out radial gradient in temperature or to test the adiabicity of operation.

An extensive survey of the literature was undertaken to arrive at the design of two experimental systems to investigate the methanation reaction in isothermal and adiabatic conditions. The development of satisfactory steady state and dynamic models for fixed bed reactors is important for a number of reasons:

a) Design, simulation and optimization of steady state reactors.

b) Design of control systems for the reactors.

c) Since the optimum of reactor performance is often near constraint boundaries imposed by the strength of the construction materials, catalyst deactivation, safety considerations, etc., the optimization is only feasible when good dynamic models for reactors are available.

d) The transient behaviour of a reactor should be known in sufficient detail for start-ups, shut-downs and changes in operating conditions caused by changes of feed or dictated by the necessity to vary product quality.

e) In some processes, catalyst activity declines relatively rapidly; this requires cyclic operation with attendant dynamic changes in concentration and temperature profiles during production and regeneration periods.

Methanation, hydrogenation of carbon oxides by nickel based catalysts, has been used as the test reaction. The reaction is by itself industrially important, being the final purification step of process gas for the manufacture of hydrogen and ammonia synthesis gas. The reaction also has a potential in the production of gaseous fuel from solid carbonaceous sources. In addition, the reaction provides an ideal exothermic system for the study of the characteristics of fixed bed reactors under varying conditions of exothermicity depending on the concentration of carbon oxides.

It was desired that the present work would involve experimental work to study the behaviour of the fixed bed reactors experimentally. The work emphasized the thermal behaviour because it is often the thermal response of the system which is of paramount importance in the control, stability and operability of these reactors.

Literature survey over a wide range of books and papers is presented in chapter 2. Mechanisms of the test reaction, kinetics of the test reaction and reactor modeling have been surveyed.

The development of experimental facilities used in this project is detailed in chapter 3. This has been done by constructing suitable laboratory reactors for adiabatic operation and isothermal operation.

In chapter 4, the results obtained during the evaluation of the capabilities of the experimental systems developed in the project are presented and discussed.

Computer programs are developed for calculation of gas analysis of gas chromatograph integrator data for adiabatic steady and unsteady state and isothermal conditions.

CHAPTER 2

LITERATURE SURVEY

2.1 Mechanism of CO methanation

The mechanism of hydrogenation of carbon monoxide to higher hydrocarbons has been the subject of an intensive study for many years. Somewhat surprisingly, relatively little work has been done on the methanation reaction and the arguments for and against various pathways have been mentioned elsewhere (Vannice, 1982). The different pathways can conveniently be divided into two general groups: one which involves hydrogenation of adsorbed CO prior to the rupture of the CO bond, and the other in which CO first dissociates to produce surface carbon which is then hydrogenated.

Vlasenko and Yuzefovich (1969) point out that the methanation reaction offers special opportunities for study since it is the simplest reaction of the series (Mills and Steffgen, 1973). The mechanism of hydrogenation of CO has been examined particularly under conditions of the Fischer-Tropsch reaction in which hydrocarbons higher than methane are formed. Here, in contrast to methane synthesis, the mechanism of chain growth is of great importance. However, despite this consideration and the fact that somewhat different catalysts are used to optimize higher hydrocarbon formation, many considerations in Fischer-Tropsch synthesis are believed applicable to the mechanism of methane synthesis.

One of the earliest proposals for hydrocarbon synthesis was the carbide theory proposed by Fischer and Tropsch. The carbide theory in its simplest form postulates that adsorbed carbon monoxide is reduced to surface carbide. The surface carbide was believed to be hydrogenated and the adsorbed methylene radicals polymerize and desorb as olefinic and paraffinic hydrocarbons. Craxford and Rideal (1939) gave a more detailed version of the carbide hypothesis, especially with respect to chain growth. The carbide hypothesis was originally based on the observation that the chief Fischer - Tropsch catalysts - iron, cobalt and nickel react with carbon monoxide to form bulk carbides and that these carbides can react with hydrogen to form hydrocarbons. The carbide theory was subsequently found to be inadequate to explain hydrocarbon synthesis by metals of the iron group. Other theories of methanation, in addition to the carbide theory, have included schemes in which oxygenated compounds such as methanol or formaldehyde are intermediates. But attempts to detect formaldehyde or methanol in the synthesis of methane on a nickel catalyst were unsuccessful. Moreover, when methanol is used as a starting material over a cobalt catalyst, it was shown that the yield of hydrocarbons is less than that obtained when a mixture of carbon monoxide and hydrogen is used.

An early suggestion put forward was that a metal carbonyl is first formed which is then reduced with the formation of methane.

Several workers have concluded that synthesis based on CO and H_2 involves the production of an unstable intermediate complex, containing C,H, and O atoms, which is the precursor of both hydrocarbons and alcohols.

At present, two related mechanisms deserve special consideration. Both involve the concept of initial formation of a HCOH surface complex but differ in subsequent steps. One mechanism involves methylene radical intermediates and emphasizes electronic charge or polarization factors.

Vlasenko and yuzefovich (1969) conclude that the most probable scheme for the mechanism of the reduction of carbon monoxide to methane on nickel, cobalt, and possibly iron catalysts is

$$[\quad] + e + H_2 \longrightarrow [H_2]\ - \qquad (7)$$

$$[\quad] + CO \longrightarrow [CO]^+ + e \qquad (8)$$

$$[CO]^+ + [H_2]^- \longrightarrow [HCOH]^+ + e(\text{Slow stage}) + [\quad] \qquad (9)$$

$$[HCOH]^+ + [H_2]^- \longrightarrow [CH_2] + H_2O + [\quad] \qquad (10)$$

$$[CH_2] + [H_2]^- \longrightarrow CH_4 + e + 2\,[\quad] \qquad (11)$$

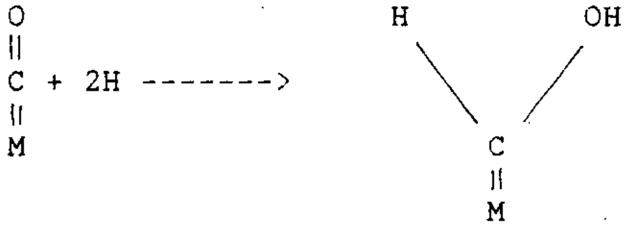
The symbol [ ] denotes a vacant active center on the catalyst surface. The symbols in square brackets represent adsorbed species. For the synthesis of higher hydrocarbons, the fifth stage of this scheme is not the reaction of methylene radicals with hydrogen, but their polymerization.

Orlov's suggestions (1908) that methylene radicals are formed in the primary stages of the hydrogenation of carbon monoxide was believed verified experimentally by the existence of CH_2 radicals in the methylation of benzene to toluene. Evidence was obtained that CH_2 species are formed from carbon monoxide and hydrogen. On the basis of the results obtained, Eidus concluded that on cobalt and nickel catalysts the primary stages of the process involves the successive hydrogenation of carbon monoxide, first to an unstable oxygen-containing group, and then to a methylene radical. Eidus (1967) has provided a recent review of his views on the mechanism of the Fischer - Tropsch reaction.

Hamai (1941) proposed a similar mechanism having an intermediate oxygenated complex, OH-C-M, which is reduced to $M-C-H_2$ groups. The $M-CH_2$ groups, in the adsorbed state, polymerize to long-chain hydrocarbons on the surface. Hamai concluded that, except at the highest temperatures, methane formation did not occur at the catalyst surface.

Storch, Golumbic, and Anderson (1951, 1959) have proposed a different mechanism for the Fischer-Tropsch reaction based on oxygenated intermediates as shown below. They assumed that (1) hydrogen is adsorbed as atoms on the surface of the metal, (2) chemisorption of carbon monoxide occurs on metal atoms with bonding similar to that in metal carbonyl, and (3) adsorbed carbon monoxide is partly hydrogenated according to Equation (12).

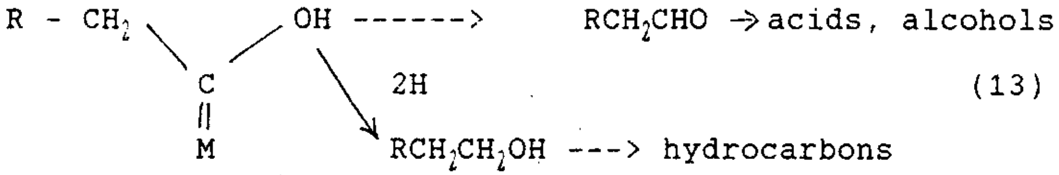
Initiation of chain:



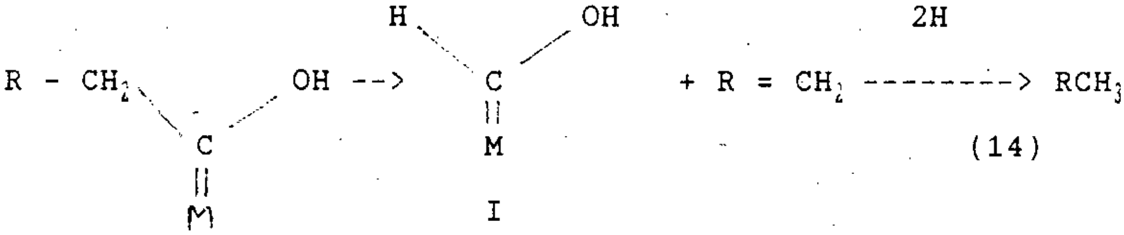
(12)

I

Termination of chain:

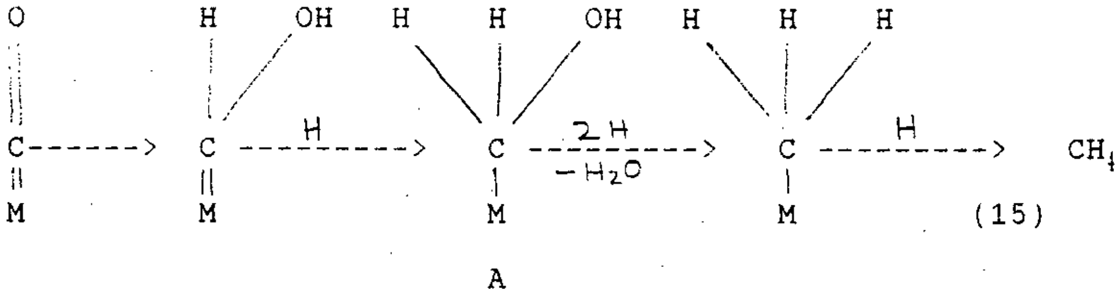


(13)



(14)

While the overall scheme proposed describes details of chain growth not applicable to methane synthesis, the initiation and termination steps are pertinent for the mechanism of the hydrogenation of carbon monoxide to methane. As shown in reactions (13) and (14), termination products are aldehydes, alcohols, and olefine but not paraffins. The complex. I has been questioned since IR spectra do not indicate a M = C bond but this does not fundamentally change the picture. For methane synthesis it is proposed that this reaction scheme may be modified to become:



(15)

In this scheme Intermediate A would form alcohol under certain circumstances and under other conditions would produce methane. The reversible dissociative sorption of methane on nickel (the reverse of the last step) was demonstrated many years ago.

Vannice (1976) postulated that the reaction occurred between molecularly absorbed carbon monoxide and hydrogen via C/H/O intermediates. Chen and et. al (1990) mentioned more recent evidence (Ponce, 1978; Happel et al., 1980; McCarty and Wise, 1979; Goodman et. al., 1980; Zagli et al., 1979), dissociative adsorption of carbon monoxide and hydrogen followed by reaction between surface carbon and hydrogen atom via CH_x- species appears to be more likely. For the latter mechanism, some researchers proposed hydrogenation of surface carbon was the rate determining step and others proposed that is proportionation of CO was. Recently two models are generally accepted. Ho and Harriot (1980) suggested that the limiting step might be the surface reaction between adsorbed carbons monoxide and hydrogen atom to form carbon and water ($CO^* + 2H^* \text{------>} C^* + H_2O$). Klose and Barens (1984) suggested that the limiting step was the hydrogenation of surface carbon to carbon species (CH_2^*) involving two adsorbed hydrogen and the surface carbon ($C^* + 2H^* \text{--->} CH_2^*$).

The latter model was preferred in this study for two reasons. The first reason is that it will be a problem to explain the deactivation of most methanation catalysts by deposited carbon. It may be better explained if the hydrogenation of surface carbon is slow and then some of active deposited carbon will become unreactive. The other reason is that adsorbed carbon monoxide it self can be easily dissociated under reaction temperature. Thompson Jr. and et. al (1989) stated that the first type of mechanism (Bell 1981) assumes the associative adsorption of CO. This mechanism allows for oxygenate formation, but does not directly account for the production of CO_2. The production of CO_2 has often been attributed to the water gas shift reaction. The following equations summarize the most important elementary reaction steps.

$$CO + * \xrightleftharpoons{k_{CO}} CO^*$$

$$H_2 + 2* \xrightleftharpoons{k_{H_2}} 2H^*$$

$$CO^* + H^* \xrightleftharpoons{k_1} HCO^* + *$$

$$HCO^* + H^* \xrightleftharpoons{k_2} HCHO^* + * \qquad \text{(r.d.s.)}$$

$$HCHO^* + H^* \xrightleftharpoons{k_3} CH^* + H_2O^*$$

$$CH^* + H^* \xrightleftharpoons{k_4} CH_2^* + *$$

$$CH_2^* + H^* \xrightleftharpoons{k_5} CH_3^* + *$$

$$CH_3^* + H^* \xrightleftharpoons{k_6} CH_4^* + *$$

$$CH_4^* \xrightleftharpoons{k_{-CH_4}} CH_4 + *$$

$$H_2O^* \xrightleftharpoons{k_{-H_2O}} H_2O + *$$

The latter type of mechanism suggested by Klose and Baerns (1984) is described as follows:

$$CO + 2^* \xrightleftharpoons{K_{CO}} C^* + O^*$$

$$H_2 + 2^* \overset{K_{H_2}}{=\!=\!=\!=\!=\!=} H^* + H^*$$

$$C^* + 2H^* \xrightarrow{k_{CH_2}} CH_2^* + 2^* \qquad \text{(r.d.s.)}$$

$$CH_2^* + 2H^* \xrightarrow{k_{CH_4}} CH_4 + 3^*$$

$$O^* + 2H^* \xrightarrow{k_{H_2O}} H_2O + 3^*$$

Carbon monoxide and hydrogen are dissociatively adsorbed and equilibrium is established. Interaction of surface carbon and adsorbed hydrogen to a carbene species is the rate determining step. Subsequently, the carbine intermediate is quickly hydrogenated to methane. Surface oxygen reacts to water in a similar manner as carbon formation. Until recently most authors seemed to prefer the view that the first group of mechanism involving some aldehydic or enolic surface intermediate is the more probable (Sachtler, 1980). This preference was based metal carbides to methane and the Boudouard reaction,

$$2\ CO \text{ ------> } C + CO_2$$

is known to be rapid only at much higher temperatures, which suggested that both the dissociation of CO and the hydrogenation of carbon are too slow to be intermediate steps in the methanation reaction. However, these arguments do not rule out the possibility that the formation of the "surface carbide" C_{ads} and its subsequent hydrogenation to CH_4 are fast enough to be preferred pathway for the formation of methane on the surface of a nickel catalyst. Indeed, in 1948, Kummer et al. had shown that labelled surface carbides can yield labelled methane under the conditions of the Fischer-Tropsch synthesis. The problem was recently reinspected by Wentruk, Wood and Wise in Stanford, by Araki and Ponec in Leiden, and by Rabo, Risch and Rabo at Union Carbide. The stanford group observed that on an alumina - supported Ni catalyst, the reaction

$$2CO \text{ ------> } C_{ads} + CO_2$$

occurs at a detectable rate at temperatures as low as 350^0K.

In pulse experiments at 553^0K CO was rapidly converted to Cads + CO_2. Subsequent pulses of hydrogen at the same temperature rapidly converted the C_{ads} quantitatively to CH_4. The stanford workers conclude that the dissociative chemisorption of CO on nickel provides an energetically possible mechanism for methanation and they stress that the surface carbon species, unlike Ni_3C, is reactive towards hydrogenation.

Ponec (1978) also found that disproportionation of CO to C_{ads} and CO_2 can be rapid. On nickel films exposed to low pressures of CO + H_2 the first product observed in the gas phase was actually CO_2, while CH_4 formation appeared to be preceded by an induction period. Which means that this CO_2 was not formed by water gas shift reaction. Evidently it was formed by disproportionation:

$$2\ CO \text{-------}> C_s + CO_2$$

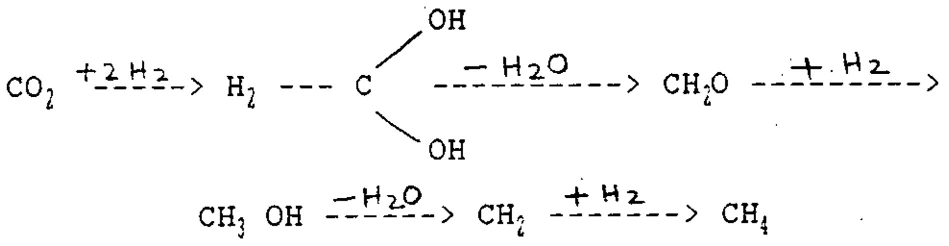
by which C_s was successively deposited and accumulated on the surface. The rate of CH_4 formation increased in the course of the reaction. Since dissociation of CO is thus demonstrated to occur under the conditions of CO hydrogenation on these film the pertinent question is: which adsorbed species is faster converted to methane, C_{ads} or CO_{ads}? To answer this question, the authors covered their film with labelled $^{13}C_{ads}$ obtained by pretreatment with ^{13}CO and exposed this film to a gas mixture of $5H_2$ + ^{12}CO at 77 pa and 523 K. It was found that initially much more $^{13}CH_4$ than $^{12}CH_4$ was formed, indicating that under these conditions methane formation via dissociation of CO seems to be thepreferred pathway. The same conclusion was drawn by Rabo et al. who found that C_{ads} on Ni is readily hydrogenated to CH_4 even at room temperature where CO + H_2 would not be converted to methane. For CO and Ru films it was observed by Sachtler and et al. (1979) that predeposited ^{13}C is hydrogenated to $^{13}CH_4$, but this carbon also undergoes a deactivation.

2.2 MECHANISM OF CO_2 METHANATION

The hydrogenation of CO_2 to methane has not been investigated extensively. Catalysts which bring about methanation of CO_2 are in general those active in methanation of CO.

Two mechanisms of methanation of carbon dioxide have been discussed in the literature (Mills and Steffgen, 1973). One of these was proposed by Bahr (1929), who considers that the methanation of CO_2 occurs with the intermediate formation of CO. This idea is supported in studies of Ru and Fe group of catalysts. Other evidence strongly indicates that the mechanism does not proceed through intermediate formation. In the presence of Ni (nickel) and cobalt catalysts it has been shown that CO_2 is converted only into CH_4 and the formation of small quantities of higher hydrocarbons was detected only in some instances when iron-cobalt and copper-cobalt catalysts where used. If has also been shown that CO_2 is not hydrogenated in the presence of significant amount of CO and does not influence the transformation of the latter.

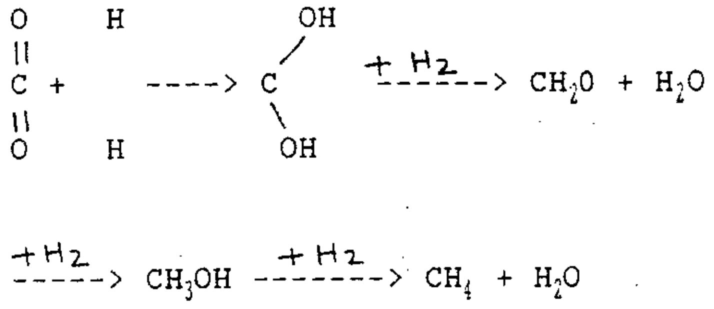
Medsford (1923) proposed the mechanism of CO_2 methanation without intermediate CO formation as the following way:



$$CO_2 \xrightarrow{+2H_2} H_2\ \text{---}\ C\begin{matrix}\diagup OH\\ \\ \diagdown OH\end{matrix} \xrightarrow{-H_2O} CH_2O \xrightarrow{+H_2}$$

$$CH_3\,OH \xrightarrow{-H_2O} CH_2 \xrightarrow{+H_2} CH_4$$

This mechanism was further developed by Pichler (1943) who proposed the following sequence:



$$\begin{matrix}O\\ \|\\ C\\ \|\\ O\end{matrix} + \begin{matrix}H\\ \\ \\ \\ H\end{matrix} \longrightarrow C\begin{matrix}\diagup OH\\ \\ \diagdown OH\end{matrix} \xrightarrow{+H_2} CH_2O + H_2O$$

$$\xrightarrow{+H_2} CH_3OH \xrightarrow{+H_2} CH_4 + H_2O$$

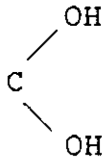
Vlasenko and Yuzefovich (1969) conclude that kinetic data cannot confirm a particular mechanism directly, and that evidence by independent method is required. They found from weighing experiments that there is no significant adsorption of CO_2 and the product of its transformation. Further, when a mixture of H_2 and CO_2 was introduced to the untreated catalyst, the work function remain unchanged relative to that in an atmosphere of hydrogen. This was taken to indicate that adsorption of CO_2 and the formation complexes influencing the electronic structure of the catalyst does not take place on the surface of the catalyst containing dissolved hydrogen. They conclude that recent experimental results refute the suggestion that the start of formation of CH_4 from CO_2 on nickel catalysts is preceded by the adsorption of both components of the reaction, and indicate that hydrogen adsorbed on the catalyst surface reacts with molecules of carbon dioxide in the gas phase.

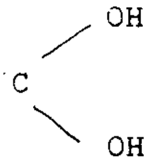
From such considerations, Vlasenko and Yuzefovich (1969) conclude that the most probable scheme for the methanation of CO_2 appears to be one in which the formation of complexes of a type corresponding to the enol form of formaldehyde takes place initially, and in which the subsequent transformations are analogous to the stages in the hydrogenation of CO, but with the significant difference that in the reduction of CO_2 these changes take place not on the catalyst surface, but in the volume of the gas.

The mechanism proposed by Vlasenko and Yuzefovich (1969) is:

$$2\ [\ ] + 2e + H_2 \text{------>} 2[H]^-$$

$$2\ [H]^- + CO_2 \text{---------->} [HCOOH] \text{---->} 2[\ ]$$

$+$  $+ 3e$ (slow)

 $+ H_2 \text{------>} HCOH + H_2O$

$$H - C - OH + H_2 \text{------>} CH_2 + H_2O$$

$$CH_2 + H_2 \text{-------->} CH_4$$

According to this scheme, the process is initiated by the activation of only the hydrogen on the catalyst surface, after which the reaction takes place in the gas volume. Mills and steffgan (1973) questioned this mechanism and concluded that the mechanism of CO_2 methanation is uncertain and that this would be a fruitful field for investigation.

In addition to the direct mechanism of CO_2, there is evidence that CO_2 is removed by the reverse water-gas-shift reaction, by conversion to carbon monoxide

$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$

If a catalyst is tested with carbon dioxide, with no carbon monoxide in the inlet gas, a trace of carbon monoxide is found in the exit gas, indicating the occurrence of the above reaction.

There have been a number of investigations on the hydrogenation of CO and CO_2 together (Seglin and et. al, 1975); it was concluded that CO_2 is not hydrogenated in the presence of CO. Such a conclusion might me erroneous because it does not take into account that simultaneous with CH_4 formation is the formation of water which reacts with CO to make CO_2 by water-gas shift reaction. This leads to the observation that the CO_2 concentration, instead of decreasing, may actually increase or at best maintain steady until the CO is substantially consumed. Thus only at low concentrations of CO would CO_2 reduction to methane be observed.

2.3 Mechanistic Rate Equation

Chen and Wu (1990) used the complete mechanism suggested by Klose and Baerns (1984) is described as follows:

$$CO+2^* \overset{K_{CO}}{\rightleftharpoons} C^*+O^* \quad \dots\dots\dots\dots\dots\dots\dots (1)$$

$$H_2+2^* \overset{K_{H_2}}{\rightleftharpoons} H^*+H^* \quad \dots\dots\dots\dots\dots\dots (2)$$

$$C^*+2H^* \xrightarrow{k_{CH_2}} CH_2^*+2^* \quad (r.d.s) \; .(3)$$

$$CH_2^*+2H^* \xrightarrow{k_{CH_4}} CH_4+3^* \quad \dots\dots\dots (4)$$

$$O^*+2H^* \xrightarrow{k_{H_2O}} H_2O+3^* \quad \dots\dots\dots (5)$$

On the basis of this mechanism, a Kinetic model was derived applying the principle of one rate determining step and assuming that the adsorption of kinetically relevant species can be described by Langmuir adsorption isotherms. The detail derivation is described as follows.

The equilibrium adsorption constants for carbon monoxide and hydrogen adsorption according to reactions of equations (1) and (2) are given by

$$K_{CO} = \frac{\theta_c \theta_o}{P_{CO}\theta^2_v} \Rightarrow \theta_o = \frac{K_{CO}P_{CO}\theta^2_v}{\theta_c} \qquad (6)$$

$$K_{H_2} = \frac{\theta H^2}{P_H \theta^2_v} \qquad \Rightarrow \theta_H = K_{H_2}^{1/2} \; P_{H_2}^{1/2} \; \theta \; v \qquad (7)$$

The reaction rates according to the reactions of equations (3), (4) and (5) are given by:

$$r^*_{CH_2} = k_{CH_2} \; \theta_c \; \theta^2_H \qquad (8)$$

$$r_{CH_4} = k_{CH_4} \; \theta^*_{CH_2} \; \theta^2_H \qquad (9)$$

$$r_{H_2O} = k_{H_2O} \; \theta_o \; \theta^2_H \qquad (10)$$

On steady state, the balance relations of carbon and oxygen are given as

$$r_{H_2O} = -r_{CO} = r_{CH_4}$$

The CO dissociation of Equation (1) is a fast and reversible reaction, therefore the rate of CO disappearance is determined by the formation of carbine.

$$-r_{CO} = r^*_{CH_2}, \; r_{H_2O} = r^*_{CH_2}, \quad r_{CH_4} = r^*_{CH_2} \qquad (11)$$

From equations (8), (9), (10) and (11), the coverage of oxygen and carbine are given as

$$r_{H_2O} = r^*_{CH_2}$$

$$k_{H_2O}\theta_O = k_{CH_2}\theta_C$$

$$=> \theta_O = \frac{k_{CH_2}}{k_{H_2O}}\theta_C \qquad (12)$$

$$\& \qquad r_{CH4} = r^*_{CH2}$$

$$k_{CH_4}\theta^*_{CH_2} = k_{CH_2}\theta_C$$

$$=> \theta^*_{CH_2} = \frac{k_{CH_2}}{k_{CH_4}}\theta_C \qquad (13)$$

From equations (6), (12) & (13) the coverage of carbon is given as

$$\frac{k_{CH_2}}{k_{H_2O}}\theta_C = \frac{k_{CO}\,P_{CO}\,\theta^2_v}{\theta_C}$$

$$=> \theta^2_c = \frac{k_{H_2O}}{k_{CH_2}} K_{CO}\,P_{CO}\,\theta^2_v$$

$$=> \theta_c = \left(\frac{k_{H_2O}}{k_{CH_2}} k_{CO}\right)^{\frac{1}{2}} P^{1/2}_{CO}\,\theta_v$$

$$\theta_c = K_c\,P^{1/2}_{CO}\,\theta_v \qquad (14)$$

$$\text{where } k_c = \left(\frac{k_{H_2O}}{k_{CH_2}} K_{CO}\right)^{1/2}$$

From equation (7), the coverage of hydrogen is given as

$$\theta_H = K_{H_2}^{1/2}\ P_{H_2}^{1/2}\ \theta_v$$

$$\theta_H = K_H\ P_{H_2}^{1/2}\ \theta_v \ldots\ldots\ldots\ldots\ldots (15)$$

$$\text{where}\quad K_H = K_{H_2}^{1/2}$$

The total surface coverage is:

$$\theta_v + \theta_c + \theta_H + \theta_O + \theta^{*}_{CH_2} = 1$$

Neglecting the coverage by oxygen and carbine, the surface balance can be approximated by

$$\theta_v + \theta_c + \theta_H = 1 \quad \ldots\ldots\ldots (16)$$

The coverage of vacant sites is calculated from equation (14), (15) & (16) as,

$$\theta_v + K_C P_{CO}^{1/2}\,\theta_v + K_H P_{H_2}^{1/2}\,\theta_v = 1$$

$$\Rightarrow \theta_v\,(1 + K_C P_{CO}^{1/2} + K_H P_{H_2}^{1/2}) = 1$$

$$\Rightarrow \theta_v = \frac{1}{1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (17)$$

Now from (13), (14) & (17)

$$\theta_{CH_2}^{*} = \frac{k_{CH_2}}{k_{CH_4}}\,\theta_C$$

$$= \frac{k_{CH_2}}{k_{CH_4}}\ X\ K_C P_{CO}^{1/2}\,\theta_v$$

$$\theta_{CH_2}^{*} = \frac{k_{CH_2}}{k_{CH_4}}\,K_C P_{CO}^{1/2}\ X\ \frac{1}{1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots (18)$$

and from (15) & (17)

$$\theta_H = K_H P_{H_2}^{1/2}\,\theta_v$$

$$= K_H P_{H_2}^{1/2}\ X\ \frac{1}{1 + K_C P_{CO}^{1/2} + K_H P_{H_2}^{1/2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (19)$$

Then the rate equation of methane formation from equations (9), (18) & (19) is given as

$$r_{CH_4} = k_{CH_4}\ \theta^{*}_{CH_2}\ \theta^{2}_{H}$$

$$= k_{CH_4}\ \frac{k_{CH_2}}{k_{CH_4}}\ K_C\ P_{CO}^{1/2}\ X\ \frac{1}{1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2}}$$

$$X\left(K_H\ P_{H_2}^{1/2}\ X\ \frac{1}{1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2}}\right)^2$$

$$=> r_{CH_4} = \frac{k_{CH_2}\ K_C\ P_{CO}^{1/2}}{(1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2}})\ X\ \frac{K_H^2\ P_{H_2}}{(1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2})^2}$$

$$r_{CH_4} = \frac{k_{CH_2} K_C K_H^2 P_{H_2} P_{CO}^{1/2}}{(1+K_C P_{CO}^{1/2}+K_H P_{H_2}^{1/2})^3} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(20)$$

Parameter estimation

For parameter estimation, a linear least square method was applied. The rate equation (20) can be rearranged as follows:

$$\left[\frac{P_{CO}^{\frac{1}{2}}}{r_{CH_4}}\right]^{\frac{1}{3}} = \left[\frac{K_C}{(k_{CH_2}\ K_C\ K_H^2)^{\frac{1}{3}}}\right] P_{CO}^{\frac{1}{2}}$$

$$+\left[\frac{K_H}{(k_{CH_2}\ K_C\ K_H^2)^{\frac{1}{3}}}\right] P_{H_2}^{\frac{1}{2}} + \frac{1}{(k_{CH_2}\ K_C\ K_H^{\frac{1}{2}})^{\frac{1}{3}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(21)$$

The plot of $[P_{CO}^{\frac{1}{2}}\ P_{H_2}/r_{CH_4}]^{\frac{1}{3}}$ versus $P_{H2}^{1/2}$ at different partial pressure of CO should be straight lines. The slopes (S_1) and intercepts (I_1) could be estimated and formulated as follows:

$$S_1 = \frac{K_H}{(k_{CH_2}\ K_c\ K_H^2)^{\frac{1}{3}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (22)$$

$$I_1 = \left[\frac{K_c}{(k_{CH_2}\ K_c\ K_H^2)^{\frac{1}{3}}} \right] P_{CO}^{\frac{1}{2}} + \frac{1}{(k_{CH_2}\ K_c\ K_H^2)^{\frac{1}{3}}}$$

Based on the above equation, the plot I_1 versus $P_{CO}^{1/2}$ should be straight lines. The slope (S_2) and intercept (I_2) could be estimated as follows:

$$S_2 = \frac{K_c}{(k_{CH_2}\ K_c\ K_H^2)^{\frac{1}{3}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (23)$$

$$I_2 = \frac{1}{(k_{CH_2}\ K_c\ K_H^2)^{\frac{1}{3}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (29)$$

From equations (22), (23) & (24), the model parameters of k_{CH}, K_c and K_H could be estimated

Mills and Steffgen (1973) concluded that the rate of methane formation must depend on the concentration of an appropriate complex of the sorbed CO and H_2. Using the static method at about 300^{0}C over nickel catalysts, the rate of formation of methane was found to be approximately proportional to the pressure of hydrogen but retarded by carbon monoxide. Using a flow method, an extensive study was made of the kinetics of methane formation at atmospheric pressure over an industrial nickel-kieselguhr catalyst in the range 300-350^{0}C at H_2/CO ratio of 1.2 to 4.0. The rate of methane formation is expressed by the equation:

$$r = \frac{P_{CC}\, P_{H_2}^{3}}{(A+BP_{CO}+DP_{CO_2}+FP_{CH_4})^{4}}$$

where A,B,D, and E are constants.

Additional kinetic expressions for nickel catalysts which reflect the inhibiting influence of CO are discussed in connection with catalyst compositions. One exception to this has been noted. The retarding influence of carbon monoxide at high concentrations is apparently due to fact that the CO covers the catalyst surface to a considerable extent, leading to a corresponding decrease in the degree of coveringwith hydrogen. Similarly, the empirical rate of methane formation over a ruthenium catalyst was found to be

$$r = kP_{H_2}^{1.33}\ P_{CO}^{-0.13}$$

indicating that here also high CO pressure inhibits catalyst activity.

This situation can be changed by the use of a low concentration of CO in a large excess of hydrogen. The kinetic relation ship obtained in this way by a flow-circulation method with a nickel - chromium catalyst at 135-175^{0}C and a concentration of CO in H_2 equal to 0.3 vol% has the form

$$W = kP_{CO}^{0}\ P_{H}^{0}$$

The zero-order of the reaction with respect to both components was attributed to the non uniformity of the nickel surface with respect to the adsorption of CO and H_2 under the given conditions.

Thermogravimetric catalyst measurements during reaction established that at 160^{0}C the degree of coverage of the nickel surface by CO amounted to about 1/3 and 2/3 of the surface being covered with hydrogen. A critical review concluded that the rate expression r = $kp_{CO}\ P_{H}^{0.5}$ correlates most of the experimental data except when excess H_2 and/or CH_4 are present. To cover the entire range of gas compositions, this equation was modified to

$$r = \frac{kP_{CO}\ P_{H_2}^{0.5}}{1+K_2\ P_{H_2}+K_3\ P_{CH_4}}$$

It is noted that this expression does not include a term in the denominator for the inhibiting effect of CO.

The extensive kinetic studies of hydrogenation of CO to higher hydrocarbons have established that carbon dioxide is a secondary product and results from the water-shift reaction.

Thompson. Jr., and et. al. (1989) stated, considering CO insertion mechanism and hydrogenation of the surface formyl group as the rate determining step, the reaction rate by the following expression:

$$N_{CH_4} = k_2\ \theta_{HCO}\ \theta_{H}$$

Based on the assumption of the thermodynamic equilibrium the fractional surface coverage would be:

$$\theta_{HCO} = K_1\theta_{CO}\theta_{H}/\theta_{v}$$

$$\theta^2_H = K_{H_2}\ P_{H_2}\ \theta^2_v$$

$$\theta_{CO} = K_{CO}\ P_{CO}\ \theta_{v}$$

where 0_v represents the fractional surface vacancy. The low activities indicate that the surface was covered predominantly by CO and H, so the fractional surface vacancy would be described by

$$\theta_v = 1-\theta_{CO}-\theta_H = \frac{1}{(1+\sqrt{K_{H_2}P_{H_2}} + K_{CO}P_{CO})}$$

Substitution into rate equation leads to an overall reaction rate in terms of the partial pressures of H_2 and CO.

$$N_{CH_4} = k_2K_1K_{H_2}P_{H_2}K_{CO}P_{CO}(\theta_v)^2$$

$$= k_2K_1 \frac{K_{H_2}P_{H_2}K_{CO}P_{CO}}{(1+\sqrt{K_{H_2}P_{H_2}} + K_{CO}P_{CO})^2}$$

Rearranging this equation into the form

$$\sqrt{\frac{P_{H_2}P_{CO}}{N_{CH_4}}} = \frac{1}{\sqrt{k_2K_1K_{H_2}K_{CO}}} + \sqrt{\frac{P_{H_2}}{k_2K_1K_{CO}}} + \frac{\sqrt{K_{CO}}}{\sqrt{k_2K_1K_{H_2}}}\,P_{CO}$$

and numerical analysis yields k_2, K_1, K_{CO} and K_{H_2} Numerical values of the coefficients were obtained from regression analysis. Negative coefficients are obviously physically impossible and the only equation with all positive co-efficient had the following form:

$$N_{CH_4} = k\,\frac{K_{H_2}P_{H_2}K_{CO}P_{CO}}{(1+\sqrt{K_{H_2}P_{H_2}}+K_{CO}P_{CO})^2}$$

If the hydrogenation of a surface methylidyne were the rate determining step, the reaction rate could be described by:

$$N_{CH_4} = k_3\theta_{CH}\theta_H$$

where the surface coverages at thermodynamic equilibrium are

$$\theta_{CH} = \frac{K_2\theta_c\theta_H}{\theta_v}$$

$$\theta_c = = \frac{K_1\theta_{CO}\theta_v}{\theta_O}$$

The surface coverage by atomic oxygen, θ_o , was estimated using the quasisteady - state approximation. With this assumption the atomic oxygen coverage would be:

$$\theta_O = \left(\frac{k_1\theta_{CO}+k_{-6}\theta_{CO_2}}{k_6\theta_{CO}+k_{-1}\theta_c}\right)$$

Under differential conditions the forward reaction rates would be more significant than the reverse reaction rates, therefore,

$$\theta_O \approx \frac{k_1\theta_v}{k_5}$$

Substitution of these expressions along with expressions for O_{CO} and O_H into above rate equation leads to the following rate equation:

$$N_{CH_4} = \frac{k_3\,(k_6/k_{-1})\,K_{H_2}P_{H_2}K_{CO}P_{CO}}{(1+\sqrt{K_{H_2}P_{H_2}} + K_{CO}P_{CO})^2}$$

Numerical analysis would yield k_3, (k_6/k_{-1}), K_H and K_{CO}.

2.4 KINETICS OF METHANATION

Van Herwijnen and et. al (1973) studied the kinetics of the methanation of CO and CO_2 in H_2 on a supported nickel catalyst. They measured the methanation of CO_2 at partial pressures below 0.02 atm and at atmospheric pressure and at temperatures between 200 and 230^{0}C. They studied the methanation of CO in the same concentration range, between 170 and 210^{0}C.

They proposed Langmuir-type rate equations as:

$$r_{CO_2} = \frac{1.36X10^{12}.\exp(-25300/RT).P_{CO_2}}{(1+1270.P_{CO_2})} mol.hr^{-1}.g^{-1}.$$

and

$$r_{CO} = \frac{2.09X10^{5}.\exp(-10100/RT).P_{CO}}{(1+4.56X10^{-4}.\exp(+12400/RT).P_{CO})^2} mol.hr^{-1}.g^{-1}.$$

In this study they used Nickel catalyst (33.6% wt NiO) of Girdlr-Sudehemic, Munich. -alumina was used as carrier material in a 4 ml tubular reactor placed in a fluid bed acting as a thermostatic bath.

Experiments at 200^{0}C showed that CO poisoned the methanation of CO_2 in concentrations larger than 200 ppm. Water and methane in small concentrations had no effect on the reaction rate. The results of this study were in good agreement with data published previously. Same mechanistic implications of the kinetic data were discussed.

Chen and Wu (1990) studied the kinetics of methanation of CO in H_2 over nickel boride catalysts. The kinetic studies were carried out in a continuous flow type reaction apparatus with a differential fixed catalyst bed U-shape reactor immersed in a controlled furnace was made of stainless-steel with 1/4 inch diameter. This investigation was under P_{CO}: 0.05 - 0.40 atm, P_H : 0.75 - 4.0 atm and T : 210-280^{0}C on nickel borides. The kinetics was explained satisfactorily by dissociative carbon monoxide and hydrogen, and hydrogenation of surface carbon to a CH^*_2 species involving two adsorbed hydrogen atom as rate determining step. Both the hydrogenation of surface oxygen to water and CH_2^* species to methane were considered to be fast processes. The rate equation of methane formation was expressed as follows:

$$r_{CH_4} = \frac{k_{CH_2} K_C K_H^2 P_{CO}^{\frac{1}{2}} P_{H_2}}{(1 + K_C P_{CO}^{\frac{1}{2}} + K_H P_{H_2}^{\frac{1}{2}})^3}$$

The investigator finally concluded that the rate of methane formation increases with partial pressure of H_2 and decreases with that of CO in the studied range.

Randhava and et. al (1969) studied the methanation of carbon monoxide at parts per million levels over 0.5% ruthenium metal catalyst, dispersed on alumina catalyst in a fixed-bed reactor. The catalyst pellets were 1/8 x 1/8 inch cylinders. The reactor was built from 1/2 inch i.d., 1-inch o.d., and 22 inch-long stainless steel 304 tubing. Gas mixtures of 3450, 1090, and 505 p.p.m. carbon monoxide in hydrogen were used within the range of 175^0 - 275^{0}C. The rate of reaction of carbon monoxide follows simple pseudo-first order kinetics. The rate constant follows the Arrhenius temperature dependence at low temperatures. The rate of CO conversion increases rapidly with a decrease in the partial pressures of CO at the same temperature. For the atmospheric pressures at which the investigation was conducted, the fractional conversion of carbon monoxide increased continuously with an increase in temperature. Evidence of diffusion control of the reaction rate was found in the higher temperature regions investigated.

Thompson. Jr. and et. al (1989) studied CO hydrogenation over alumina supported sulfide cluster catalysts. Kinetic experiments were carried out in a glass-lined, stainless steel U-tube reactor (6.35 mm OD). Bimetallic Mo-Fe and Mo-CO sulfide clusters were anchored on Al_2O_3 and used for CO hydrogenation. In addition to methane, significant amounts of dimethyl ether were produced. The reaction orders obtained from power rate laws for methanation indicated that the surfaces of the catalytic ensembles were not completely saturated by CO in contrast to the observations for most conventional CO hydrogenation catalysts. A kinetic analysis and parameter estimation was performed to identify the rate determining step for methanation. A catalytic cycle was postulated that could account not only for the formation of methane and higher hydrocarbons, but also for dimethylether as a primary product. The result showed that the partial pressure dependencies were positive for both H_2 and CO. Over CO hydrogenation catalysts such as Fe, Co and Ni, the reaction rate was near first order in H_2 and zero order in CO. Evidently CO did not inhibit methanation over sulfide cluster derived catalysts also it did over late transition metals.

Van Ho and Harriott (1980) studied the kinetics of methanation of carbon monoxide with 2% Ni/SiO_2 and 10% Ni/SiO_2 catalysts in a differential reactor. Kinetic measurements were made using a 3/8 in. diam. stainless-steel reactor immersed in a fluidized-bed sand bath. The range of temperature was 200^0 to 450^0C. The role of carbon as an intermediate was explored by making transient tests of carbon deposition, carbon gasification, and methane formation. If carbon is an intermediate, neither the normal dissociation of CO nor reactions of H with C seem to be controlling. The limiting step may be the surface reaction between adsorbed carbon monoxide and hydrogen atoms to form carbon and water. The methanation rate was almost independent of P_{CO} from 0.01 to 0.50 atm. at 275^0C. At 255^0C, the reaction became negative order to CO at P_{CO} = 0.05 atm. and 212_0C, the inhibiting effect of CO was still more pronounced. Data for the 10% Ni catalyst showed that the order with respect to CO changed from strongly negative at 200^0C to slightly negative at 247^0C and almost zero at 300 and 330^0C. The reaction rate increased with hydrogen pressure, but the effect changed with gas composition. The apparent reaction order decreased at higher hydrogen pressure. The results suggest that CO is more strongly adsorbed but may be displaced at high hydrogen pressures. The data also suggest surface heterogeneity with over a 10 fold range in activity for adsorbed CO.

When the H_2 / CO ratio is between 1 and 3, Karn and et. al. and Dry and coworkers have shown that the Fischer-Tropsch reaction is close to first order in H_2 partial pressure and zero order in CO partial pressure. Under similar conditions, the exponential dependence of the methanation reaction is usually close to first order in H_2 and between zero and -1/2 in CO as shown by McKee, Schoubye and Luyten and Jungers.

Dalla Betta and et al. also utilized a differential batch reactor to study initial rates for both methane formation and total CO conversion at a pressure of 0.75 atm. It was assumed that no loss of metal surface area occurred under reaction conditions; therefore hydrogen adsorption on fresh catalyst samples was used for the calculation of metal dispersion and turnover numbers. They showed that the rate of the synthesis reaction was independent of ruthenium particle size in a series of Ru/Al_2O_3 catalysts. The turnover numbers calculated for these supported Ru catalysts were lower than those measured for a 5% Ni/ZrO_2 catalyst.

Fitzharris and et. al (1982) studied sulphur deactivation of supported Ni in CO hydrogenation was studied in all quartz internal recycle reactor with a feed containing 4% CO in H_2 . Thirteen ppb H_2S reduced the steady state methanation activity of Ni/ Al_2O_3 about 200-fold at 661 K; 100 ppb H_2S reduced the activity 5000 fold. A dual site langmuir-Hinshelwood rate expression predicts both the CO partial pressure dependence and the S poisoning. Poisoning and chemisorption data indicate formation of a stable two-dimensional, surface sulfide with a S; Ni surface atom ratio of 1:2 for 13 ppb H_2S in H_2 at 661^0K. The surface sulfide has a free energy of formation of at least -26 kcal/mole which is 15 kcal/mole more stable than bulk Ni_2S_3. Sulfur poisoning is due to geometric effects, i.e., site blockage, rather than electronic effects since the activation energy for methanation over s-poisoned Ni was the same as that over unpoisoned Ni, 24 kcal/mole.

When hydrogenating CO on nickel Vlasenko, Yuzefovich, and Rusov found a zero order dependency of the rate on the partial pressure of carbon monoxide between 135 and 175^{0}C and at concentrations below 0.3% in hydrogen. The total pressure was always 1 atm.

J. Happel and et. al (1980) studied multiple isotope tracing of methanation over nickel catalyst. The methanation of mixtures of carbon monoxide and hydrogen over a supported nickel catalyst was studied by transient isotope tracing with ^{13}C, ^{18}O, and D.A mechanism was proposed based on computer modeling which takes into account results from a wide variety of data. Evidence was presented that rate controlling steps involved hydrogenolysis of chemisorbed CH_x species (x=0-3) rather than only the splitting of carbon monoxide or the formation of an "enolic" intermediate. Carbon dioxide formation appeared to occur directly rather than through the water gas shift reaction. The computer program enabled estimates to be made of concentrations of intermediates as well as velocities of individual steps in the mechanism. Under reaction conditions predominant adsorbed species appeared to be carbidic carbon plus hydrogenated hydrocarbon intermediates.

DeBruijn, and et. al studied the methanation of carbon dioxide in hydrogen at atmospheric pressure in a Parallel Passage Reactor. The experiment was carried out with the temperature: 190-240^{0}C concentration: 0.19-4 vol% and the catalyst: Girdler G-65 Ni/Al_2O_3;

NiO/Al_2O_3 = 3:3 w/w particle size = 0.35 - 0.42 mm; S_{BET} = 42.4 m^2/g. S_{Ni} = 6.6 m^2/g. The PPR was immersed in a fluidized bed thermostat. They proposed the rate equation as

$$r_{CO_2} = -\frac{K_\infty \exp.(-Ea/RT)\,P_{CO_2}}{1+K_{CO_2}P_{CO_2}}\ mol.h^{-1},g^{-1}.$$

The result showed that at high space velocities, the ratio of mass transport by flow through the channel to the mass transport by diffusion into the catalyst bed is relatively high, resulting in low CO_2 conversion. As the flow rate of the gas in the channel is decreased, the above ratio diminishes and a larger proportion of CO_2 is then converted. At very low space velocities the residence time apparently is long enough to give complete conversion. Operation at pressures higher than atmospheric gives improved reactor performance.

A model reactor has been built and studied using the methanation of carbon dioxide as the test reaction. Calculated results of a simple, mathematical model agree well with the experimental data except at low temperatures. The conversions obtained are sufficiently promising to warrant further exploration of the parallel passage reactor as a tool in SNG production, the more so because exploratory calculations show that operation at higher pressures results in much improved performance.

Chlang and Hopper (1983) studied the kinetics of the hydrogenation of carbon dioxide to methane using a 58% nickel catalyst supported on kieselguhr. The kinetic studies were conducted in continuous flow tubular reactor system immersed in a fluidized sand bath. The reactor was constructed of 1/4 in. 316 stainless steel tubing, and normally about 0.15 g of catalyst was contained in the reactor between two 15 μm inline filters. The volume percentages of carbon dioxide and hydrogen in feed mixture were varied from 20 to 30% and 67 to 80% respectively. A total pressure range of 100 to 250 psig and a temperature range of 276 to 318^0C was covered. The catalyst was reduced at a temperature, 427^0C and 500 psig for 48 hr., greater than any used in the kinetic experiments to minimize thermal effects of catalyst activity. To minimize external transport resistances superficial mass velocity (183 - 1179 lb/h ft^2) were used and to minimize intraparticle transport effects, particle sizes of 140 - 200 mesh were used. Experimental data were correlated with the power rate model to give the following relationship:

$$r_{CH_4} = 1.19x10^6 \exp[-14600/RT]\, P_{H_2}^{0.21} P_{CO_2}^{0.66}$$

Binder and White (1950) acknowledged the significance of CO_2 alone and observed the methanation-rate for CO_2 to be two orders of magnitude less than that for CO. This work at the University of Michigan was continued by Dew et al. (1955). Solc (1962) and Pour (1969) studied the kinetics of carbon dioxide hydrogenation on a chromium-nickel catalyst using a large excess of hydrogen in the flow system feed gas. Both reported to be half-order with respect to carbon dioxide. In a study using pure CO_2 the rate of methanation was observed to be first order with respect to CO_2 and no appreciable adsorption of CO_2 was observed. Methane and water did not influence the rate. Saletore and Thomson (1977) reported on a study including all five components present in the methanation reactions. The presence and absence of CO_2 and water in the system feed was demonstrated to have a significant role in methanation kinetics and it was proposed that CO_2 methanation might actually proceed via the water gas shift reaction. At the higher concentrations of carbon oxides, water reduced the rate of both the shift reaction and CO methanation, but methane had little effect. An increase in carbon dioxide increased the CO methanation rate slightly but decreased the shift reaction rate significantly. Moore (1977) made an extensive study of the hydrogenation of carbon monoxide, with some experiments including the addition of carbon dioxide methane, and water to the feed. He observed that an increase in carbon dioxide concentration increased the rate of disappearance of carbon dioxide and simultaneously a slight increase in the rate of formation of methane. Methane concentration upto 57% had little influence on the CO methanation rate, while the addition of water caused a significant decrease in methane formation but only a slight increase in CO_2 formation.

Dew and et. al (1955) studied hydrogenation of carbon dioxide on nickel-kieselguhr catalyst. The reactor was a 36 x 3/4 inch stainless steel pipe. The catalyst used in this investigation was supplied by Harshaw Chemical Co. and was designated as reduced Nickel 88, Lot No. 219-1-14. The catalyst pellets were approximately 3/8 x 3/8 inch cylinders and had an average weight of 0.0495 g. Their bulk density in the reactor was 94 pounds per cubic foot. An approximate analysis of catalyst was nickel, 59.4; silica, 18.2; carbon, 5.0; sulfur, 0.06% and traces of iron and alumina. They reduced the catalyst at a pressure of 30 atmosphere and a temperature of 320^{0}C for 48 hours. They used a feed gas containing 20% CO_2 and 80% hydrogen, and a pressure of 30 atmosphere to determine the effect of temperature on reaction rate. They increased the temperature incrementally starting from 193^{0}C until the maximum rate in methane formation had been covered. The temperature was then decreased incrementally to observe the thermal deactivation resulting from high temperatures. They presented the obtained results at a plot of reaction rate vs. catalyst temperatures.

They obtained a maximum reaction rate at 426^{0}C and this maximum reaction rate continued upto 515^{0}C and then decreased. During decreasing of temperature from a maximum of 665^{0}C they observed that a threshold temperature does not exist. They conclude that the resistance to diffusion of the reactants into the catalyst pores consumes some of the driving potential for the overall reaction. This resistance may become appreciable for small catalyst pores. The diameters of the catalyst pores decreased in size during exposure to higher temperatures. The effect of smaller pores on rate of reaction would be somewhat equivalent to the effect of lower total pressure since in either case the effective partial pressures of the reactants at the reaction sites would be lowered.

Zagli and et al (1979) studied methanation on supported nickel catalysts. The techniques of temperature programmed desorption and temperature programmed reaction were used to study methanation of carbon monoxide on three high-weight loading, supported nickel catalysts. A flow system at atmospheric pressure and a mass spectrometer detector was used to continuously monitor the products leaving the surface. The desorption spectra of adsorbed CO and of CO_2 were dependent on the catalyst properties. On all three catalysts CO and CO_2 desorbed from the surface during heating following CO adsorption. Products were observed leaving the surface upto temperatures in excess of 500^0C. The reaction of coadsorbed CO and H_2 as well as the reaction of adsorbed CO with flowing H_2 were studied on each of the catalysts. Both CH_4 and H_2O were observed leaving the catalyst surface at the same temperature indicating that C-O bond breaking was rate determining. The results show that temperature desorption is a very useful technique for studying reaction mechanisms as well as characterizing catalysts.

Wedler and et al. (1975) studied the interaction of hydrogen and carbon monoxide on polycrystalline nickel films at temperatures 77, 273 and 353 K by measurements of thermal desorption, electrical resistance and changes in work function. For the purpose the adsorption of H_2 on nickel films partially covered with CO, the adsorption of CO on nickel films partially covered with H_2, and alternating adsorption of H_2 and CO were studied.

Although reaction products of H_2 and CO could not be found under experimental conditions chosen, clear evidence for their interaction could be seen. This interaction could be recognized by an increase in the heat of adsorption of H_2 due to the presence of

CO, an increase in the amount of CO adsorbed on nickel films due to the presence of H_2 and the CO induced transformation of H_2 adsorbed in the β_2 phase, into another phase.

2.5 REACTOR MODELLING

Modelling (mathematical modelling) implies the representation of a physical system by a set of equations which in a limited way can represent the system under study. Rose (1981) stated that relevant in reactor design is a mathematical description that can predict reactor out let concentrations and temperature from inlet concentrations, flow, and reactor dimensions. These equations are usually, though not always, solved by computer.

The models used to simulate fixed bed reactors range from the very simple ones to some very sophisticated ones. The justification for using a more refined model can only be on the basis of showing that they predict significantly different behaviour. Hossain (1983) stated that the factors on which the sophistication of a model should depend are the reaction or the process, the sensitivity of the process to perturbations in the operating conditions and the degree of accuracy with which the kinetic and transport parameters are known.

The models can be divided into two broad groups namely the Pseudo homogeneous and the heterogeneous models. A pseudo-homogeneous model is obtained when one recognizes the packing as only having an effect of the fluid flow so that the bulk temperature and bulk concentration are the same as that on the surface. In a heterogenous model separate conservation equations for fluid and catalyst results in the bulk temperature and concentration being different from those at the surface, with in each category further classifications are made in order of increasing complexity. In the ideal pseudo homogeneous plug flow is generally assumed. By superposing some types of mixing in the axial direction the non-ideal flow condition is somewhat accounted for. A two-dimensional model results when one accounts for the radial gradients. In the radial mixing may also be included. The basic heterogeneous model considers transport by plug flow only. Two kinds of gradients are introduced due to the catalyst; the interfacial and intraparticle gradient. Accounting for one or both of these the one dimensional model may be increased in complexity. Similar to pseudo homogeneous models axial mixing, radial gradient and radial mixing may be introduced to gradually increase the heterogeneous model in sophistication. The most general models used today are the two-dimensional heterogeneous models.

The first models to be proposed have obviously been pseudo homogeneous ones. Froment & Bischoff (1979) stated that the basic model is the pseudo homogeneous one dimensional model, which only considers transport by plug flow in the axial direction. This model assumes that concentration and temperature gradients occur only in the axial direction and the only transport mechanism operating in this direction is the overall flow itself. Several assumptions involved in the pseudohomogeneous model are subject to criticism. The flow in a packed bed reactor deviates from the ideal pattern because of radial variations flow velocity and mixing effects due to the presence of packing. Also because of external cooling it is a gross simplification to assume that the temperature is uniform in a cross section. Velocity profile is seldom accounted for because it introduces serious complications and few data are available to date and no general correlation could be set up for the velocity profile. The mixing in axial direction is accounted for by superposing an "effective" transport mechanism by the introduction of the "effective" diffusivities and conductivities. This whole field has been reviewed and organized by Levenspiel and Bischoff (1963), Yagi, Kunii, and Wakao (1960) determined the "effective" conductivity experimentally, while Bischoff (1963) derived it from the analogy between heat and mass transfer in packed beds. It has been shown several times that for the flow velocities used in industrial practice-the effect of axial dispersion of heat and mass on conversion is negligible when the bed depth exceeds about 50 particle diameter. In spite of this the model has been used because with axial mixing the possibility of multiple steady states come in. For reactions with a pronounced heat effect a model is required that predicts the detailed temperature and conversion pattern in the reactor so that the design can be directed towards avoiding eventual detrimental over-temperatures on the axis. For this a two-dimensional model is required. The two dimensional pseudo homogeneous model uses the effective transport concept to formulate the flux of heat or mass in the radial direction.

Valstar (1969) refined the two dimensional model by introducing a velocity profile published by Schwartz and Smith (1953) that exhibit a maximum at 1.5 dp of the wall. Lerou and

Froment (1977) concluded from a simulation of experimental radial temperature profiles that a radial velocity profile inversely proportional to the radial porosity profile led to the best fit. Such a radial velocity profile exhibits more than one peak. Thus in simulation of severe operating conditions accounting for velocity profile are worthwhile until more knowledge of the packing pattern and hydrodynamics of fixed beds become available, this aspect has to be leftout of usable models.

For very rapid reactions with an important heat effect it is necessary to distinguish between conditions in the fluid and on the catalyst surface even inside the catalyst. The heterogeneous system consisting of the solid catalyst and reacting gas where temperature and concentration gradients exist both in the axial and radial direction can be represented by a quasi-continuum where a smooth variations of all quantities and dependent variables in the bed is assumed. Writing the heat and mass fluxes in the axial and radial directions in the form analogous to the Fourier's and Fick's law, the balances for a simple A ----> B reaction results in a set of non linear elliptic partial differential equations which are extremely complicated even for numerical solution. Assumptions and simplifications therefore follow logically. The coefficient in the transport equations can be approximated by average values. Beek (1961), Carberry and Wendel (1963) have shown that the effect of axial mixing term can be omitted in the majority of industrially operated reactors. This results in a set of parabolic partial differential equations which is more amenable to solution. However

Hlavacek (1973) by experimental and theoretical investigation of the effect of heat transfer in packed catalytic adiabatic reactors has shown that this assumption is in question.

In the majority of industrially important cases for exothermic reactions gas to solid heat and mass transfer also play an important role so that one has to write a two phase heat and mass balance. Froment(1972) has suggested possibilities of writing elaborate governing equations for the two dimensional two phase mode.

McGreavy and Cresswell(1969) proceeded by adding to the one-dimensional model accounting for interfacial and intraparticle gradients the terms accounting for radial heat and mass transfer in the bed. They however assumed heat transfer in the radial direction occurs only through the fluid phase. But it has been shown that even for typical industrial flow rates the solid and stagnant films contribute for at least 25 percent in the radial heat flux.

For radial heat and mass transfer in addition to the terms for interfacial and intraparticle gradients a two dimensional model is required which distinguishes between the effective thermal conductivity for the fluid phase and that for the solid phase.

Van Doesburg and DeJong (1974) studied the dynamic behaviour of an adiabatic fixed-bed methanator containing Ni/Al_2O_3 catalyst. They used the hydrogenation of small amounts of CO and CO_2 to methane, a purification step in hydrogen synthesis, as the test reaction. They studied the response of a 0.5 liter methanator to step changes in inlet conditions in the parameter space 0.6-2.5

vol% CO or CO_2 in hydrogen, 180-250^{0}C inlet temperature, and space velocity 5000 - 32000 hr^{-1}.

A pseudo homogeneous plug flow model was selected to compare the experimental results with calculations, integrating the partial differential equations with a finite difference approximation containing the Crank - Nicholson algorithm. The results show that the model gives a good description of the measurements.

Van Doesburg and De Jong. (1976) studied the transient behaviour of an adiabatic fixed-bed methanator using the hydrogenation of mixtures of CO and CO_2 at concentrations upto 2.7 vol. % carbon oxide in hydrogen as the test reactions. Responses to disturbances in feed conditions were studied by measuring the axial temperature profile as a function of time. The results show that the dynamic behaviour of the reactor is complicated by the inhibition by CO of the methanation of CO_2.

The agreement between theory and experiment was again quite satisfactory; the pseudo homogeneous plug flow model which applied to experiments using binary mixtures of hydrogen and a carbon oxide applies to the data obtained with mixtures of CO, CO_2 and H_2, provided that the successive hydrogenation of CO and CO_2 is taken into account. It is improbable that the pseudo homogeneous model can be applied to industrial methanation, when the higher temperatures and consequent faster rates of methanation are likely to cause heat and mass transfer limitations. But there is no doubt that response times of a few seconds must be expected in industrial methanation.

Sharma and Hughes (1978) studied the effect of perturbations on the performance of an adiabatic reactor used for processing the exothermic catalytic oxidation of carbon monoxide. Perturbations study included, step changes in concentration and temperature, pulse changes in concentration hysteresis effects and addition of CO_2 to the feed stream. Intraparticle temperatures were measured for some of these perturbations. The heterogeneous dispersion model was suitable for steady state predictions but was not adequate for transient behaviour.

Hoiberg, and et. al. (1971) studied the experimental evaluation of dynamic models for a fixed-bed catalytic reactor. Experimental observations of a reactor's frequency response when compared with mathematical models of the reactor revealed the need for accurate modeling of heat generation, heat exchange, and heat storage processes. The experiments were performed in a laboratory reactor with the exothermic reaction between hydrogen and oxygen catalyzed by platinum on granules of silicagel. This system permitted observation of several non linear effects. One-and two-dimensional, locally linear, plug flow models of the continuum type were used for the comparison. One of the models included the effects of intraparticle diffusion of reactants. However, models that neglected intraparticle dynamic effects were found suitable here because the decay time for the diffusion process within the catalyst was short compared to the reactors major thermal time constant. A two dimensional model was found to give an excellent representation of the very complex movement of concentration and temperature waves in this type of reactor, while a one dimensional model was found to serve well when radial gradients are small. Van Doesburg and De Jong (1976) studied the transient behaviour of an adiabatic fixed-bed catalytic reactor has been studied experimentally as well as theoretically using the hydrogenation of small amounts of CO and CO_2 to methane as the test reactions. The axial temperature profile in a 0.5 liter reactor containing a Ni/Al_2O_3 catalyst was measured as a function of time after applying changes of the carbon oxide concentration in the feed and of the feed temperature. Besides, a quasi-homogeneous model was developed to simulate the transient behaviour of the reactor; its partial differential equations were solved numerically using the Crank-Nicholson algorithm.

The agreement between measured and calculated reactor responses was quite good at carbon oxide concentrations upto 2.2 vol%, an inlet temperature below 250°C and in the space velocity range of 5000-25000 hr^{-1}, under which conditions the reaction is so slow that mass and heat transfer limitations do not occur.

CHAPTER 3

EXPERIMENTAL SYSTEMS

Two flow diagrams, one for adiabatic reactor and the other for isothermal reactor of the experimental setups are shown in figure 3.1 and 3.7 respectively. Figure 3.2 shows a photograph of a section of the experimental systems. Each apparatus has three main sections:

1. Feed preparation
2. Reactor
3. Sampling and analysis

3.1 Feed preparation

The feed preparation section consists of feed purification and drying, flow measurement, preheating and mixing. All the gases needed for the reaction such as CO, CO_2, H_2 and N_2 are supplied from gas cylinders. The purity of the gases as supplied is better than 99.9%. These gases are dried by passing through silicagel and molecular sieve columns. The gases are then metered by rotameters which are calibrated to measure the flow rates of the respective gases using soap bubble flow meter. The nitrogen and hydrogen gases, before they are metered, pass through heated columns of copper turnings for the removal of trace amounts of oxygen that may be present. The reactant gases are then mixed in a mixing column and sent to the preheater. Two preheaters have been installed in

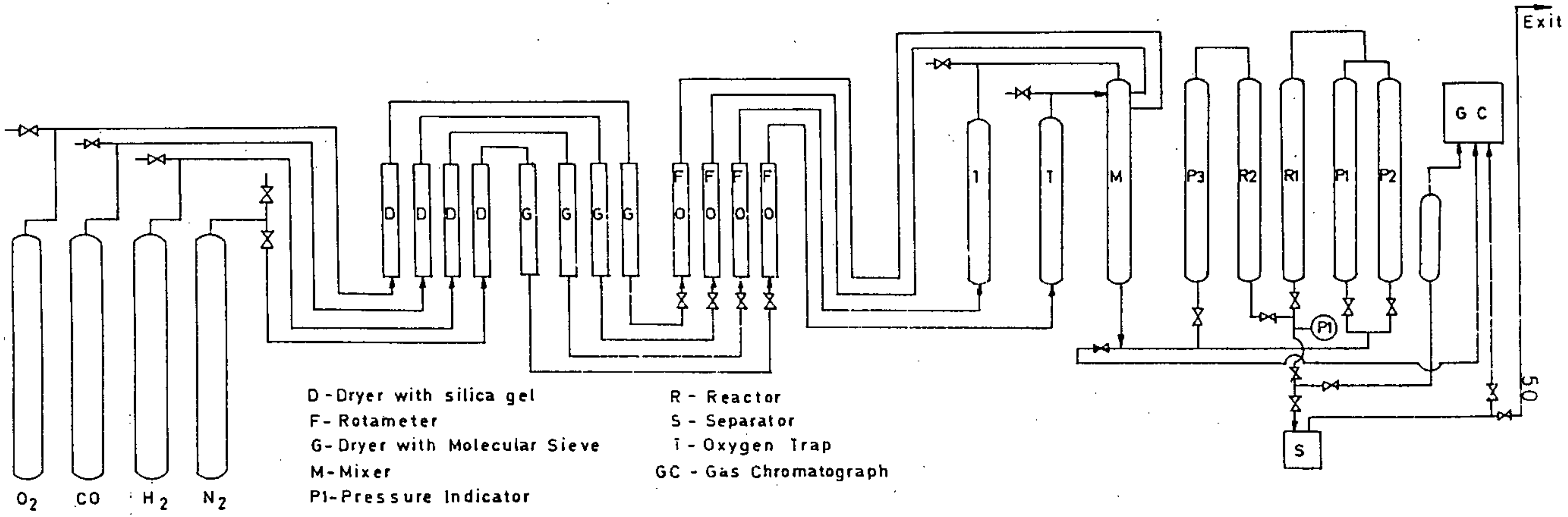


Figure 3.1: Schematic Diagram for Laboratory Adiabatic Reactor System

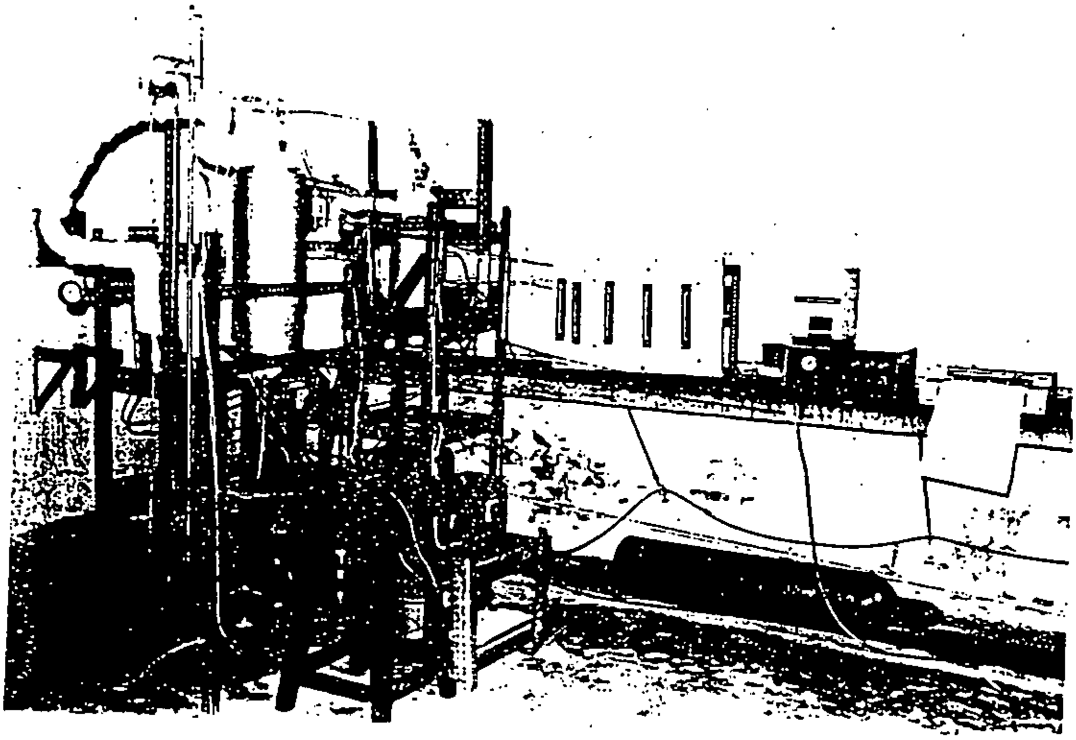


Fig. 3.2 A Photograph of a Section of the Experimental System

parallel and either one or both of them may be used. The dryers, oxygen traps, mixers and preheaters are simple in construction and their dimensions and sketches are given in figures 3.3 to 3.5.

3.2 Reactor

3.2.1 Adiabatic reactor

A tubular reactor is placed in a cylindrical oven installed with temperature controller. It had thermocouples for measurement of axial and wall temperatures. The general construction and dimensions of the reactor is given in figure 3.6.

3.2.1.1 Reduction procedure

Nitrogen purified in an oxygen trap is allowed to pass through the reactor for half an hour. The reactor is then heated upto a temperature of 300^0C with the nitrogen stream and the reducing gas, hydrogen, was introduced at a low flow rate. The flow rate of nitrogen was 51.5 l/h and of hydrogen was 39.5 l/h. The reduction was continued for four hours. The completion of reduction was tested by gas chromatographic analysis till successive samples did not produce any change in the hydrogen content of the exit gas. The reactor is then used for a specified run or cooled in stream of nitrogen and kept in a nitrogen environment.

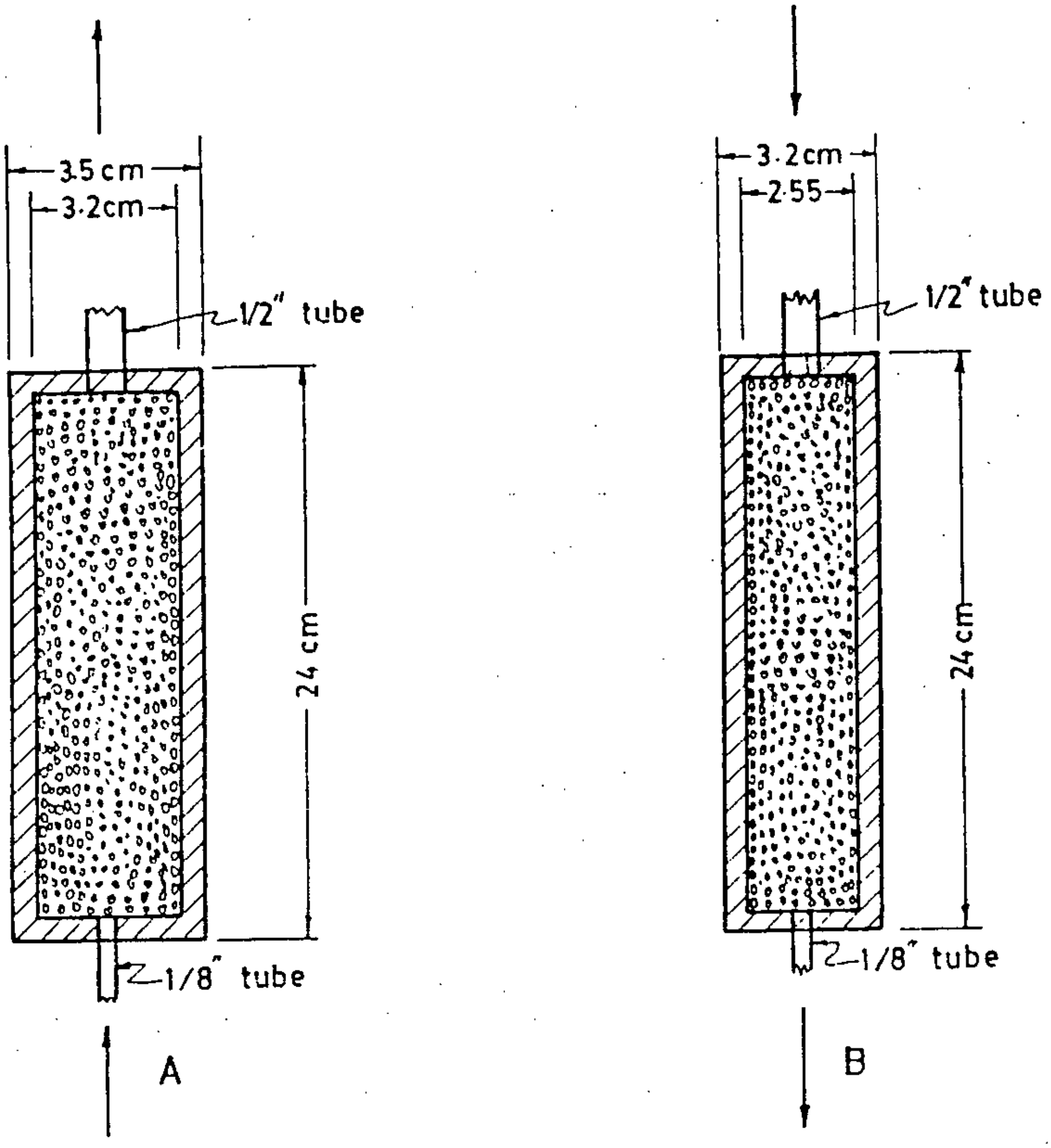


Fig. 3.3 (A) Dryer packed with silica gel,
(B) Dryer with molecular sievs.

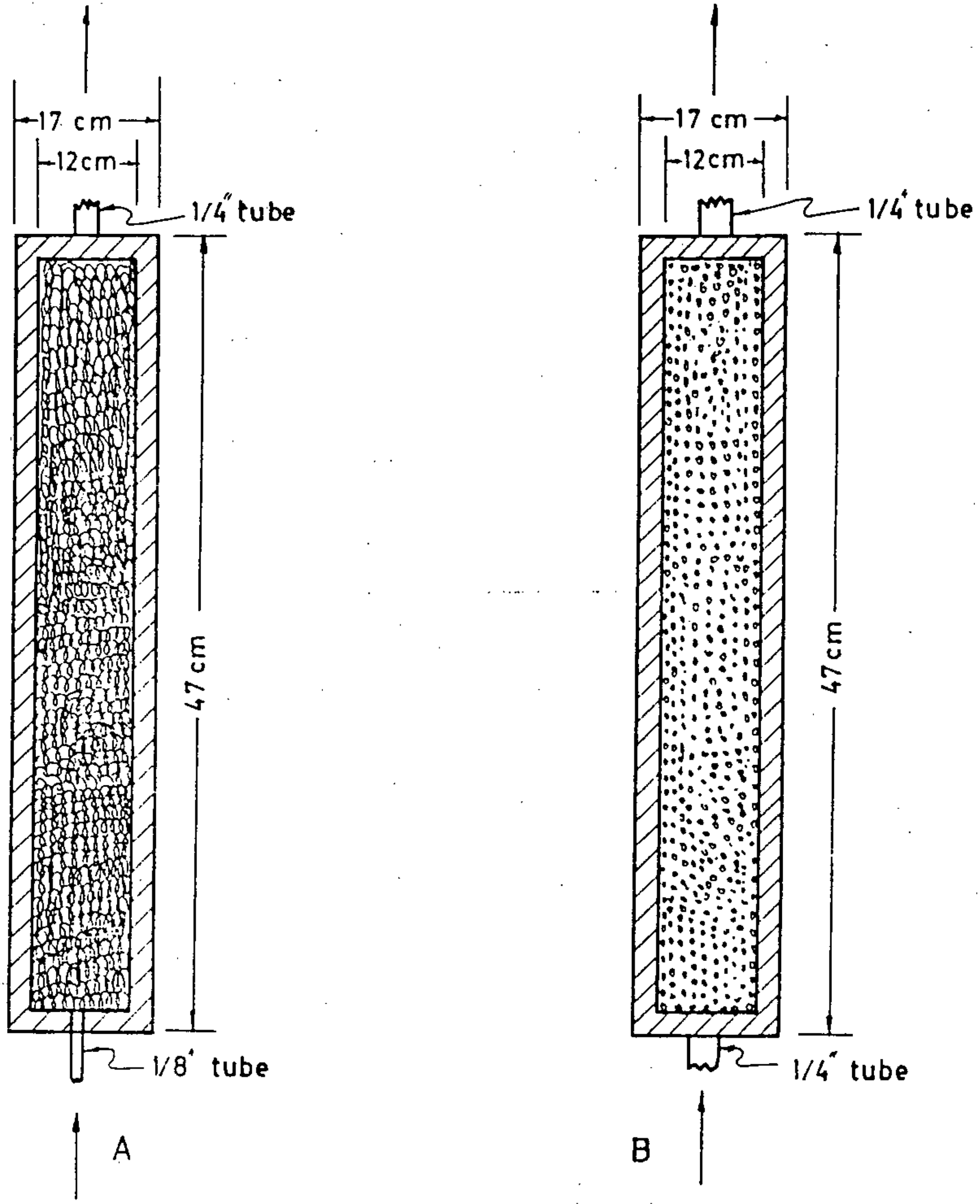


Fig.3.4 (A) Oxygen trap packed with copper turning,
(B). Preheater packed with alumina.

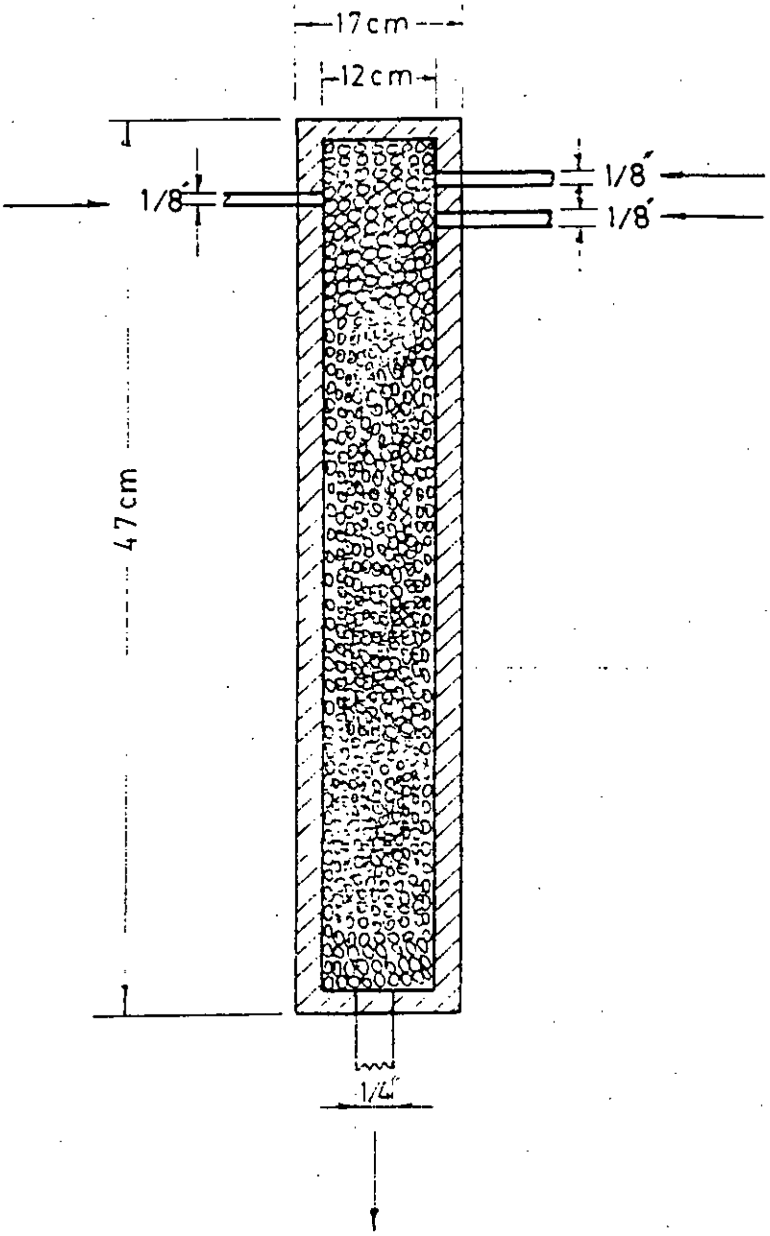


Fig. 3.5: Mixer packed with alumina.

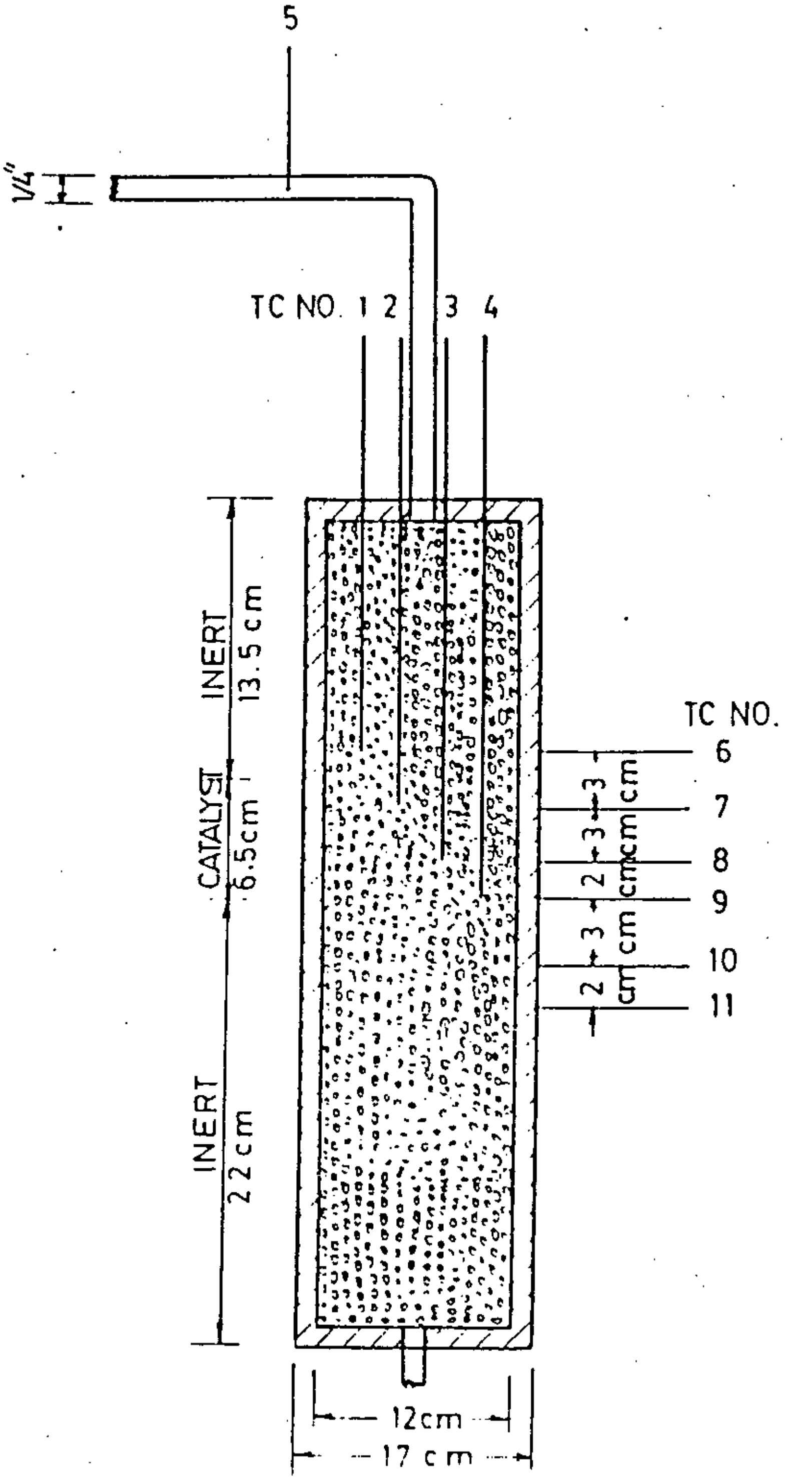


Figure 3.6 Details of the Adiabatic Reactor

3.2.1.2 Procedure for operation

In order to carry out an experimental run, the reduced catalyst kept in nitrogen environment is slowly heated upto the reaction temperature with nitrogen flow in the system. Hydrogen was then allowed to pass together with nitrogen for one hour. Carbon monoxide or carbon dioxide was introduced in desired proportion and the reaction was allowed to take place till steady state was reached. The attainment of steady state was tested by two successive analysis of the product gas as well as by the steady values of temperatures in the reactor. Both the product and reactant gases were analyzed at steady state. The reactor was then either set at new operating conditions or cooled in a nitrogen stream and kept in the nitrogen environment till the next experiment was carried out.

3.2.2 Isothermal Reactor

A tubular reactor was constructed for the purpose of carrying out methanation reaction in isothermal condition. The reactor was placed in a fluidized sand bath and heated by electrical heater operated by variacs. The inlet gases were preheated in a preheater attached to the reactor. The reactor had thermocouples for measurement of axial and wall temperatures. A manometer was set up on the air line for measuring flowrate of air. The fluidizing air was preheated in a preheater. The preheater was also heated by electrical heater. The reactor was filled with 1:8 diluted catalyst of 40-60 mesh. The reactor bed length was 5 cm. Both sides of

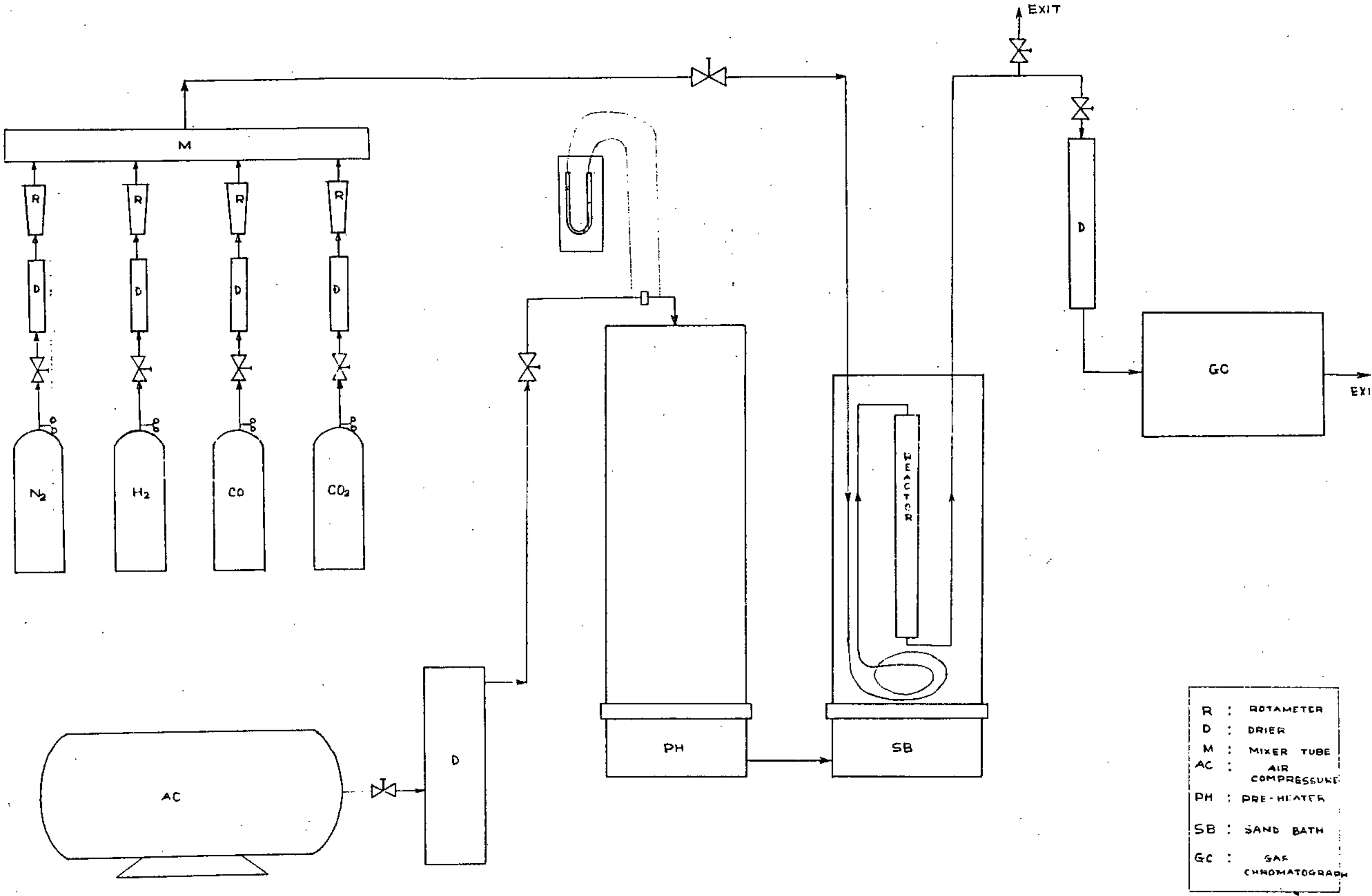


Figure 3.7: Schematic Diagram for Laboratory Isothermal Reactor immersed in a Fluidized sand bath .

catalyst bed were filled by inert. The details of the preheater, sand bath and reactor are in fig. 3.8 to 3.10.

3.2.2.1 Reduction procedure

The reduction procedure is same as the adiabatic reactor.

3.2.2.2 Operating Procedure

Temperature control in the reactor immersed in the fluidized sand bath to maintain isothermality is the principal matter of the operating procedure.

Isothermality was maintained in the reactor by adjusting fluidizing air flow rate, variac voltage and reactor position.

Rest of the operating procedure is same as the adiabatic reactor.

3.3 Sampling and Analysis

A Shimadzu model 8C-3A gas chromatograph connected with Shimadzu model C-R6A chromatopac was used for the analysis of the reactant and product gases. Details of the calibration of gas chromatographic peaks for the quantitative analysis of the gases are given in Appendix A.

The exit gases from the reactor pass through different columns before being discharged to the atmosphere. A stream is allowed to pass through two columns of silicagel for drying and then sent to the gas chromatograph for on line analysis of the products. The products are analyzed using two columns, a porapak column and a molecular sieve column. The relevant information for gas chromatographic analysis is given in Appendix A.

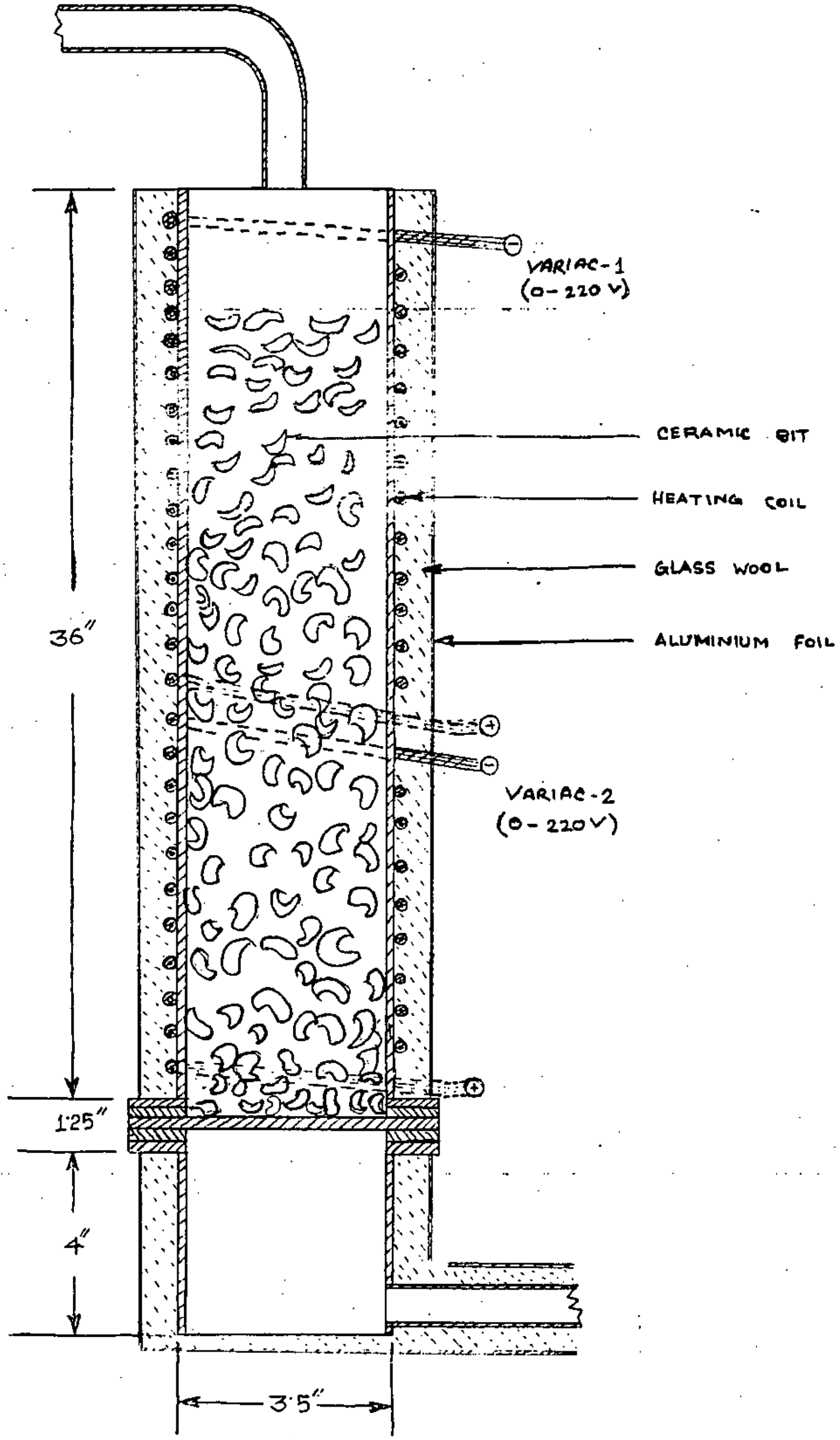


Figure 3.8: Preheater packed with ceramic beat

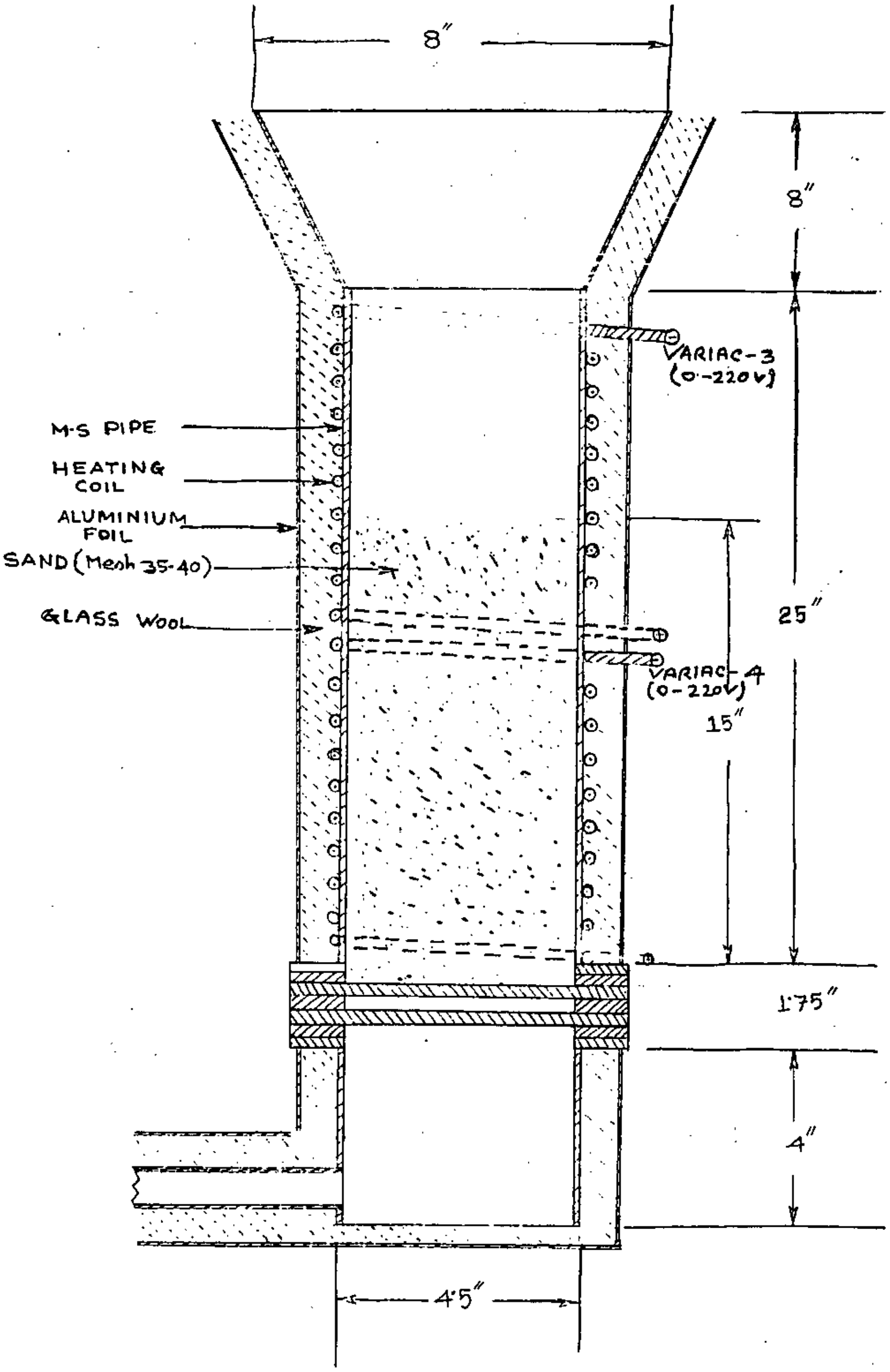


Figure 3.9 Sand bath with sand, insulation and heating coil.

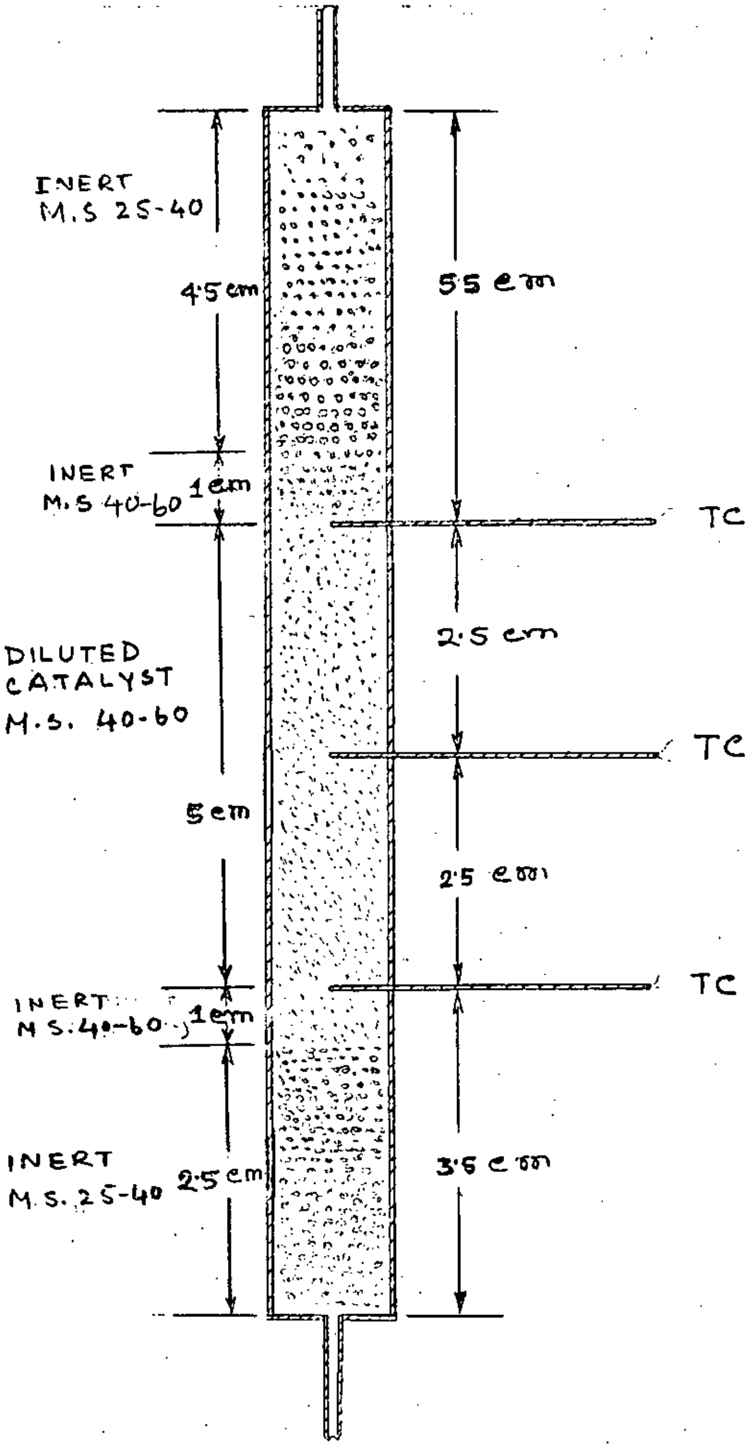


Figure 3.10: Details of the Isothermal Reactor.

CHAPTER 4

RESULTS AND DISCUSSIONS

4.1 Adiabatic steady state Methanation

A large number of experiments were carried out in the adiabatic reactor for the methanation of carbon dioxide, carbon monoxide and mixture of carbon oxides to study the steady state behabiour of the fixed bed Reactor. The catalyst without dilution was used in the reactor. The results are tabulated in Table 4.1 to 4.3. The details of the reactor with the catalyst beds are presented with the results in the appendices C to E.

The reactions were carried out at different temperatures using different concentrations of carbon oxides individually. The reactor showed an initial temperature profile and it was somewhat difficult to obtain the same profile for different runs. From the figures 4.58 to 4.60, it was clear that an isothermal temperature can not be reached in the reactor even without reaction nor an adiabatic condition can be achieved. Some of the runs were repeated, most of them gave similar results but a few did not. The figures 4.1 to 4.34 show the steady state behaviour of the reactor.

4.1.1 Study on CO_2 Methanation

4.1.1.1 Effect of inlet temperature on the temperature profiles:

Figures 4.1 to 4.4 show the general pattern of temperature profile in the reactor. The temperature profile remains nearly flat for low inlet temperature, the profiles getting sharper as the inlet temperature is increased. For example, for an inlet temperature of 270^{0}C in figure 4.1, the rise in temperature is only about 15^{0}C while it is nearly 30^{0}C with inlet temperature of 292^{0}C when the concentration of inlet CO_2 is 0.9385 mol % CO_2. The effect is more pronounced at higher concentration of CO_2 as seen in figure 4.4.

4.1.1.2 Effect of inlet concentration on the temperature profiles:

Figure 4.5 to 4.7 show the same runs plotted as a function of inlet temperature with inlet CO_2 concentration as parameter. The figures show milder profiles at low inlet concentration and low inlet temperatures. The profiles become sharper with rise in both inlet concentration and inlet temperatures.

At a given inlet temperature, it is seen that the profiles rise with increase in inlet CO_2 concentration upto a certain limit, beyond which the profile shows a downward trend. For example, in figure 4.5, the profiles increase as the inlet concentration of CO_2 rises from 0.9385 mol% to 1.7241 mol%, but for 2.5308 mol% CO_2 run, the profile is lower. Similar results were obtained in figure 4.6 (for run with 2.5308 mol% CO_2). However, for run with 2.5308 mol% CO_2 at inlet temperature 290^{0}C, the profile was higher. This shows that the peculiarity in the temperature profile occurs only in the case of lower inlet temperatures. At higher inlet temperatures, the rates are high and the reaction goes to near completion as indicated by a rapid rise in temperature followed by a drop in temperature.

The temperature drop occurs because the system is not adiabatic and there is loss of heat to the surrounding and the generation of heat is low or zero because of the depletion of reactants.

4.1.1.3 Effect of inlet temperature on conversion of CO_2

Figure 4.8 shows the effect of inlet temperature on conversion of CO_2 at different inlet concentrations of CO_2. The figure shows nearly complete conversion of CO_2 for both high and low inlet concentration at higher inlet temperature, 290°C. At low inlet temperature conversion of CO_2 varies inversely with inlet concentration of CO_2. For example, in Figure 4.8, conversion of CO_2 is 21% with inlet concentration of 2.5308 mol% CO_2 while it is 56% with inlet concentration of 0.9385 mol% CO_2. When inlet temperature is 247°C. But at higher inlet temperature conversion of CO_2 does not vary largely. At higher inlet concentration of CO_2 the conversion profile becomes sharper than that at lower inlet concentration of CO_2 with the increasing inlet temperature.

4.1.1.4 Effect of inlet concentration on conversion of CO_2:

Figure 4.9 shows the effect of inlet concentration on conversion of CO_2. The figure shows concentration of CO_2 has almost no effect on conversion of CO_2 at higher temperature. For example, in figure 4.9, conversion of CO_2 is 100% with inlet concentration of 0.9385 mol% CO_2 and it is 98% with inlet concentration of 2.5308 mol% CO_2 when inlet temperature is 290^0C. At higher inlet temperature the conversion profile is almost flat but it is sharper with negative slope at lower inlet temperature. The rise in conversion at higher inlet concentration is more than that at lower inlet concentration.

4.1.1.5 Effect of space velocity on the temperature profiles in the reactor

Figure 4.10 shows the temperature profiles in the reactor at different space velocities. It shows that the profiles with lower space velocity is sharper than that with higher space velocity. It also shows that the peak temperature moves towards right with increasing space velocity. This is because of heat generated in the reactor is swept out by excess flow. So that temperature could not be risen as before and peak temperature moves toward right.

4.1.1.6 Effect of space velocity on conversion of CO_2

Figure 4.11 shows the effect of space velocity on CO_2 conversion at constant flow of CO_2. It describes that conversion of CO_2 decreases with increasing space velocity or decreasing ***residence time.***

Table 4.1: Experimental Results of Steady State Methanation of Carbon Dioxide

Run No.	Inlet condition							Outlet condition		
	Temp. ^{0}K	Flow rate, mol/hr				Space velocity hr^{-1}	Peak temp. ^{0}C	Exit temp. ^{0}C	% conversion	
		H_2	N_2	CO_2	Total				CO_2	H_2
2001.1	520	1.7634	4.5982	0.0603	6.4219	0.2519	251	241	56.15	43.47
2001.2	520	1.7634	4.5982	0.0603	6.4219	0.2519	251	241	58.57	44.89
2001.3	520	1.7634	4.5982	0.0603	6.4219	0.2519	251	241	59.12	46.59
2002.1	520	1.7634	4.5982	0.1116	6.4732	0.2539	251	244	41.48	49.55
2002.2	520	1.7634	4.5982	0.1116	6.4732	0.2539	251	244	42.24	50.46
2003.0	520	1.7634	4.5982	0.1652	6.5268	0.2560	251	243	20.87	53.19
2004.1	543	1.7634	4.5982	0.0603	6.4219	0.2630	285	282	79.39	52.45
2004.2	543	1.7634	4.5982	0.0603	6.4219	0.2630	285	282	79.59	54.54
2005	543	1.7634	4.5982	0.1116	6.4732	0.2651	288	286	68.12	52.31
2006	543	1.7634	4.5982	0.1652	6.5268	0.2673	290	288	53.75	57.68
2007.1	543	3.0357	4.5982	0.1652	7.7991	0.3194	289	289	44.85	29.64
2007.2	543	3.0357	4.5982	0.1652	7.7991	0.3194	289	289	45.41	30.61
2008	543	3.0357	4.5982	0.0826	7.7165	0.3160	285	283	63.82	27.17

Run No.	Inlet condition							Outlet condition		
	Temp. ^{0}K	Flow rate, mol/hr				Space velocity hr^{-1}	Peak temp. ^{0}C	Exit temp. ^{0}C	% conversion	
		H_2	N_2	CO_2	Total				CO_2	H_2
2009	563	1.7634	4.5982	0.0469	6.4085	0.2721	314	301	100	44.60
2010	563	1.7634	4.5982	0.0915	6.4531	0.2740	328	316	99.34	48.21
2011	557	1.7634	4.5982	0.1205	6.4821	0.2723	325	312	98.75	62.10
2012.1	556	1.7634	4.5982	0.1652	6.5268	0.2737	338	325	96.87	70.73
2012.2	557	1.7634	4.5982	0.1652	6.5268	0.2742	340	331	96.11	71.52
2013.1	559	3.0357	4.5982	0.1652	7.7991	0.3288	343	336	97.36	43.19
2013.2	561	3.0357	4.5982	0.1652	7.7991	0.3300	345	336	96.82	43.63
2014.0	563	1.7634	4.5982	0.1116	6.4732	0.2749	332	318	98.53	21.97
2015	565	1.7634	4.5982	0.0603	6.4219	0.2737	319	304	100.00	31.15
2016	564	3.0357	4.5982	0.0826	7.7165	0.3282	325	311	99.30	28.90
2017.1	563	1.7634	4.5982	0.0915	6.4531	0.2740	329	315	99.66	48.74
2017.2	561	1.7634	4.5982	0.0915	6.4531	0.2740	327	313	99.63	55.42
2018.0	557	1.7634	4.5982	0.1652	6.5268	0.2742	342	335	95.34	70.52
2019	559	3.0357	4.5982	0.1652	7.7991	0.3288	341	330	96.21	41.16

Run No.	Inlet condition							Outlet condition		
	Temp. °K	Flow rate, mol/hr				Space velocity hr^{-1}	Peak temp. °C	Exit temp. °C	% conversion	
		H_2	N_2	CO_2	Total				CO_2	H_2
2020	559	3.0357	4.5982	0.1853	7.8192	0.3297	352	336	97.14	48.00
2021	559	3.0357	4.5982	0.1451	7.7790	0.3280	336	323	98.11	37.41
2022	561	3.0357	4.5982	0.1272	7.7612	0.3284	334	318	98.47	40.18
2023	563	3.0357	4.5982	0.1027	7.7366	0.3285	321	305	99.68	33.49
2024	552	1.7634	4.5982	0.1652	6.5268	0.2717	323	319	90.27	76.27
2026	543	1.7634	3.6384	0.1116	5.5134	0.2258	312	294	94.90	57.80
2027	543	1.7634	2.7679	0.1116	4.6429	0.1901	312	286	95.58	49.52
2028	573	1.7634	4.5982	0.1853	6.5469	0.2829	389	345	99.72	84.21
2029	573	1.7634	4.5982	0.1652	6.5268	0.2821	381	338	100.0	75.31
2030	573	1.7634	4.5982	0.1384	6.500	0.2809	371	332	100.0	75.44
2031	573	1.7634	4.5982	0.2054	6.5670	0.2838	401	351	99.67	83.93
2032	555	1.7634	4.5982	0.1384	6.500	0.2721	339	322	95.76	71.27
2040	543	1.7634	4.5982	0.0603	6.4219	0.2630	290	285	89.87	64.88
2041	543	1.7634	4.5982	0.1384	6.50	0.2662	302	299	81.45	74.08

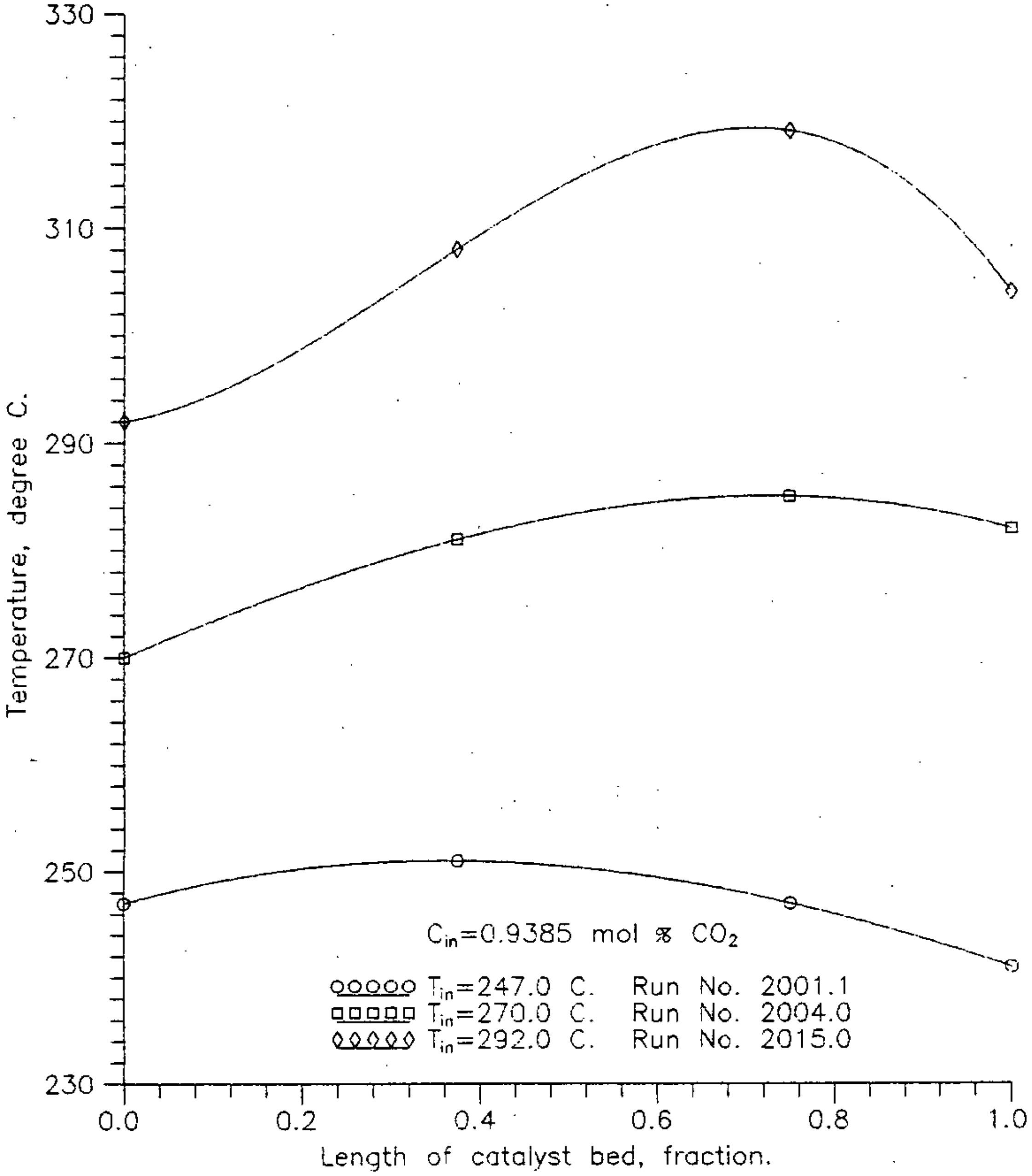


Figure 4.1 Temperature profiles in the reactor at different inlet temperatures.

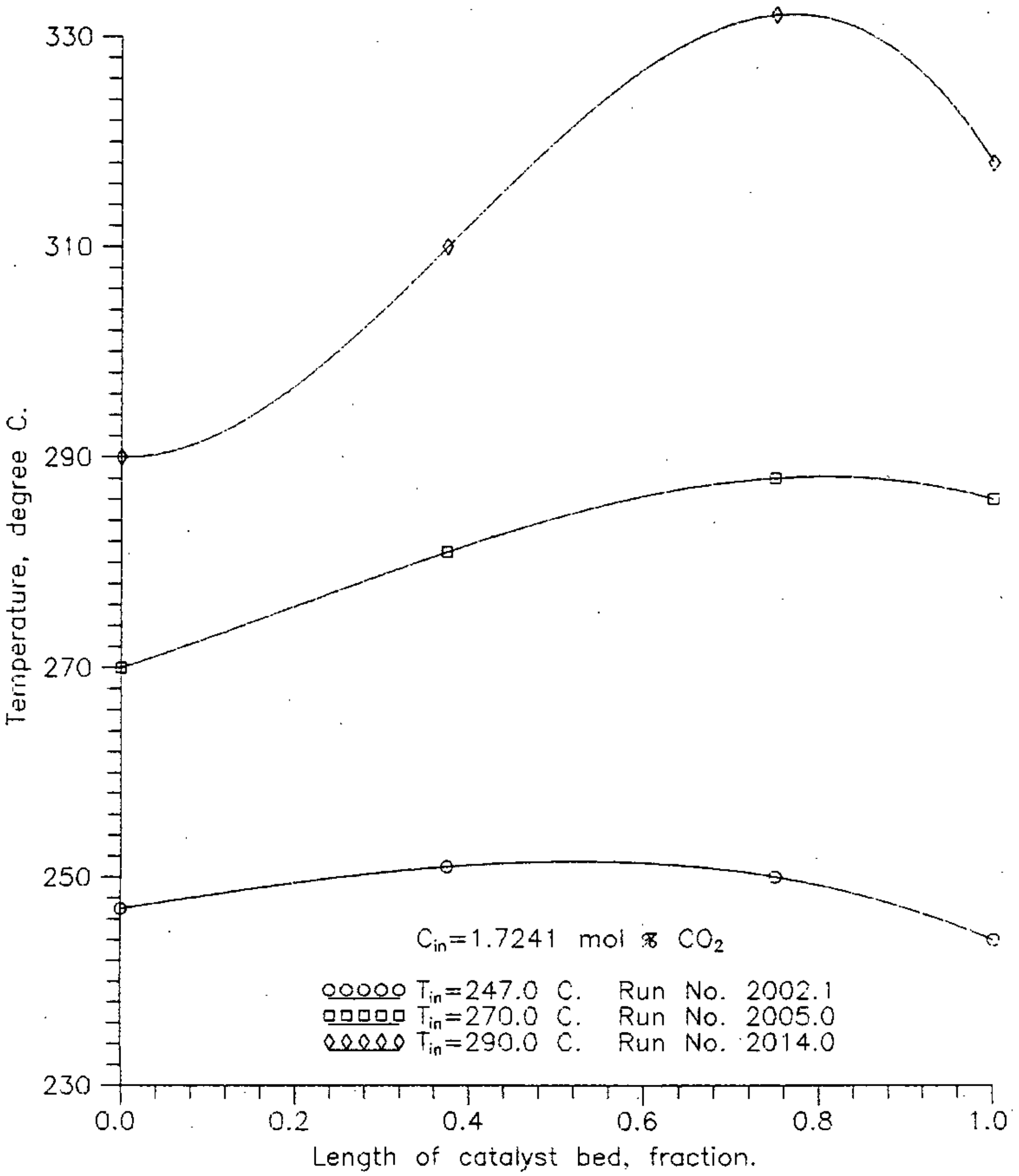


Figure 4.2 Temperature profiles in the reactor at different inlet temperatures.

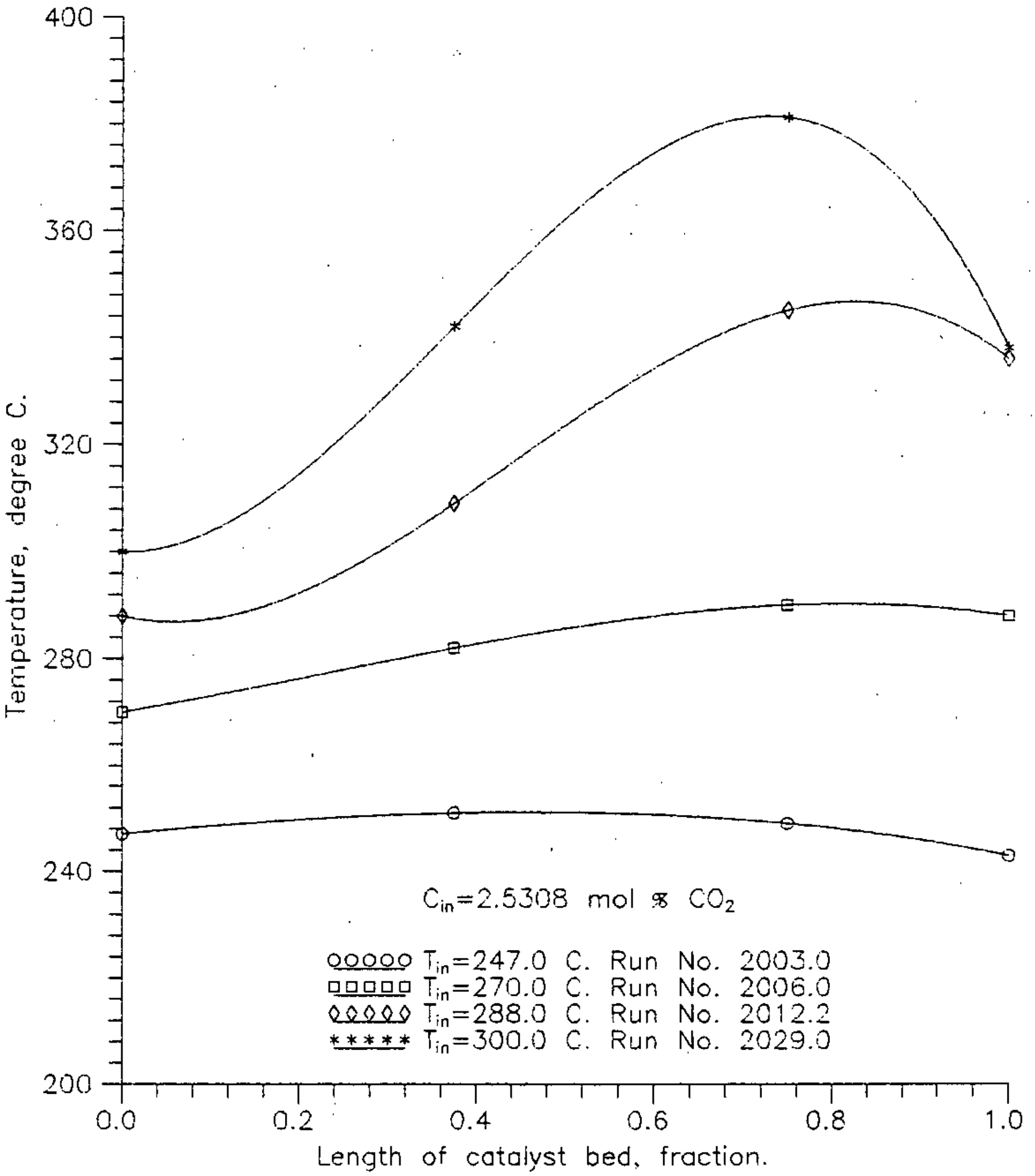


Figure 4.3 Temperature profiles in the reactor at different inlet temperatures.

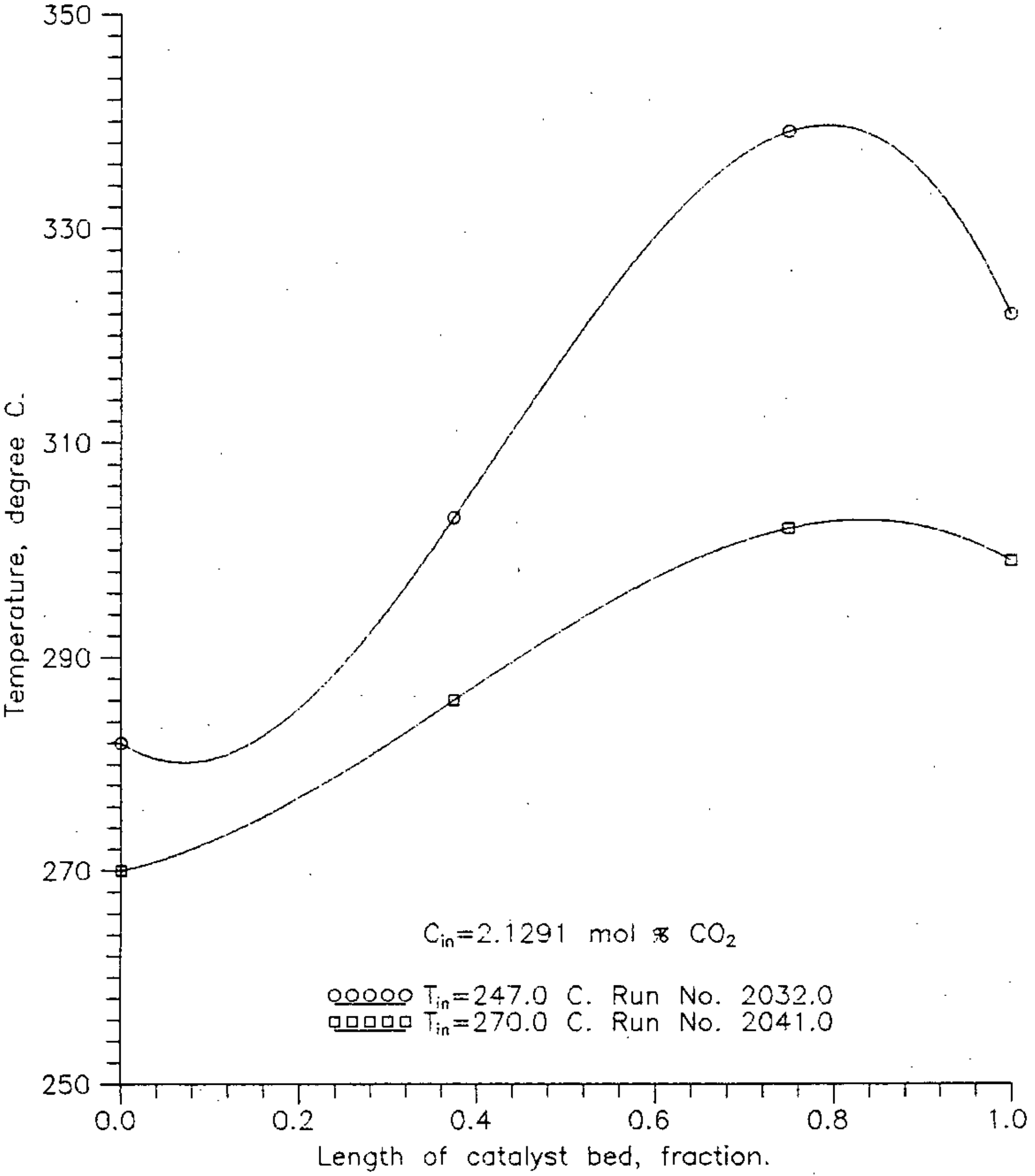


Figure 4.4 Temperature profiles in the reactor at different inlet temperatures.

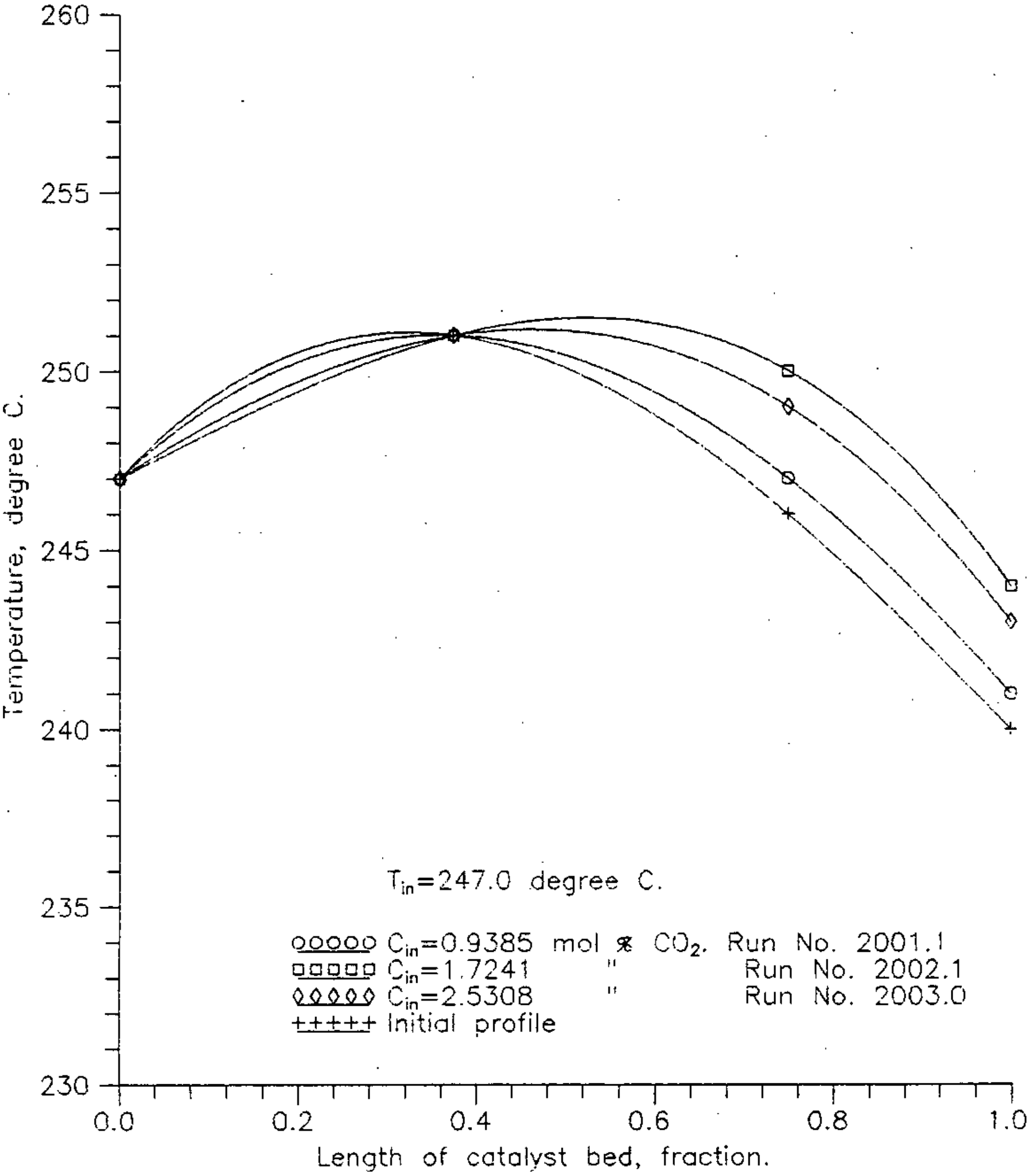


Figure 4.5 Temperature profiles in the reactor at different inlet concn. of CO_2.

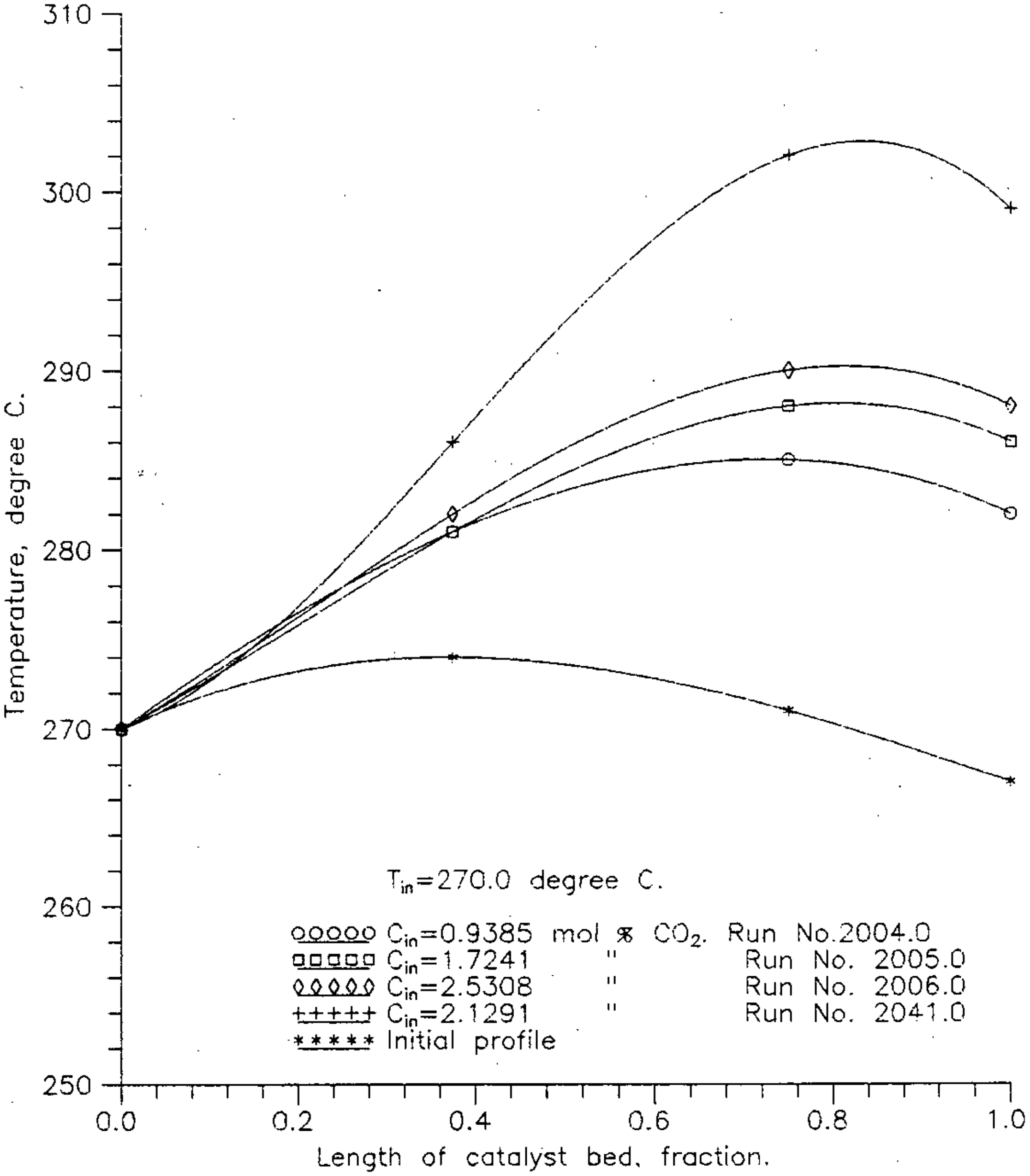


Figure 4.6 Temperature profiles in the reactor at different inlet concn. of CO_2.

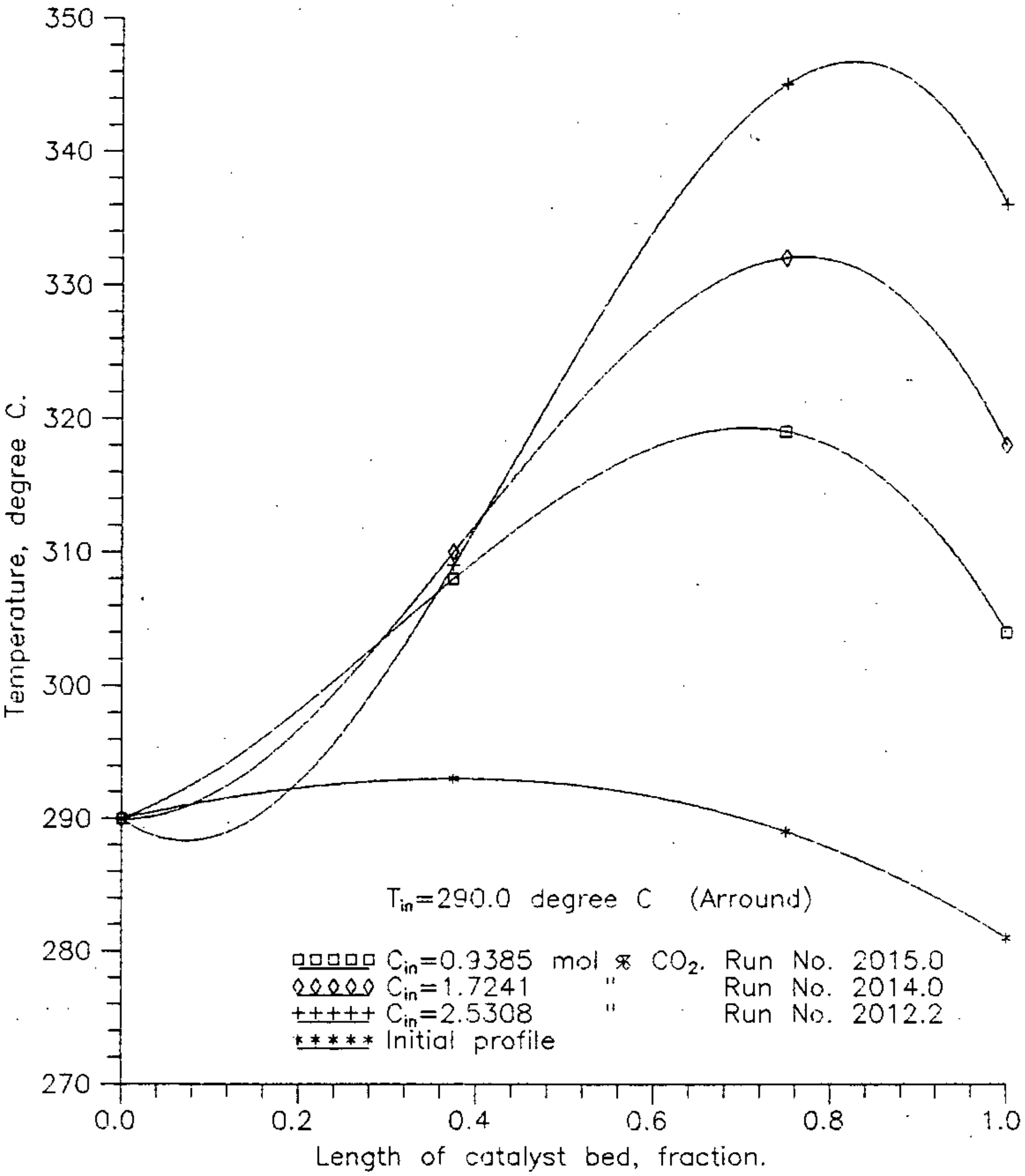


Figure 4.7 Temperature profiles in the reactor at different inlet concn. of CO_2.

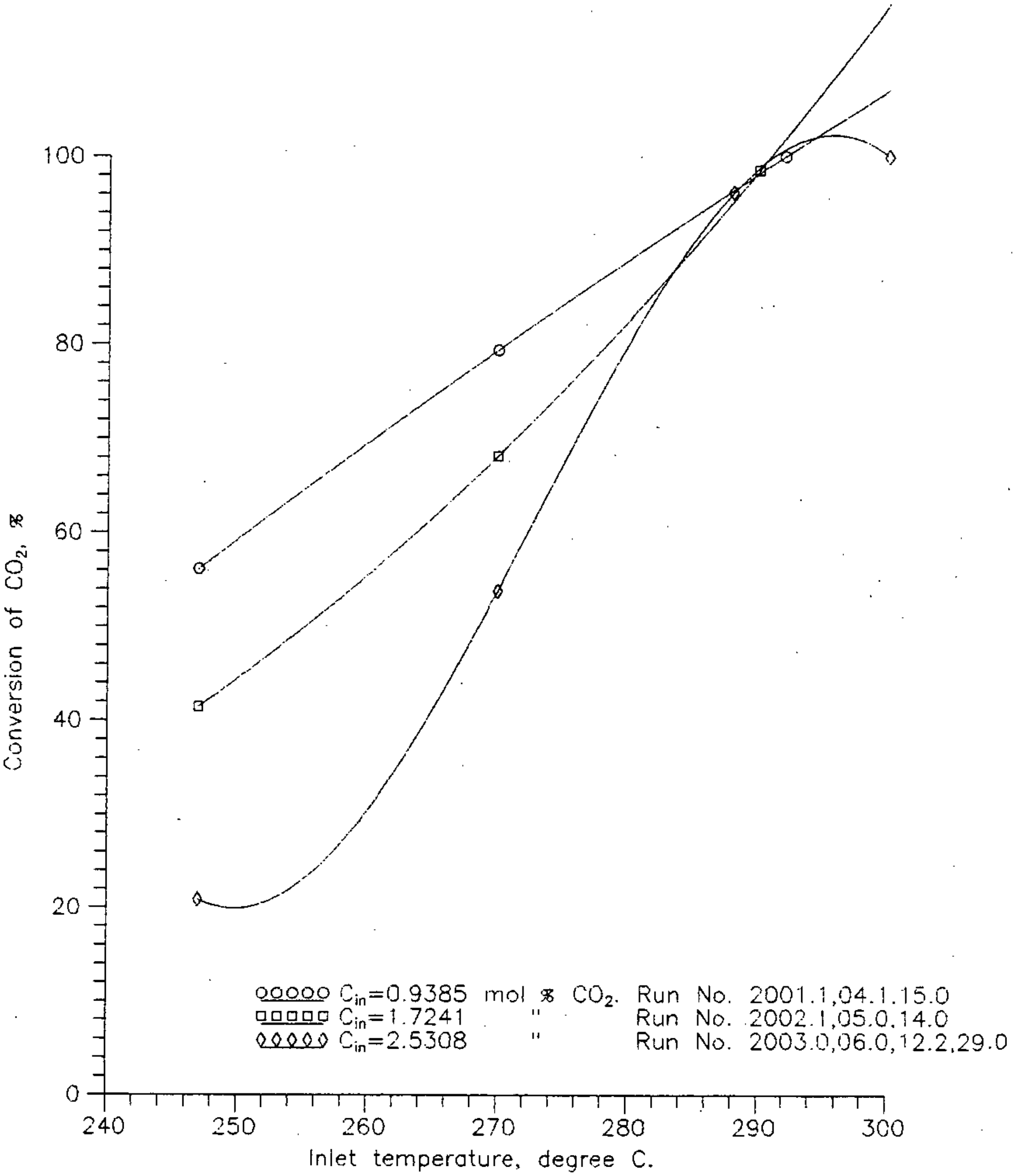


Figure 4.8 Effect of inlet temp. on conversion of CO_2 at different inlet conc. of CO_2.

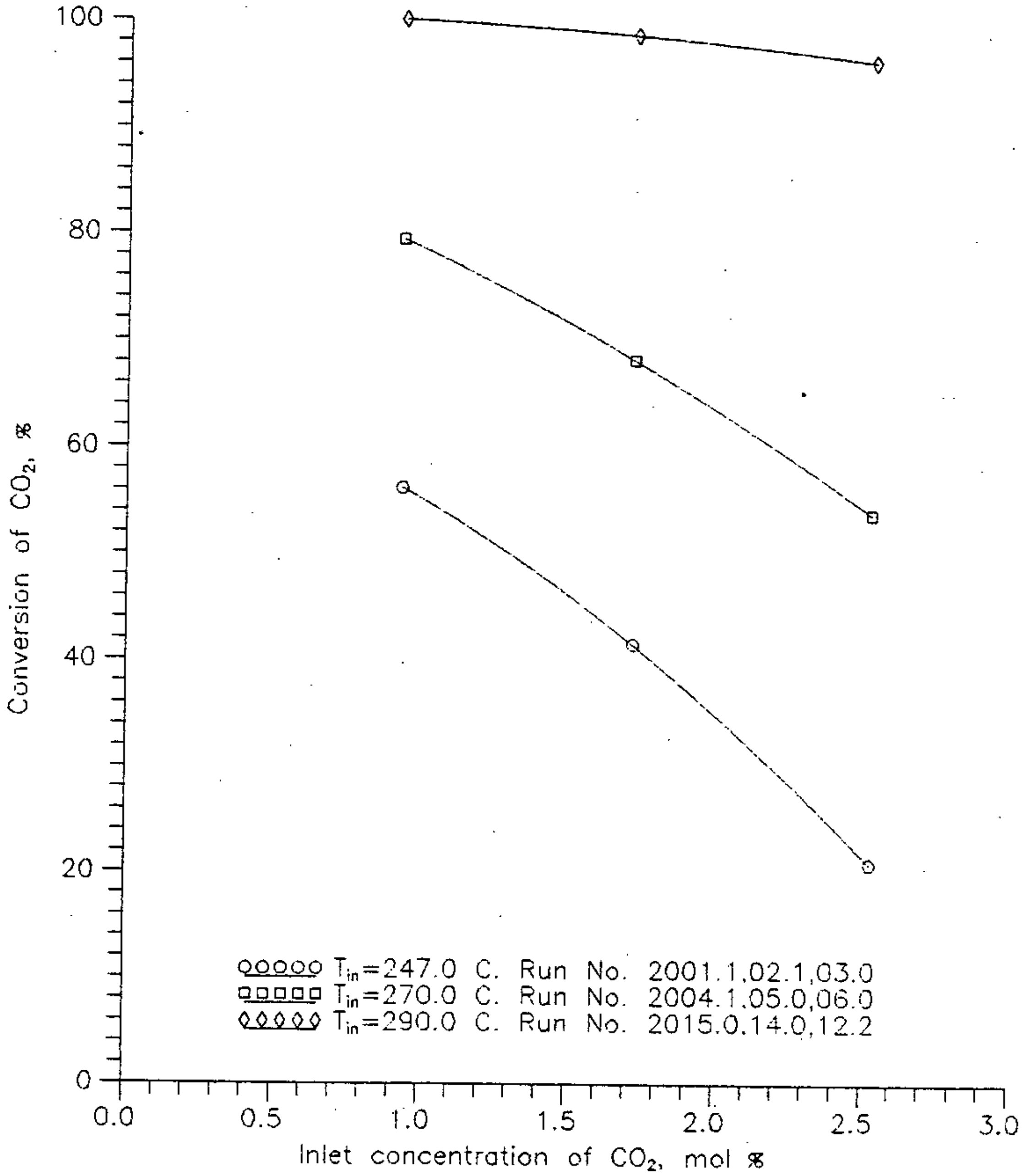


Figure 4.9 Effect of inlet concn. on conversion at CO_2 at different inlet temperatures.

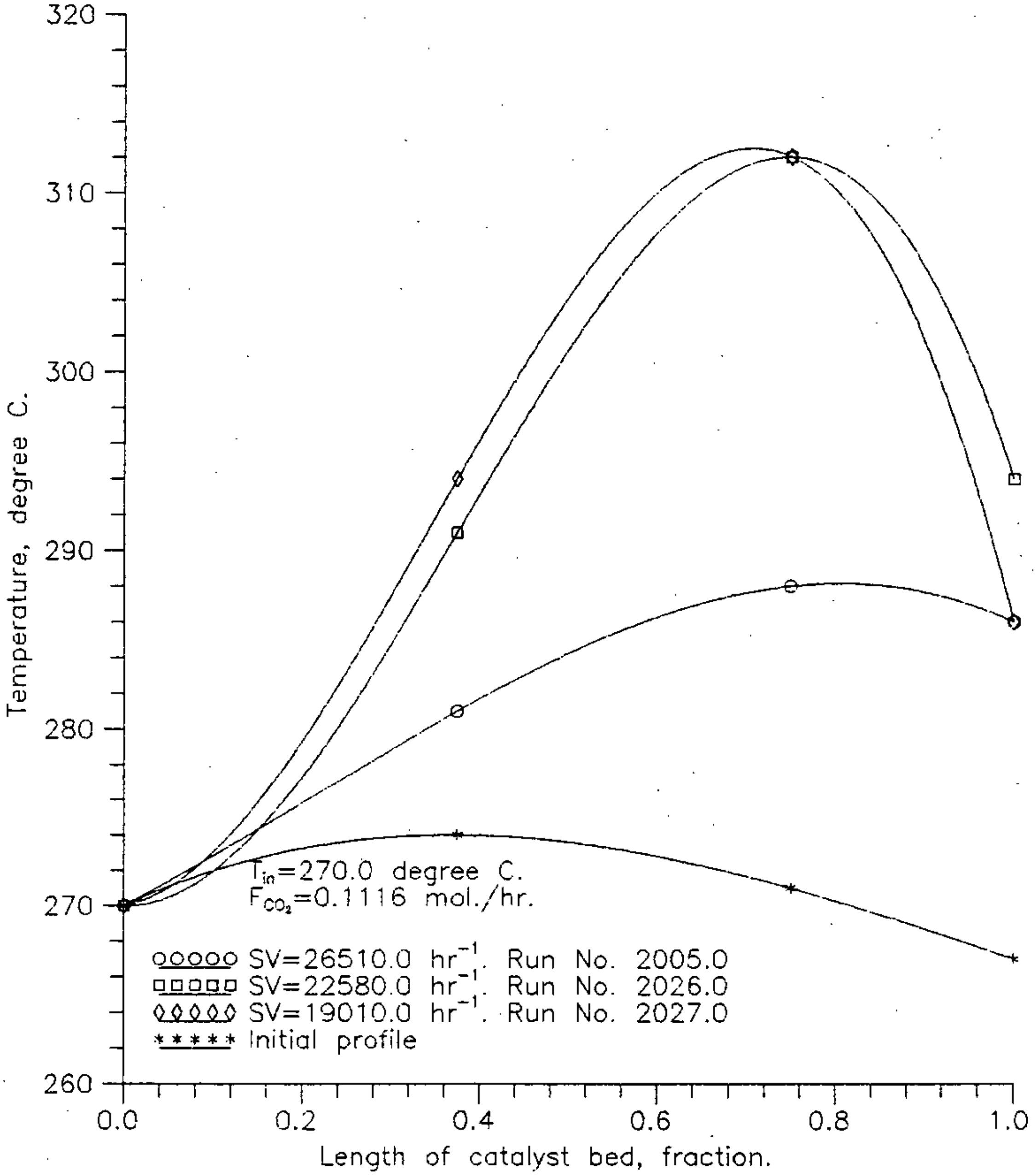


Figure 4.10 Temperature profiles in the reactor at different space velocities.

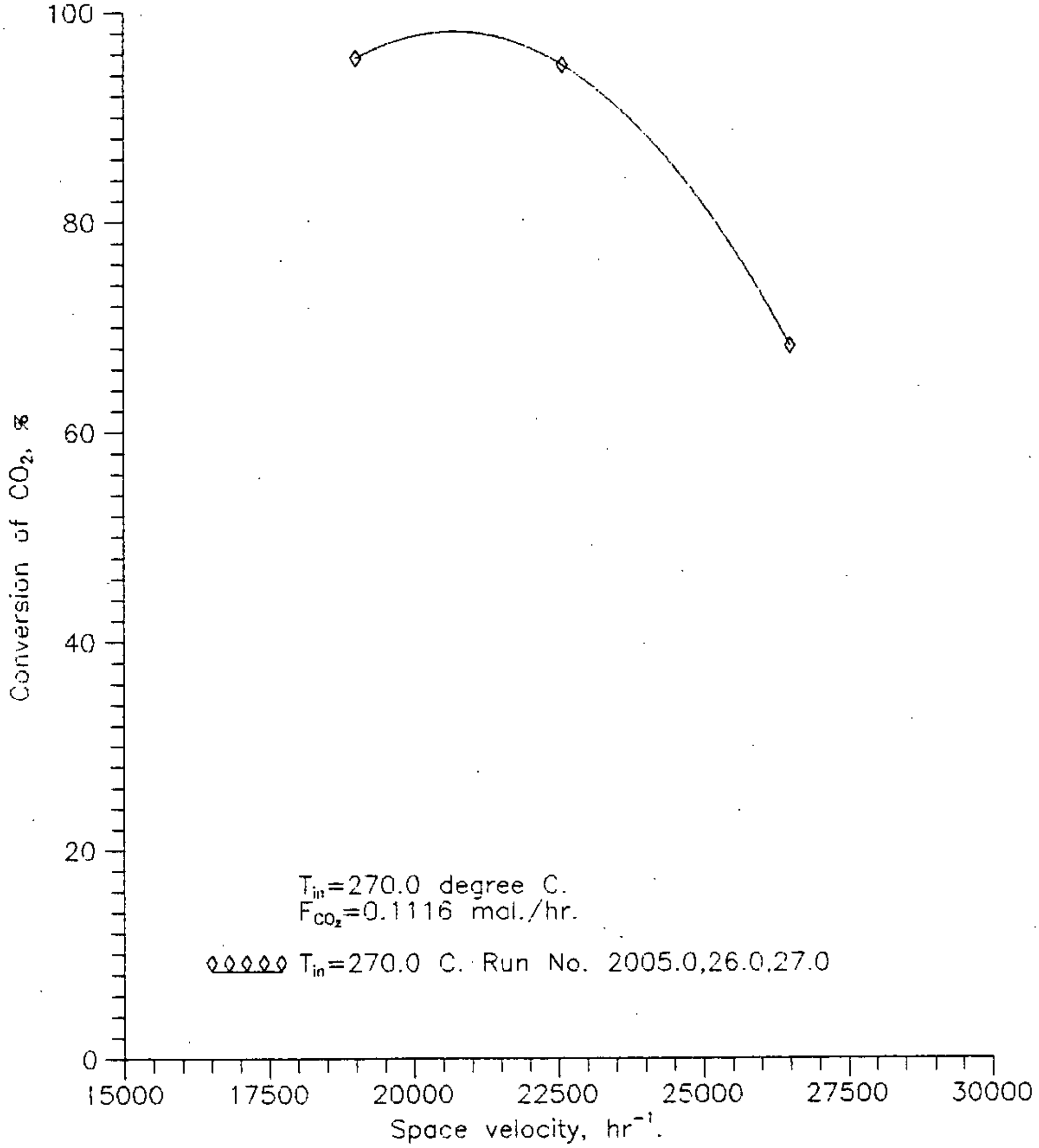


Figure 4.11 Effect of space velocity on conversion of CO_2 at constant CO_2 flow rate.

4.1.2 Study on CO methanation

4.1.2.1 Effect of inlet temperature on the temperature profiles.

Figures 4.12 to 4.14 show the general trend of temperature profile in the reactor. The initial profile of the reactor was of negative shope. For this reason the profiles show that the exit temperature is lower than the inlet temperature though exothermic reaction taking place in the reactor. The temperature profile remains downward trend for low inlet temperature, the profiles getting upward trend as the inlet temperature is increased. This effect is more pronounced at higher concentration of CO_2 as seen in figure 4.14.

4.1.2.2 Effect of inlet concentration on the temperature profiles

Figure 4.15 to 4.19 show the previous runs plotted as a function of inlet temperature with inlet CO concentration as parameter. The figures show milder profiles at low inlet concentration and low inlet temperature. The profiles become sharper with rise in both inlet concentrations and inlet temperatures. At a given inlet temperature, it is seen that the profiles rise with increase in inlet CO concentration upto a certain for certain inlet temperature, beyond which the profile shows a downward trend. For example in figure 4.15, the profiles increase as the inlet concentration of CO rises from 0.5971 mol% to 1.5588 mol%, but for 1.6448 mol% CO run the profile is lower with inlet temperature of 270^{0}C.

In figure 4.17, for 1.2950 and higher mol% CO run, the profile is lower with inlet temperature of 240^{0}C. In figure 4.18, for 1.5589 mol% CO run, the profile is lower with inlet temperature of 210^{0}C. However, for run with 1.5589 mol% CO at inlet temperature 270^{0}C, 250^{0}C, the profile is higher. These show that the peculiarity in the temperature profile occurs only in the case of lower inlet temperature and higher inlet concentration. At higher inlet temperatures, the rates are high and the reaction goes to near completion as indicated by a rise in temperature followed by a drop in temperature. The temperature drop occurs because the system is not adiabatic and there is loss of heat to the surrounding and the generation of heat is low or zero because of the depletion of reactants.

4.1.2.3 Effect of inlet temperature on conversion of CO

Figure 4.20 shows the effect of inlet temperature on conversion of CO at different inlet concentration of CO. The figure shows nearly complete conversion of CO for both high and low inlet concentration at higher inlet temperature. At low inlet temperature conversion of CO varies inversely with inlet concentration of CO. For example, in figure 4.20, conversion of CO is 15% with inlet concentration of 1.5589 mol% CO while it is 82% with inlet concentration of 0.5971 mol% CO when inlet temperature is 210^{0}C. But at higher inlet temperature conversion of CO does not vary largely. At low inlet concentration conversion is maximum over the range of inlet temperatures. At high inlet concentration conversion is minimum at lower inlet temperature. At higher inlet concentration of CO the conversion profile becomes sharper than that at lower inlet concentration of CO with the increasing inlet temperature.

4.1.2.4 Effect of inlet concentration on conversion of CO

Figure 4.21 shows the effect of inlet concentration on conversion. The figure shows concentration of CO has almost no effect on conversion of CO_2 at higher temperature. At higher inlet temperature the conversion profile is almost flatter but it is sharper with negative slope at lower inlet temperature. The rise in conversion of CO at higher inlet concentration of CO is more than that at lower inlet concentration of CO.

4.1.2.5 Effect of space velocity on the temperature profiles

Figure 4.22 shows the temperature profiles in the reactor at different space velocities. The figure shows that the profiles with lower space velocity is sharper than that with higher space velocity. It also shows that the peak temperature moves towards right with increasing space velocity. This is because of heat generated in the reactor is swept out by excess flow so that temperature could not be risen as before and peak temperature moves towards right.

4.1.2.6 Effect of space velocity on conversion of CO

Figure 4.23 shows the effect of space velocity on CO conversion at constant CO flow rate. The figure describes that conversion of CO decreases slightly with increasing space velocity

Table 4.2: Experimental Results of Steady State Methanation of Carbon Monoxide

Run No.	Inlet condition							Exit condition		
	Temp. ^{0}K	Flow rate, mol/hr				Space velocity hr^{-1} X 10^{-5}	Peak temp. ^{0}C	Exit temp. ^{0}C	% conversion	
		H_2	N_2	CO	Total				CO	H_2
3001.0	543	1.7634	4.7768	0.0393	6.5795	0.2695	273	250	100.00	47.32
3002.0	543	1.7634	4.7768	0.0732	6.6134	0.2708	289	255	100.00	55.18
3003.0	543	1.7634	4.7768	0.1036	6.6438	0.2721	299	267	100.00	56.44
3004.0	523	1.7634	4.7768	0.1036	6.6438	0.2621	280	259	99.15	61.55
3005.0	523	1.7634	4.7768	0.0732	6.6134	0.2609	258	246	100.00	51.76
3006.0	523	1.7634	4.7768	0.0393	6.5795	0.2595	251	233	100.00	48.05
3007.0	508	1.7634	4.7768	0.0732	6.6134	0.2534	235	226	74.08	53.48
3008.0	513	1.7634	4.7768	0.0393	6.5795	0.2546	245	220	100.00	53.89
3009.0	513	1.7634	4.7768	0.0732	6.6134	0.2559	250	236	96.03	55.34
3010.0	513	1.7634	4.7768	0.1036	6.6438	0.2571	244	242	75.67	57.89
3011.0	513	1.7634	3.817	0.0732	5.6536	0.2187	246	233	99.40	40.79
3012	513	1.7634	2.9464	0.0732	4.7830	0.1851	246	227	99.46	31.25

Run No.	Inlet condition							Exit condition		
	Temp. ^0K	Flow rate, mol/hr				Space velocity hr^{-1} X 10^{-5}	Peak temp. ^0C	Exit temp. ^0C	% conversion	
		H_2	N_2	CO	Total				CO	H_2
3018	513	3.0357	4.7768	0.0732	7.8857	0.3051	246	233	98.75	20.32
3019	513	1.7634	4.7768	0.0393	6.5795	0.2546	240	222	100.00	42.47
3024.1	543	1.7634	4.7768	0.1094	6.6496	0.2723	292	273	99.88	57.24
3024.2	543	1.7634	4.7768	0.1094	6.6496	0.2723	292	273	99.96	57.69
3039	483	1.7634	4.7768	0.0393	6.5795	0.2397	210	191	82.05	60.48
3040	483	1.7634	4.7768	0.0732	6.6134	0.2409	211	190	35.44	41.91
3041	483	1.7634	4.7768	0.1036	6.6438	0.2420	210	188	15.06	27.48
3042	497	1.7634	4.7768	0.1036	6.6438	0.2490	228	206	16.86	45.37
3043	497	1.7634	4.7768	0.0732	6.6134	0.2479	224	206	38.24	26.57
3044	497	1.7634	4.7768	0.0393	6.5795	0.2466	228	207	98.97	44.60

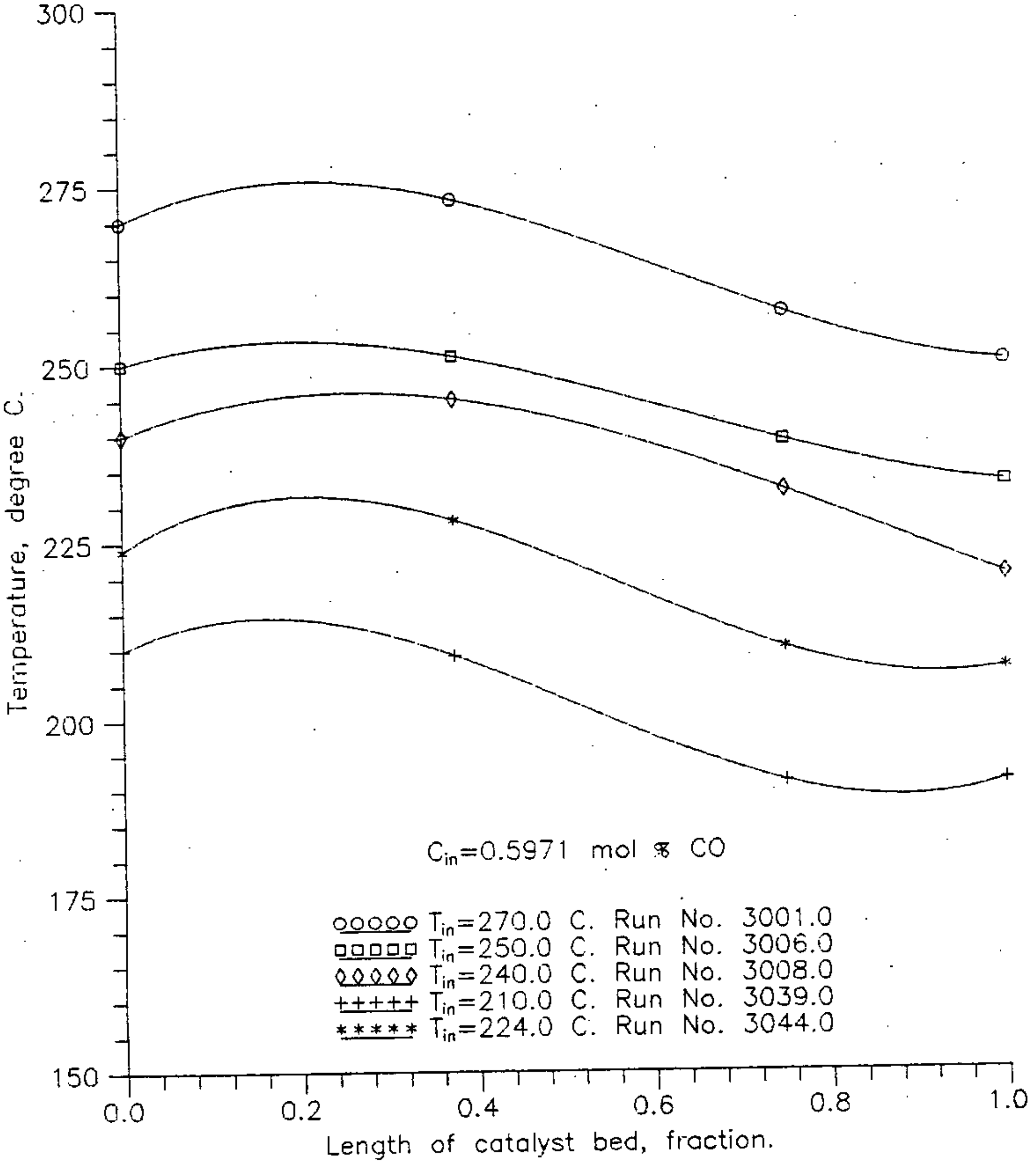


Figure 4.12 Temperature profiles in the reactor at different inlet temperatures.

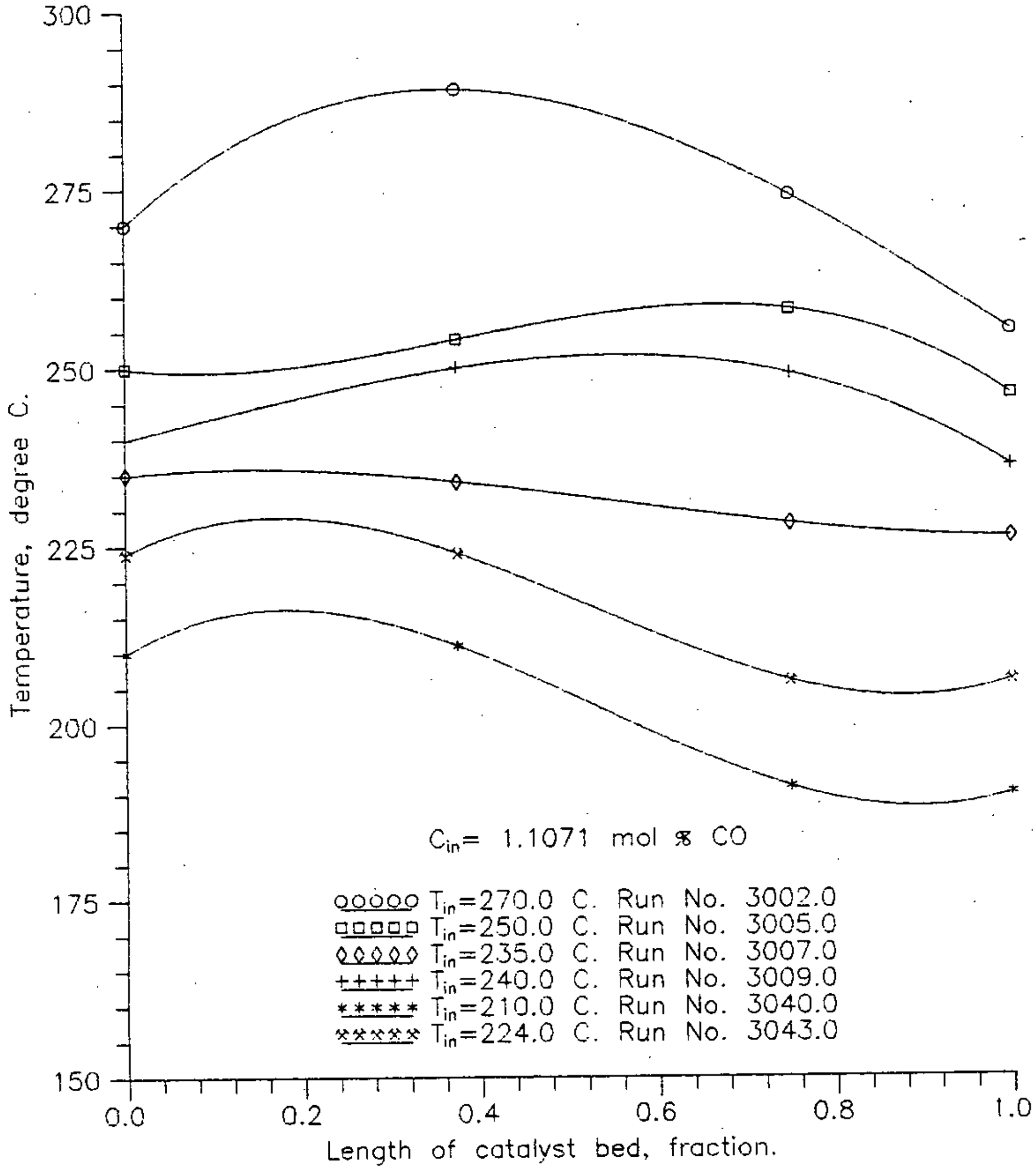


Figure 4.13 Temperature profiles in the reactor at different inlet temperatures.

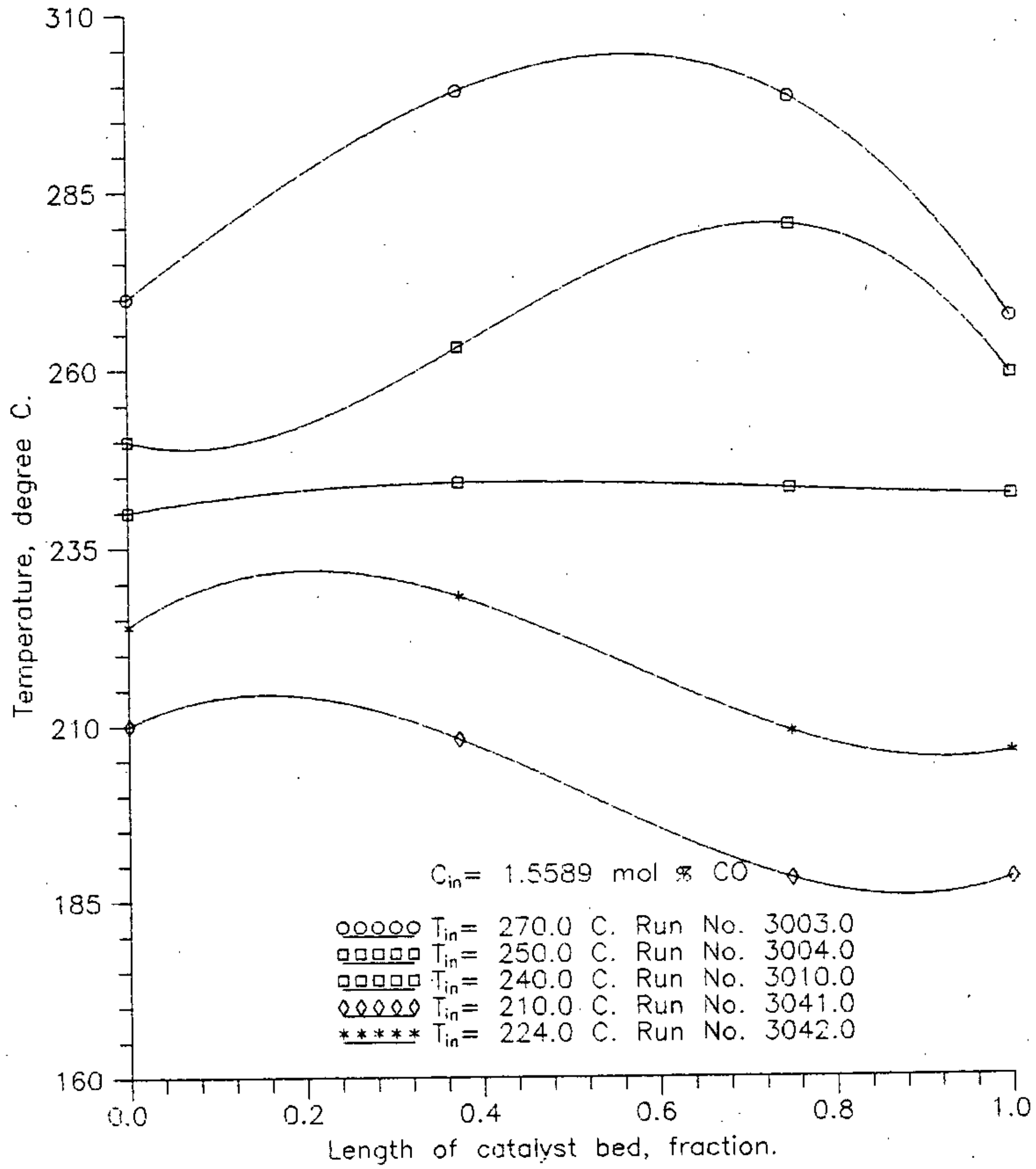


Figure 4.14 Temperature profiles in the reactor at different inlet temperatures.

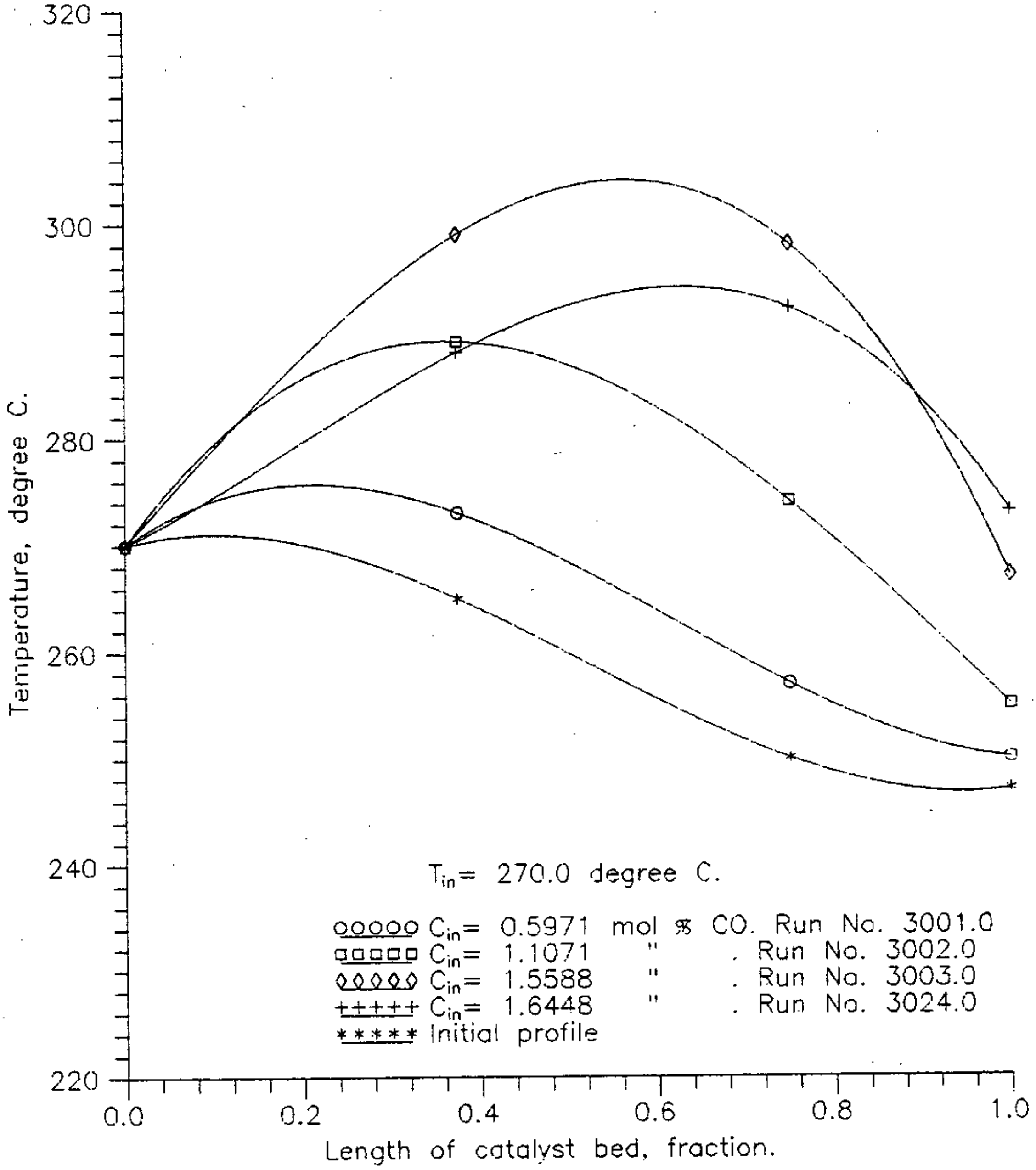


Figure 4.15 Temperature profiles in the reactor at different inlet concentrations of CO.

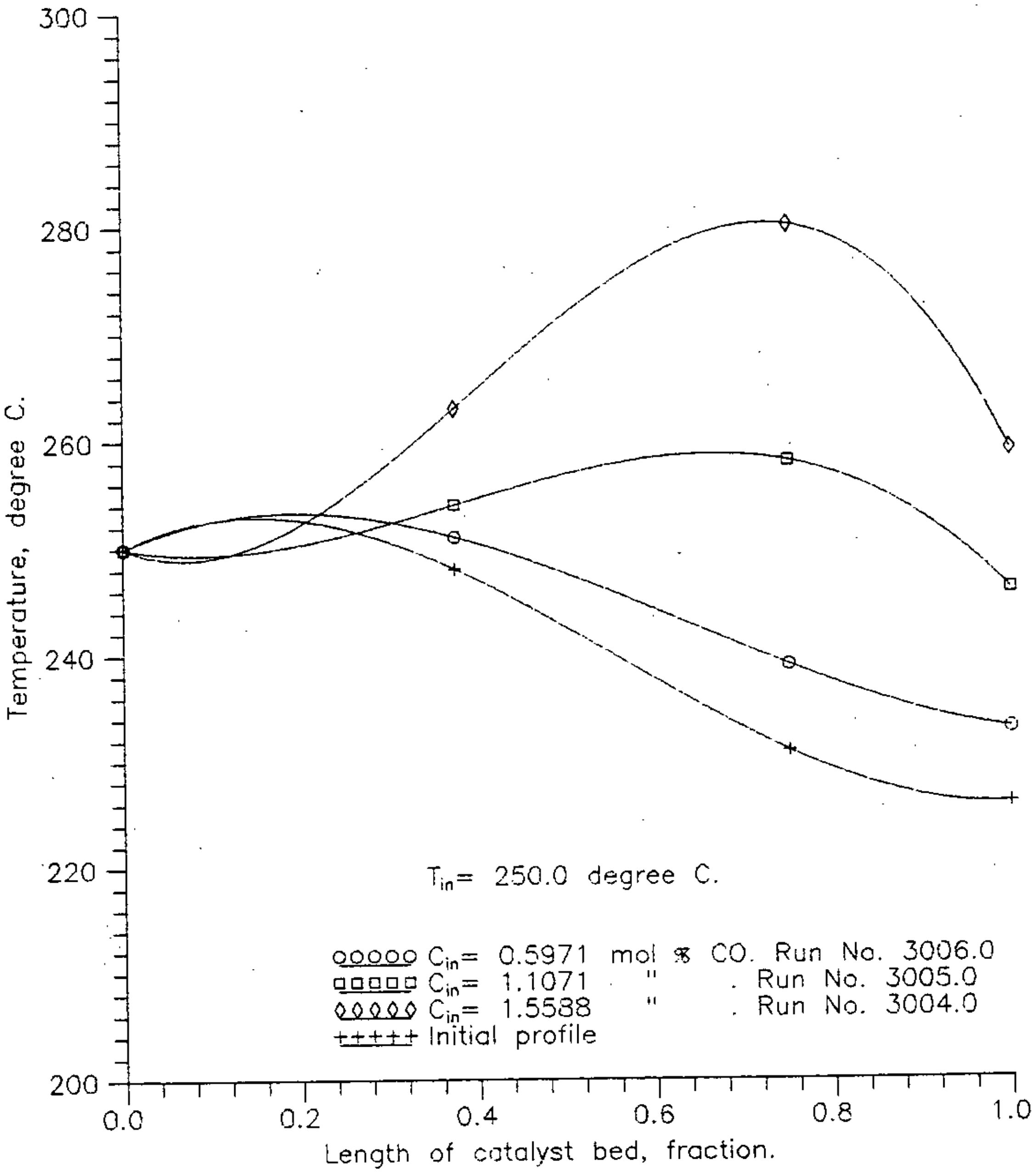


Figure 4.16 Temperature profiles in the reactor at different inlet concentrations of CO.

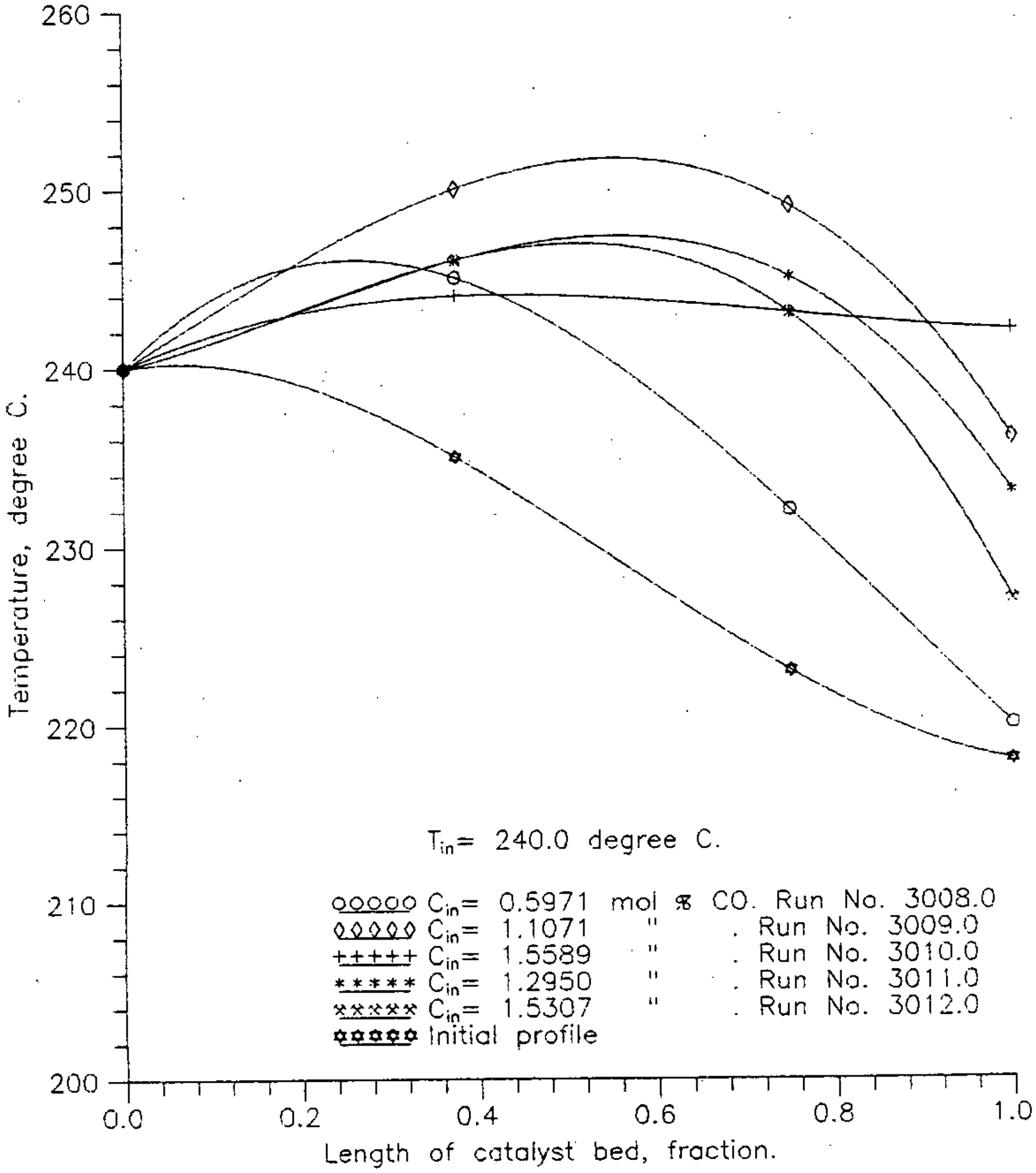


Figure 4.17 Temperature profiles in the reactor at different inlet concentrations of CO.

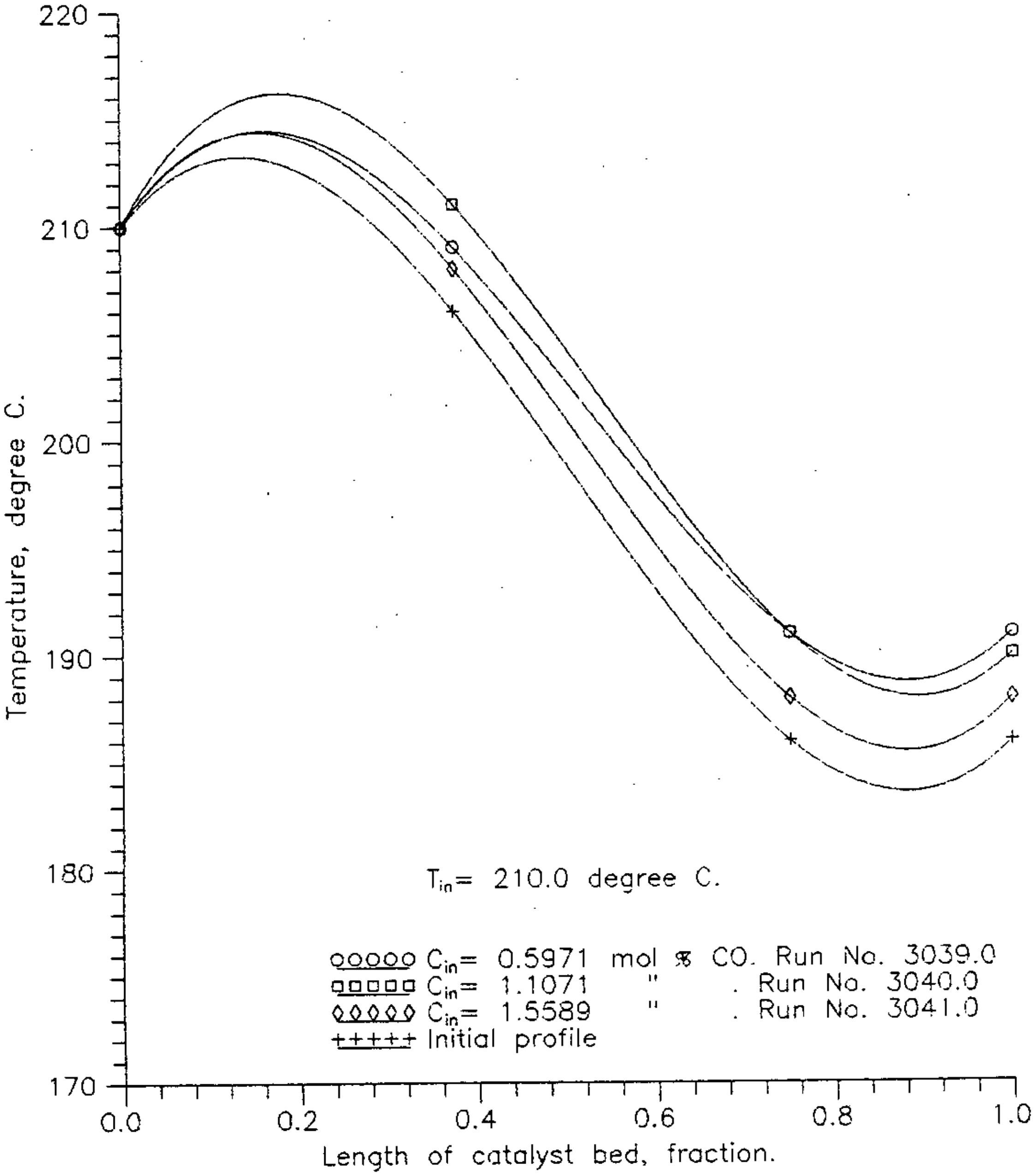


Figure 4.18 Temperature profiles in the reactor at different inlet concentrations of CO.

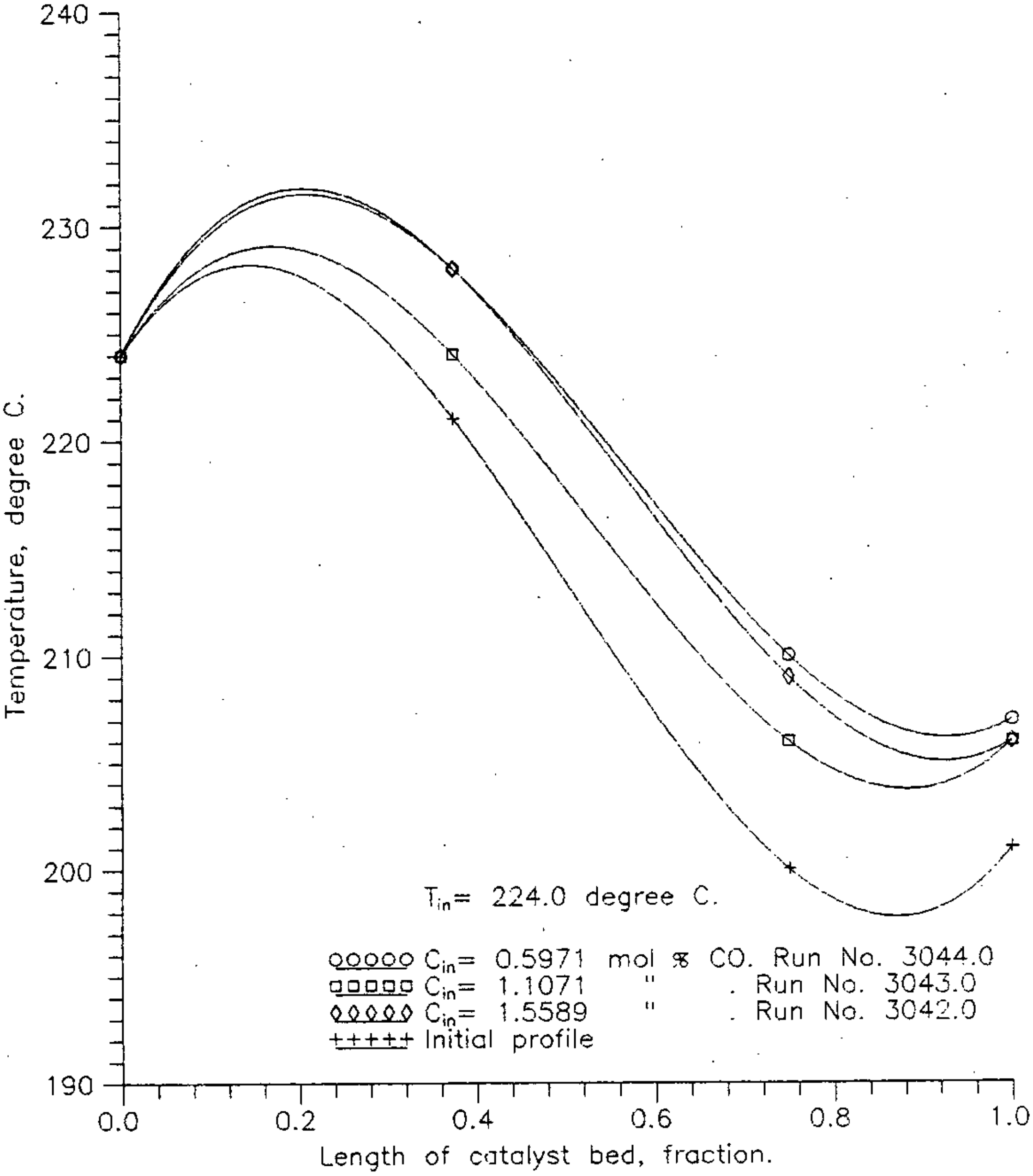


Figure 4.19 Temperature profiles in the reactor at different inlet concentrations of CO.

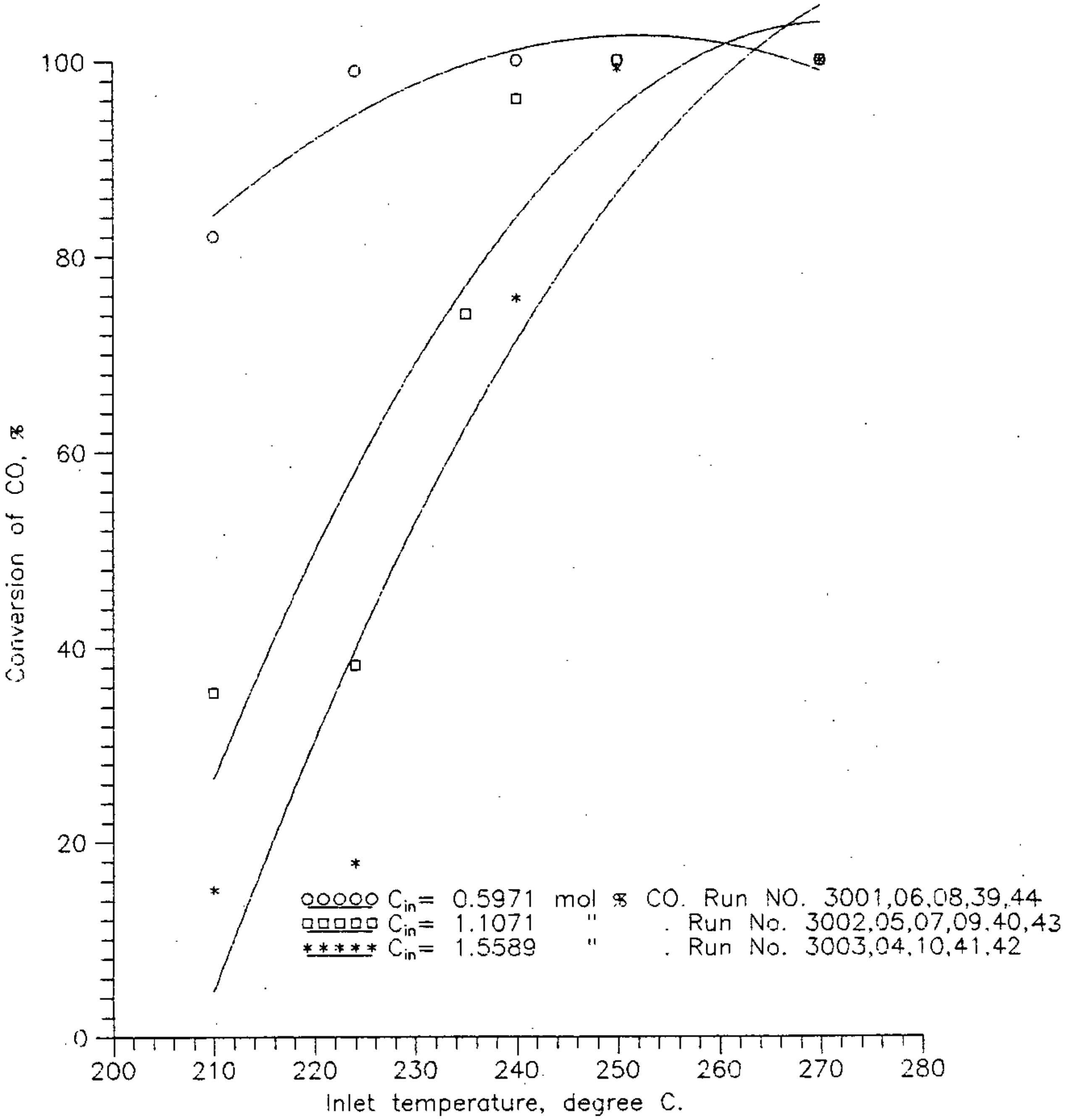


Figure 4.20 Effect of inlet temp. on conversion of CO at different inlet conc. of CO.

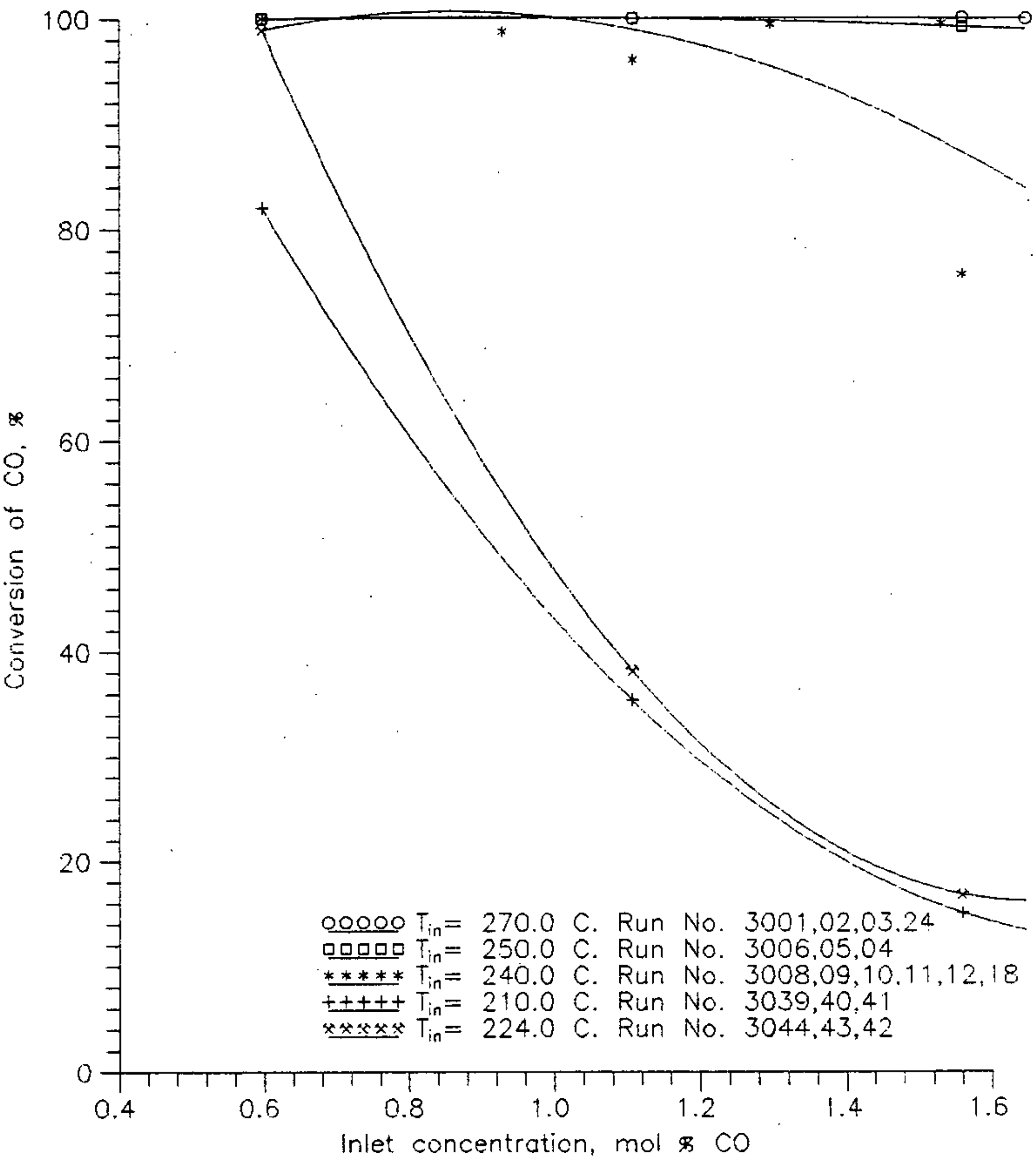


Figure 4.21 Effect of inlet concn. of CO on convn. of CO at different inlet temperatures.

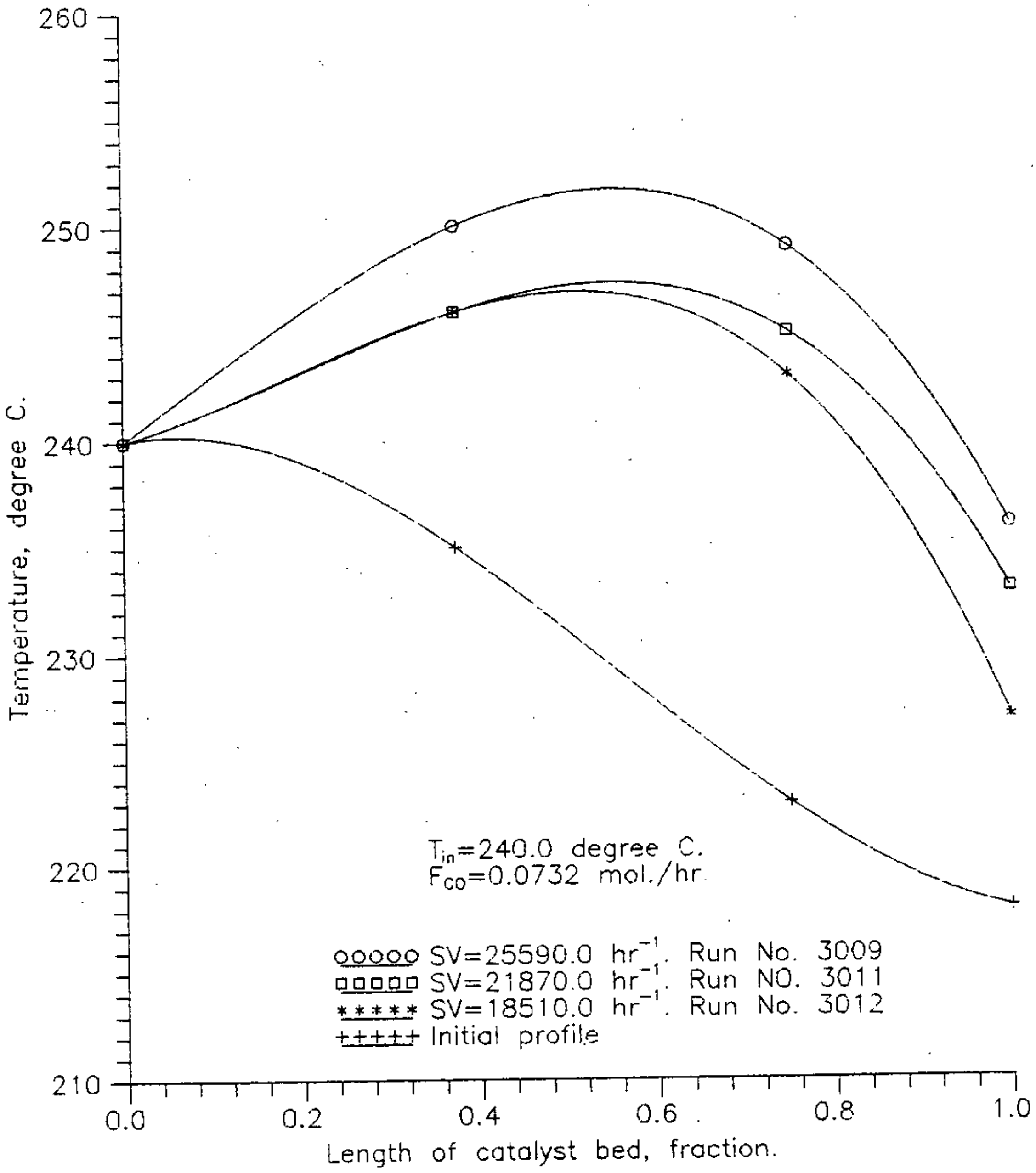


Figure 4.22 Temperature profiles in the reactor at different space velocities.

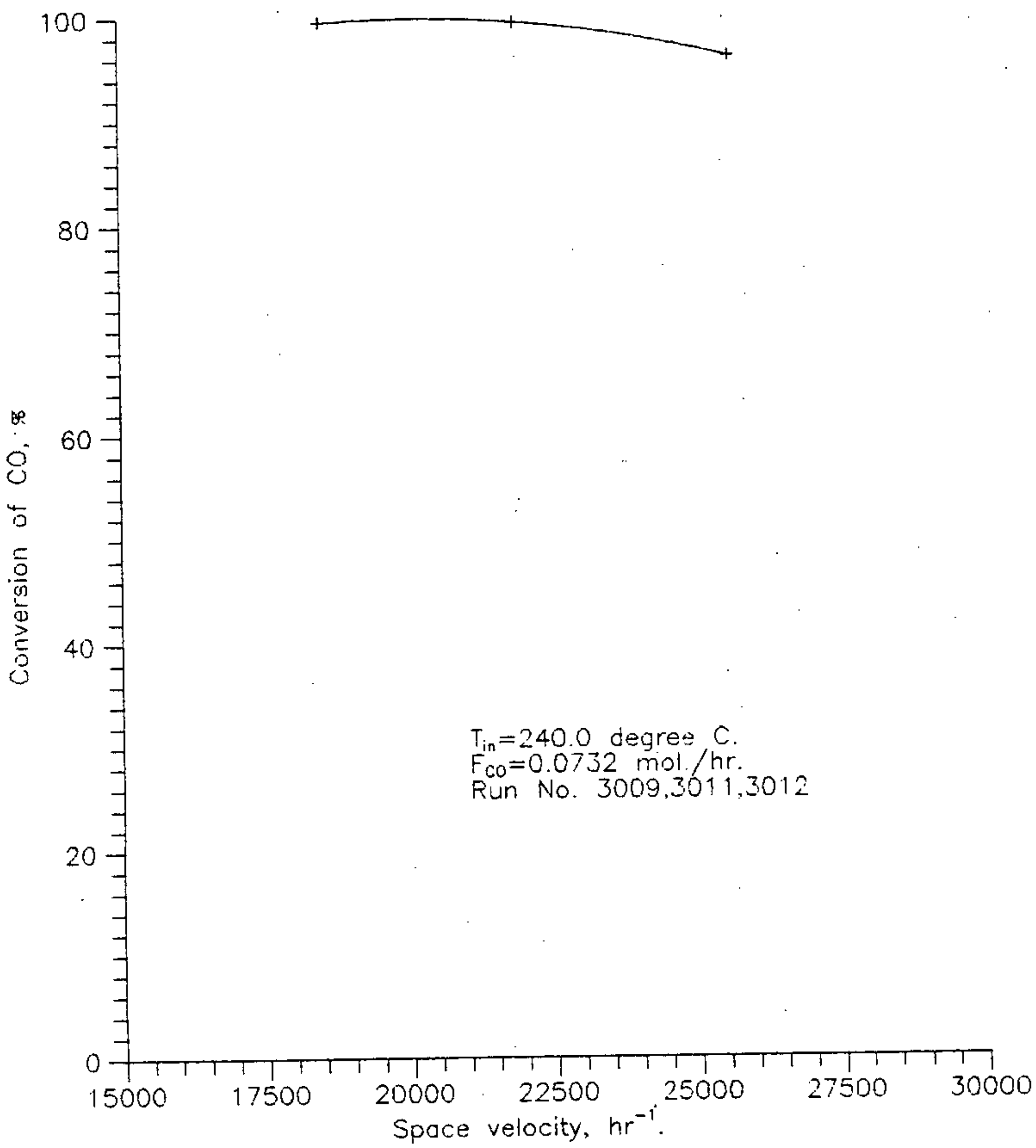


Figure 4.23 Effect of space velocity on conversion of CO at constant CO flow rate.

or decreasing residence time. This figure also shows space velocity has small effect on conversion of CO.

4.1.3 Study on mixture of CO & CO_2 methanation

Figure 4.24 to 4.34 are plotted for mixture of CO and CO_2. In case of concentration variation, flow rate of CO_2 is varied but flow rate of CO is kept constant. Also in this case the reactor shows the initial profile of downward trend.

4.1.3.1 Effect of inlet temperature on the temperature profiles

Figure 4.24 to 4.26 show the usual pattern of temperature profile in the reactor. The temperature profile remains flat or downward trend for low inlet temperature, the profiles getting upward trend as the inlet temperature is increased. This effect is more pronounced at higher concentration of CO_2 keeping CO flowrate constant as seen in figure 4.26.

4.1.3.2 Effect of inlet concentration on the temperature profiles

Figure 4.27 to 4.30 show the same runs plotted as a function of inlet temperature with inlet CO_2 concentration is parameter, but CO flow rate is kept constant. The figures show profiles of downward trend at low inlet concentration and low inlet temperature. The profiles become sharper and upward trend with the rise in both inlet concentration and inlet temperature. At a given inlet temperature, it is seen that the profiles rise with increase in inlet concentration upto a certain limit, beyond which the profile shows a downward trend. For example, in figure 4.28, the profiles increase as the inlet concentration of CO_2 rises from 0.7074 mol% to 1.2066 mol% and flowrate of CO is 0.0393 mol/hr., but for 1.6352 mol% CO_2 run, the profile is lower. Similar results were obtained in figure 4.29 (for run with 1.6352 mol%). However, for run with 1.6352 mol% CO_2 at inlet temperature 260^0C, the profile was higher. This shows that the peculiarity in the temperature profile occurs only in the case of lower inlet temperature.

At higher inlet temperature the rates are high and the reaction goes to near completion as indicated by a rapid rise in temperature followed by a drop in temperature. The temperature drop occurs because the system is not adiabatic and there is loss of heat to the surrounding and the generation of heat is low or zero because of the depletion of reactants.

4.1.3.3 Effect of inlet temperature on conversion of CO & CO_2

Figure 4.31 shows the effect of inlet temperature on conversion of CO and CO_2. The figure shows nearly complete conversion of CO for both high and low inlet concentration at higher inlet temperature. The figure also shows that the conversion of CO & CO_2 increases with the increasing inlet temperature.

4.1.3.4 Effect of inlet concentration on conversion of CO & CO_2

Figure 4.32 shows the effect of inlet concentration on conversion of CO & CO_2. The figure shows concentration of CO_2 has less effect on conversion of CO & CO_2 at higher temperature, 260^0C.

At low temperature conversion of CO decreases highly with the increasing concentration of CO_2. At lower temperature conversion of CO_2 decreases more than that of CO.

4.1.3.5 Effect of space velocity on the temperature profiles

Figure 4.33 shows the temperature profiles in the reactor at different space velocities. The figure shows that the profiles rise with increasing space velocity upto a certain limit beyond which the profile shows a downward trend. For example, in figure 4.33 the profiles increase as the space velocity from 19050.0 hr^{-1} 26270.0 hr^{-1}, but for 31290.0 hr^{-1}. run, the profile is lower.

4.1.3.6 Effect of space velocity on conversion of CO & CO_2

Figure 4.34 shows the effect of space velocity on conversion of CO and CO_2. The figure shows that conversion of CO decreases very little with the increasing space velocity and shows almost complete conversion of CO. It also shows that conversion of CO_2 initially increases with the increasing space velocity then decreases. Here another thing is to describe that at the same inlet temperature, inlet concentration of CO & CO_2 and space velocity conversion of CO is higher than that of CO_2.

Table 4.3: Experimental Results of Steady State Methanation of the mixture of Carbon Monoxide and Carbon Dioxide

Run No.	Inlet condition								Exit condition			
	Temp. ^{0}K	Flow rate, mol/hr					Space velocity hr^{-1} X 10^{-5}	Peak temp. ^{0}C	Exit temp. ^{0}C	% conversion		
		H_2	N_2	CO	CO_2	Total				H_2	CO_2	CO
3027	533	1.7634	4.7768	0.0393	0.0469	6.6263	0.2664	273	248	52.57	81.82	99.43
3028	533	1.7634	4.7768	0.0393	0.0804	6.6598	0.2677	278	254	51.03	80.04	98.69
3029	533	1.7634	4.7768	0.0393	0.1094	6.6888	0.2689	276	249	62.43	74.27	97.5
3030	523	1.7634	4.7768	0.0393	0.1094	6.6888	0.2638	258	244	48.02	46.44	97.62
3031	523	1.7634	4.7768	0.0393	0.0804	6.6598	0.2627	264	244	52.75	56.77	98.23
3032	523	1.7634	4.7768	0.0393	0.0469	6.6263	0.2614	260	239	26.23	53.18	99.02
3033	523	1.7634	3.8170	0.0393	0.0804	5.700	0.2248	266	242	45.16	62.31	98.75
3034	523	1.7634	2.9464	0.0393	0.0804	4.8295	0.1905	264	239	31.97	53.59	99.15
3035	523	3.0357	4.7768	0.0393	0.0804	7.9321	0.3129	257	244	19.71	35.75	96.77
3036	513	1.7634	4.7768	0.0393	0.0804	6.6598	0.2577	244	232	44.45	21.93	94.93
3037	513	1.7634	4.7768	0.0393	0.1094	6.6888	0.2588	243	233	44.18	27.65	93.13
3038	513	1.7634	4.7768	0.0393	0.0469	6.6263	0.2564	242	231	42.01	28.24	97.89
3045	543	1.7634	4.7768	0.0393	0.0804	6.6598	0.2727	285	271	60.83	91.09	99.18

Run No.	Inlet condition								Exit condition			
	Temp.	Flow rate, mol/hr					Space velocity	Peak temp.	Exit temp.	% conversion		
	^{0}K	H_2	N_2	CO	CO_2	Total	hr^{-1} X 10^{-5}	^{0}C	^{0}C	H_2	CO_2	CO
3046.1	553	1.7634	4.7768	0.0393	0.0804	6.6598	0.2778	297	280	61.29	96.88	99.62
3046.2	553	1.7634	4.7768	0.0393	0.0804	6.6598	0.2778	297	280	62.77	96.90	99.74
3047	497	1.7634	4.7768	0.0393	0.0804	6.6598	0.2496	224	206	50.40	33.95	57.01
3048	497	1.7634	4.7768	0.0393	0.0869	6.6263	0.2484	225	206	46.77	26.22	81.15
3049	497	1.7634	4.7768	0.0393	0.1094	6.6888	0.2507	225	205	48.40	27.07	39.44

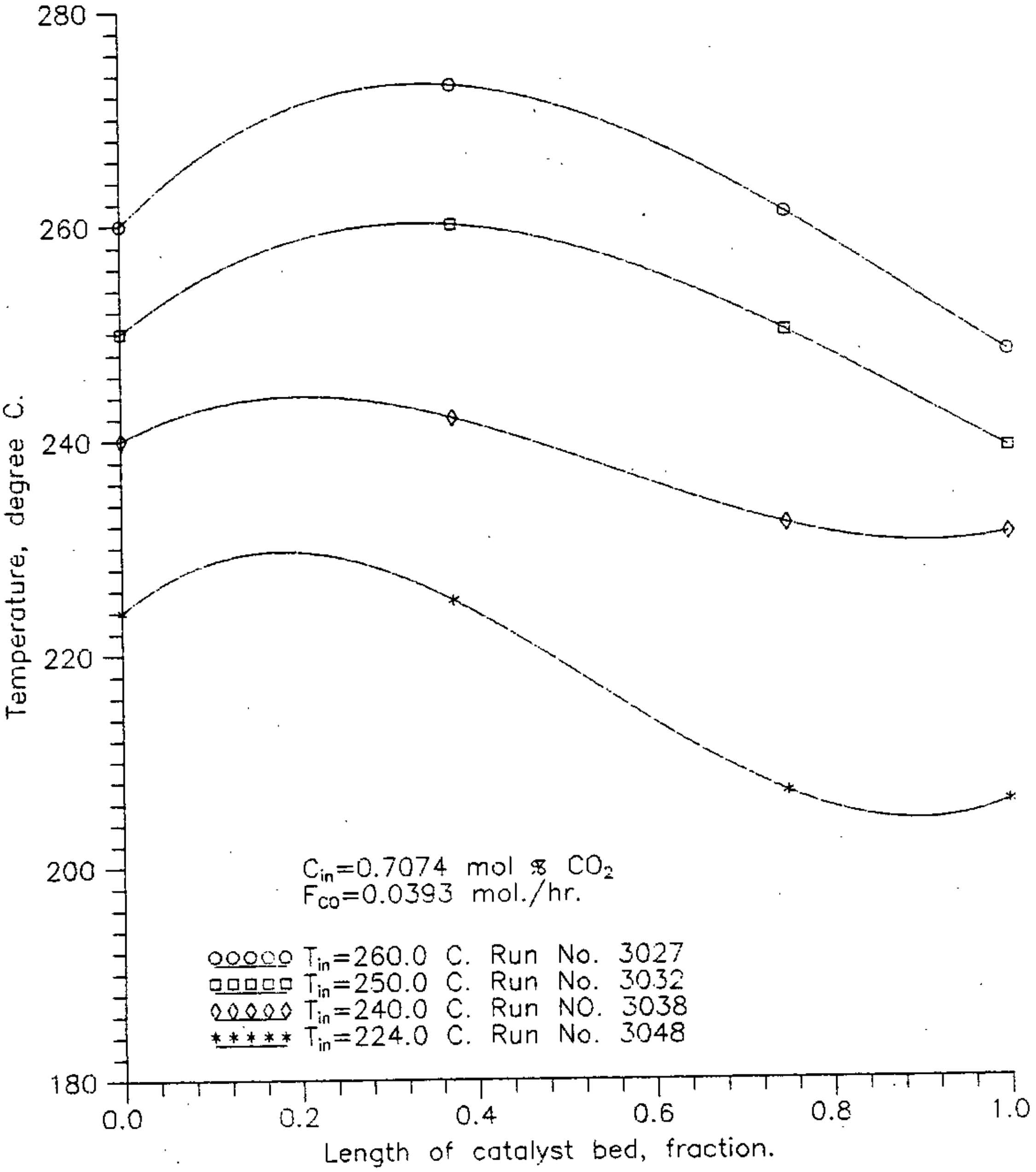


Figure 4.24 Temperature profiles in the reactor at different inlet temperatures.

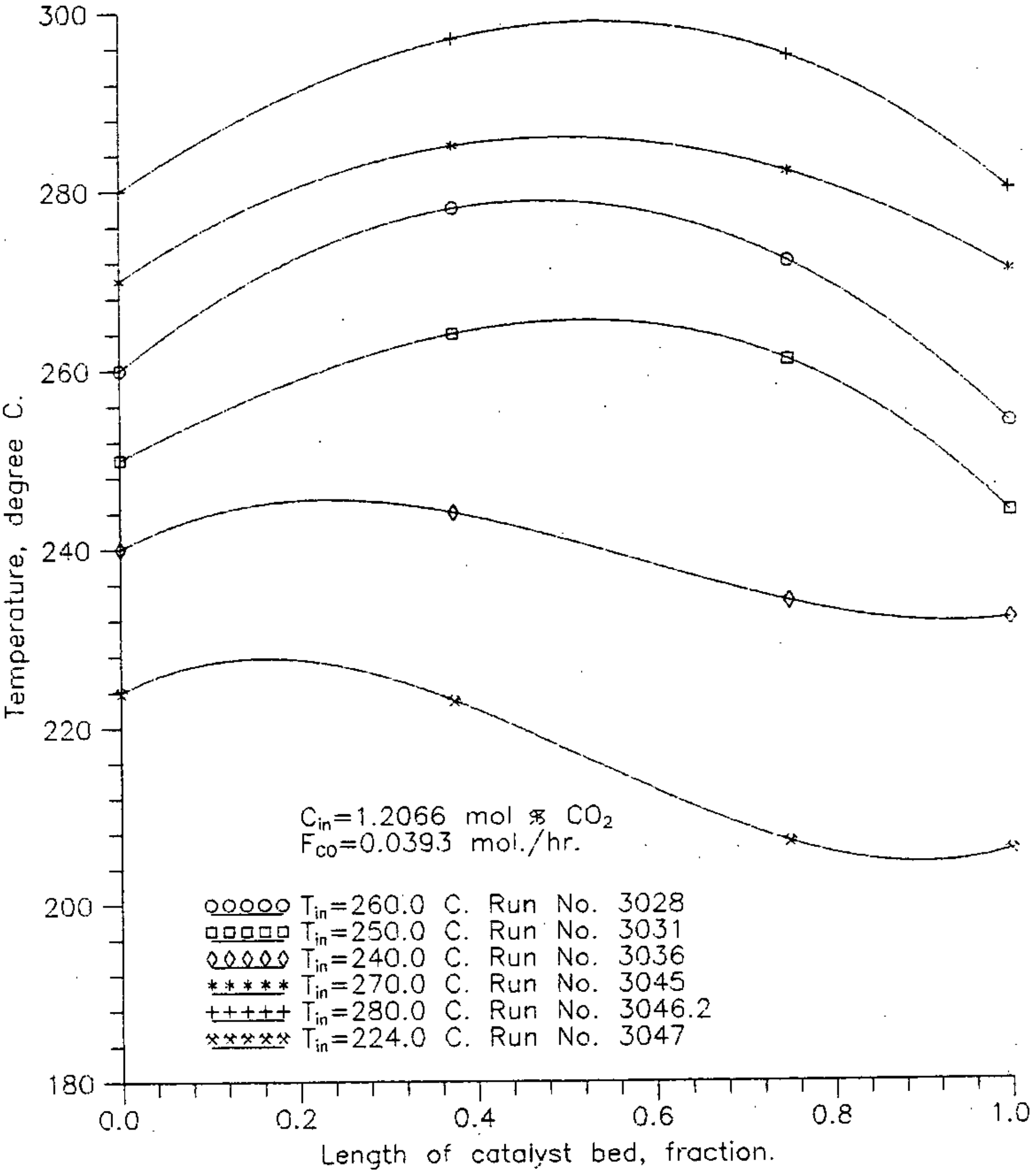


Figure 4.25 Temperature profiles in the reactor at different inlet temperatures.

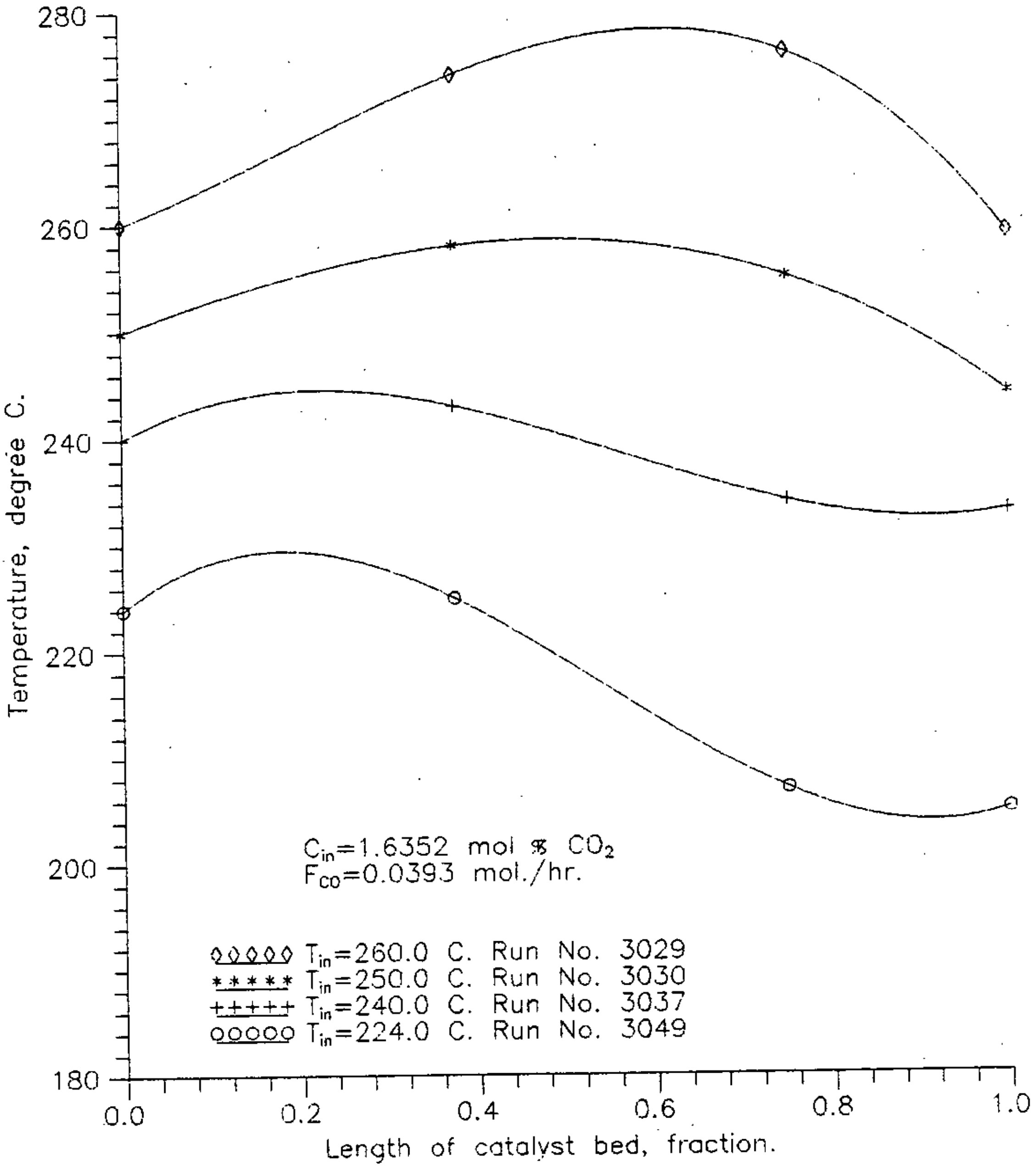


Figure 4.26 Temperature profiles in the reactor at different inlet temperatures.

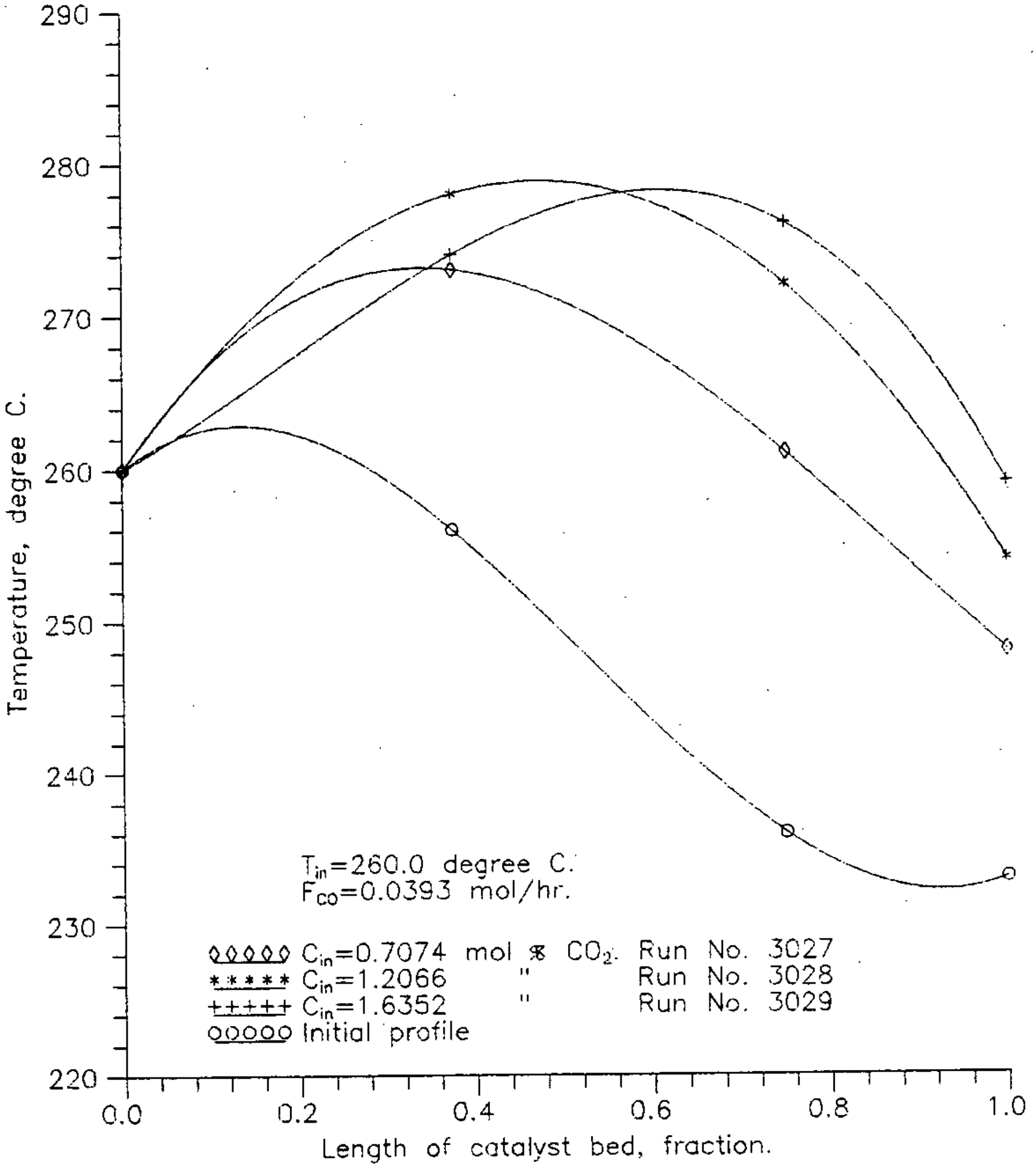


Figure 4.27 Temperature profiles in the reactor at different inlet concentrations of CO_2.

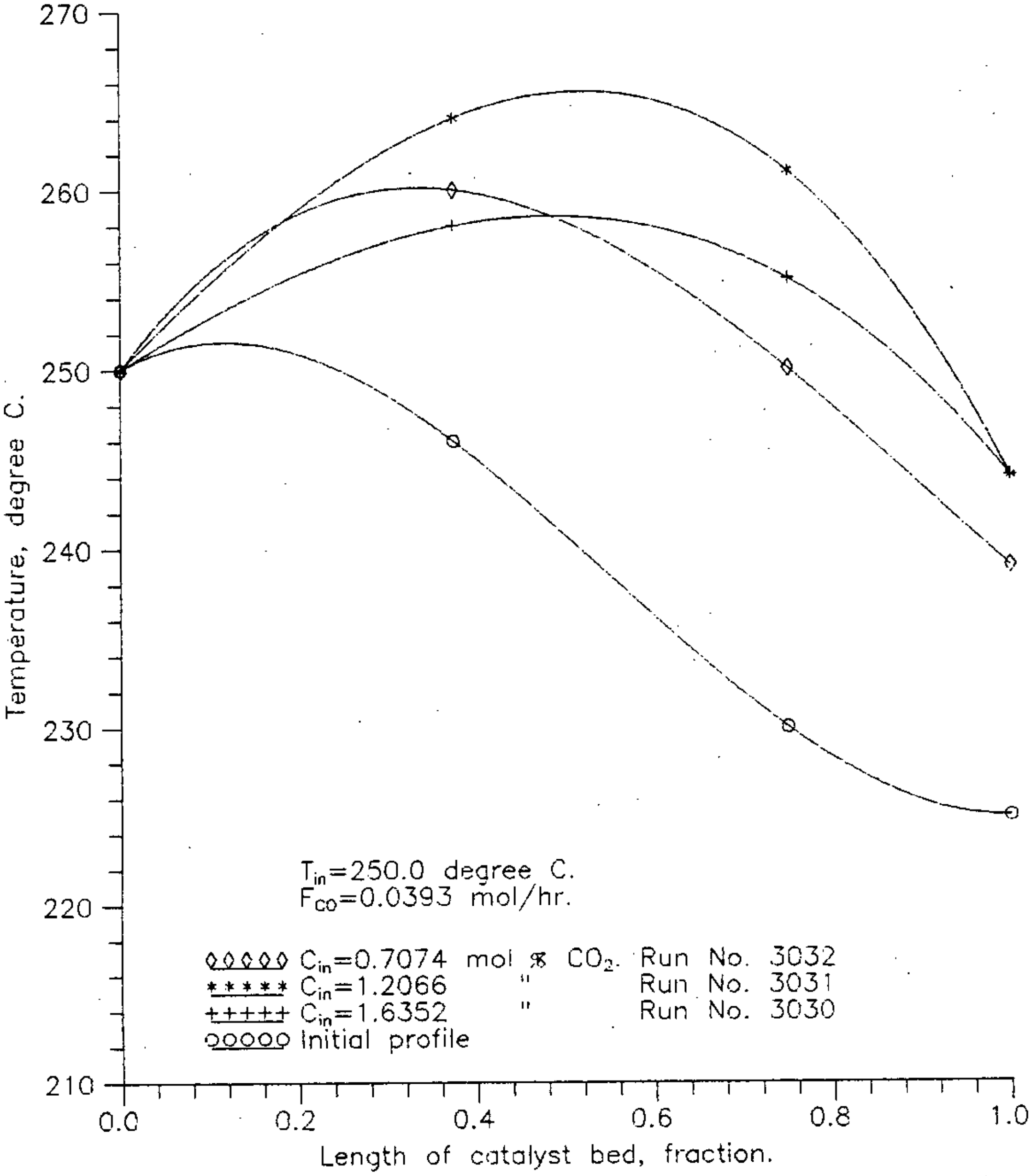


Figure 4.28 Temperature profiles in the reactor at different inlet concentrations of CO_2.

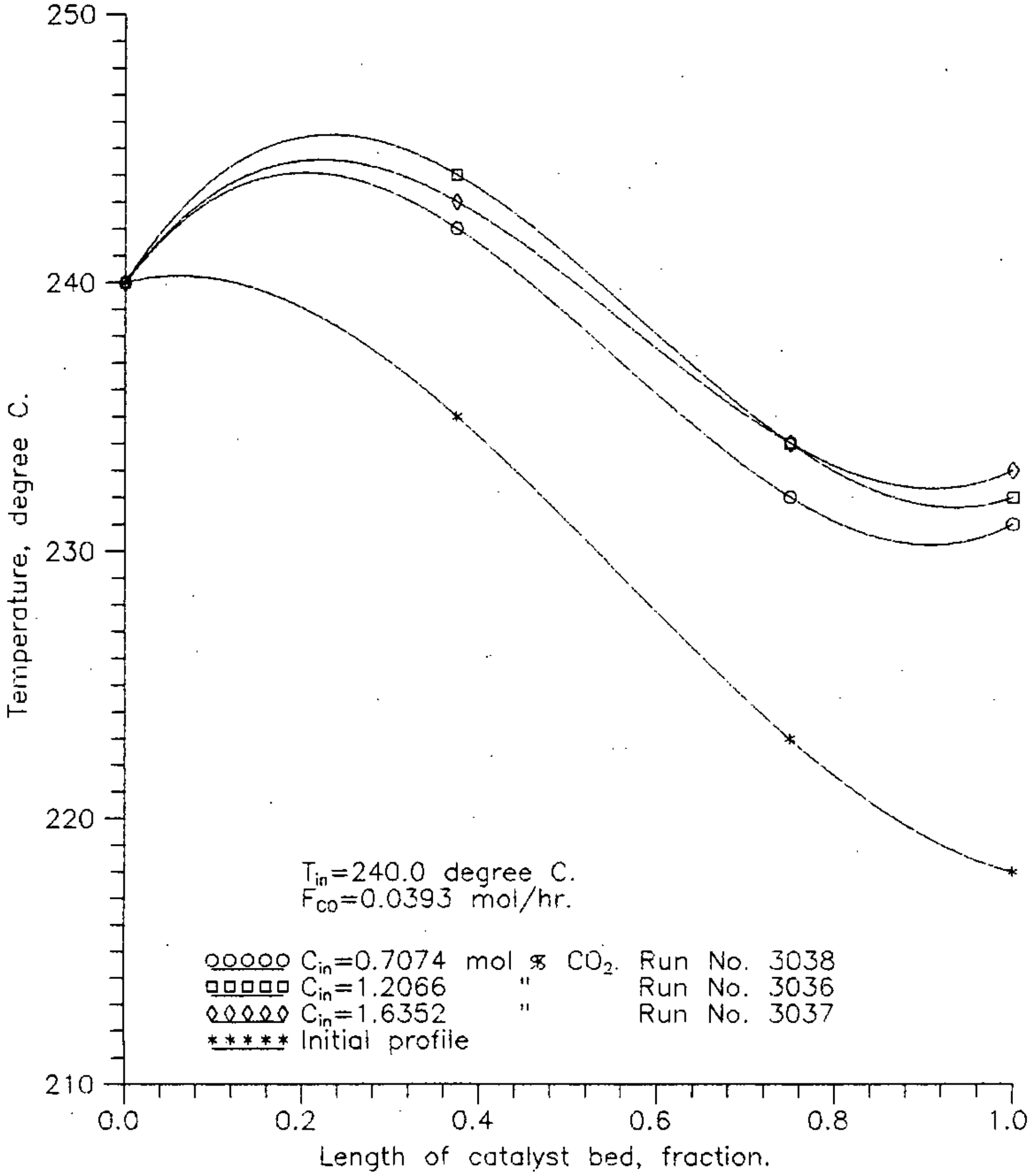


Figure 4.29 Temperature profiles in the reactor at different inlet concentrations of CO_2.

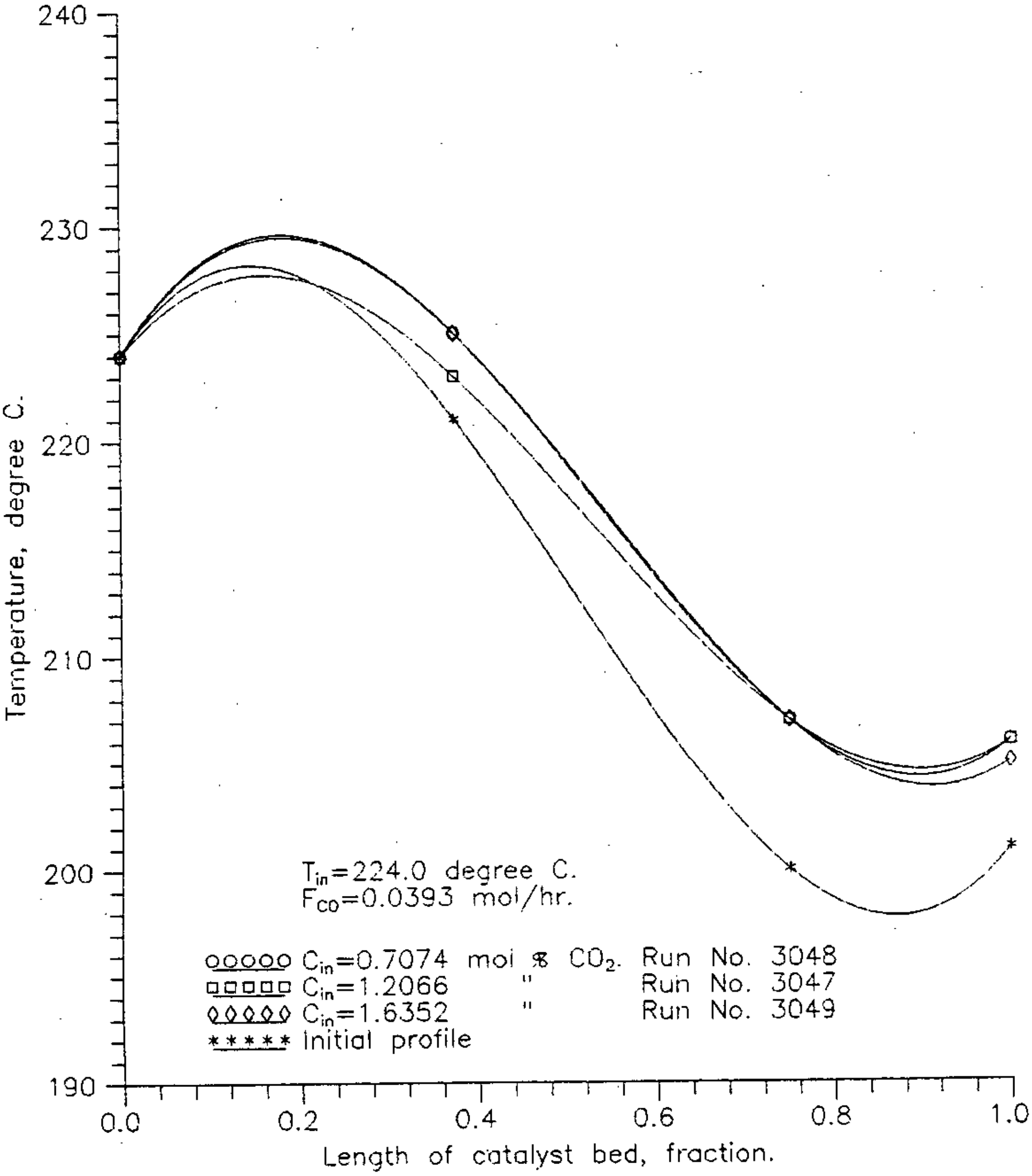


Figure 4.30 Temperature profiles in the reactor at different inlet concentrations of CO$_2$.

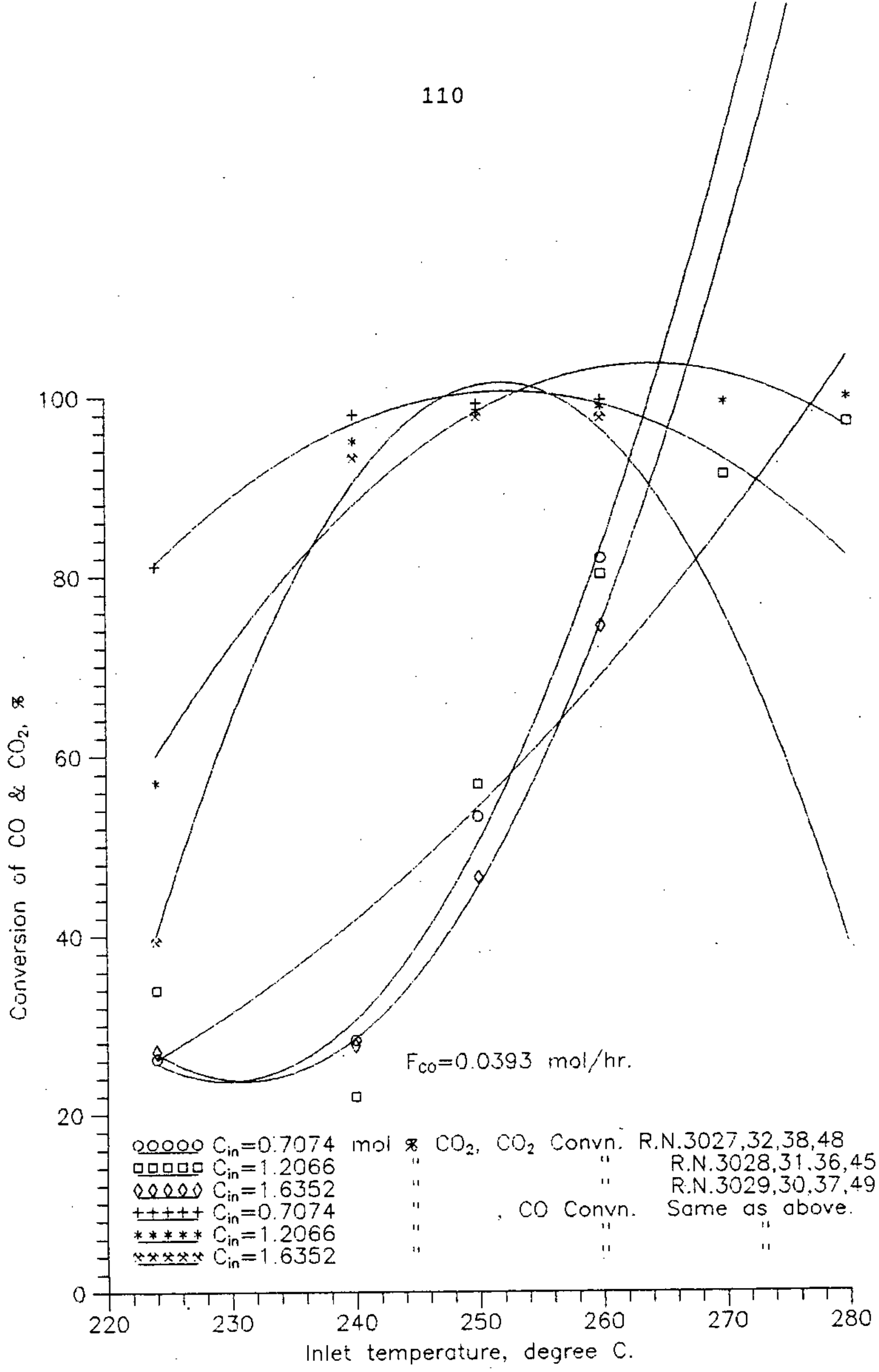


Figure 4.31 Effect of inlet temp. on conversion of CO & CO_2 at different inlet concn. of CO_2.

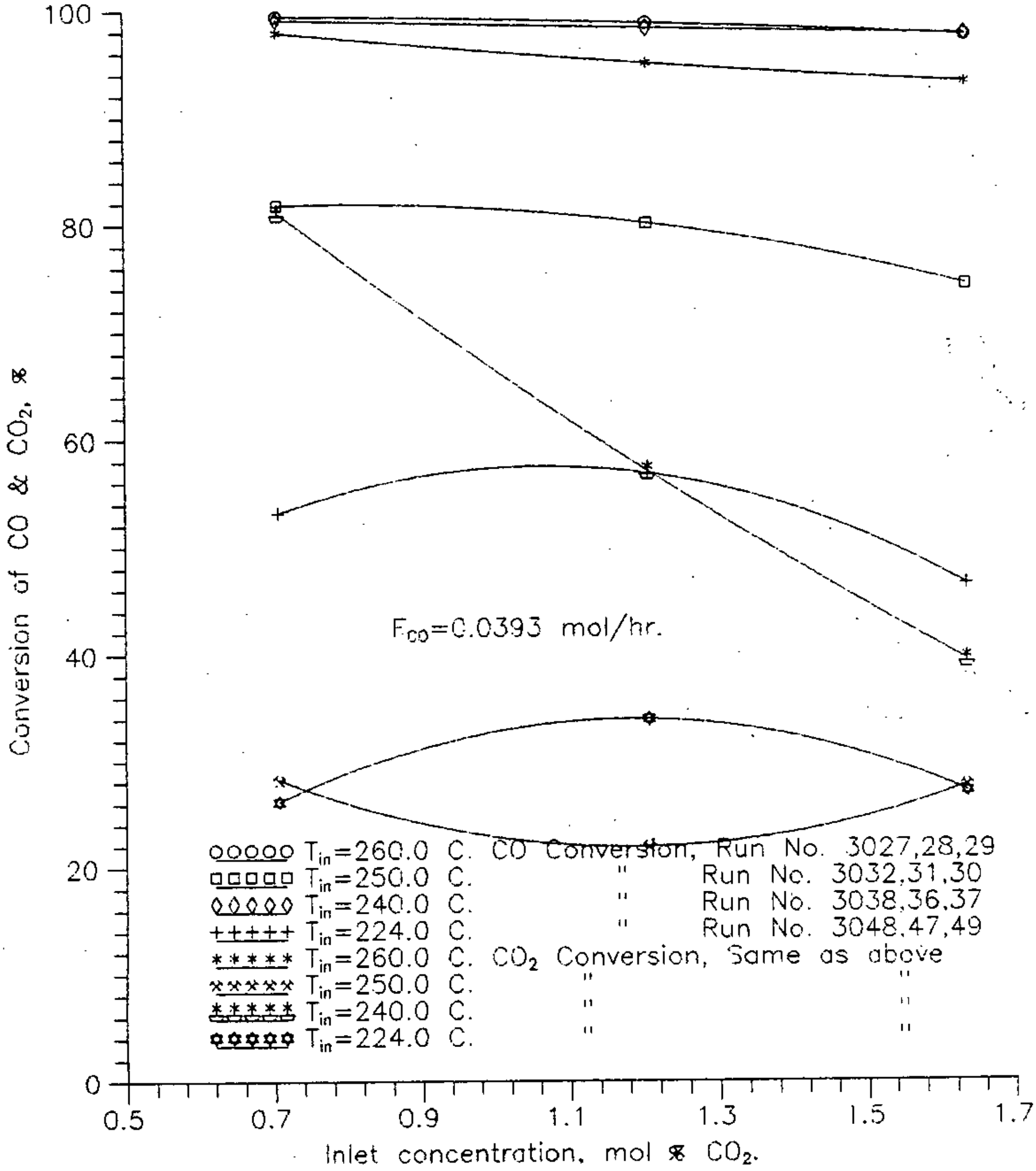


Figure 4.32 Effect of inlet concn. on conversion of CO & CO_2 at different inlet temps.

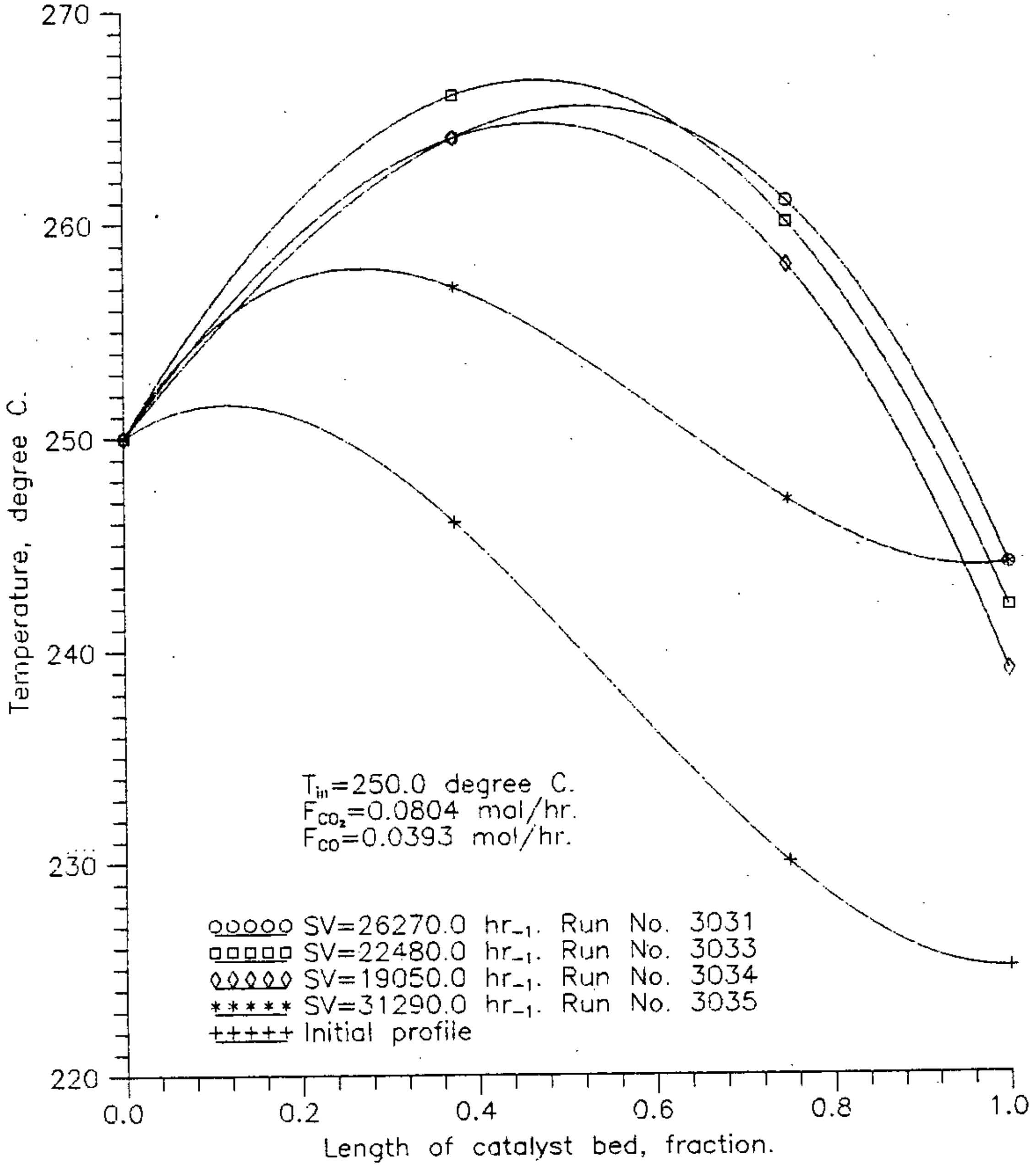


Figure 4.33 Temperature profiles in the reactor at different space velocities.

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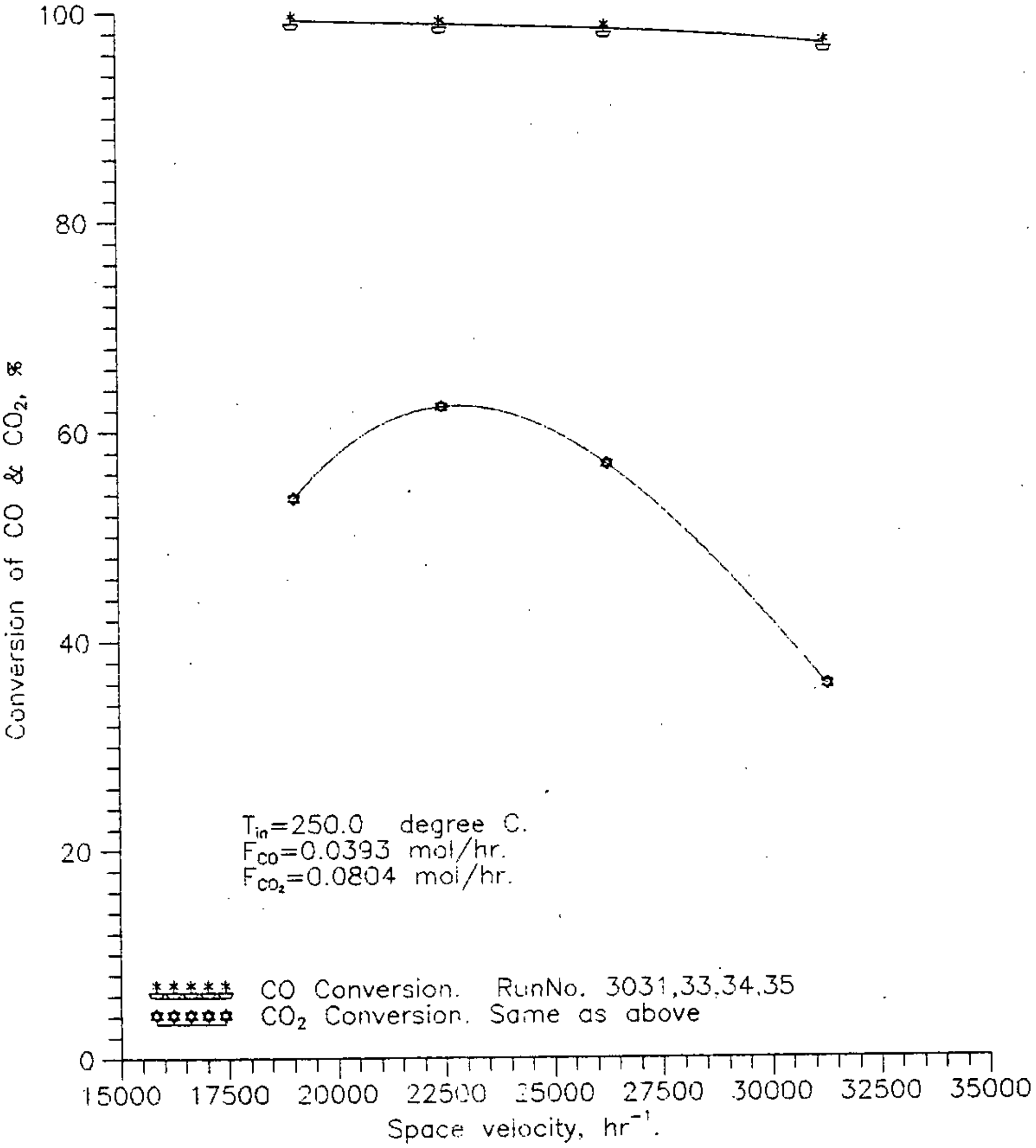

Figure 4.34 Effect of space velocity on convn. of CO & CO_2 at constant flow rate of CO & CO_2

4.2 Adiabatic Unsteady state methanation

A large number of experiments were carried out in the same reactor for the methanation of carbon oxides to study the unsteady state behaviour of the reactor. The catalyst was also undiluted.

The detailed results of the experiments to disturbances in inlet conditions are presented in the appendices F to ~~G~~ H. The figures 4.35 to 4.57 show the unsteady state behaviour of the reactor.

4.2.1 Using binary feeds of CO or CO_2 with hydrogen

The results of experiments of the reactor to disturbances in inlet conditions using binary feeds, i.e., CO or CO_2 in hydrogen are given here. Depending on the inlet conditions varied, several types of disturbances can be distinguished, three of which were studied viz Type-1, step increase of the carbon oxide concentration in the feed to an isothermal reactor; Type 2, similar concentration steps in the feed to a reactor with a temperature profile; Type 3, flow changes in the feed to a reactor with a temperature profile.

4.2.1.1 Type 1 disturbance:

At time t<o the catalyst bed is showing a temperature profile, the feed to the reactor consisting of hydrogen and nitrogen: Nitrogen is used as carrier gas. Because of constructional limitations the reactor could not be made isothermal and this condition of the reactor is assumed as isothermal. At time t=0 the carbon oxide is added to the feed. The disturbance obtained in this way is of interest in connection with start up procedures. When

analyzing the behaviour of the reactor for a type 1 disturbance one finds that immediately after the addition of carbon oxide to the feed i.e. within 1 or 2 gas residence times in the reactor, a carbon oxide concentration profile is established. Here it was not possible to measure the concentration at different thermocouple points of the reactor and concentration profile could not be drawn. The heat of reaction then causes the temperature profile gradually i.e., much more slowly than the initial change of the axial concentration profile. These effects are referred to as Fast concentration Responses, FCR, followed by Slow Temperature Responses, STR.

Figures 4.37 to 4.39 are plotted for carbon dioxide and figure 4.42 is for carbon monoxide. In case of carbon dioxide step decrease or reverse action is also shown. Step increase of carbon dioxide shows upward temperature profile and step decrease of carbon dioxide shows downward temperature profile.

The physical significance of the above findings is that a change in concentration travels through the reactor with substantially the same velocity as the gas flow because there is virtually no net accumulation of carbon oxide in the solid phase. On the other hand, an appreciable amount of heat is absorbed by the catalyst bed and the reactor wall, the heat capacity of which is about 1000 times the heat capacity of the gas phase. Since the temperature equilibrium between gas phase and solid is established instantaneously, it follows that the temperature profile changes much more slowly than the initial concentration profile during the

FCR because accumulation of heat in the catalyst bed now determines the response speed. After some time of adding carbon oxide a zone is established in which the temperature does not change any further and where the CO_2 is converted completely, whereas the second part of the bed has not yet reached the final steady-state temperature. From then on the latter section of the bed is heated by the constant heat flow generated by the chemical reaction in the first half of the bed, during this second period the change in temperature of the tail end of the reactor is identical with the behaviour of any packed bed heated by a hotter fluid flowing through if, heat transport to the bed being proportional with time.

4.2.1.2 Type-2 disturbance:

When the reactor operates at a steady state with a hydrogen feed containing CO or CO_2 an axial temperature profile is present. This situation is taken as the starting point for creating type 2 disturbance, a step increase of the concentration in the feed to a non-isothermal reactor.

Figure 4.35 & 36 show a decrease & an increase of the inlet concentration of CO_2 in hydrogen respectively.

Figure 4.43 & 44 show an increase and a decrease of the inlet concentration of CO in hydrogen respectively.

In case of CO hydrogenation, a somewhat different behaviour is observed when changing the CO inlet concentration. When CO partial pressure is above maximum the reaction rate decreases with increasing partial pressure. The decrease of the reaction rate with increasing partial pressure also shows up the transient behaviour for type 2 disturbance. Where the inlet concentration of CO was lowered with a sharp step.

4.2.1.3 Type 3 disturbance:

When the reactor operates at a steady state with a hydrogen and nitrogen feed containing CO or CO_2, an axial temperature profile is present. This situation is taken as the starting point for creating a type 3 disturbance, a step increase or decrease of nitrogen flow in the feed to a non isothermal reactor.

The figure 4.45 shows step decrease of nitrogen flow where the peak temperature increases and the exit temperature decreases. The physical significance of this finding is that heat evolved from the methanation reaction travels through the reactor with substantially the same velocity as the gas flow. After decreasing nitrogen flow heat evolved from the reaction could not be flown as before and more amount of heat is absorbed by the middle of the catalyst bed and wall which increases peak temperature. because less amount of heat reaches to the exit of the reactor. The exit temperature decreases.

Figure 4.40, 41 and 4.47, 48 are plotted for CO_2 and CO respectively. These figures show the reasonable behaviour, when the CO or CO_2 step up then the exit hydrogen concentration decreases but methane concentration increases. This finding can be explained as CO or CO_2 reacts with hydrogen and produces methane so in the exit stream hydrogen decreases and methane increases.

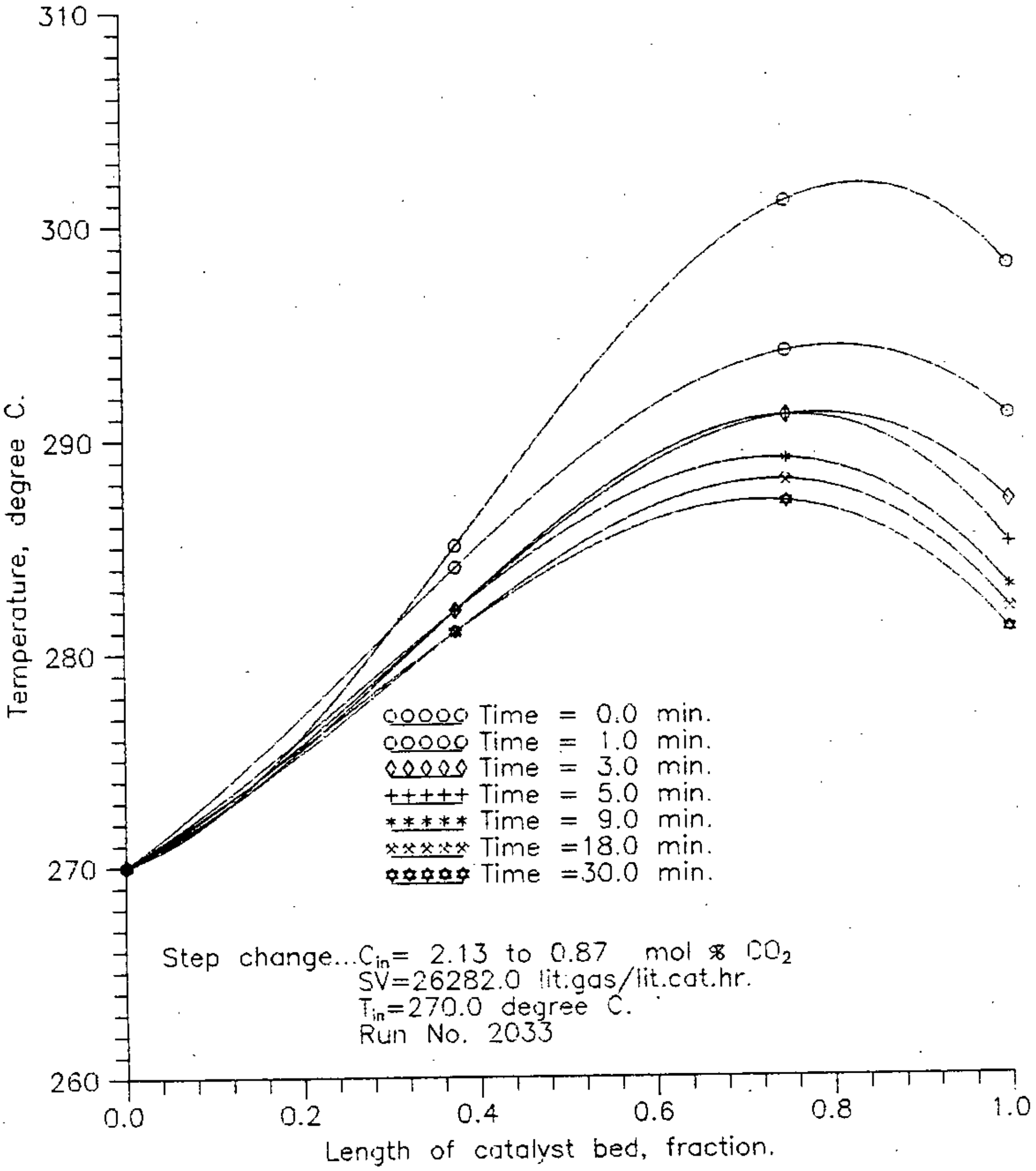

Figure 4.35 Temperature profiles in the reactor at different times.

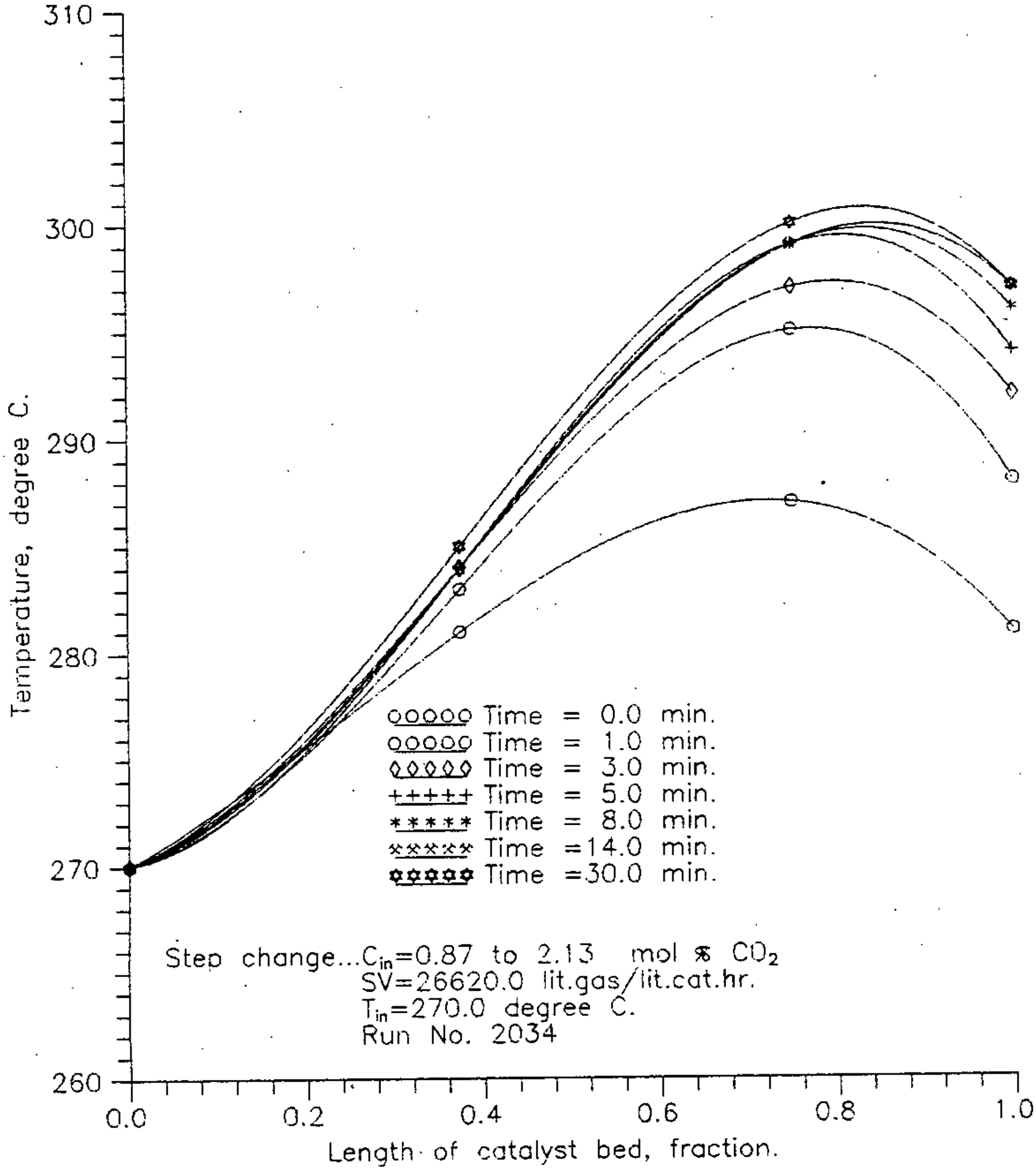

Figure 4.36 Temperature profiles in the reactor at different times.

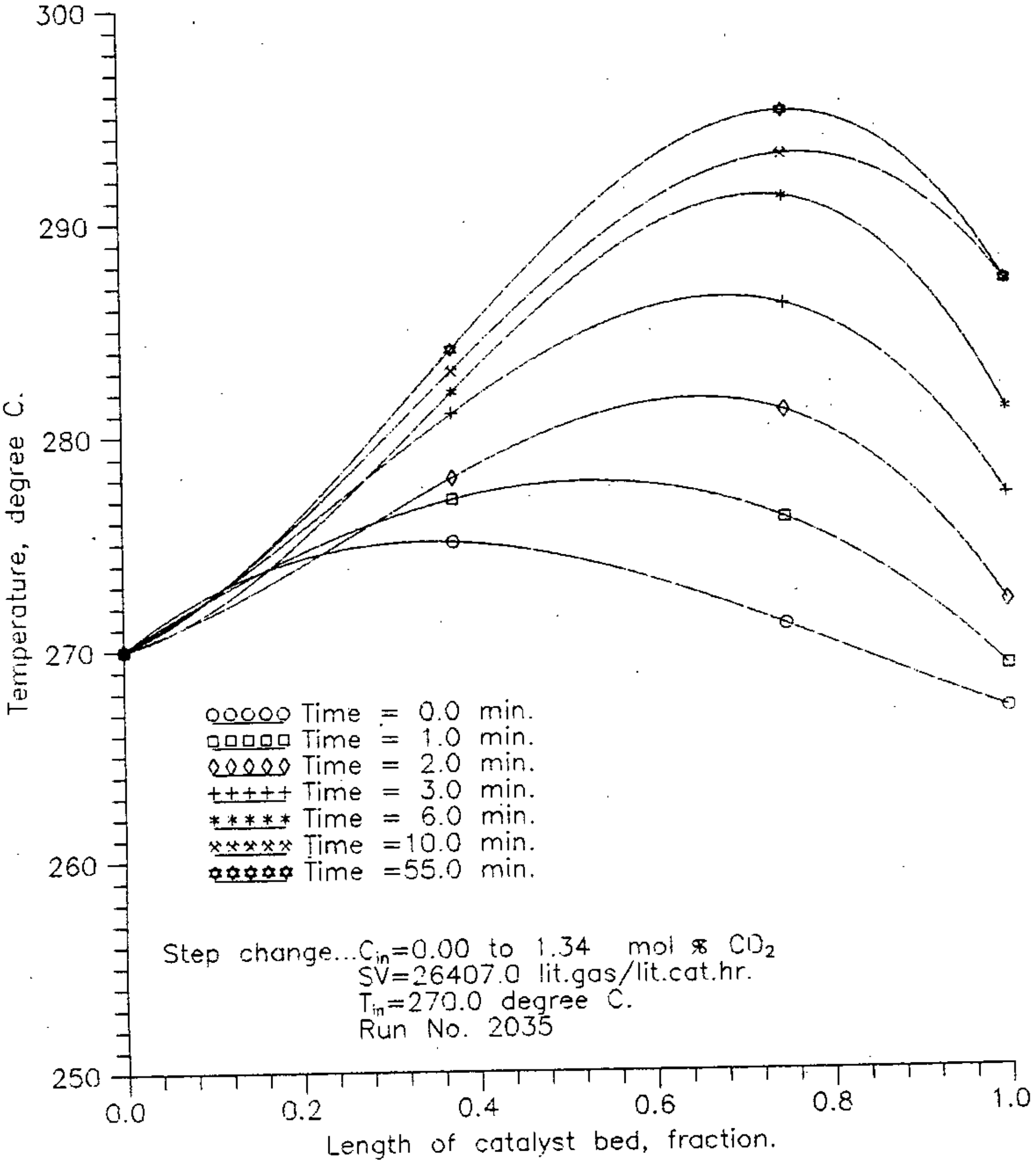

Figure 4.37 Temperature profiles in the reactor at different times.

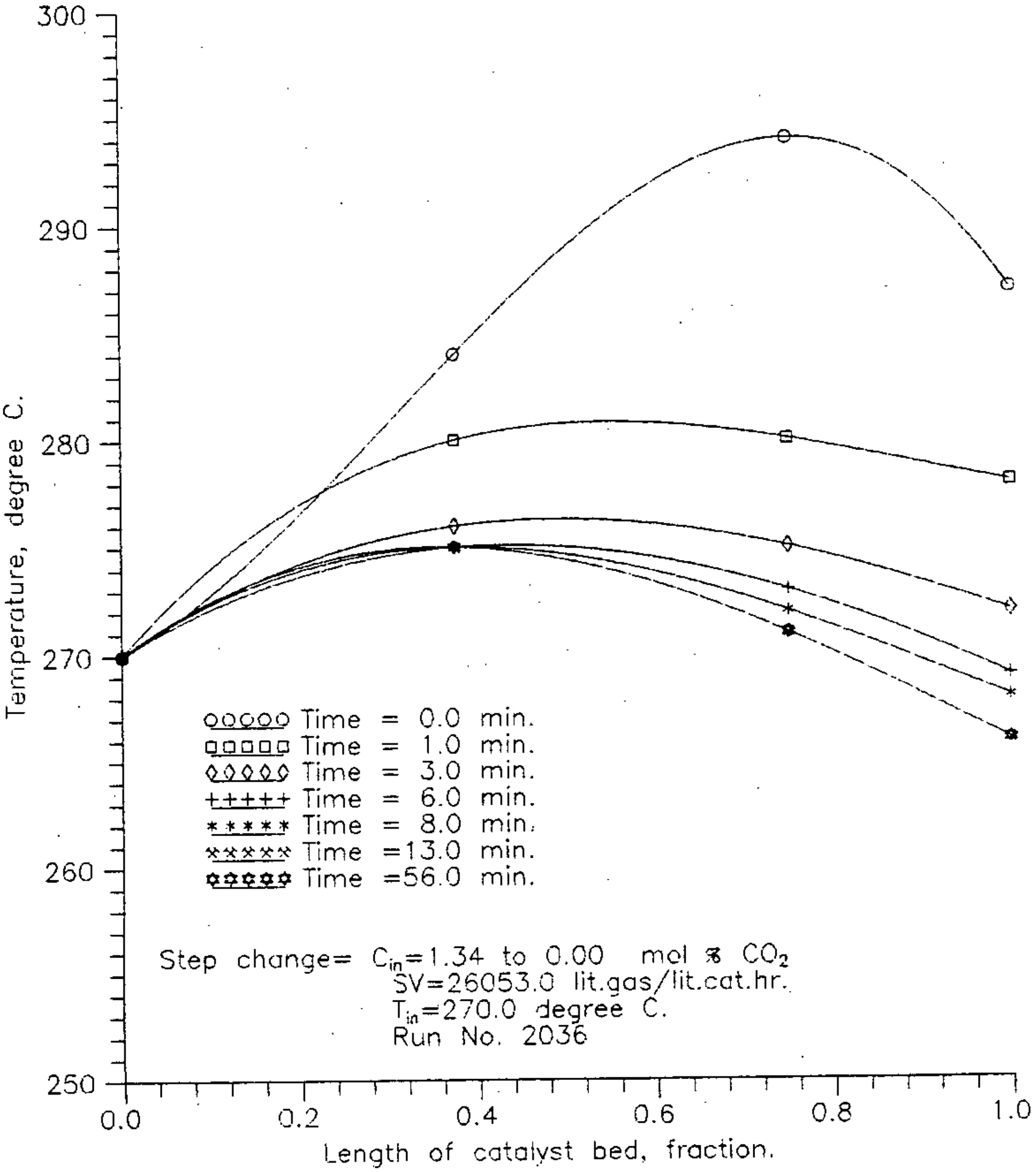

Figure 4.38 Temperature profiles in the reactor at different times.

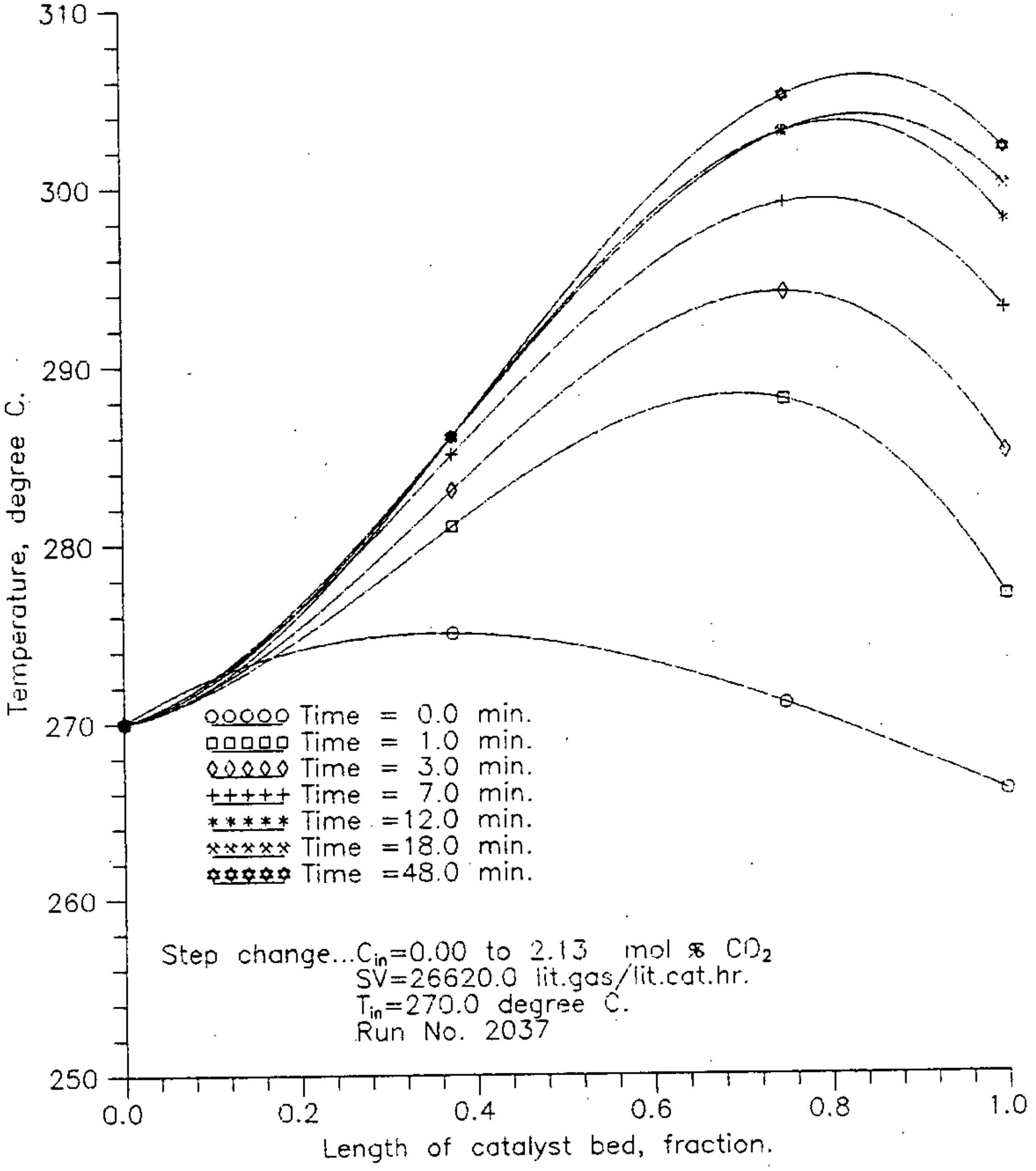

Figure 4.39 Temperature profiles in the reactor at different times.

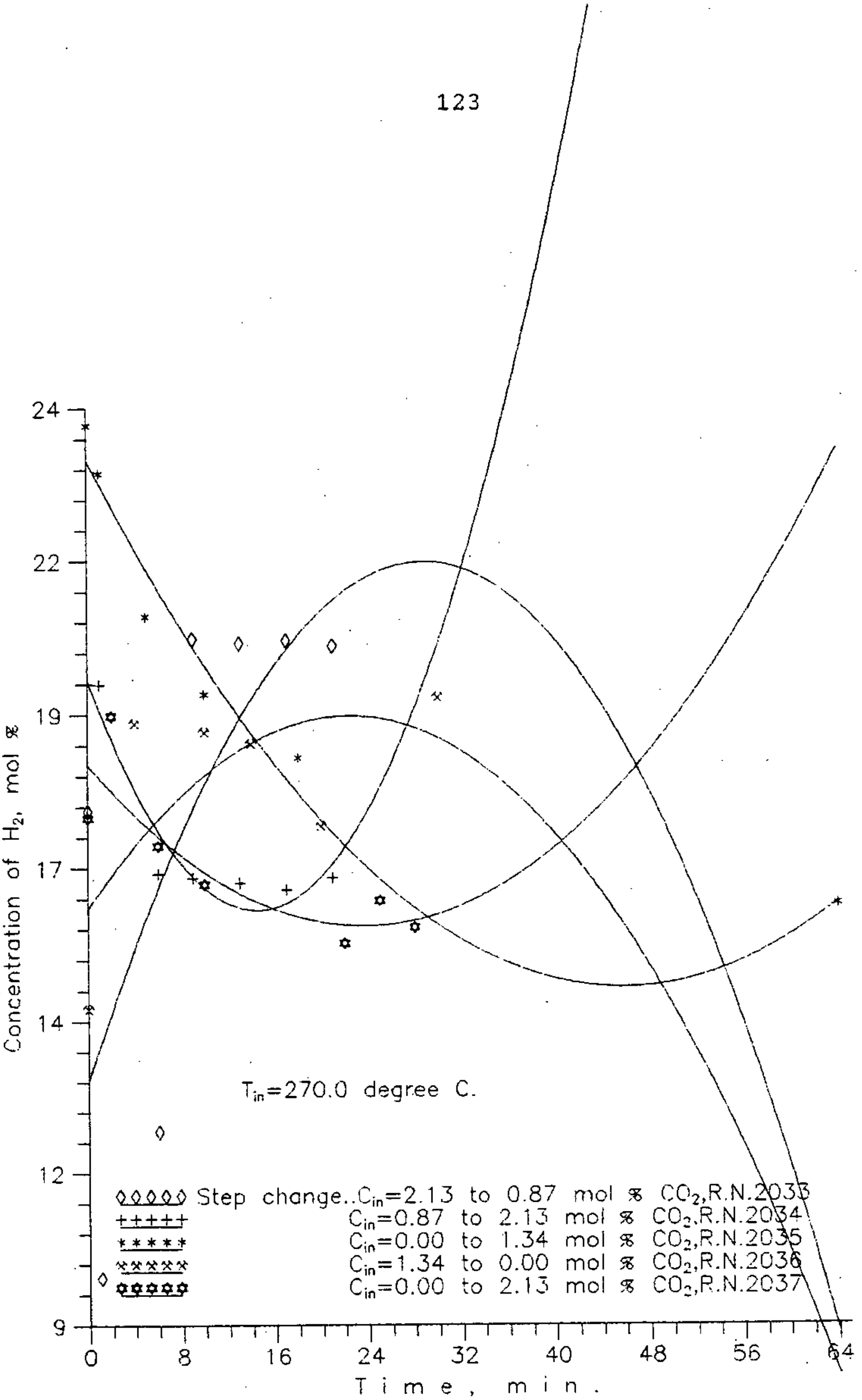

Figure 4.40 Variation of outlet H_2 concn. with time at diff. disturbances of inlet CO_2 concn.

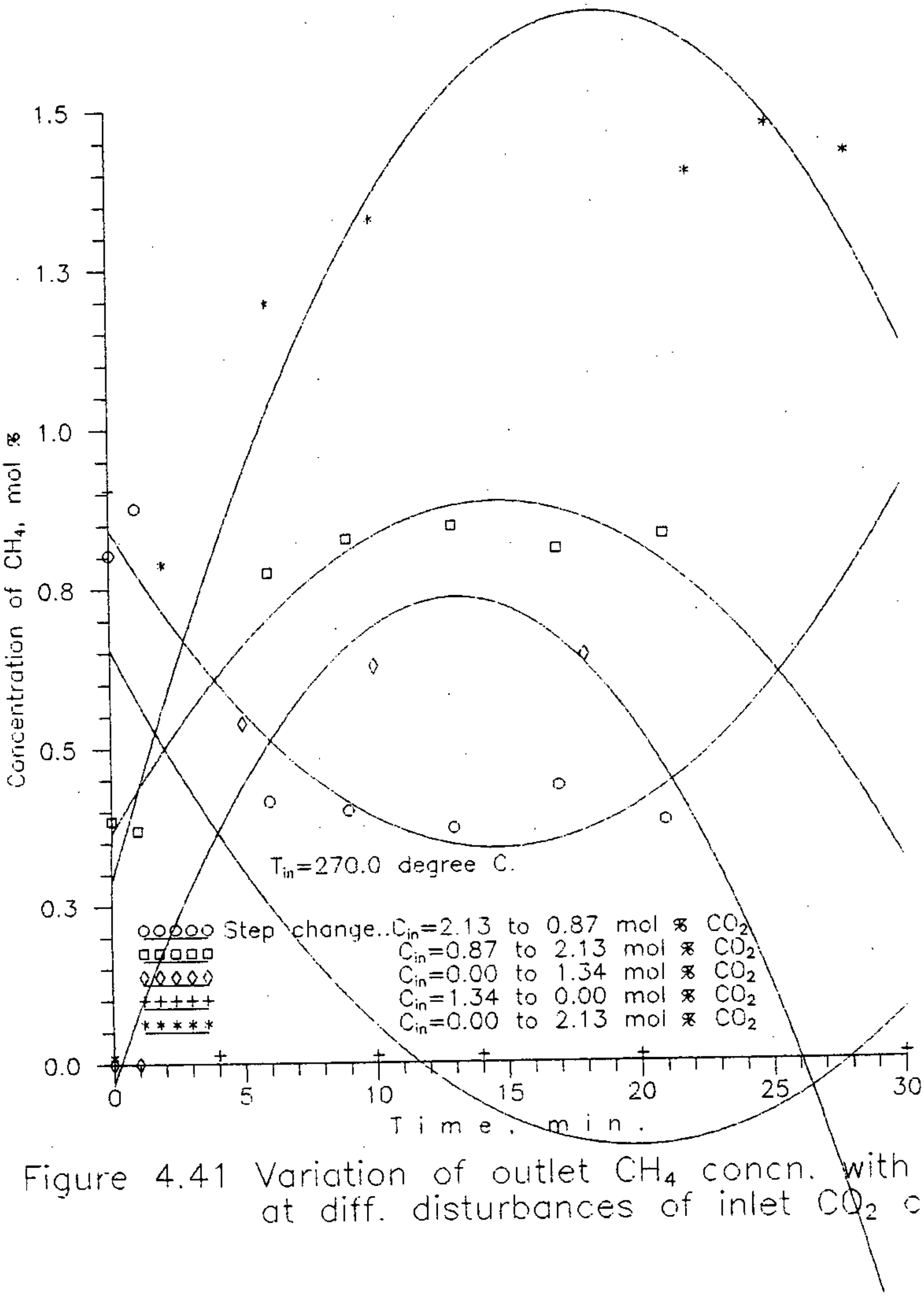

Figure 4.41 Variation of outlet CH_4 concn. with time at diff. disturbances of inlet CO_2 concn.

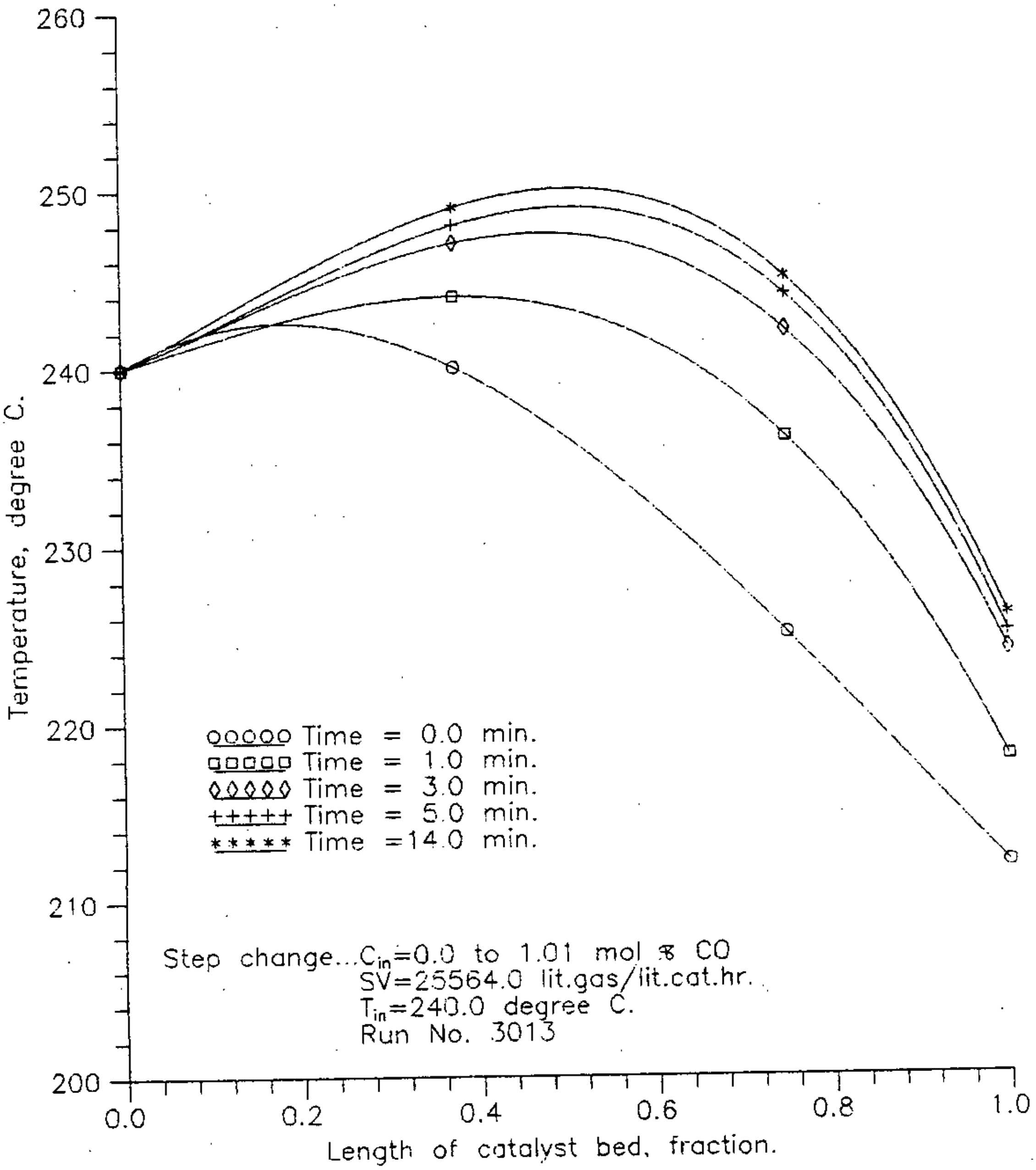

Figure 4.42 Temperature profiles in the reactor at different times.

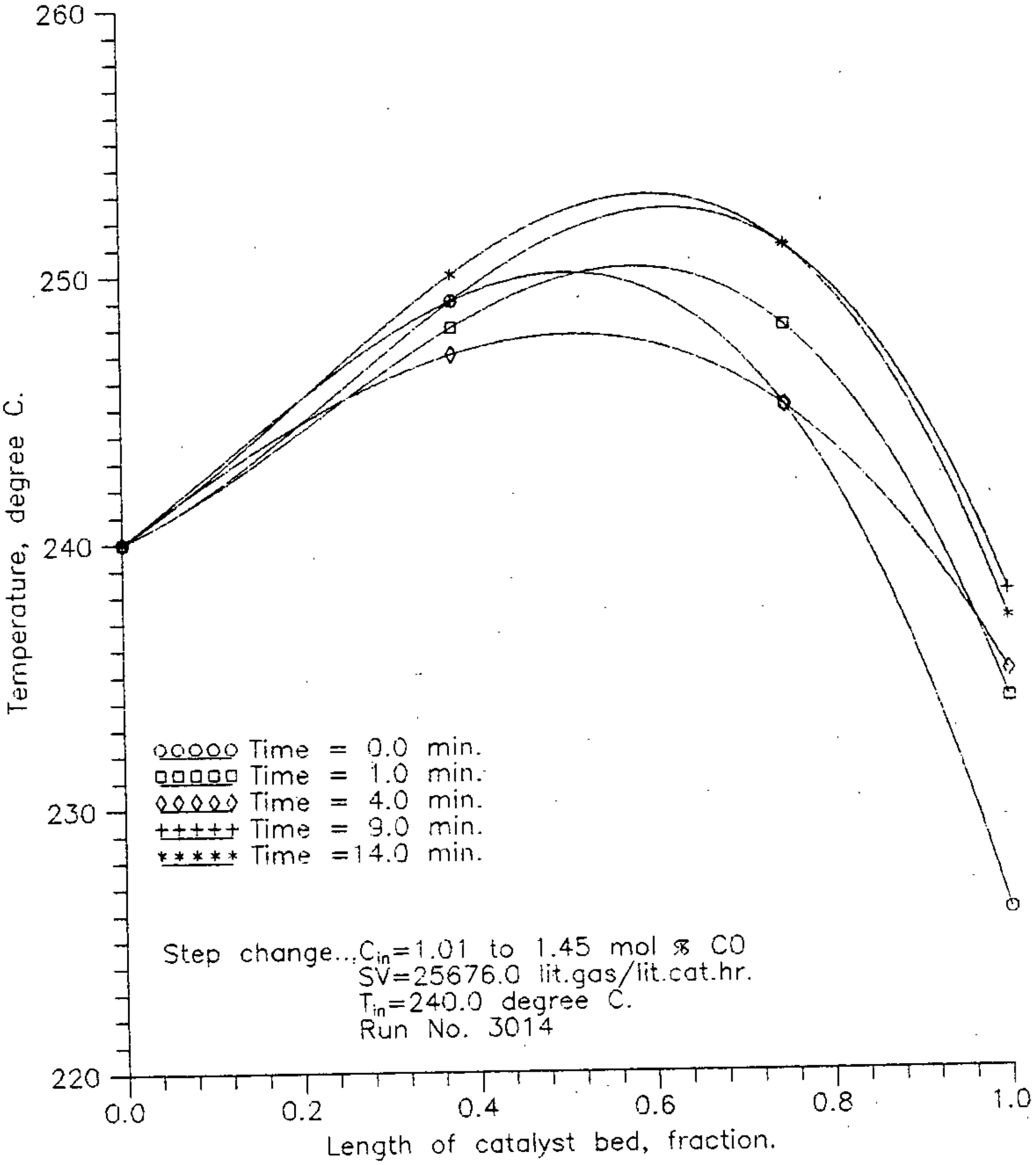

Figure 4.43 Temperature profiles in the reactor at different times.

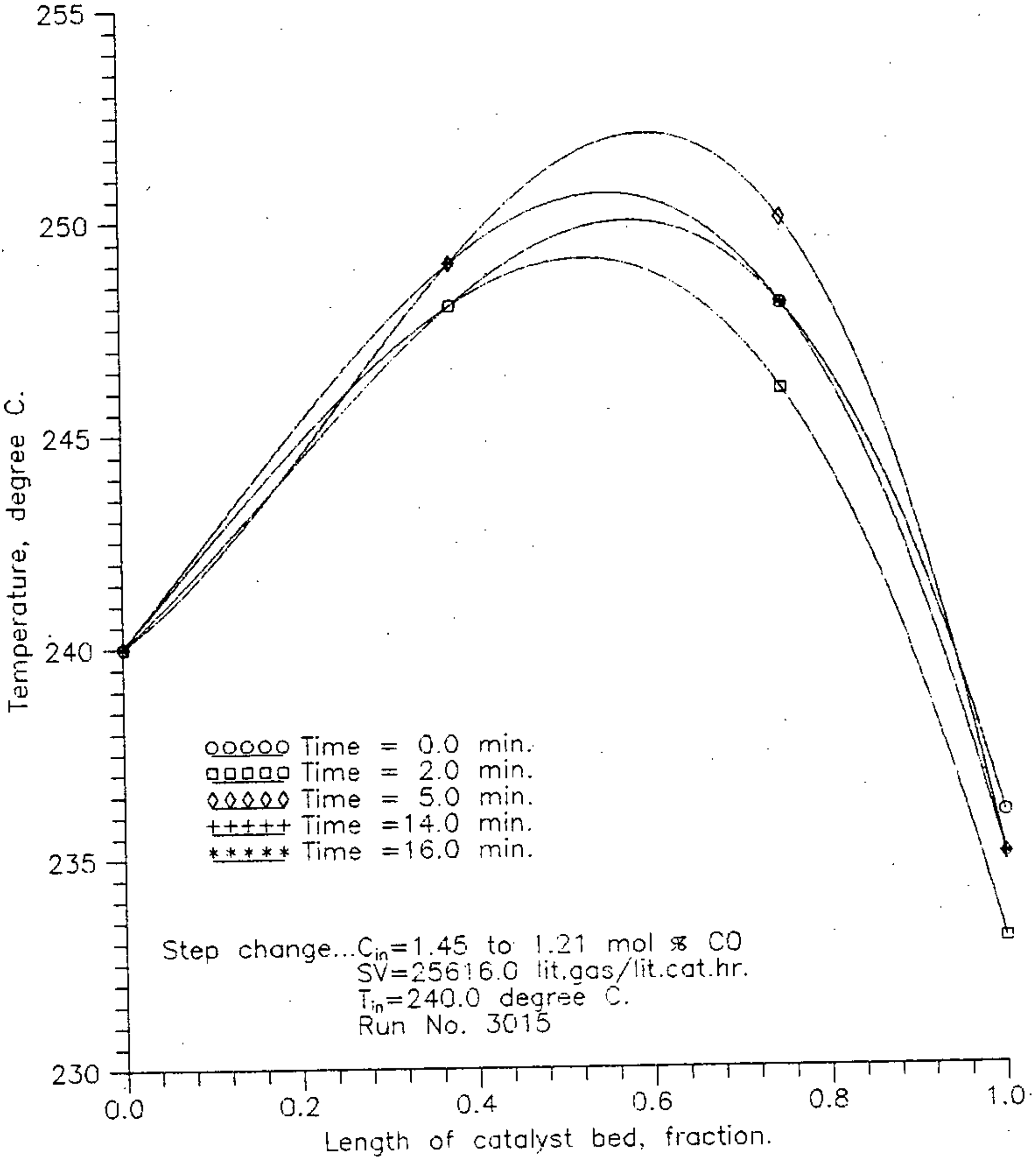

Figure 4.44 Temperature profiles in the reactor at different times.

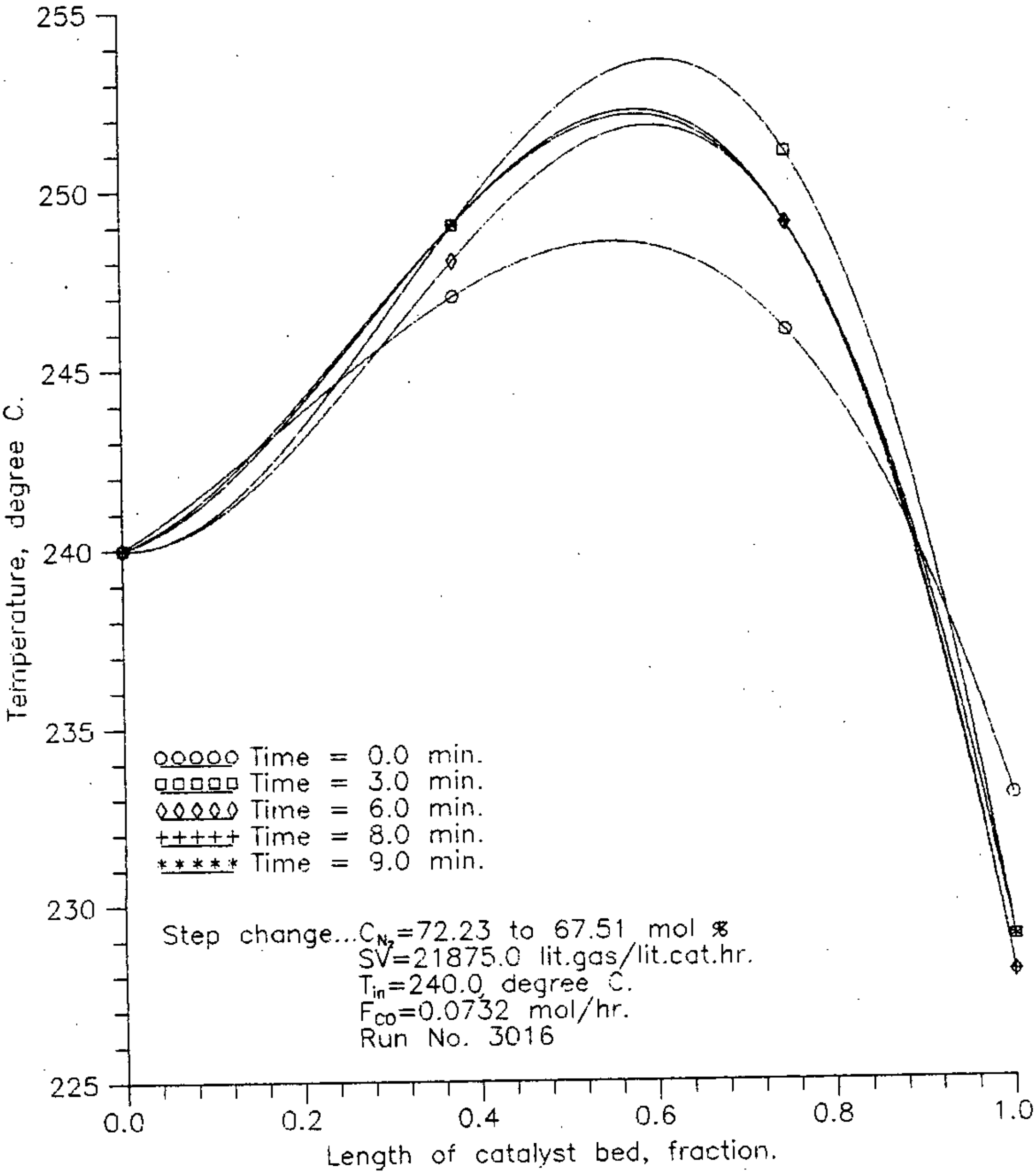

Figure 4.45 Temperature profiles in the reactor at different times.

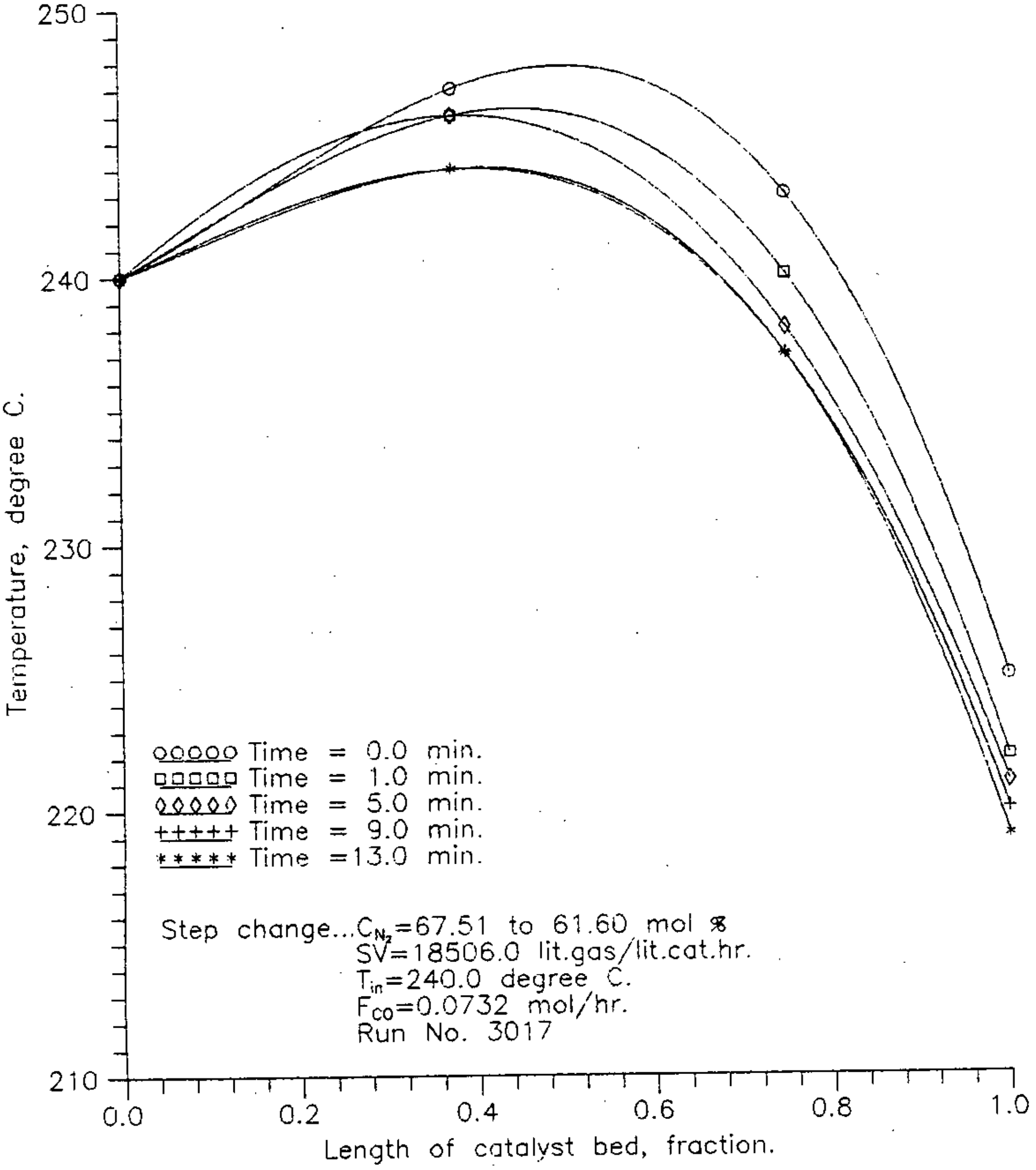

Figure 4.46 Temperature profiles in the reactor at different times.

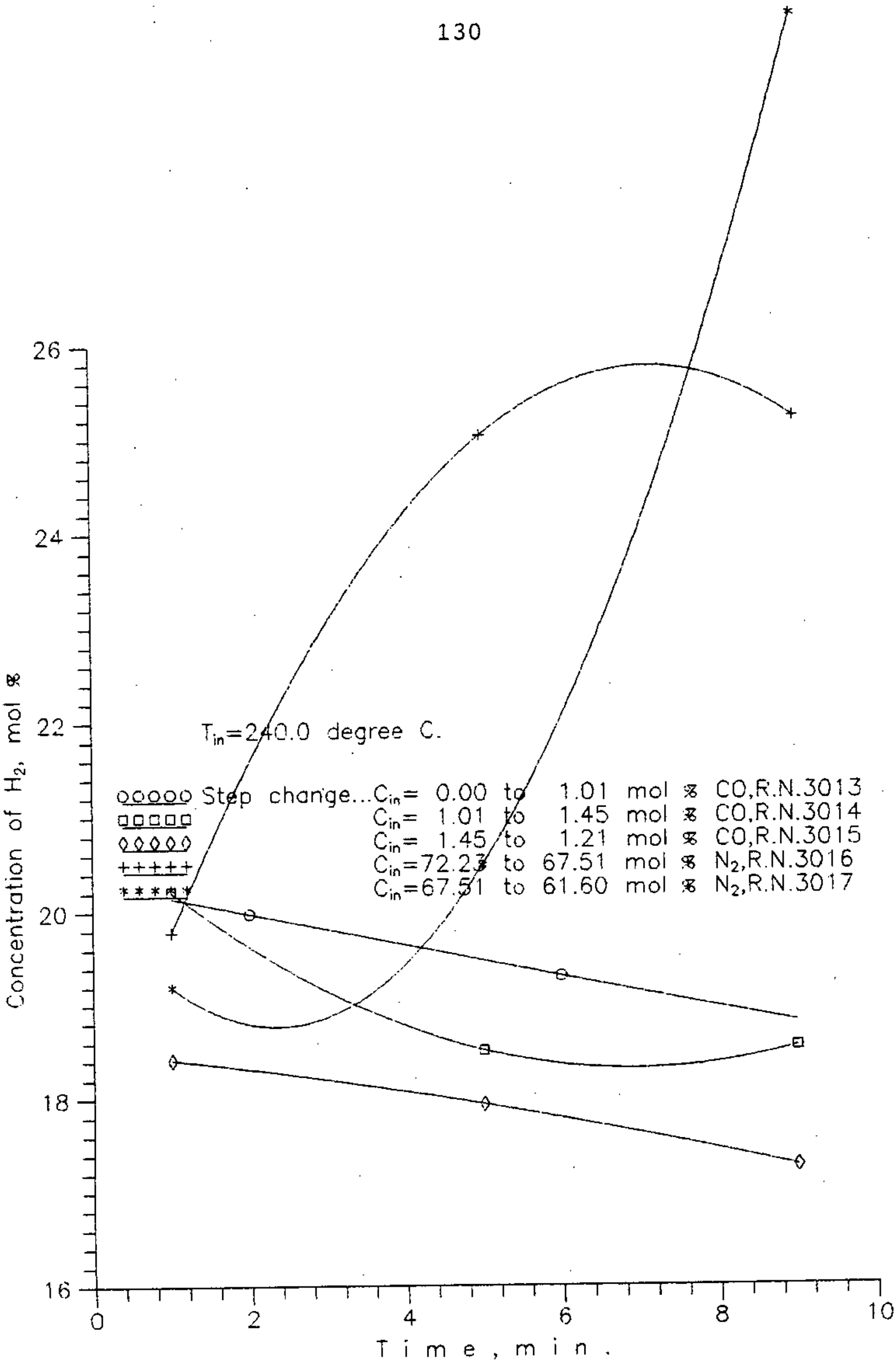

Figure 4.47 Variation of outlet H_2 concn. with time at diff. disturbances of inlet CO concn.

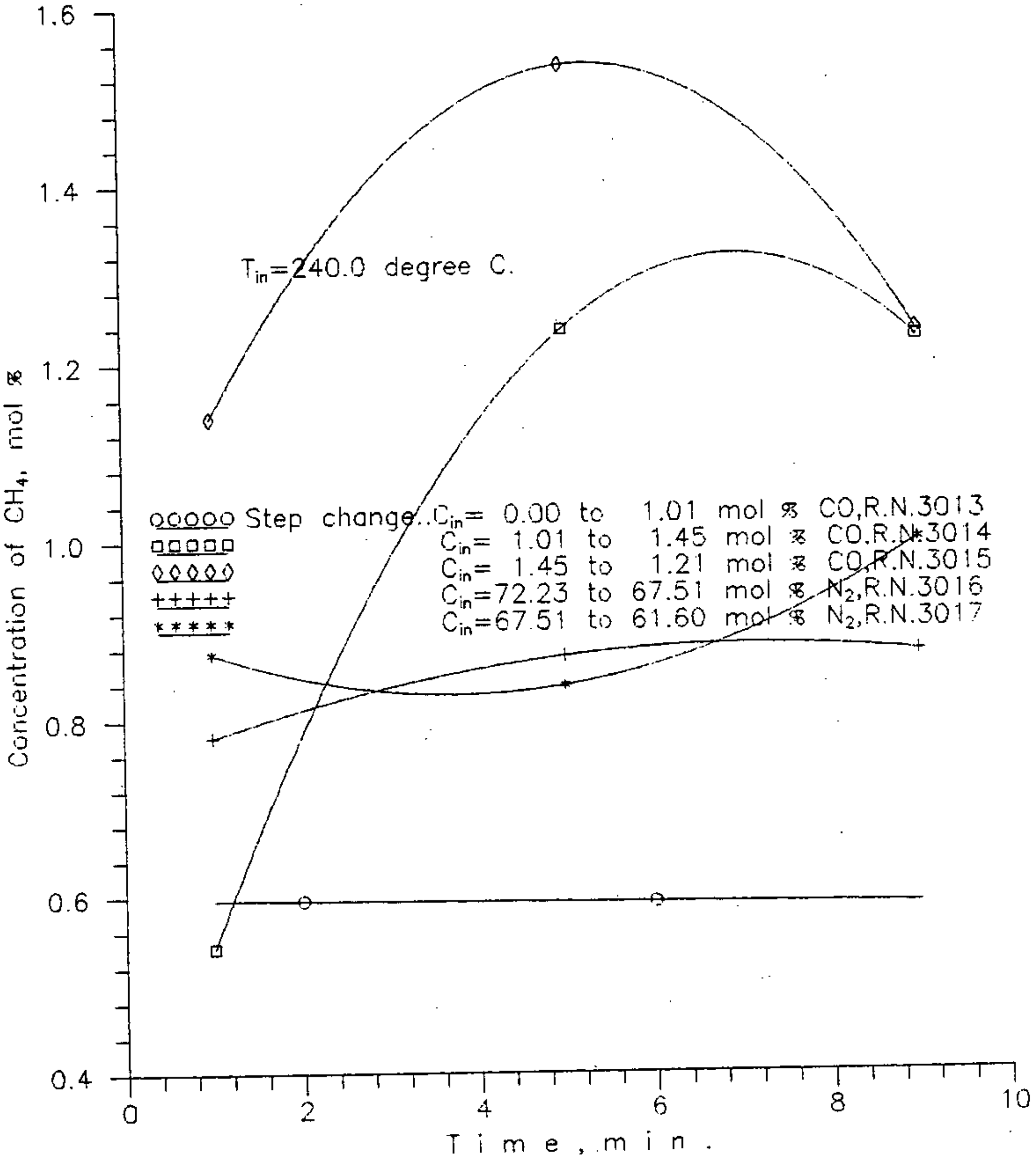

Figure 4.48 Variation of outlet CH_4 concn. with time at diff. disturbances of inlet CO concn.

4.2.2 Using mixed feed of CO and CO_2 in hydrogen:

The experiments of the reactor responses to disturbances in inlet conditions using mixed feeds of CO and CO_2 in hydrogen can be studied with more types of disturbances than with binary feeds. Three types of disturbances are considered in this discussion viz. Type 1 - step increase in CO_2 in assumed isothermal reactor. Type 2 - step change in CO_2 concentration, reactor with a CO & CO_2 temperature profile. Type 3 - step change in nitrogen flow, reactor with a CO, CO_2 temperature profile.

From the point of view of plant scale operation the most interesting types of disturbances are type-1 (for start up purposes) and type-2 (the amount of CO_2 at the methanator inlet can increase suddenly because of failure of the CO_2 absorber).

4.2.2.1 Type 1 disturbances:

Immediately after the introduction of the mixture in the feed gas, a Fast concentration Responses (FCR) occurs until a pseudo-stationary isothermal concentration profile is reached.

Figure 4.49 shows the measured responses of the axial temperature profile. Comparisons with the results for binary feeds show that new dynamic phenomena are not observed.

4.2.2.2 Type 2 disturbances:

Figure 4.50 shows the responses to an increase of the CO_2 concentration in the feed to a reactor containing an initial temperature profile due to conversion of a mixture of CO and CO_2.

In this case the response of the second part of the level is quite similar to type-2 disturbances for single feed and the first part of the bed is not affected because CO hydrogenated preferentially.

4.2.2.3 Type 3 disturbances:

Figure 4.51, 52 and 4.53, 54 shows the responses to the step decrease of the nitrogen flow in the feed to the reactor containing an initial temperature profile due to conversion of a mixture of CO and CO_2. In this case the responses are quite similar to type-3 disturbances for single feed.

Because of the instrumental limitations it was not possible to measure the concentration of CO or CO_2 at the different thermocouple points of the reactor. It was also not possible to take the complete analysis of a single run by the laboratory GC by less than 5 mins. and so unsteady state concentration profiles could not be drawn. There is another type of disturbance which can be made by changing feed temperature. It is important to learn how the reactor behaves after disturbance in feed temperature, because this is a common type of disturbance in practice. A step wise increase or decrease of the feed temperature could not be obtained with the equipment used in this work because of the relatively large heat capacity of the piping and the flanges of the reactor tube.

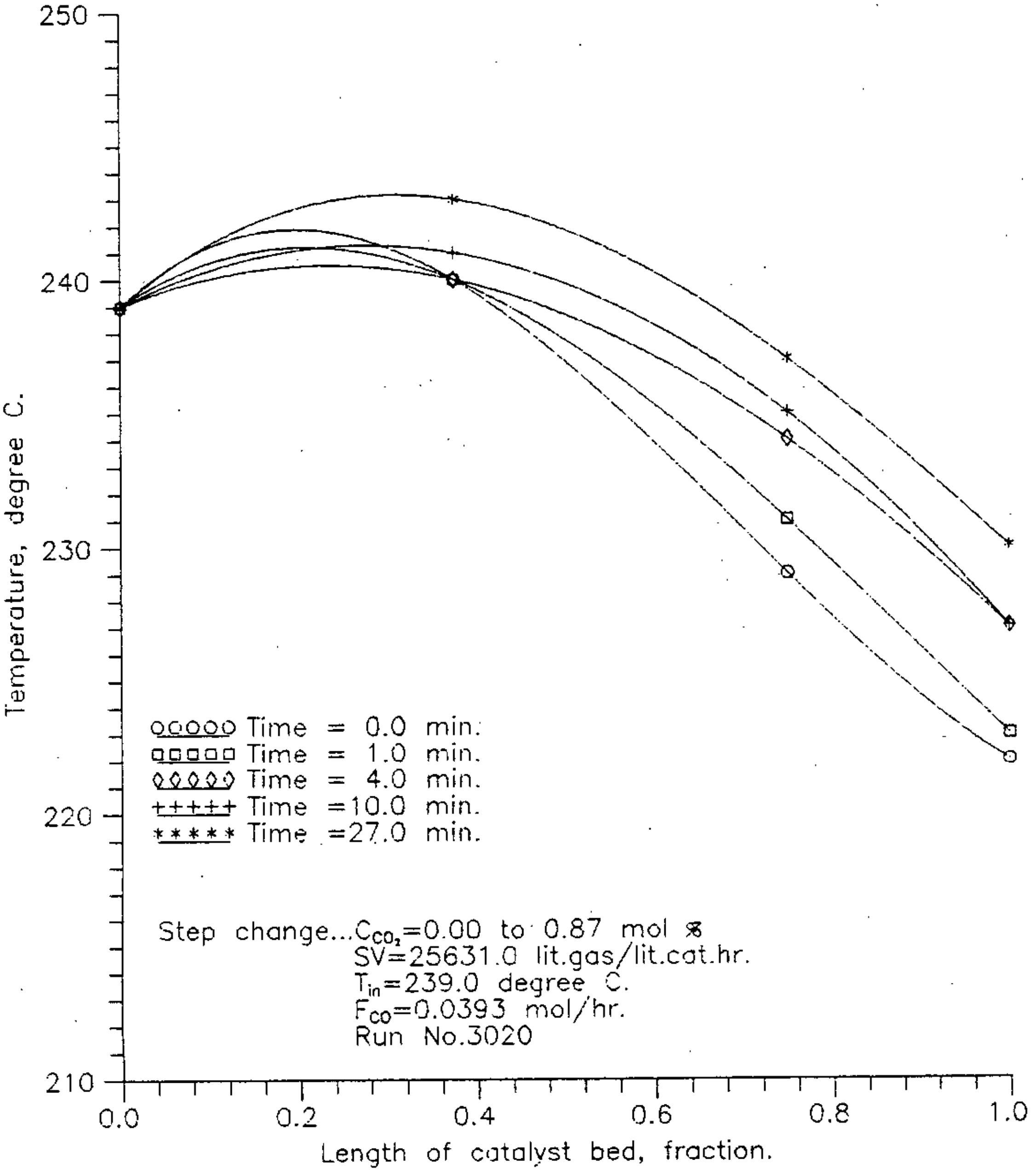

Figure 4.49 Temperature profiles in the reactor at different times.

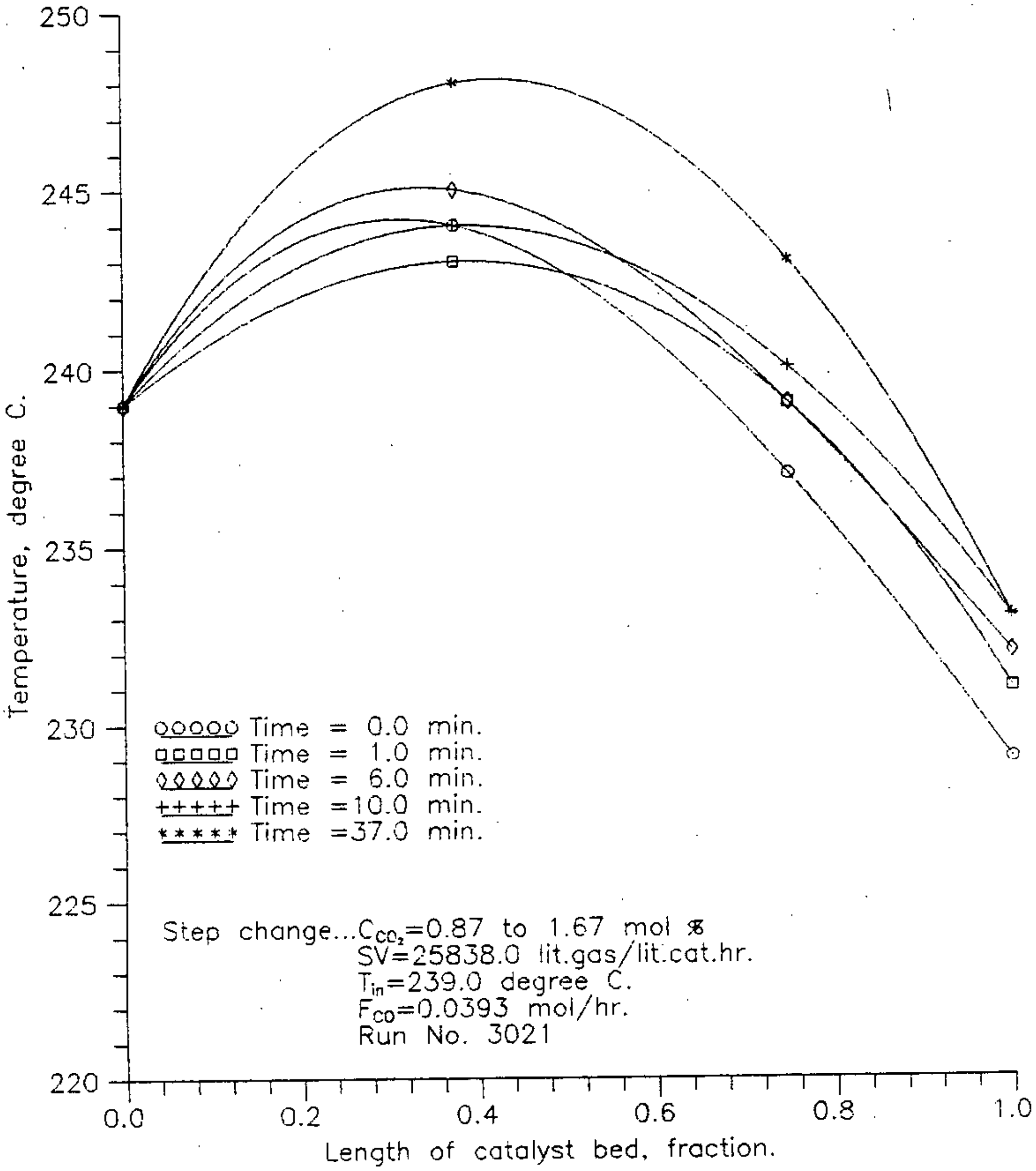

Figure 4.50 Temperature profiles in the reactor at different times.

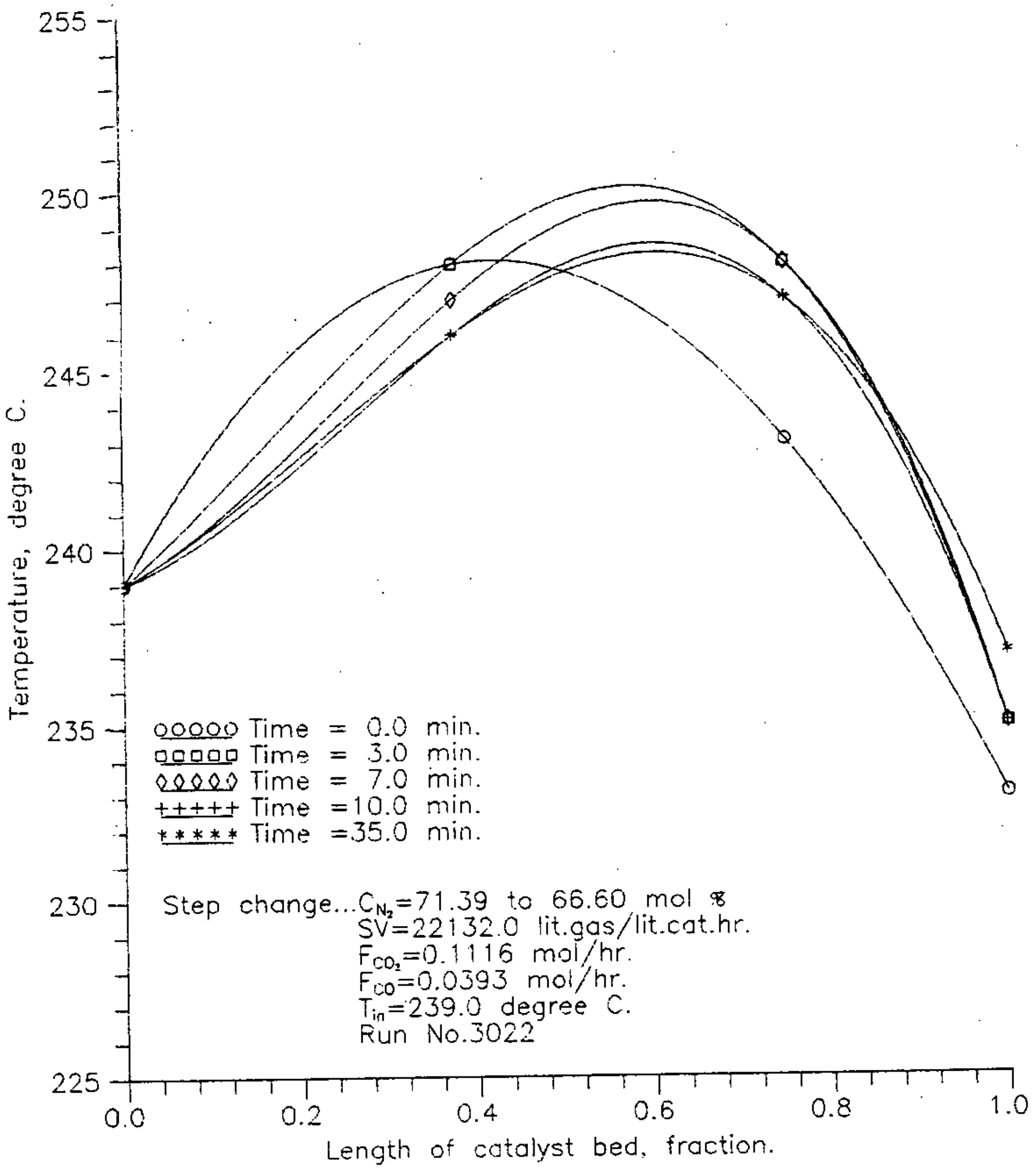

Figure 4.51 Temperature profiles in the reactor at different times.

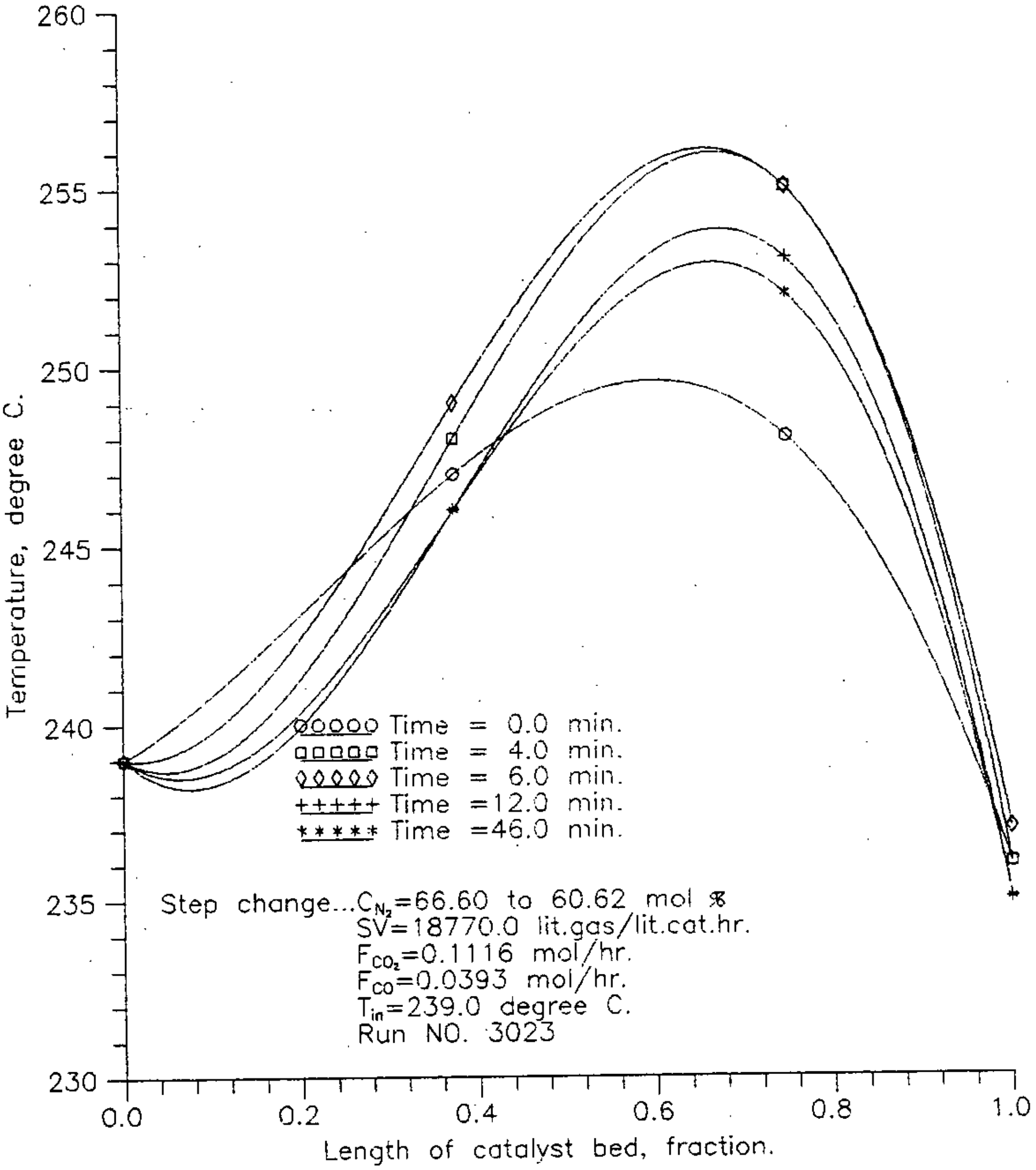

Figure 4.52 Temperature profiles in the reactor at different times.

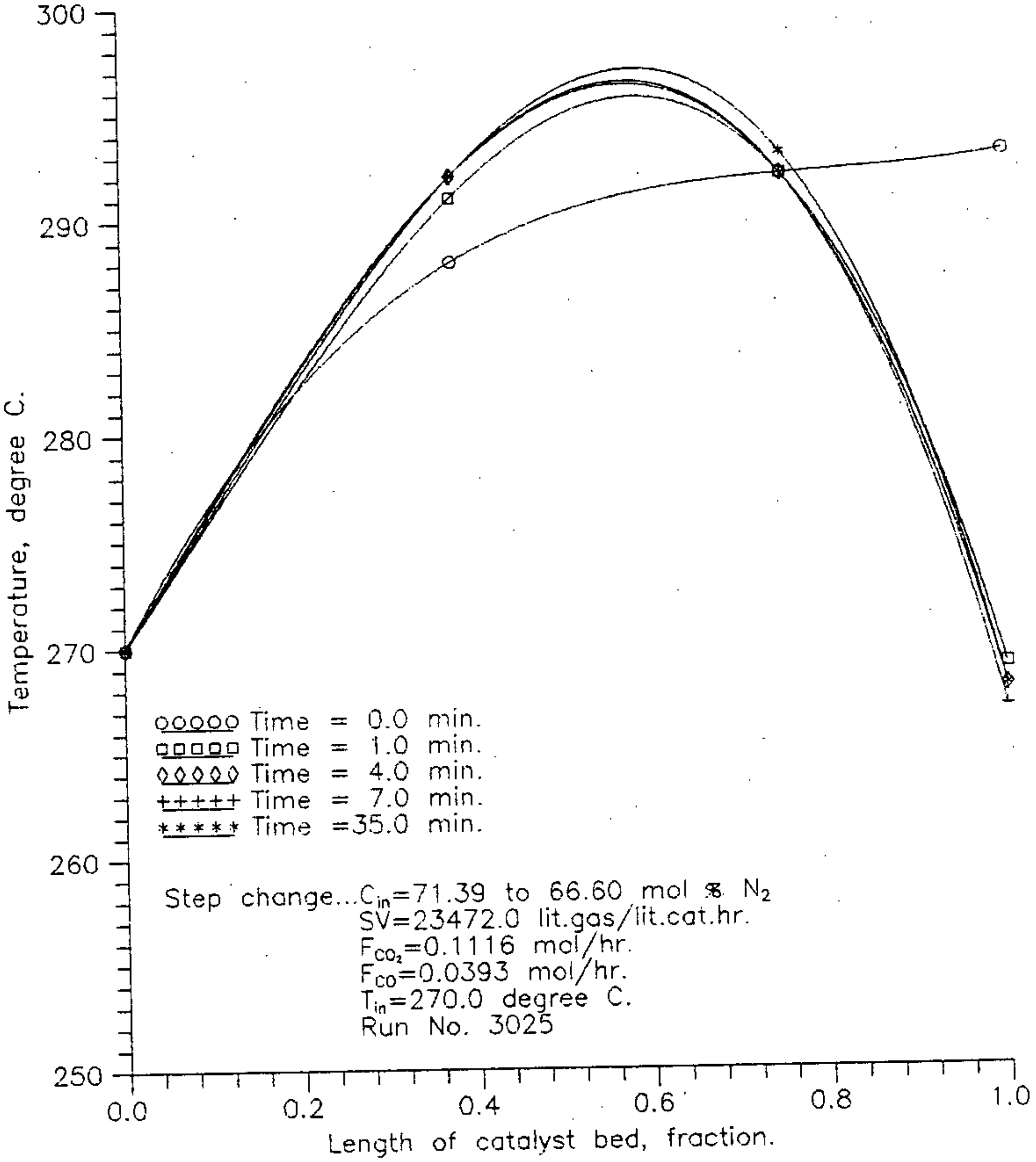

Figure 4.53 Temperature profiles in the reactor at different times.

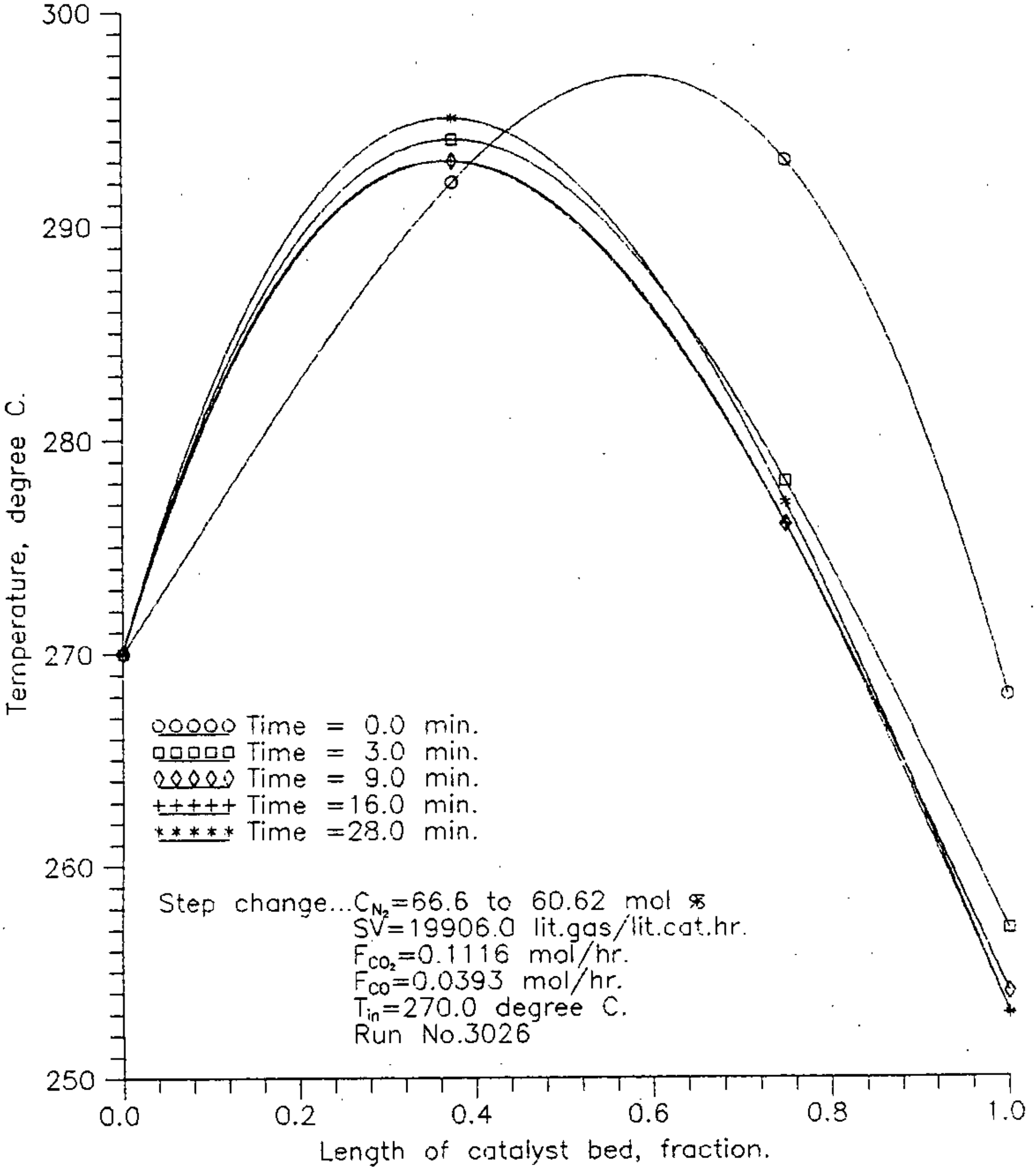

Figure 4.54 Temperature profiles in the reactor at different times.

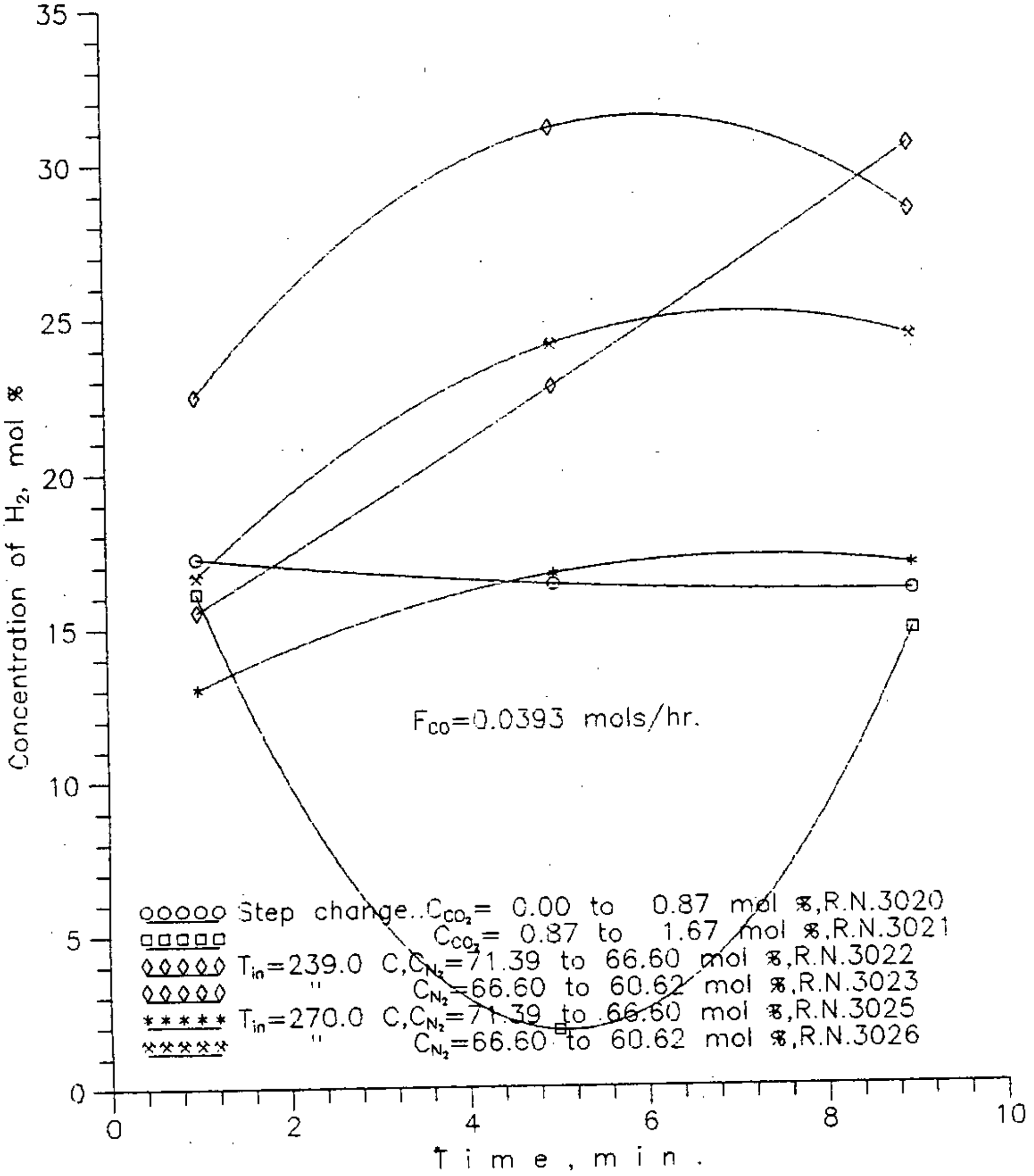

Figure 4.55 Variation of outlet H_2 concn. with time at diff. disturbances of inlet CO_2 concn.

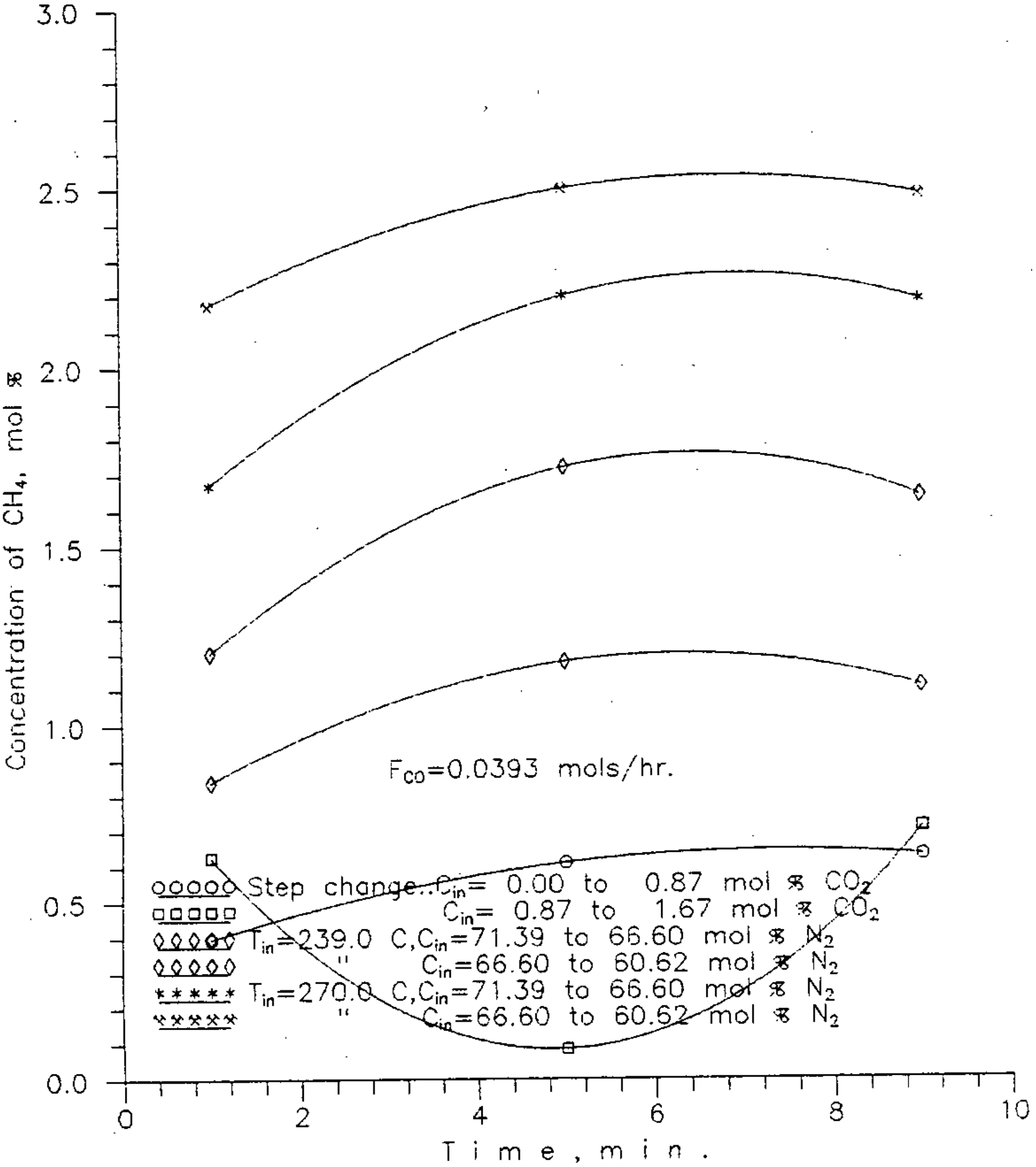

Figure 4.56 Variation of outlet CH_4 concn. with time at diff. disturbances of inlet CO_2 concn.

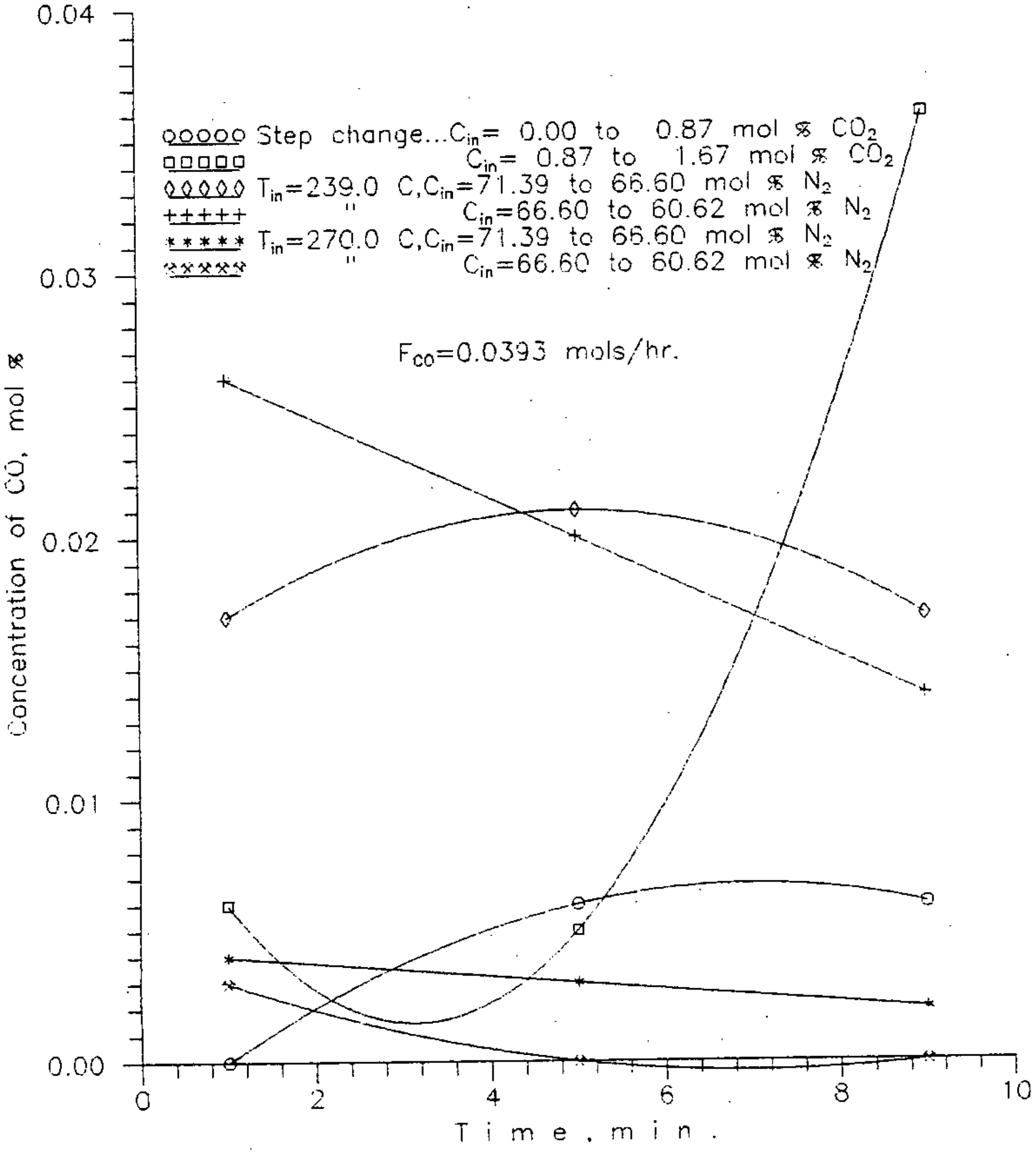

Figure 4.57 Variation of outlet CO concn. with time at diff. disturbances of inlet CO_2 concn.

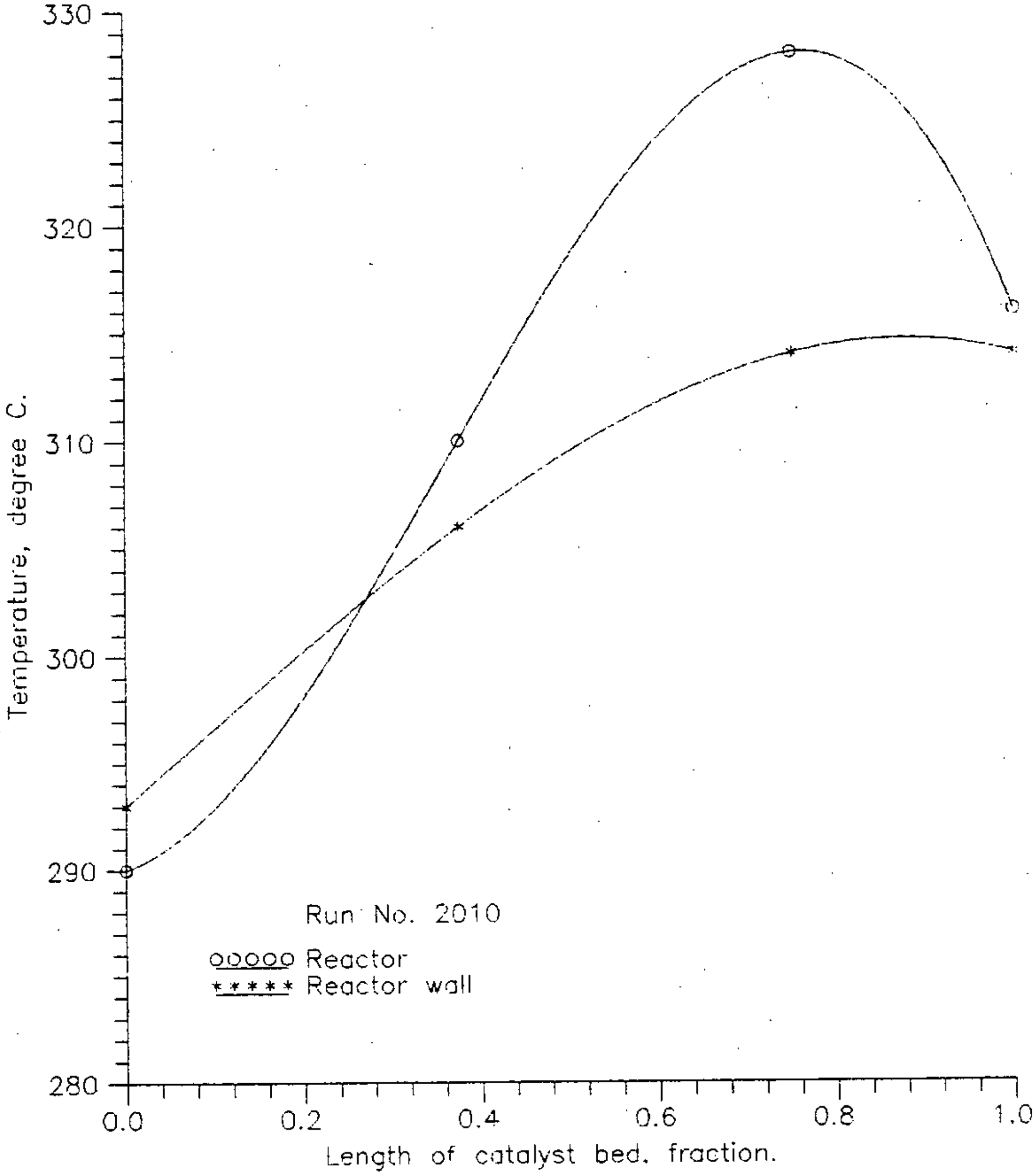

Figure 4.58 Temperature profiles of the reactor and reactor wall (During reaction).

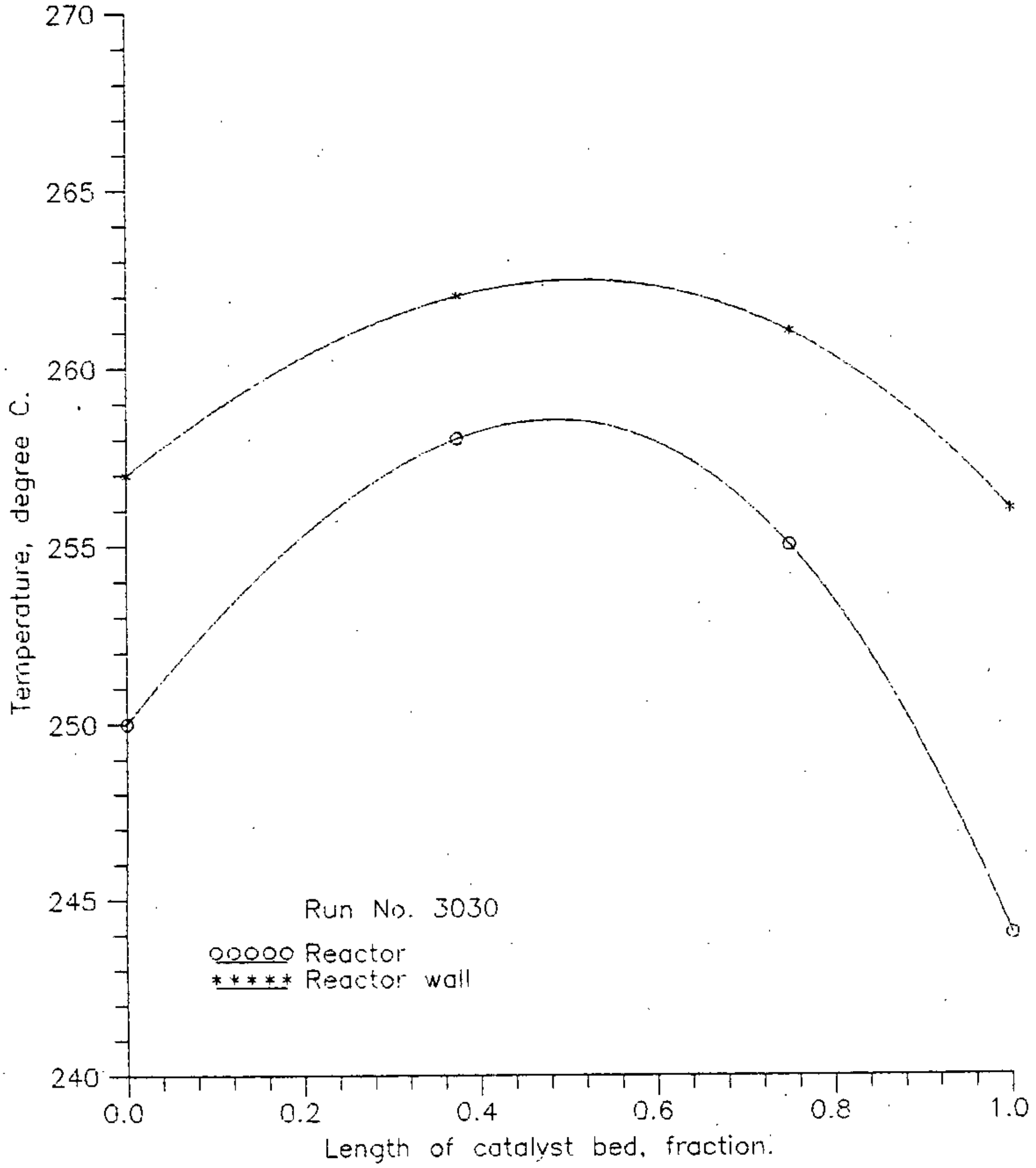

Figure 4.59 Temperature profiles of the reactor and reactor wall (During reaction).

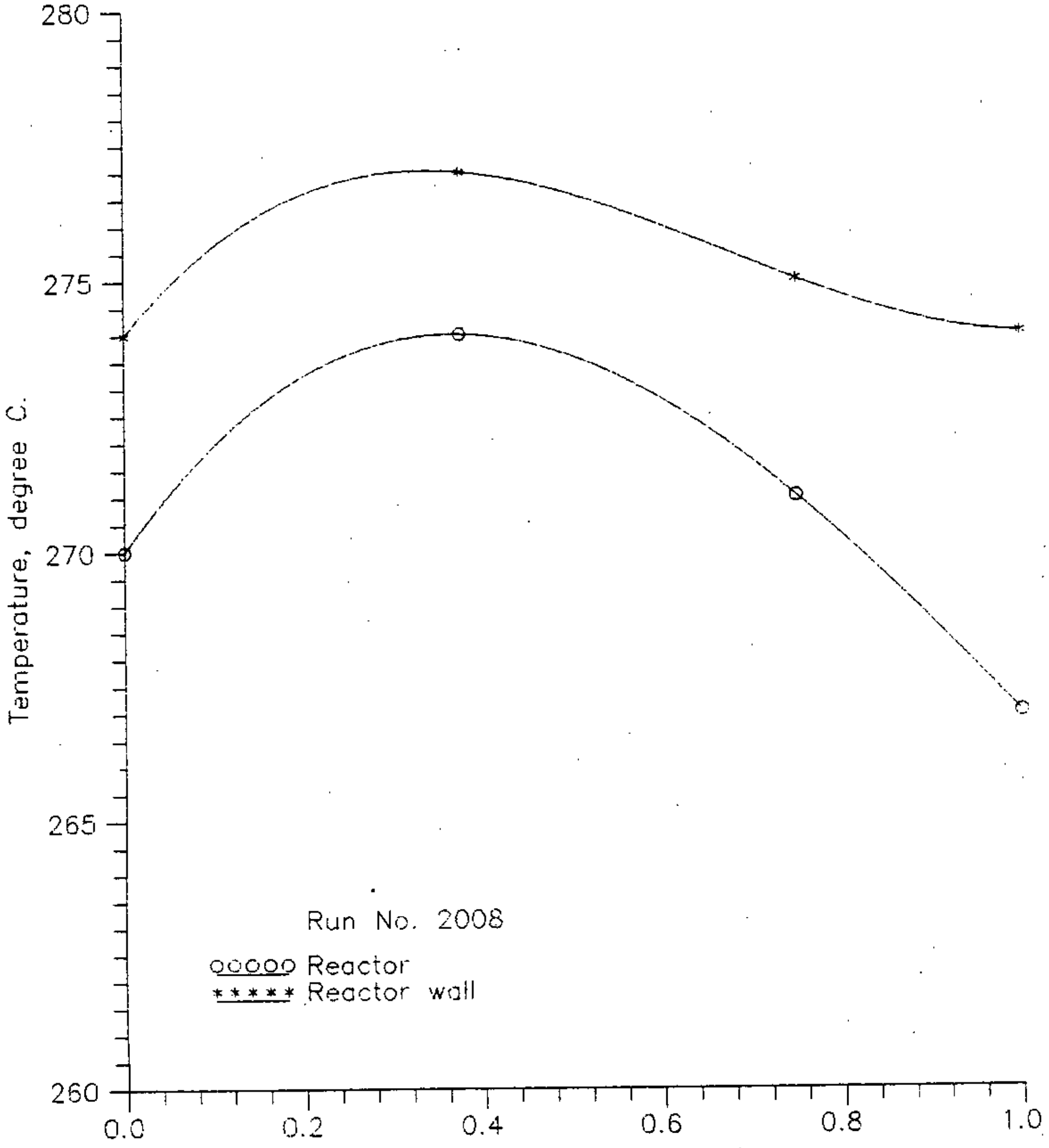

Figure 4.60 Temperature profiles of the reactor and reactor wall (Without reaction).

4.3 Isothermal methanation

To determine the rate equation of the test reaction, hydrogenation of carbon oxides, a fluidized sand bath had been erected to maintain isothermality in the reactor but actually it was not possible due to different limitations. It was decided to use the technique of measuring initial reaction rates to determine the rate equation by processing data produced from the experiments. It involves a series of rate measurements (at least three) at different initial reactant concentrations but restricted to very small conversions of the limiting reagent. Each rate measurement involves a new experiment. This method combines the advantages of the differential method and the integral method by measuring several points of the curve of the conversion, vs. the space time, W/F, followed by extrapolation of this line to the origin. For plotting the curve, conversion vs space time, several space times and conversions for several initial concentrations are necessary. For single concentration of carbon oxide, several space times and conversions could be made by varying Nitrogen and hydrogen flow to the feed. It is further necessary to take runs for at least three different concentrations and temperatures in this method. The slope of the curve at the origin, i.e., the reaction rate corresponding to the feed conditions, is determined by fitting a straight line through the origin to those points which, by visual inspection, are still in the linear region. The reciprocal space velocity, W/F, is defined as the quotient of the catalyst weight, W, divided by the molar flow, F, of the carbon oxide. The best slope for a straight line through the origin one can drive: $r = \frac{\sum \zeta (W/F)_i}{\sum (W/F)^2_i}$

After calculating the initial rates for different concentrations or partial pressures and temperatures by the above equation a figure of the rates as a function of partial pressures could be plotted. It can be described with langmuir isotherm by the equation

$$r = \frac{k.P_{CO}}{1+K_{CO}.P_{CO}}$$

$$= \quad 1/r = 1/kP_{CO} + K_{CO} /k$$

To test the applicability of this equation a polynomial regression analysis is made for 1/r as a function of $1/P_{CO}$ and compare the best description at the different temperatures. From the slope of the lines and the intercepts the values of k and k_{CO} can be calculated.

Some figures were tried to plot as measured conversion vs reciprocal space velocity for CO and CO_2 hydrogenation individually. But those showed that the conversion was less at higher temperature than that at lower temperature. The experiments were carried out at three different concentrations and two different inlet temperatures. But actually at least three different concentrations and three different inlet temperatures are necessary to determine the rate equation in this method. The details of the reactor with the catalyst bed are presented with the data and results in the appendices I to J.

It was not possible to take the runs for another temperature due to the failure of the air blower. For those abnormal behaviour of the conversion vs space time plots and for the shortage of the runs it was not possible to determine the rate equation of the test reaction.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

1. The thermal behaviour of the fixed bed reactor has been studied at steady and unsteady state conditions in an experimental system developed in the department. A separate fixed bed reactor immersed in a fluidized sand bath for isothermal operation has also been designed and operated over a range of experimental conditions.
2. The experiments were conducted for the methanation of carbon monoxide, carbon dioxide and the mixture of carbon oxides at various temperatures, concentrations and flow rates. The temperature profiles in the reactor rise sharply with the increasing inlet temperature. The profiles show downward trend at higher inlet concentration but lower inlet temperature. But at higher inlet temperature the reactor overcomes this peculiarity in the temperature profile.
3. The conversion of carbon oxides varies inversely with the inlet concentrations at lower inlet temperatures. But at higher inlet temperatures, concentration has almost no effect on the conversion of carbon oxides and the reaction goes to completion. The conversion of carbon oxides varies inversely with the space velocity.
4. The conversion of carbon monoxide is higher than that of carbon dioxide at the same inlet temperature, inlet concentration and

space velocity. This means that the catalyst is more effective for the methanation of carbon monoxide. This is in conformity with results in the literature for similar catalysts.

5. The dynamic behaviour has been studied by introducing step disturbances in inlet conditions using binary and ternary feeds of carbon oxides in hydrogen with three types of disturbances. Immediately after the introduction of carbon oxides in the feed gas a Fast Concentration Response (FCR) followed by a Slow Temperature Response (STR) occurs until a new stationary situation is reached. Comparison of the results of ternary feeds with the binary feeds does not show any new dynamic phenomena. The results of the dynamic experiments show general agreement with the information available in the literature.

5.2 <u>Recommendations</u>

1. An on-off temperature controller controls the inlet temperature of the reactor. In this case a 220V volt controller can't control inlet temperature effectively; a low voltage output controller could give better result in controlling the inlet temperature. It would be more desirable to instal a PID controller for temperature.
2. Further work should be undertaken to carry out the isothermal experiments and establish a rate equation.
3. With the rate equation developed for the system, the reactor can be modelled and the model parameters evaluated from the experimental runs.

NOMENCLATURE

K	equilibrium constant
k	rate constant
N	turn over frequency
p, P_i	partial pressure of i component
$*$	surface site
r, R_i	rate of i formation
R	gas constant
T	temperature
ξ	conversion of carbon oxide
S	slope of the curve
I	Intercept of coordinate
E_a	activation energy

Greek letters

θ_i = fractional surface coverage of i th component

θ_v = fractional surface vacency

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APPENDIX A

GAS CHROMATOGRAPHIC CALIBRATION

APPENDIX A

PROCEDURE OF ANALYSIS BY GAS CHROMATOGRAPH

CALIBRATION OF GAS CHROMATOGRAPH

Introduction

The chromatographic peaks are the measure of the proportions of the different chemical components present in the sample. There are a number of methods for the evaluation of the composition of the gas mixture from the areas of the peaks. In this work the peak areas were obtained directly from the integrator. Denoting the peak area as a_i and the respective response factors as F_i the mole fraction x_i is obtained from the following equation:

$$x_i = \left(\frac{a_i F_i}{\sum_{i=1}^{N} a_i F_i}\right), \quad i = 1,2,......N..........(A.1)$$

Where N is the number of components in the sample.

Determination of F_i

In order to determine the response factors F_i for the different components in a gas mixture, two known samples were analyzed and F_i values were found out using the following procedure.

Two gas mixtures with known compositions were fed to the chromatograph. The gas mixtures had five and six components respectively. Each component or a group of components gave one peak on the integrator chart. The component was identified by its retention time in the column. Area percentages, a_i were calculated by the following equation:

$$a_i = \left(\frac{a_i}{\sum_{i=1}^{N} a_i}\right) 100.....(A.2)$$

Each of the known compositions C_i was divided by area percentage a_i and a set of C_i/a_i was obtained. A reference component, r was chosen (preferably, the one with the lowest $C_{i/ai}$). Then F_1 was obtained with the following equation:

$$F_1 = \frac{(C_1/a_1)}{C_1/a_1)}.....(A.3)$$

Tables A.1 and A.2 show the retention times for the different components in the Porapak and Molecular Sieve columns together with the F values.

Method of Calculation of Composition

The following procedure is used to calculate the composition of the reactor effluent using the peak areas for Porapak and Molecular Sieve columns.

1. For Porapak column, calculate $(x_i)_{PR}$ using equation (A.1).
2. For Molecular Sieve Column, calculate $(x_i)_{MS}$ using equation (A.1).
3. The first peak in Porapak contains H_2, N_2, CH_4 and CO. These are the first four peaks in the Molecular Sieve column. Hence the $(x_i)_{MS}$ values give the multiplying

factors for the components in $(x_1)_{PR}$. Hence, multiply $(x_i)_{MS}$ by $(x_1)_{PR}$ to obtain the compositions of H_2, N_2, CH_4 and CO.

4. The second peak in the Porapak column is CO_2 and hence the CO_2 composition is given by $(x_2)_{PR}$.

TABLE A.1: RETENTION TIME AND F VALUES FOR DIFFERENT COMPONENTS IN PORAPAK COLUMN

Temperature = 100^0C

He pressure = 1.6 kg /cm^2

He flow rate = 13.3 cc/min

Component	Retention time min	F values
H_2	4.5	1.0
N_2		
CH_4		
CO		
CO_2	7.75	0.795

TABLE A.2 RETENTION TIME AND F VALUES FOR DIFFERENT COMPONENTS IN MOLECULAR SIEVE COLUMN

Temperature = 100^0C

He pressure = 1.6 kg /cm^2

He flow rate = 26.7 cc/min

Component	Retention time min	F values
H_2	1.5	1.043
N_2	2.65	1.043
CH_4	4.5	1.043
CO	6.25	1.049

APPENDIX B

CALIBRATION CURVES FOR ROTAMETERS

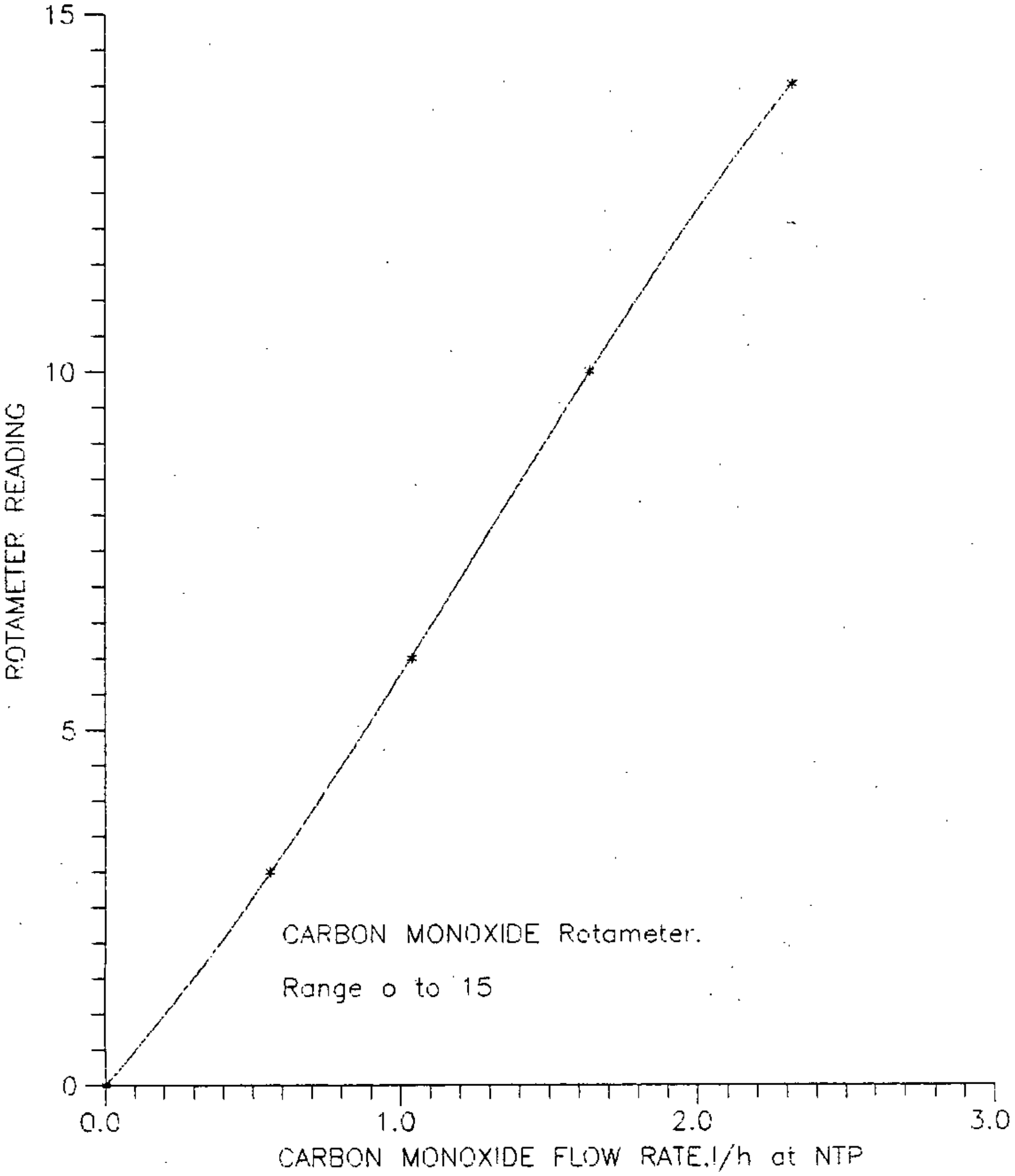

Figure B.1 Calibration curve for CARBON MONOXIDE.

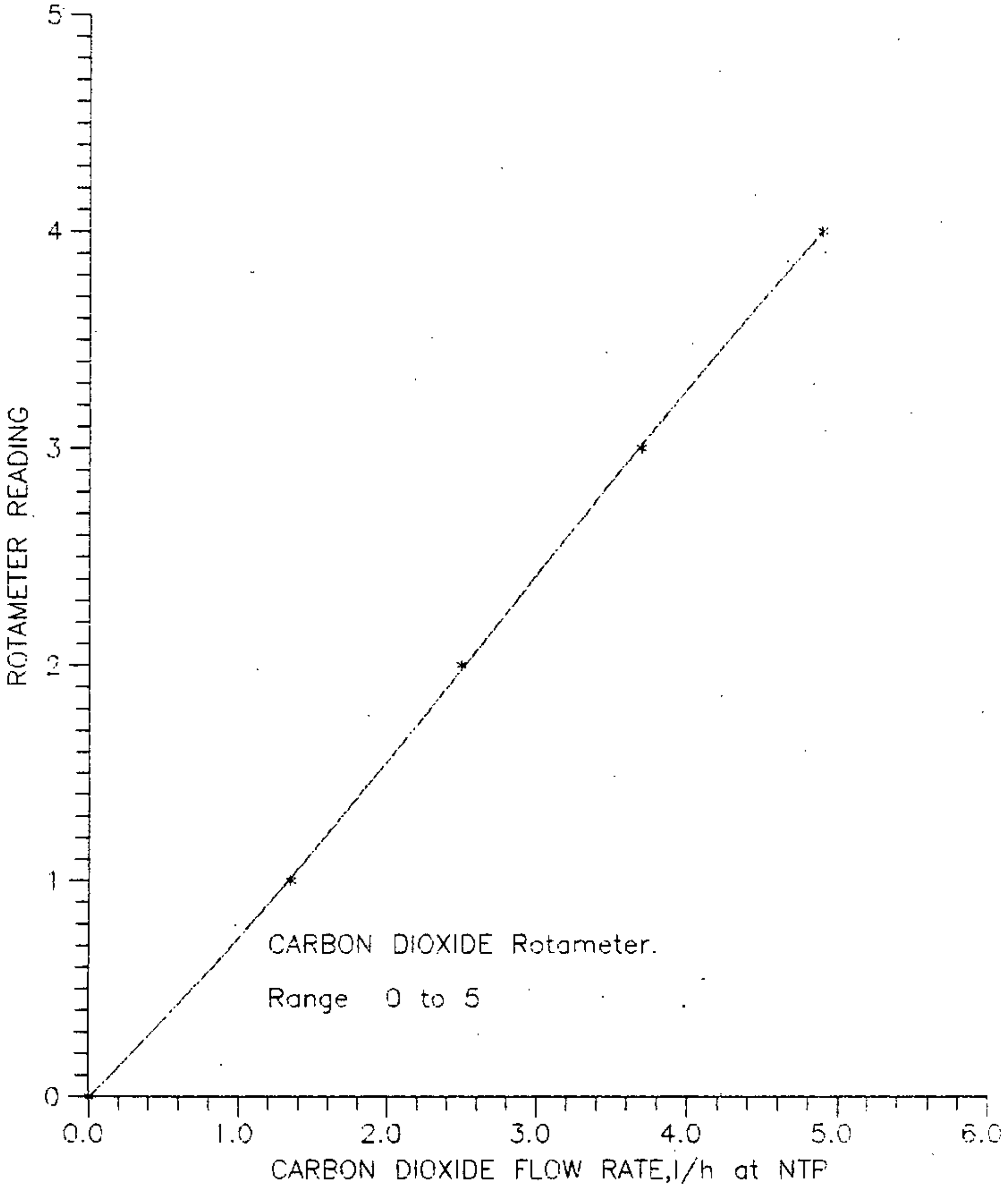

Figure B.2 Calibration curve for CARBON DIOXIDE.

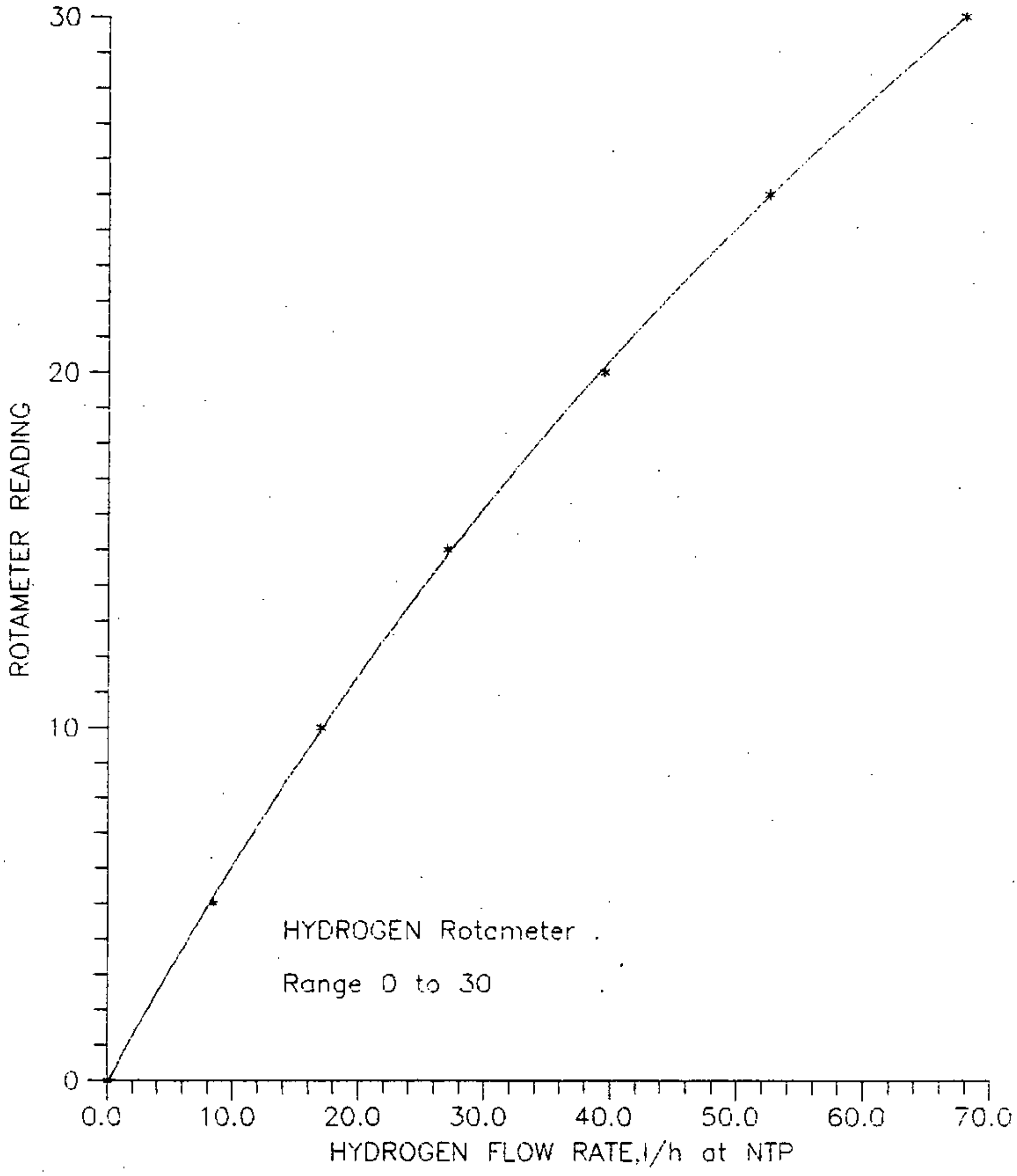

Figure B.3 Calibration curve for HYDROGEN.

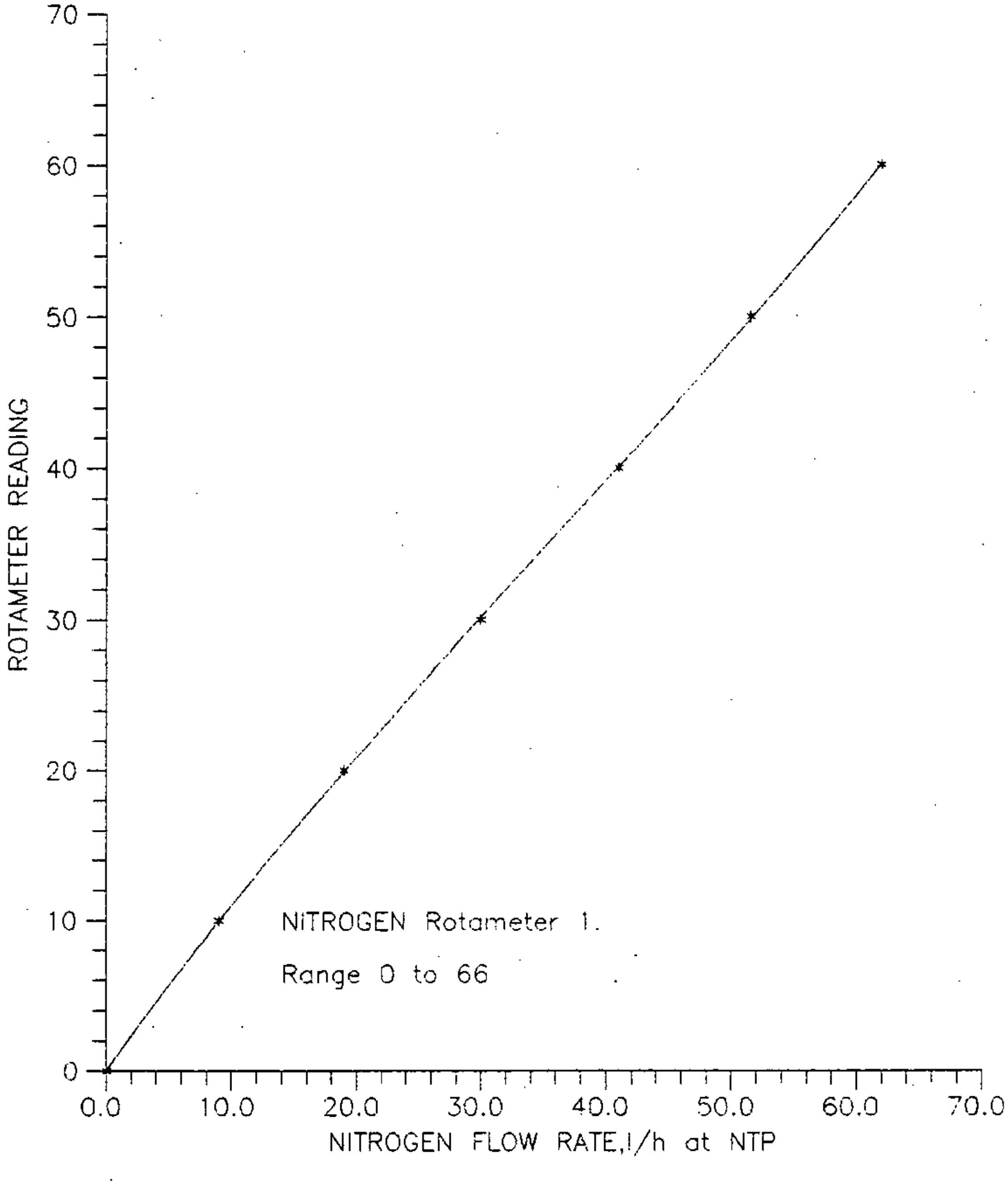

Figure B.4 Calibration curve for NITROGEN−1

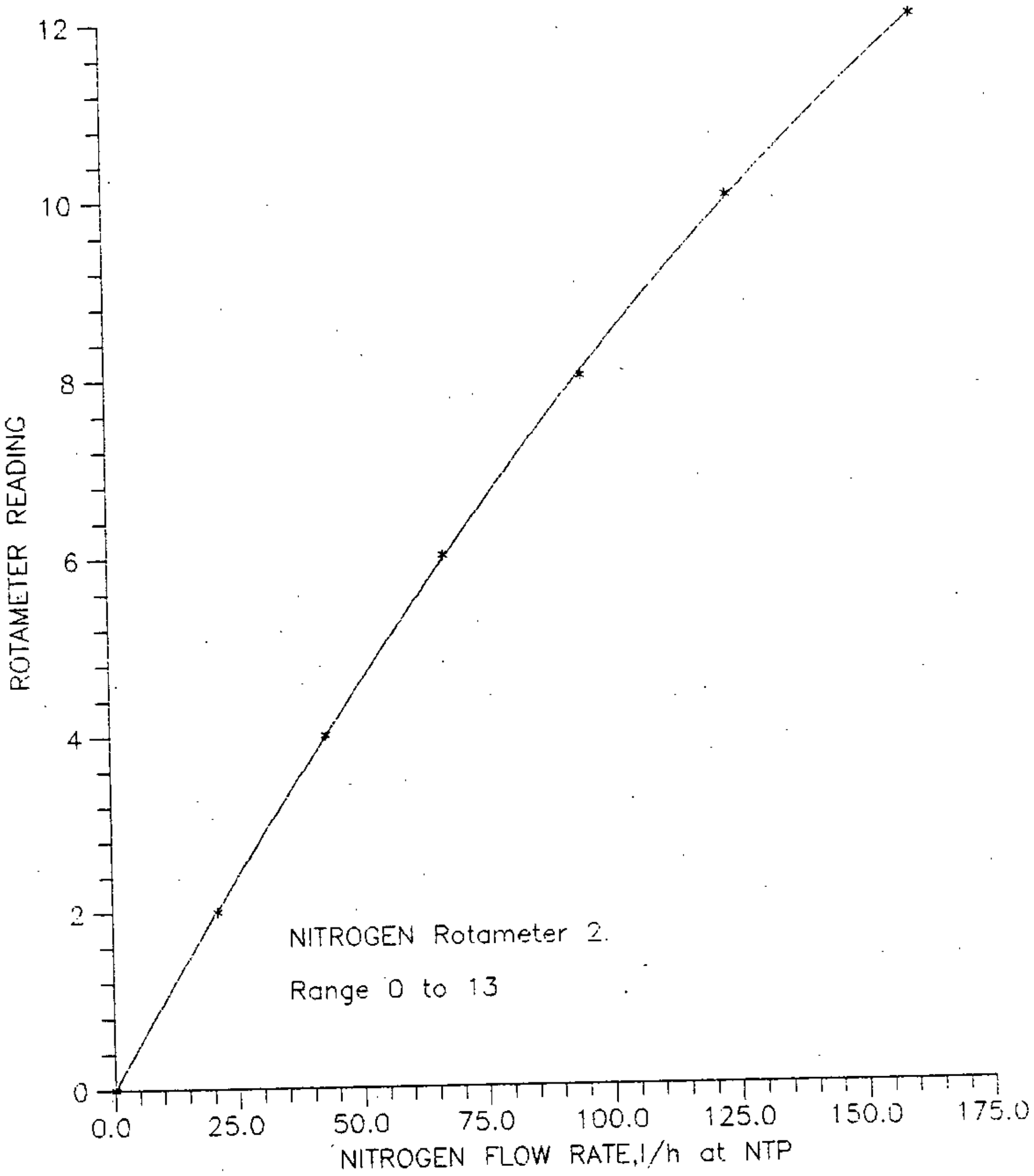

Figure B.5 Calibration curve for NITROGEN-2

APPENDIX C

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF STEADY STATE METHANATION OF CO_2 IN ADIABATIC REACTOR

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C                      COMPUTER PROGRAM (CO2.FOR)
C   FOR STEADY STATE METHANATION OF CO2 IN THE FIXED BED REACTOR
C  *  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C  *  THIS PROGRAM CALCULATES THE PRODUCT COMPOSITIONS AND TABULATES *
C  *  THE RESULTS BY TAKING THE INITIAL CONDITIONS OF OPERATION AND  *
C  *  THE GAS CHROMATOGRAPH PEAK AREAS FOR THE PRODUCTS               *
C  *  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C   *******************************************************
C   * NT          NUMBER OF RUNS                              *
C   * FRUN        RUN NUMBER                                  *
C   * NP          NUMBER OF PEAKS IN PORAPAK COLUMN           *
C   * NC          NUMBER OF PEAKS IN MOLECULAR SIEVE          *
C   * JP          NUMBER OF COMPOUNDS ANALYZED                *
C   * JPK         TOTAL NUMBER OF COMPOUNDS PRESENT           *
C   *******************************************************
C   * RSP         RESPONSE FACTOR IN PORAPAK COLUMN           *
C   * RSC         RESPONSE FACTOR IN MOLECULAR SIEVE COLUMN   *
C   * HYDCON      HYDROGEN CONVERSION                         *
C   * PCNT        MOL PERCENT OF PRODUCT GASES                *
C   * PR          FLOW RATE OF WATER FREE COMPOUND            *
C   *******************************************************

C   * ****************************************************
C   * CWT      WT. OF CATALYST,GM.                          *
C   * FD       DIAMETER OF REACTOR,CM.                      *
C   * FBD      BULK DENSITY OF CATALYST PELLET,GM/CC.       *
C   * FDP      DIAMETER OF CATALYST PELLETS,CM.             *
C   * FN2P     MOL PERCENT N2 IN FEED                       *
C   * TPK      PEAK TEMPERATURE OF REACTOR                  *
C   * TEX      EXIT TEMPERATURE OF REACTOR                  *
C   ******************************************************
C   * TNH      INITIAL TEMPERATURE PROFILE OF REACTOR       *
C   * TNHW     INITIAL TEMPERATURE PROFILE OF REACTOR WALL  *
C   * TR       FINAL TEMPERATURE PROFILE OF REACTOR         *
C   * TW       FINAL TEMPERATURE PROFILE OF REACTOR WALL    *
C   * *****************************************************

      DIMENSION RSP(6),RSC(6),RPN(6),PR(6)
      DIMENSION PRA(6),PRH(6),PRW(6),CPH(6),CHW(6),CHA(6)
      DIMENSION PRAM(6),CHAM(6),CHAP(6),PCNT(6)

      OPEN(UNIT=1,FILE = 'CO2DATA',STATUS = 'UNKNOWN')
      OPEN(UNIT=3,FILE = 'CO2OUT',STATUS = 'UNKNOWN')

      READ(1,*)NP,NC,JP,JPK,NT
      READ(1,*)(RSP(I),I=1,NP)
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)TC1,PC1,FM1,ZC1,FMUE1
      READ(1,*)TC2,PC2,FM2,ZC2,FMUE2
      READ(1,*)TC3,PC3,FM3,ZC3,FMUE3
      READ(1,*)FD,FBD,CWT,FDP

      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)

 200  FORMAT(/,'EXPERIMENTAL RESULTS OF METHENATION OF CO2 IN A FIXED BE
     ?D REACTOR',/,25x,'Steady state')
 201  FORMAT('--------------------------------------------------------------
     ?-------')
```

```
204    FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'8.23 gm',///,'DILUTION
      ? RATIO, CATALYST:INERT',5X,':',3X,'Undiluted',///,'CATALYST SIZE',
      ?22X,':',3X,'25-40 mesh.',///,'INERT SIZE',25X,':',3X,'25-40 mesh.'
      ?,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (ZFCL)')
205    FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'8.0 cm.',///,'LENGT
      ?H OF INERT BED BEFORE CATALYST:',3X,'13.5 cm.',///,'LENGTH OF INER
      ?T BED AFTER CATALYST :',3X,'22.0 cm.',///,'BULK DENSITY OF CATALYS
      ?T',11X,':',3X,'0.7565 gm./c.c.')
210    FORMAT(//,'BULK DENSITY OF INERT',14X,':',3X,'1.821 gm./c.c.',///,
      ?'OD OF REACTOR',22X,':',3X,'17.00 mm.',///,'ID OF REACTOR',22X,':'
      ?,3X,'12.00 mm.',///,'THERMO COUPLE LOCATIONS FROM INLET :',3X,'0.0
      ? cm. 3.0 cm. 6.0 cm. 8.0 cm.',////////////////////)
140    FORMAT('>>>>>>>>>>>>>>>        RUN NUMBER:',1X,F6.1,5X,'<<<<<<<<<<<<
      ?<<<')
220    FORMAT(/,'**********   INLET CONDITION:-')
207    FORMAT('TEMPRATURE:',F8.2,1X,'K',12X,'PRESSURE:',F8.2,1X,'mm.')
251    FORMAT(10X,'FLOW RATE,lit/hr.',6X,'FLOW RATE,mol/hr.',9X,'mol %')
224    FORMAT('H2',8X,F10.2,12X,F10.3,12X,F10.2)
212    FORMAT('N2',8X,F10.2,12X,F10.3,12X,F10.2)
214    FORMAT('CO2',7X,F10.2,12X,F10.3,12X,F10.2)
213    FORMAT('TOTAL',5X,F10.2,12X,F10.3,12X,F10.2)
246    FORMAT(/,'SPACE VELOCITY,lit.gas/lit.cat.hr.                 =',E1
      ?0.4,/,'CO2:H2 RATIO    = 1:',F8.4,7X,'W/FCO2 gm.hr./mol=',F10.4)
234    FORMAT('RE(superficial)=',F7.2,12X,'RE(particle)     =',F8.2)
226    FORMAT('INITIAL TEMPERATURE PROFILE:-')
227    FORMAT('REACTOR  :',4F10.2,1X,'C')
228    FORMAT('WALL     :',4F10.2,1X,'C')
215    FORMAT(/,'!!!!!!!!!!      EXIT CONDITION:-')
293    FORMAT('GAS FLOW RATE, mol/hr. :',F8.4)
222    FORMAT('GAS COMPOSITION (mol %):-')
223    FORMAT(6X,'H2',9X,'N2',9X,'CH4',9X,'CO',9X,'CO2',9X,'H2O')
100    FORMAT(F10.4,1X,F10.4,1X,F10.4,1X,F10.4,2X,F10.4, 2X,F10.4)
105    FORMAT(/,'$$$$$$$$$       ','CONV.OF H2:',F8.2,1X,'%',5X,'CONV.OF C
      ?O2:',F8.2,1X,'%')
261    FORMAT(/,'TEMPERATURE PROFILE:-')
97     FORMAT('REACTOR   :',4F10.2,1X,'C')
260    FORMAT('WALL      :',4F10.2,1X,'C')
221    FORMAT('PEAK TEMP.:',F10.2,1X,'C',8X,'EXIT TEMP:',F10.2,1X,'C',/)

       DO 75 LPN=1,NT

       READ(1,*)FRUN
       READ(1,*)T,P.FY1,FY2.FY3
       READ(1,*)TNH1,TNH2,TNH3,TNH4
       READ(1,*)TNHW1,TNHW2,TNHW3.TNHW4
       READ(1,*)(PRH(I),PRW(I),PRA(I),I=1,NP)
       READ(1.*)(CPH(I),CHW(I),CHA(I),I=1,NC)
       READ(1,*)TPK,TEX
       READ(1,*)RT1,RT2,RT3.RT4
       READ(1,*)WT1,WT2,WT3,WT4

C **   CALCULATE INLET COMPOSITIONS **************************************
C      HERE COMPONENT NO. 1=N2, 2=H2, 3=CO2

       FA=0.785*FD**2.0
       FW1=FY1/22.4
       FW2=FY2/22.4
       FW3=FY3/22.4
       FY4=FY1+FY2+FY3
       FW4=FW1+FW2+FW3
       FN2P=FW1*100.0/FW4
       FH2P=FW2*100.0/FW4
```

```
      FCO2P=FW3*100.0/FW4
      Y1=FW1/FW4
      Y2=FW2/FW4
      Y3=FW3/FW4
      AMW=Y1*FM1+Y2*FM2+Y3*FM3
      FTL=FN2P+FH2P+FCO2P
      RCH=FH2P/FCO2P
      RH2N=FH2P/FN2P
      RCO2N=FCO2P/FN2P
      WRCO2=CWT/FW3
      VO=FY4*T/273.0
      V=CWT/(FBD*1000.0)
      U=VO*1000.0/(3600.0*FA)
      RO=AMW*P/(82.05*760.0*T)
      ST=V/VO
      SV=1.0/ST

C   * CALCULATE VISCOSITIES OF PURE COMPONENTS BY LUCUS METHODS   *

      TR1=T/TC1
      FJITA1=0.176*(TC1/((FM1**3.0)*(PC1**4.0)))**(1.0/6.0)
      FJ1=1.0/FJITA1
      FMUER1=52.46*(FMUE1**2.0)*PC1/TC1**2.0
      FP=1.0
      FE1=(0.807*(TR1**0.618)-0.357*EXP(-0.449*TR1)+0.34*EXP(-4.058*TR1)
     ?+0.018)*FP*FJ1
      TR2=T/TC2
      FJITA2=0.176*(TC2/((FM2**3.0)*(PC2**4.0)))**(1.0/6.0)
      FJ2=1.0/FJITA2
      FMUER2=52.46*(FMUE2**2.0)*PC2/TC2**2.0
      Q=0.76
      FOQ2=1.22*(Q**0.15)*(1.0+0.00385*((TR2-12.0)**2.0)**(1.0/FM2)+1.0)
      FE2=(0.807*(TR2**0.618)-0.357*EXP(-0.449*TR2)+0.34*EXP(-4.058*TR2)
     ?+0.018)*FP*FOQ2*FJ2
      TR3=T/TC3
      FJITA3=0.176*(TC3/((FM3**3.0)*(PC3**4.0)))**(1.0/6.0)
      FJ3=1.0/FJITA3
      FMUER3=52.46*(FMUE3**2.0)*PC3/TC3**2.0
      FE3=(0.807*(TR3**0.618)-0.357*EXP(-0.449*TR3)+0.34*EXP(-4.058*TR3)
     ?+0.018)*FP*FJ3

C  ** CALCULATE MIXTURE VISCOSITY BY WILKE'S METHODS *******************

      F12=(1.0+((FE1/FE2)**0.5)*(FM2/FM1)**0.25)**2.0/(8.0*(1.0+FM1/FM2)
     ?)**0.5
      F13=(1.0+(FE1/FE3)**0.5*(FM3/FM1)**0.25)**2.0/(8.0*(1.0+FM1/FM3))*
     ?*0.5
      F21=FE2*FM1*F12/(FE1*FM2)
      F23=(1.0+(FE2/FE3)**0.5*(FM3/FM2)**0.25)**2.0/(8.0*(1.0+FM2/FM3))*
     ?*0.5
      F31=FE3*FM1*F13/(FE1*FM3)
      F32=FE3*FM2*F23/(FE2*FM3)
      F1=Y1*FE1/(Y1+Y2*F12+Y3*F13)
      F2=Y2*FE2/(Y1*F21+Y2+Y3*F23)
      F3=Y3*FE3/(Y1*F31+Y2*F32+Y3)
      FT=F1+F2+F3
      FTT=FT*1.0E-06
      FRE1=FD*U*RO/FTT
      FRE2=FDP*U*RO/FTT

C  ** CALCULATE EXIT COMPOSITION **************************************
```

```
C     HERE COMPONENT NO. 1=H2, 2=N2, 3=CH4, 4=CO, 5=CO2, 6=H2O
C  ** PRAM = MOL PERSENT IN PORAPAK COLUMN

      PRAS=0.0
      DO 10 I=1,NP
      PRAM(I)=PRH(I)*PRW(I)*PRA(I)*RSP(I)
      PRAS=PRAS+PRAM(I)
10    CONTINUE
      DO 11 I=1,NP
11    PRAM(I)=PRAM(I)/(PRAS)*100.0

C   * * CHAM = MOL PERCENT IN MOLECULAR SIEVE COLUMN * * * * * * * * * *

      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CPH(I)*CHW(I)*CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
13    CHAP(I)=CHAM(I)/(CHAS)*100.0

C     ****************************************************************
C     FIND MOL PERCENT IN EXIT GAS FOR MOLECULAR SIEVE COLUMN. PEAK 1 IN
C     PORAPAK COLUMN STANDS FOR ALL THE PEAKS IN MOLECULAR SIEVE COLUMN.
C     THERE ARE ONLY TWO PEAKS IN PORAPAK COLUMN. THE SECOND PEAK IS
C     COMPONENT NUMBER JP (CARBON DIOXIDE).
C     ****************************************************************

      TCNT=0.0
      DO 14 I=1,NC
      PCNT(I)=CHAP(I)*PRAM(1)/100.0
      TCNT=TCNT+PCNT(I)
14    CONTINUE
      PCNT(JP)=PRAM(NP)
      FR=FW1/PCNT(2)*100.0
      DO 21 I=1,JP
21    PR(I)=FR*PCNT(I)/100.0

C     ****************************************************************
C        FR=FLOW RAT OF WATER FREE PRODUCT , PR=FLOW RATE OF WATER FREE
C        COMPOUNDS . THE AMOUNT OF WATER FORMED IS FOUND OUT BY MATERIAL
C        BALANCE CALCULATIONS
C     ****************************************************************

      R1=PR(3)
      R2=PR(4)
      TCO2R=R1+R2
      TH2R=4.0*R1+R2
      TH2OP=2*R1+R2
      PR(6)=TH2OP
      PTOT=FR+PR(6)
      DO 23 I=1,JPK
      PCNT(I)=PR(I)/(PTOT)*100.0
23    CONTINUE

C     ****************************************************************
C                    PTOT=TOTAL FLOW RATE OF PRODUCT
C     THE CALCULATION FOR PRODUCT GAS COMPOSITION HAS BEEN COMPLETED
C                 RPN => MOL COMPONENT/MOL N2 IN PRODUCT
C     * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *

      DO 26 I=1,JPK
```

```
      RPN(I)=PCNT(I)/PCNT(2)
26    CONTINUE
      CO2CON=(RCO2N-RPN(5))/(RCO2N)*100.0
      HYDCON=(RH2N-RPN(1))/(RH2N)*100.0

      WRITE(3,140)FRUN
      WRITE(3,220)
      WRITE(3,207)T,P
      WRITE(3,251)
      WRITE(3,224)FY2,FW2,FH2P
      WRITE(3,212)FY1,FW1,FN2P
      WRITE(3,214)FY3,FW3,FCO2P
      WRITE(3,213)FY4,FW4,FTL
      WRITE(3,246)SV,RCH,WRCO2
      WRITE(3,234)FRE1,FRE2
      WRITE(3,226)
      WRITE(3,227)TNH1,TNH2,TNH3,TNH4
      WRITE(3,228)TNHW1,TNHW2,TNHW3,TNHW4
      WRITE(3,215)
      WRITE(3,293)PTOT
      WRITE(3,222)
      WRITE(3,223)
      WRITE(3,100)(PCNT(I),I=1,JPK)
      WRITE(3,105)HYDCON,CO2CON
      WRITE(3,261)
      WRITE(3,97)RT1,RT2,RT3,RT4
      WRITE(3,260)WT1,WT2,WT3,WT4
      WRITE(3,221)TPK,TEX

75    CONTINUE
      STOP
      END
```

```
    2     4     5     6    41
1.00        0.800
36.0        1.00        1.00        1.13
126.2       33.90       28.00       0.29        0.00
33.2        13.00        2.00       0.303       0.00
304.10      73.80       44.00       0.274       0.00
1.2         0.7565       8.23       0.0564
2001.1
520.00      760.00      103.00      39.50       1.35
248.00      251.00      246.00      240.00
250.00      251.00      247.00      245.00
11587941.00      1.00               1.00
68338.00         1.00               1.00
29514.00         1.00               1.00
4901164.00       1.00               1.00
6185.00          1.00               1.00
228.00           1.00               1.00
251.00      241.00
247.00      251.00      247.00      241.00
249.00      250.00      248.00      246.00
2001.2
520.00      760.00      103.00      39.50       1.35
248.00      251.00      246.00      240.00
250.00      251.00      247.00      245.00
11573529.00      1.00               1.00
64780.00         1.00               1.00
28956.00         1.00               1.00
4931950.00       1.00               1.00
5851.00          1.00               1.00
308.00           1.00               1.00
251.00      241.00
247.00      251.00      247.00      241.00
249.00      251.00      248.00      246.00
2001.3
520.00      760.00      103.00      39.50       1.35
248.00      251.00      246.00      240.00
250.00      251.00      247.00      245.00
11622648.00      1.00               1.00
64548.00         1.00               1.00
28248.00         1.00               1.00
4964988.00       1.00               1.00
5827.00          1.00               1.00
292.00           1.00               1.00
251.00      241.00
247.00      251.00      247.00      241.00
249.50      250.00      248.50      246.00
2002.1
520.00      760.00      103.00      39.50       2.50
248.00      251.00      246.00      240.00
250.00      251.00      247.00      245.00
11674628.00      1.00               1.00
173440.00        1.00               1.00
26594.00         1.00               1.00
4948089.00       1.00               1.00
7575.00          1.00               1.00
598.00           1.00               1.00
251.00      244.00
247.00      251.00      250.00      244.00
248.00      250.00      249.00      246.00
2002.2
520.00      760.00      103.00      39.50       2.50
```

```
248.00      251.00      246.00      240.00
250.00      251.00      247.00      245.00
11680217.00     1.00                1.00
171770.00       1.00                1.00
26319.00        1.00                1.00
4986927.00      1.00                1.00
7822.00         1.00                1.00
615.00          1.00                1.00
251.00      244.00
247.00      251.00      250.00      244.00
249.00      250.00      249.00      247.00
2003.00
520.00      760.00      103.00      39.50       3.7
248.00      251.00      246.00      240.00
250.00      251.00      247.00      245.00
11689655.00     1.00                1.00
351555.00       1.00                1.00
24866.00        1.00                1.00
4986818.00      1.00                1.00
8669.00         1.00                1.00
1066.00         1.00                1.00
251.00      243.00
247.00      251.00      249.00      243.00
250.00      251.00      249.00      247.00
2004.1
543.00      760.00      103.00      39.50       1.35
270.00      274.00      271.00      267.00
274.00      277.00      275.00      274.00
15831643.00     1.00                1.00
44964.00        1.00                1.00
33439.00        1.00                1.00
6602189.00      1.00                1.00
41620.00        1.00                1.00
0.00            1.00                1.00
285.00      282.00
270.00      281.00      285.00      282.00
275.00      282.00      286.00      286.00
2004.2
543.00      760.00      103.00      39.50       1.35
270.00      274.00      271.00      267.00
274.00      277.00      275.00      274.00
15980689.00     1.00                1.00
45027.00        1.00                1.00
32913.00        1.00                1.00
6797088.00      1.00                1.00
80264.00        1.00                1.00
4906.00         1.00                1.00
285.00      282.00
270.00      281.00      285.00      282.00
275.00      282.00      286.00      286.00
2005.0
543.00      760.00      103.00      39.50       2.50
270.00      274.00      271.00      267.00
274.00      277.00      275.00      274.00
15994779.00     1.00                1.00
128852.00       1.00                1.00
34388.00        1.00                1.00
6769237.00      1.00                1.00
108705.00       1.00                1.00
10899.00        1.00                1.00
288.00      286.00
270.00      281.00      288.00      286.00
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274.00     281.00     286.00     288.00
2006.0
543.00     760.00     103.00     39.50      3.70
270.00     274.00     271.00     267.00
274.00     277.00     275.00     274.00
16160993.00     1.00             1.00
283882.00       1.00             1.00
30422.00        1.00             1.00
6748810.00      1.00             1.00
118228.00       1.00             1.00
14354.00        1.00             1.00
290.00     288.00
270.00     282.00     290.00     288.00
274.00     282.00     288.00     288.00
2007.1
543.00     760.00     103.00     68.00      3.7
270.00     274.00     271.00     267.00
274.00     277.00     275.00     274.00
12944283.00     1.00             1.00
215355.00       1.00             1.00
73100.00        1.00             1.00
5665318.00      1.00             1.00
118770.00       1.00             1.00
14658.00        1.00             1.00
289.00     289.00
270.00     282.00     289.00     289.00
273.00     282.00     288.00     290.00
2007.2
543.00     760.00     103.00     68.00      3.7
270.00     274.00     271.00     267.00
274.00     277.00     275.00     274.00
12994341.00     1.00             1.00
214907.00       1.00             1.00
72638.00        1.00             1.00
5708024.00      1.00             1.00
120300.00       1.00             1.00
15573.00        1.00             1.00
289.00     289.00
270.00     282.00     289.00     289.00
273.00     282.00     288.00     290.00
2008.0
543.00     760.00     103.00     68.00      1.85
270.00     274.00     271.00     267.00
274.00     277.00     275.00     274.00
12969976.00     1.00             1.00
70206.00        1.00             1.00
76556.00        1.00             1.00
5732265.00      1.00             1.00
100796.00       1.00             1.00
11493.00        1.00             1.00
285.00     283.00
270.00     280.00     285.00     283.00
275.00     282.00     286.00     288.00
2009.0
563.00     760.00     103.00     39.50      1.05
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
11313260.00     1.00             1.00
0.0             1.00             1.00
28412.00        1.00             1.00
4814440.00      1.00             1.00
46647.00        1.00             1.00
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0.00           1.00           1.00
314.00    301.00
290.00    307.00    314.00    301.00
298.00    309.00    312.00    309.00
2010.0
563.00    760.00    103.00    39.50     2.05
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
11474784.00    1.00           1.00
1543.00        1.00           1.00
26906.00       1.00           1.00
4876640.00     1.00           1.00
74455.00       1.00           1.00
265.00         1.00           1.00
328.00    316.00
290.00    310.00    328.00    316.00
293.00    306.00    314.00    314.00
2011.0
557.00    760.00    103.00    39.50     2.70
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
12136976.00    1.00           1.00
4272.00        1.00           1.00
20404.00       1.00           1.00
5054004.00     1.00           1.00
103705.00      1.00           1.00
469.00         1.00           1.00
325.00    312.00
284.00    308.00    325.00    312.00
295.00    311.00    323.00    323.00
2012.1
556.00    760.00    103.00    39.50     3.70
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
12586940.00    1.00           1.00
15511.00       1.00           1.00
16161.00       1.00           1.00
5182629.00     1.00           1.00
136116.00      1.00           1.00
1796.00        1.00           1.00
338.00    325.00
283.00    307.00    338.00    325.00
295.00    313.00    330.00    331.00
2012.2
557.00    760.00    103.00    39.50     3.70
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
12622468.00    1.00           1.00
19376.00       1.00           1.00
15807.00       1.00           1.00
5210397.00     1.00           1.00
143825.00      1.00           1.00
1139.00        1.00           1.00
340.00    331.00
288.00    309.00    345.00    336.00
292.00    311.00    330.00    330.00
2013.1
559.00    760.00     103.00   68.00     3.70
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
10046119.00    1.00           1.00
8462.00        1.00           1.00
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45500.00       1.00           1.00
4367408.00     1.00           1.00
131577.00      1.00           1.00
880.00         1.00           1.00
343.00    336.00
286.00    309.00    343.00    336.00
293.00    309.00    328.00    331.00
2013.2
561.00    760.00     103.00   68.00      3.70
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
10064596.00    1.00           1.00
10235.00       1.00           1.00
45422.00       1.00           1.00
4393600.00     1.00           1.00
130704.00      1.00           1.00
956.00         1.00           1.00
345.00    336.00
288.00    310.00    345.00    336.00
292.00    308.00    327.00    331.00
2014.0
563.00    760.00    103.00    39.5       2.50
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
9606876.00     1.00           1.00
2872.00        1.00           1.00
54899.00       1.00           1.00
4225280.00     1.00           1.00
84378.00       1.00           1.00
234.00         1.00           1.00
332.00    318.00
290.00    310.00    332.00    318.00
295.00    308.00    318.00    318.00
2015.0
565.00    760.00    103.00    39.50      1.35
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
9366475.00     1.00           1.00
0.0            1.00           1.00
58425.00       1.00           1.00
4181985.00     1.00           1.00
49451.00       1.00           1.00
0.0            1.00           1.00
319.00    304.00
292.00    308.00    319.00    304.00
297.00    307.00    313.00    311.00
2016.0
564.00    760.00    103.00    68.00      1.85
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
9506881.00     1.00           1.00
1000.00        1.00           1.00
55559.00       1.00           1.00
4260764.00     1.00           1.00
66703.00       1.00           1.00
138.00         1.00           1.00
325.00    311.00
291.00    309.00    325.00    311.00
296.00    307.00    314.00    313.00
2017.1
563.00    760.00    103.00    39.50      2.05
290.00    293.00    289.00    281.00
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292.00     293.00     291.00     288.00
11561934.00     1.00                 1.00
800.00          1.00                 1.00
26111.00        1.00                 1.00
4781535.00      1.00                 1.00
72677.00        1.00                 1.00
00.00           1.00                 1.00
329.00     315.00
290.00     310.00     329.00     315.00
295.00     309.00     315.00     314.00
2017.2
561.00     760.00     103.00     39.50      2.05
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
11718718.00     1.00                 1.00
900.00          1.00                 1.00
24020.00        1.00                 1.00
5057708.00      1.00                 1.00
73787.00        1.00                 1.00
176.00          1.00                 1.00
327.00     313.00
288.00     309.00     327.00     313.00
293.00     306.00     314.00     313.00
2018.0
557.00     760.00     103.00     39.50      3.70
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
12718460.00     1.00                 1.00
23342.00        1.00                 1.00
16441.00        1.00                 1.00
5235048.00      1.00                 1.00
142025.00       1.00                 1.00
1583.00         1.00                 1.00
342.00     335.00
284.00     307.00     342.00     335.00
291.00     308.00     325.00     329.00
2019.0
559.00     760.00     103.00     68.00      3.7
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
10147610.00     1.00                 1.00
12161.00        1.00                 1.00
47562.00        1.00                 1.00
4408000.00      1.00                 1.00
132691.00       1.00                 1.00
808.00          1.00                 1.00
341.00     330.00
286.00     309.00     341.00     330.00
292.00     308.00     322.00     322.00
2020.0
559.00     760.00     103.00     68.00      4.15
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
10451751.00     1.00                 1.00
10915.00        1.00                 1.00
43357.00        1.00                 1.00
4546419.00      1.00                 1.00
157361.00       1.00                 1.00
857.00          1.00                 1.00
352.00     336.00
286.00     310.00     352.00     336.00
291.00     308.00     329.00     332.00
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2021.0
559.00     760.00     103.00     68.00      3.25
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
10012268.00    1.00              1.00
5183.00        1.00              1.00
50519.00       1.00              1.00
4401459.00     1.00              1.00
118877.00      1.00              1.00
371.00         1.00              1.00
336.00     323.00
286.00     307.00     336.00     323.00
293.00     309.00     323.00     323.00
2022.0
561.00     760.00     103.00     68.00      2.85
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
9987612.00     1.00              1.00
3720.00        1.00              1.00
48292.00       1.00              1.00
4401943.00     1.00              1.00
104529.00      1.00              1.00
343.00         1.00              1.00
334.00     318.00
288.00     308.00     334.00     318.00
293.00     308.00     321.00     321.00
2023.0
563.00     760.00     103.00     68.00      2.30
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
9778641.00     1.00              1.00
600.00         1.00              1.00
53976.00       1.00              1.00
4425136.00     1.00              1.00
80991.00       1.00              1.00
75.00          1.00              1.00
321.00     305.00
290.00     308.00     321.00     305.00
299.00     311.00     318.00     315.00
2024.00
552.00     760.00     103.00     39.5       3.70
290.00     293.00     289.00     281.00
292.00     293.00     291.00     288.00
13767004.00    1.00              1.00
53950.00       1.00              1.00
14177.00       1.00              1.00
5609440.00     1.00              1.00
131861.00      1.00              1.00
3021.00        1.00              1.00
323.00     319.00
279.00     297.00     323.00     319.00
284.00     296.00     310.00     314.00
2026.0
543.00     760.00     81.50      39.50      2.50
270.00     274.00     271.00     267.00
274.00     277.00     275.00     274.00
12578180.00    1.00              1.00
20061.00       1.00              1.00
29800.00       1.00              1.00
5245752.00     1.00              1.00
118796.00      1.00              1.00
526.00         1.00              1.00
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312.00     294.00
270.00     291.00     312.00     294.00
272.00     285.00     293.00     291.00
2027.0
543.00     760.00     62.00      39.50      2.50
270.00     274.00     271.00     267.00
274.00     277.00     275.00     274.00
10733804.00     1.00             1.00
17673.00        1.00             1.00
41413.00        1.00             1.00
4635321.00      1.00             1.00
144246.00       1.00             1.00
359.00          1.00             1.00
312.00     286.00
270.00     294.00     312.00     286.00
272.00     286.00     290.00     283.00
2028.0
573.00     760.00     103.00     39.50      4.15
300.00     305.00     302.00     299.00
305.00     308.00     306.00     304.00
14559902.00     1.00             1.00
1877.00         1.00             1.00
9970.00         1.00             1.00
5927876.00      1.00             1.00
190469.00       1.00             1.00
0.0             1.00             1.00
389.00     345.00
300.00     343.00     389.00     345.00
308.00     334.00     345.00     338.00
2029.0
573.00     760.00     103.00     39.50      3.70
300.00     305.00     302.00     299.00
305.00     308.00     306.00     304.00
14202374.00     1.00             1.00
0.0             1.00             1.00
15006.00        1.00             1.00
5705035.00      1.00             1.00
170868.00       1.00             1.00
0.0             1.00             1.00
381.00     338.00
300.00     342.00     381.00     338.00
308.00     331.00     340.00     332.00
2030.0
573.00     760.00     103.00     39.50      3.10
300.00     305.00     302.00     299.00
305.00     308.00     306.00     304.00
13936060.00     1.00             1.00
00.00           1.00             1.00
14981.00        1.00             1.00
5726933.00      1.00             1.00
147348.00       1.00             1.00
00.00           1.00             1.00
371.00     332.00
300.00     338.00     371.00     332.00
308.00     328.00     336.00     330.00
2031.0
573.00     760.00     103.00     39.50      4.60
300.00     305.00     302.00     299.00
305.00     308.00     306.00     304.00
14687148.00     1.00             1.00
2487.00         1.00             1.00
10134.00        1.00             1.00
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5918720.00     1.00               1.00
213937.00      1.00               1.00
00.00          1.00               1.00
401.00    351.00
300.00    349.00    401.00    351.00
306.00    335.00    348.00    340.00
2032.0
555.00    760.00    103.00    39.50     3.10
290.00    293.00    289.00    281.00
292.00    293.00    291.00    288.00
13694784.00    1.00               1.00
19264.00       1.00               1.00
17350.00       1.00               1.00
5668114.00     1.00               1.00
131108.00      1.00               1.00
1083.00        1.00               1.00
339.00    322.00
282.00    303.00    339.00    322.00
285.00    299.00    315.00    315.00
2040.0
543.00    760.00    103.00     39.50     1.35
270.00    274.00    271.00    267.00
274.00    277.00    275.00    274.00
14024366.00    1.00               1.00
20355.00       1.00               1.00
22027.00       1.00               1.00
5887390.00     1.00               1.00
52374.00       1.00               1.00
00.00          1.00               1.00
290.00    285.00
270.00    283.00    290.00    285.00
275.00    283.00    288.00    288.00
2041.0
543.00    760.00    103.00     39.50     3.10
270.00    274.00    271.00    267.00
274.00    277.00    275.00    274.00
14701376.00    1.00               1.00
91946.00       1.00               1.00
17075.00       1.00               1.00
6184365.00     1.00               1.00
98268.00       1.00               1.00
3452.00        1.00               1.00
302.00    299.00
270.00    286.00    302.00    299.00
275.00    285.00    295.00    297.00
```

EXPERIMENTAL RESULTS OF METHENATION OF CO2 IN A FIXED BED REACTOR
Steady state

WEIGHT OF CATALYST : 8.23 gm

DILUTION RATIO, CATALYST:INERT : Undiluted

CATALYST SIZE : 25-40 mesh.

INERT SIZE : 25-40 mesh.

CATALYST TYPE : Ni on Alumina (ZFCL)

LENGTH OF CATALYST BED : 8.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 13.5 cm.

LENGTH OF INERT BED AFTER CATALYST : 22.0 cm.

BULK DENSITY OF CATALYST : 0.7565 gm./c.c.

BULK DENSITY OF INERT : 1.821 gm./c.c.

OD OF REACTOR : 17.00 mm.

ID OF REACTOR : 12.00 mm.

THERMO COUPLE LOCATIONS FROM INLET : 0.0 cm. 3.0 cm. 6.0 cm. 8.0 cm

```
>>>>>>>>>>>>>>>        RUN NUMBER: 2001.1      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  520.00 K                  PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.            FLOW RATE,mol/hr.              mol %
H2             39.50                        1.763                     27.46
N2            103.00                        4.598                     71.60
CO2             1.35                        0.060                      0.94
TOTAL         143.85                        6.422                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2519E+05
CO2:H2 RATIO    = 1: 29.2593           W/FCO2 gm.hr./mol=   136.5570
RE(superficial)= 143.70                 RE(particle)     =     6.75
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      248.00     251.00     246.00     240.00 C
WALL     :      250.00     251.00     247.00     245.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6394
GAS COMPOSITION (mol %):-
     H2           N2          CH4          CO          CO2          H2O
   17.6763    81.5379      0.1029      0.0043       0.4686       0.2101

$$$$$$$$$$      CONV.OF H2:    43.47 %      CONV.OF CO2:    56.15 %

TEMPERATURE PROFILE:-
REACTOR    :      247.00     251.00     247.00     241.00 C
WALL       :      249.00     250.00     248.00     246.00 C
PEAK TEMP.:       251.00 C          EXIT TEMP:     241.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 2001.2      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  520.00 K                  PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.            FLOW RATE,mol/hr.              mol %
H2             39.50                        1.763                     27.46
N2            103.00                        4.598                     71.60
CO2             1.35                        0.060                      0.94
TOTAL         143.85                        6.422                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2519E+05
CO2:H2 RATIO    = 1: 29.2593           W/FCO2 gm.hr./mol=   136.5570
RE(superficial)= 143.70                 RE(particle)     =     6.75
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      248.00     251.00     246.00     240.00 C
WALL     :      250.00     251.00     247.00     245.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6121
GAS COMPOSITION (mol %):-
     H2           N2          CH4          CO          CO2          H2O
   17.3176    81.9343      0.0972      0.0058       0.4449       0.2002

$$$$$$$$$$      CONV.OF H2:    44.89 %      CONV.OF CO2:    58.57 %

TEMPERATURE PROFILE:-
REACTOR    :      247.00     251.00     247.00     241.00 C
WALL       :      249.00     251.00     248.00     246.00 C
PEAK TEMP.:       251.00 C          EXIT TEMP:     241.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2001.3     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  520.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.               mol %
H2              39.50                       1.763                     27.46
N2             103.00                       4.598                     71.60
CO2              1.35                       0.060                      0.94
TOTAL          143.85                       6.422                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                             =0.2519E+05
CO2:H2 RATIO     = 1: 29.2593           W/FCO2 gm.hr./mol=   136.5570
RE(superficial)= 143.70                  RE(particle)     =     6.75
INITIAL TEMPERATURE PROFILE:-
REACTOR   :     248.00     251.00     246.00     240.00 C
WALL      :     250.00     251.00     247.00     245.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5815
GAS COMPOSITION (mol %):-
      H2           N2          CH4          CO          CO2          H2O
   16.8738     82.3837     0.0967      0.0055      0.4414      0.1988

$$$$$$$$$$     CONV.OF H2:    46.59 %     CONV.OF CO2:    59.12 %

TEMPERATURE PROFILE:-
REACTOR    :     247.00     251.00     247.00     241.00 C
WALL       :     249.50     250.00     248.50     246.00 C
PEAK TEMP.:     251.00 C          EXIT TEMP:     241.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2002.1     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  520.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.               mol %
H2              39.50                       1.763                     27.24
N2             103.00                       4.598                     71.03
CO2              2.50                       0.112                      1.72
TOTAL          145.00                       6.473                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                             =0.2539E+05
CO2:H2 RATIO     = 1: 15.8000           W/FCO2 gm.hr./mol=    73.7408
RE(superficial)= 146.24                  RE(particle)     =     6.87
INITIAL TEMPERATURE PROFILE:-
REACTOR   :     248.00     251.00     246.00     240.00 C
WALL      :     250.00     251.00     247.00     245.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5756
GAS COMPOSITION (mol %):-
      H2           N2          CH4          CO          CO2          H2O
   15.9568     82.4705     0.1263      0.0113      1.1714      0.2638

$$$$$$$$$$     CONV.OF H2:    49.55 %     CONV.OF CO2:    41.48 %

TEMPERATURE PROFILE:-
REACTOR    :     247.00     251.00     250.00     244.00 C
WALL       :     248.00     250.00     249.00     246.00 C
PEAK TEMP.:     251.00 C          EXIT TEMP:     244.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2002.2     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  520.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol %
H2              39.50                    1.763                   27.24
N2             103.00                    4.598                   71.03
CO2              2.50                    0.112                    1.72
TOTAL          145.00                    6.473                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2539E+05
CO2:H2 RATIO    = 1: 15.8000          W/FCO2 gm.hr./mol=    73.7408
RE(superficial)= 146.24                RE(particle)     =     6.87
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     248.00     251.00     246.00     240.00 C
WALL     :     250.00     251.00     247.00     245.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5592
GAS COMPOSITION (mol %):-
      H2          N2          CH4         CO          CO2          H2O
   15.7150    82.7131     0.1297     0.0115      1.1597      0.2710

$$$$$$$$$$      CONV.OF H2:    50.46 %      CONV.OF CO2:    42.24 %

TEMPERATURE PROFILE:-
REACTOR    :     247.00     251.00     250.00     244.00 C
WALL       :     249.00     250.00     249.00     247.00 C
PEAK TEMP.:      251.00 C         EXIT TEMP:      244.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2003.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  520.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol %
H2              39.50                    1.763                   27.02
N2             103.00                    4.598                   70.45
CO2              3.70                    0.165                    2.53
TOTAL          146.20                    6.527                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2560E+05
CO2:H2 RATIO    = 1: 10.6757          W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 148.90                RE(particle)     =     7.00
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     248.00     251.00     246.00     240.00 C
WALL     :     250.00     251.00     247.00     245.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5805
GAS COMPOSITION (mol %):-
      H2          N2          CH4         CO          CO2          H2O
   14.7910    82.3973     0.1432     0.0199      2.3422      0.3064

$$$$$$$$$$      CONV.OF H2:    53.19 %      CONV.OF CO2:    20.87 %

TEMPERATURE PROFILE:-
REACTOR    :     247.00     251.00     249.00     243.00 C
WALL       :     250.00     251.00     249.00     247.00 C
PEAK TEMP.:      251.00 C         EXIT TEMP:      243.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2004.1      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
             FLOW RATE,lit/hr.        FLOW RATE,mol/hr.            mol %
H2                39.50                     1.763                  27.46
N2               103.00                     4.598                  71.60
CO2                1.35                     0.060                   0.94
TOTAL            143.85                     6.422                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2630E+05
CO2:H2 RATIO    = 1: 29.2593          W/FCO2 gm.hr./mol=  136.5570
RE(superficial)= 139.52                RE(particle)      =    6.56
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     270.00     274.00     271.00     267.00 C
WALL     :     274.00     277.00     275.00     274.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5360
GAS COMPOSITION (mol %):-
      H2           N2           CH4          CO           CO2          H2O
   15.1447     83.0602      0.5236      0.0000       0.2243       1.0472

$$$$$$$$$$      CONV.OF H2:    52.45 %      CONV.OF CO2:    79.39 %

TEMPERATURE PROFILE:-
REACTOR   :     270.00     281.00     285.00     282.00 C
WALL      :     275.00     282.00     286.00     286.00 C
PEAK TEMP.:     285.00 C          EXIT TEMP:     282.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2004.2      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
             FLOW RATE,lit/hr.        FLOW RATE,mol/hr.            mol %
H2                39.50                     1.763                  27.46
N2               103.00                     4.598                  71.60
CO2                1.35                     0.060                   0.94
TOTAL            143.85                     6.422                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2630E+05
CO2:H2 RATIO    = 1: 29.2593          W/FCO2 gm.hr./mol=  136.5570
RE(superficial)= 139.52                RE(particle)      =    6.56
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     270.00     274.00     271.00     267.00 C
WALL     :     274.00     277.00     275.00     274.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5825
GAS COMPOSITION (mol %):-
      H2           N2           CH4          CO           CO2          H2O
   14.3585     82.3688      0.9727      0.0672       0.2204       2.0125

$$$$$$$$$$      CONV.OF H2:    54.54 %      CONV.OF CO2:    79.59 %

TEMPERATURE PROFILE:-
REACTOR   :     270.00     281.00     285.00     282.00 C
WALL      :     275.00     282.00     286.00     286.00 C
PEAK TEMP.:     285.00 C          EXIT TEMP:     282.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2005.0     <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   543.00 K                PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.            mol %
H2             39.50                       1.763                  27.24
N2            103.00                       4.598                  71.03
CO2             2.50                       0.112                   1.72
TOTAL         145.00                       6.473                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2651E+05
CO2:H2 RATIO    = 1: 15.8000          W/FCO2 gm.hr./mol=    73.7408
RE(superficial)= 141.97                RE(particle)     =     6.67
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      270.00     274.00     271.00     267.00 C
WALL     :      274.00     277.00     275.00     274.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7130
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   14.7196     80.4871     1.2925      0.1464       0.6229       2.7315

$$$$$$$$$$      CONV.OF H2:    52.31 %      CONV.OF CO2:    68.12 %

TEMPERATURE PROFILE:-
REACTOR    :      270.00     281.00     288.00     286.00 C
WALL       :      274.00     281.00     286.00     288.00 C
PEAK TEMP.:       288.00 C          EXIT TEMP:     286.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2006.0     <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   543.00 K                PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.            mol %
H2             39.50                       1.763                  27.02
N2            103.00                       4.598                  70.45
CO2             3.70                       0.165                   2.53
TOTAL         146.20                       6.527                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2673E+05
CO2:H2 RATIO    = 1: 10.6757          W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 144.54                RE(particle)     =     6.79
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      270.00     274.00     271.00     267.00 C
WALL     :      274.00     277.00     275.00     274.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6846
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   13.1267     80.8895     1.4171      0.1944       1.3438       3.0285

$$$$$$$$$$      CONV.OF H2:    57.68 %      CONV.OF CO2:    53.75 %

TEMPERATURE PROFILE:-
REACTOR    :      270.00     282.00     290.00     288.00 C
WALL       :      274.00     282.00     288.00     288.00 C
PEAK TEMP.:       290.00 C          EXIT TEMP:     288.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2007.1      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol %
H2             68.00                     3.036                   38.92
N2            103.00                     4.598                   58.96
CO2             3.70                     0.165                    2.12
TOTAL         174.70                     7.799                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3194E+05
CO2:H2 RATIO    = 1: 18.3784         W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 144.51               RE(particle)     =     6.79
INITIAL TEMPERATURE PROFILE:-
REACTOR  :    270.00     274.00     271.00     267.00 C
WALL     :    274.00     277.00     275.00     274.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  7.1413
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  29.9094     64.3890     1.3499      0.1883      1.2756        2.8880

$$$$$$$$$$     CONV.OF H2:    29.64 %      CONV.OF CO2:    44.85 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     282.00     289.00     289.00 C
WALL       :     273.00     282.00     288.00     290.00 C
PEAK TEMP.:      289.00 C         EXIT TEMP:      289.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2007.2      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol %
H2             68.00                     3.036                   38.92
N2            103.00                     4.598                   58.96
CO2             3.70                     0.165                    2.12
TOTAL         174.70                     7.799                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3194E+05
CO2:H2 RATIO    = 1: 18.3784         W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 144.51               RE(particle)     =     6.79
INITIAL TEMPERATURE PROFILE:-
REACTOR  :    270.00     274.00     271.00     267.00 C
WALL     :    274.00     277.00     275.00     274.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  7.1140
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  29.6111     64.6360     1.3622      0.1993      1.2676        2.9238

$$$$$$$$$$     CONV.OF H2:    30.61 %      CONV.OF CO2:    45.41 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     282.00     289.00     289.00 C
WALL       :     273.00     282.00     288.00     290.00 C
PEAK TEMP.:      289.00 C         EXIT TEMP:      289.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2008.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol %
H2             68.00                     3.036                   39.34
N2            103.00                     4.598                   59.59
CO2             1.85                     0.083                    1.07
TOTAL         172.85                     7.717                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3160E+05
CO2:H2 RATIO    = 1: 36.7568          W/FCO2 gm.hr./mol=   99.6497
RE(superficial)= 140.62                RE(particle)    =    6.61
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     270.00     274.00     271.00     267.00 C
WALL     :     274.00     277.00     275.00     274.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  7.1023
GAS COMPOSITION (mol %):-
      H2          N2           CH4          CO           CO2           H2O
   31.1277    64.7429      1.1384       0.1467       0.4207        2.4236

$$$$$$$$$$       CONV.OF H2:    27.17 %      CONV.OF CO2:    63.82 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     280.00     285.00     283.00 C
WALL       :     275.00     282.00     286.00     288.00 C
PEAK TEMP.:      285.00 C          EXIT TEMP:     283.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2009.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  563.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol %
H2             39.50                     1.763                   27.52
N2            103.00                     4.598                   71.75
CO2             1.05                     0.047                    0.73
TOTAL         143.55                     6.408                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2721E+05
CO2:H2 RATIO    = 1: 37.6190          W/FCO2 gm.hr./mol=  175.5733
RE(superficial)= 135.52                RE(particle)    =    6.37
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7088
GAS COMPOSITION (mol %):-
      H2          N2           CH4          CO           CO2           H2O
   17.1122    80.5466      0.7804       0.0000       0.0000        1.5608

$$$$$$$$$$       CONV.OF H2:    44.60 %      CONV.OF CO2:   100.00 %

TEMPERATURE PROFILE:-
REACTOR    :     290.00     307.00     314.00     301.00 C
WALL       :     298.00     309.00     312.00     309.00 C
PEAK TEMP.:      314.00 C          EXIT TEMP:     301.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2010.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  563.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2              39.50                      1.763                     27.33
N2             103.00                      4.598                     71.26
CO2              2.05                      0.092                      1.42
TOTAL          144.55                      6.453                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2740E+05
CO2:H2 RATIO    = 1: 19.2683          W/FCO2 gm.hr./mol=    89.9278
RE(superficial)= 137.59                RE(particle)     =     6.47
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      290.00     293.00     289.00     281.00 C
WALL     :      292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7233
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO           CO2          H2O
  15.9578    80.3419     1.2266     0.0049       0.0105       2.4582

$$$$$$$$$$      CONV.OF H2:    48.21 %      CONV.OF CO2:    99.34 %

TEMPERATURE PROFILE:-
REACTOR    :     290.00     310.00     328.00     316.00 C
WALL       :     293.00     306.00     314.00     314.00 C
PEAK TEMP.:      328.00 C         EXIT TEMP:      316.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2011.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  557.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2              39.50                      1.763                     27.20
N2             103.00                      4.598                     70.94
CO2              2.70                      0.121                      1.86
TOTAL          145.20                      6.482                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2723E+05
CO2:H2 RATIO    = 1: 14.6296          W/FCO2 gm.hr./mol=    68.2785
RE(superficial)= 139.96                RE(particle)     =     6.58
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      290.00     293.00     289.00     281.00 C
WALL     :      292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5520
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO           CO2          H2O
  12.0370    82.8202     1.6994     0.0087       0.0272       3.4075

$$$$$$$$$$      CONV.OF H2:    62.10 %      CONV.OF CO2:    98.75 %

TEMPERATURE PROFILE:-
REACTOR    :     284.00     308.00     325.00     312.00 C
WALL       :     295.00     311.00     323.00     323.00 C
PEAK TEMP.:      325.00 C         EXIT TEMP:      312.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2012.1     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  556.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.            mol %
H2              39.50                     1.763                    27.02
N2             103.00                     4.598                    70.45
CO2              3.70                     0.165                     2.53
TOTAL          146.20                     6.527                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2737E+05
CO2:H2 RATIO    = 1: 10.6757          W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 142.23                RE(particle)     =     6.68
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      290.00     293.00     289.00     281.00 C
WALL     :      292.00     293.00     291.00     288.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.4855
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO           CO2           H2O
   9.4101    83.8254     2.2016      0.0328       0.0941        4.4360

$$$$$$$$$$       CONV.OF H2:    70.73 %      CONV.OF CO2:    96.87 %

TEMPERATURE PROFILE:-
REACTOR     :      283.00     307.00     338.00     325.00 C
WALL        :      295.00     313.00     330.00     331.00 C
PEAK TEMP.:        338.00 C           EXIT TEMP:    325.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2012.2     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  557.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.            mol %
H2              39.50                     1.763                    27.02
N2             103.00                     4.598                    70.45
CO2              3.70                     0.165                     2.53
TOTAL          146.20                     6.527                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2742E+05
CO2:H2 RATIO    = 1: 10.6757          W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 142.05                RE(particle)     =     6.68
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      290.00     293.00     289.00     281.00 C
WALL     :      292.00     293.00     291.00     288.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.4899
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO           CO2           H2O
   9.1476    83.7580     2.3120      0.0207       0.1170        4.6447

$$$$$$$$$$       CONV.OF H2:    71.52 %      CONV.OF CO2:    96.11 %

TEMPERATURE PROFILE:-
REACTOR     :      288.00     309.00     345.00     336.00 C
WALL        :      292.00     311.00     330.00     330.00 C
PEAK TEMP.:        340.00 C           EXIT TEMP:    331.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2013.1      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   559.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.            FLOW RATE,mol/hr.          mol %
H2              68.00                      3.036                  38.92
N2             103.00                      4.598                  58.96
CO2              3.70                      0.165                   2.12
TOTAL          174.70                      7.799                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.3288E+05
CO2:H2 RATIO    = 1: 18.3784         W/FCO2 gm.hr./mol=   49.8249
RE(superficial)= 141.69               RE(particle)     =     6.66
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      290.00     293.00     289.00     281.00 C
WALL     :      292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.7448
GAS COMPOSITION (mol %):-
     H2           N2           CH4          CO           CO2          H2O
   25.5687     68.1740      2.0539      0.0155       0.0646       4.1233

$$$$$$$$$$      CONV.OF H2:    43.19 %     CONV.OF CO2:    97.36 %

TEMPERATURE PROFILE:-
REACTOR    :      286.00     309.00     343.00     336.00 C
WALL       :      293.00     309.00     328.00     331.00 C
PEAK TEMP.:       343.00 C          EXIT TEMP:     336.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2013.2      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   561.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.            FLOW RATE,mol/hr.          mol %
H2              68.00                      3.036                  38.92
N2             103.00                      4.598                  58.96
CO2              3.70                      0.165                   2.12
TOTAL          174.70                      7.799                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.3300E+05
CO2:H2 RATIO    = 1: 18.3784         W/FCO2 gm.hr./mol=   49.8249
RE(superficial)= 141.34               RE(particle)     =     6.64
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      290.00     293.00     289.00     281.00 C
WALL     :      292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.7274
GAS COMPOSITION (mol %):-
     H2           N2           CH4          CO           CO2          H2O
   25.4383     68.3502      2.0333      0.0168       0.0780       4.0835

$$$$$$$$$$      CONV.OF H2:    43.63 %     CONV.OF CO2:    96.82 %

TEMPERATURE PROFILE:-
REACTOR    :      288.00     310.00     345.00     336.00 C
WALL       :      292.00     308.00     327.00     331.00 C
PEAK TEMP.:       345.00 C          EXIT TEMP:     336.00 C
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>>>>>>>>>>>>>>>        RUN NUMBER: 2014.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  563.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.              mol %
H2             39.50                      1.763                      27.24
N2            103.00                      4.598                      71.03
CO2             2.50                      0.112                       1.72
TOTAL         145.00                      6.473                     100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                        =0.2749E+05
CO2:H2 RATIO    = 1: 15.8000          W/FCO2 gm.hr./mol=    73.7408
RE(superficial)= 138.53                RE(particle)      =     6.51
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  7.0267
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO           CO2           H2O
   30.6090    65.4391     1.3068     0.0041       0.0233        2.6177

$$$$$$$$$$      CONV.OF H2:  -21.97 %     CONV.OF CO2:    98.53 %

TEMPERATURE PROFILE:-
REACTOR   :     290.00    310.00     332.00     318.00 C
WALL      :     295.00    308.00     318.00     318.00 C
PEAK TEMP.:     332.00 C        EXIT TEMP:      318.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 2015.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  565.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.              mol %
H2             39.50                      1.763                      27.46
N2            103.00                      4.598                      71.60
CO2             1.35                      0.060                       0.94
TOTAL         143.85                      6.422                     100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                        =0.2737E+05
CO2:H2 RATIO    = 1: 29.2593          W/FCO2 gm.hr./mol=   136.5570
RE(superficial)= 135.81                RE(particle)      =     6.38
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  7.0740
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO           CO2           H2O
   32.6922    65.0019     0.7686     0.0000       0.0000        1.5373

$$$$$$$$$$      CONV.OF H2:  -31.15 %     CONV.OF CO2:   100.00 %

TEMPERATURE PROFILE:-
REACTOR   :     292.00    308.00     319.00     304.00 C
WALL      :     297.00    307.00     313.00     311.00 C
PEAK TEMP.:     319.00 C        EXIT TEMP:      304.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2016.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  564.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol %
H2              68.00                    3.036                    39.34
N2             103.00                    4.598                    59.59
CO2              1.85                    0.083                     1.07
TOTAL          172.85                    7.717                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3282E+05
CO2:H2 RATIO    = 1: 36.7568          W/FCO2 gm.hr./mol=   99.6497
RE(superficial)= 137.05                RE(particle)     =    6.44
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.9736
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  30.9528    65.9373     1.0323      0.0024       0.0082       2.0669

$$$$$$$$$$     CONV.OF H2:    28.90 %      CONV.OF CO2:    99.30 %

TEMPERATURE PROFILE:-
REACTOR    :     291.00     309.00     325.00     311.00 C
WALL       :     296.00     307.00     314.00     313.00 C
PEAK TEMP.:      325.00 C         EXIT TEMP:      311.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2017.1      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  563.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol %
H2              39.50                    1.763                    27.33
N2             103.00                    4.598                    71.26
CO2              2.05                    0.092                     1.42
TOTAL          144.55                    6.453                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2740E+05
CO2:H2 RATIO    = 1: 19.2683          W/FCO2 gm.hr./mol=   89.9278
RE(superficial)= 137.59                RE(particle)     =    6.47
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7122
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  15.8252    80.4988     1.2235      0.0000       0.0054       2.4471

$$$$$$$$$$     CONV.OF H2:    48.74 %      CONV.OF CO2:    99.66 %

TEMPERATURE PROFILE:-
REACTOR    :     290.00     310.00     329.00     315.00 C
WALL       :     295.00     309.00     315.00     314.00 C
PEAK TEMP.:      329.00 C         EXIT TEMP:      315.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2017.2      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  561.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol %
H2             39.50                    1.763                    27.33
N2            103.00                    4.598                    71.26
CO2             2.05                    0.092                     1.42
TOTAL         144.55                    6.453                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2730E+05
CO2:H2 RATIO    = 1: 19.2683         W/FCO2 gm.hr./mol=   89.9278
RE(superficial)= 137.92               RE(particle)     =    6.48
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5863
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   14.0729    82.3120      1.2009      0.0032      0.0060       2.4049

$$$$$$$$$$     CONV.OF H2:    55.42 %      CONV.OF CO2:    99.63 %

TEMPERATURE PROFILE:-
REACTOR    :     288.00     309.00     327.00     313.00 C
WALL       :     293.00     306.00     314.00     313.00 C
PEAK TEMP.:     327.00 C          EXIT TEMP:     313.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2018.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  557.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol %
H2             39.50                    1.763                    27.02
N2            103.00                    4.598                    70.45
CO2             3.70                    0.165                     2.53
TOTAL         146.20                    6.527                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2742E+05
CO2:H2 RATIO    = 1: 10.6757         W/FCO2 gm.hr./mol=   49.8249
RE(superficial)= 142.05               RE(particle)     =    6.68
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5032
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
    9.4468    83.5556      2.2668      0.0286      0.1399       4.5622

$$$$$$$$$$     CONV.OF H2:    70.52 %      CONV.OF CO2:    95.34 %

TEMPERATURE PROFILE:-
REACTOR    :     284.00     307.00     342.00     335.00 C
WALL       :     291.00     308.00     325.00     329.00 C
PEAK TEMP.:     342.00 C          EXIT TEMP:     335.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2019.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  559.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol %
H2             68.00                     3.036                   38.92
N2            103.00                     4.598                   58.96
CO2             3.70                     0.165                    2.12
TOTAL         174.70                     7.799                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3288E+05
CO2:H2 RATIO    = 1: 18.3784          W/FCO2 gm.hr./mol=    49.8249
RE(superficial)= 141.69                RE(particle)      =    6.66
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.8077
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   26.2366     67.5439     2.0332      0.0140      0.0919       4.0804

$$$$$$$$$$     CONV.OF H2:    41.16 %     CONV.OF CO2:   96.21 %

TEMPERATURE PROFILE:-
REACTOR    :     286.00     309.00     341.00     330.00 C
WALL       :     292.00     308.00     322.00     322.00 C
PEAK TEMP.:      341.00 C        EXIT TEMP:       330.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2020.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  559.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol %
H2             68.00                     3.036                   38.82
N2            103.00                     4.598                   58.81
CO2             4.15                     0.185                    2.37
TOTAL         175.15                     7.819                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3297E+05
CO2:H2 RATIO    = 1: 16.3855          W/FCO2 gm.hr./mol=    44.4222
RE(superficial)= 142.61                RE(particle)      =    6.70
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.6616
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   23.6977     69.0261     2.3891      0.0147      0.0795       4.7930

$$$$$$$$$$     CONV.OF H2:    48.00 %     CONV.OF CO2:   97.14 %

TEMPERATURE PROFILE:-
REACTOR    :     286.00     310.00     352.00     336.00 C
WALL       :     291.00     308.00     329.00     332.00 C
PEAK TEMP.:      352.00 C        EXIT TEMP:       336.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2021.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  559.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol %
H2             68.00                     3.036                  39.02
N2            103.00                     4.598                  59.11
CO2             3.25                     0.145                   1.87
TOTAL         174.25                     7.779                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3280E+05
CO2:H2 RATIO   = 1: 20.9231          W/FCO2 gm.hr./mol=   56.7237
RE(superficial)= 140.76               RE(particle)     =    6.62
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.8744
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   27.6386    66.8891      1.8066     0.0064       0.0399       3.6195

$$$$$$$$$$      CONV.OF H2:    37.41 %      CONV.OF CO2:    98.11 %

TEMPERATURE PROFILE:-
REACTOR    :     286.00     307.00     336.00     323.00 C
WALL       :     293.00     309.00     323.00     323.00 C
PEAK TEMP.:      336.00 C         EXIT TEMP:      323.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2022.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  561.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol %
H2             68.00                     3.036                  39.11
N2            103.00                     4.598                  59.25
CO2             2.85                     0.127                   1.64
TOTAL         173.85                     7.761                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3284E+05
CO2:H2 RATIO   = 1: 23.8597          W/FCO2 gm.hr./mol=   64.6849
RE(superficial)= 139.60               RE(particle)     =    6.56
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.7446
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   26.9258    68.1766      1.6189     0.0060       0.0288       3.2439

$$$$$$$$$$      CONV.OF H2:    40.18 %      CONV.OF CO2:    98.47 %

TEMPERATURE PROFILE:-
REACTOR    :     288.00     308.00     334.00     318.00 C
WALL       :     293.00     308.00     321.00     321.00 C
PEAK TEMP.:      334.00 C         EXIT TEMP:      318.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2023.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  563.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol %
H2             68.00                       3.036                  39.24
N2            103.00                       4.598                  59.43
CO2             2.30                       0.103                   1.33
TOTAL         173.30                       7.737                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3285E+05
CO2:H2 RATIO   = 1: 29.5652         W/FCO2 gm.hr./mol=   80.1530
RE(superficial)= 138.14              RE(particle)    =    6.49
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.8703
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   29.3892    66.9286     1.2250      0.0013      0.0048       2.4512

$$$$$$$$$$     CONV.OF H2:    33.49 %     CONV.OF CO2:    99.68 %

TEMPERATURE PROFILE:-
REACTOR   :      290.00     308.00     321.00     305.00 C
WALL      :      299.00     311.00     318.00     315.00 C
PEAK TEMP.:      321.00 C         EXIT TEMP:      305.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2024.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  552.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol %
H2             39.50                       1.763                  27.02
N2            103.00                       4.598                  70.45
CO2             3.70                       0.165                   2.53
TOTAL         146.20                       6.527                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2717E+05
CO2:H2 RATIO   = 1: 10.6757         W/FCO2 gm.hr./mol=   49.8249
RE(superficial)= 142.93              RE(particle)    =    6.72
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.3625
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
    7.8017    85.7472     2.0157      0.0522      0.2998       4.0835

$$$$$$$$$$     CONV.OF H2:    76.27 %     CONV.OF CO2:    90.27 %

TEMPERATURE PROFILE:-
REACTOR   :      279.00     297.00     323.00     319.00 C
WALL      :      284.00     296.00     310.00     314.00 C
PEAK TEMP.:      323.00 C         EXIT TEMP:      319.00 C
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>>>>>>>>>>>>>>>        RUN NUMBER: 2026.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.            mol %
H2             39.50                      1.763                    31.98
N2             81.50                      3.638                    65.99
CO2             2.50                      0.112                     2.02
TOTAL         123.50                      5.513                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2258E+05
CO2:H2 RATIO   = 1: 15.8000          W/FCO2 gm.hr./mol=   73.7408
RE(superficial)= 113.38               RE(particle)    =    5.33
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     270.00     274.00     271.00     267.00 C
WALL     :     274.00     277.00     275.00     274.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  4.6362
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   16.0494    78.4782     1.7772      0.0089       0.1229       3.5633

$$$$$$$$$$     CONV.OF H2:   57.80 %     CONV.OF CO2:   94.90 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     291.00     312.00     294.00 C
WALL       :     272.00     285.00     293.00     291.00 C
PEAK TEMP.:     312.00 C        EXIT TEMP:      294.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 2027.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.            mol %
H2             39.50                      1.763                    37.98
N2             62.00                      2.768                    59.62
CO2             2.50                      0.112                     2.40
TOTAL         104.00                      4.643                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1901E+05
CO2:H2 RATIO   = 1: 15.8000          W/FCO2 gm.hr./mol=   73.7408
RE(superficial)=  87.55               RE(particle)    =    4.11
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     270.00     274.00     271.00     267.00 C
WALL     :     274.00     277.00     275.00     274.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  3.9219
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   22.6990    70.5743     2.1962      0.0062       0.1258       4.3986

$$$$$$$$$$     CONV.OF H2:   49.52 %     CONV.OF CO2:   95.58 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     294.00     312.00     286.00 C
WALL       :     272.00     286.00     290.00     283.00 C
PEAK TEMP.:     312.00 C        EXIT TEMP:      286.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 2028.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  573.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.           mol %
H2              39.50                     1.763                   26.93
N2             103.00                     4.598                   70.24
CO2              4.15                     0.185                    2.83
TOTAL          146.65                     6.547                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2829E+05
CO2:H2 RATIO    = 1:  9.5181          W/FCO2 gm.hr./mol=   44.4222
RE(superficial)= 140.27                RE(particle)     =    6.59
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     300.00     305.00     302.00     299.00 C
WALL     :     305.00     308.00     306.00     304.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.3204
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
    5.2329    86.4264     2.7770     0.0000      0.0097       5.5539

$$$$$$$$$$      CONV.OF H2:    84.21 %     CONV.OF CO2:    99.72 %

TEMPERATURE PROFILE:-
REACTOR    :     300.00     343.00     389.00     345.00 C
WALL       :     308.00     334.00     345.00     338.00 C
PEAK TEMP.:      389.00 C         EXIT TEMP:      345.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 2029.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  573.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.           mol %
H2              39.50                     1.763                   27.02
N2             103.00                     4.598                   70.45
CO2              3.70                     0.165                    2.53
TOTAL          146.20                     6.527                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2821E+05
CO2:H2 RATIO    = 1: 10.6757          W/FCO2 gm.hr./mol=   49.8249
RE(superficial)= 139.34                RE(particle)     =    6.55
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     300.00     305.00     302.00     299.00 C
WALL     :     305.00     308.00     306.00     304.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.4468
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
    7.9939    84.4208     2.5284     0.0000      0.0000       5.0569

$$$$$$$$$$      CONV.OF H2:    75.31 %     CONV.OF CO2:  100.00 %

TEMPERATURE PROFILE:-
REACTOR    :     300.00     342.00     381.00     338.00 C
WALL       :     308.00     331.00     340.00     332.00 C
PEAK TEMP.:      381.00 C         EXIT TEMP:      338.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 2030.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  573.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol %
H2             39.50                     1.763                    27.13
N2            103.00                     4.598                    70.74
CO2             3.10                     0.138                     2.13
TOTAL         145.60                     6.500                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2809E+05
CO2:H2 RATIO    = 1: 12.7419         W/FCO2 gm.hr./mol=    59.4684
RE(superficial)= 138.11               RE(particle)     =     6.49
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     300.00     305.00     302.00     299.00 C
WALL     :     305.00     308.00     306.00     304.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.3862
GAS COMPOSITION (mol %):-
      H2         N2          CH4          CO           CO2           H2O
    8.0395    85.3709     2.1965      0.0000       0.0000        4.3930

$$$$$$$$$$     CONV.OF H2:   75.44 %     CONV.OF CO2:  100.00 %

TEMPERATURE PROFILE:-
REACTOR    :     300.00     338.00     371.00     332.00 C
WALL       :     308.00     328.00     336.00     330.00 C
PEAK TEMP.:      371.00 C         EXIT TEMP:      332.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2031.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  573.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol %
H2             39.50                     1.763                    26.85
N2            103.00                     4.598                    70.02
CO2             4.60                     0.205                     3.13
TOTAL         147.10                     6.567                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2838E+05
CO2:H2 RATIO    = 1:  8.5870         W/FCO2 gm.hr./mol=    40.0765
RE(superficial)= 141.19               RE(particle)     =     6.64
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     300.00     305.00     302.00     299.00 C
WALL     :     305.00     308.00     306.00     304.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.3809
GAS COMPOSITION (mol %):-
      H2         N2          CH4          CO           CO2           H2O
    5.2673    85.4536     3.0888      0.0000       0.0127        6.1776

$$$$$$$$$$     CONV.OF H2:   83.93 %     CONV.OF CO2:   99.67 %

TEMPERATURE PROFILE:-
REACTOR    :     300.00     349.00     401.00     351.00 C
WALL       :     306.00     335.00     348.00     340.00 C
PEAK TEMP.:      401.00 C         EXIT TEMP:      351.00 C
```

```
>>>>>>>>>>>>>>>       RUN NUMBER: 2032.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  555.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2             39.50                       1.763                     27.13
N2            103.00                       4.598                     70.74
CO2             3.10                       0.138                      2.13
TOTAL         145.60                       6.500                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2721E+05
CO2:H2 RATIO    = 1: 12.7419           W/FCO2 gm.hr./mol=   59.4684
RE(superficial)= 141.14                 RE(particle)     =    6.63
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     290.00     293.00     289.00     281.00 C
WALL     :     292.00     293.00     291.00     288.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.4318
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   9.3284     84.6528     1.9581      0.0183      0.1080       3.9345

$$$$$$$$$$     CONV.OF H2:    71.27 %     CONV.OF CO2:    95.76 %

TEMPERATURE PROFILE:-
REACTOR    :     282.00     303.00     339.00     322.00 C
WALL       :     285.00     299.00     315.00     315.00 C
PEAK TEMP.:      339.00 C          EXIT TEMP:     322.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 2040.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2             39.50                       1.763                     27.46
N2            103.00                       4.598                     71.60
CO2             1.35                       0.060                      0.94
TOTAL         143.85                       6.422                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2630E+05
CO2:H2 RATIO    = 1: 29.2593           W/FCO2 gm.hr./mol=  136.5570
RE(superficial)= 139.52                 RE(particle)     =    6.56
INITIAL TEMPERATURE PROFILE:-
REACTOR  :     270.00     274.00     271.00     267.00 C
WALL     :     274.00     277.00     275.00     274.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.3464
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
  11.5842     86.0063     0.7651      0.0000      0.1142       1.5302

$$$$$$$$$$     CONV.OF H2:    64.88 %     CONV.OF CO2:    89.87 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     283.00     290.00     285.00 C
WALL       :     275.00     283.00     288.00     288.00 C
PEAK TEMP.:      290.00 C          EXIT TEMP:     285.00 C
```

```
>>>>>>>>>>>>>>>       RUN NUMBER: 2041.0      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   543.00 K                 PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.            FLOW RATE,mol/hr.                mol %
H2             39.50                       1.763                        27.13
N2            103.00                       4.598                        70.74
CO2             3.10                       0.138                         2.13
TOTAL         145.60                       6.500                       100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2662E+05
CO2:H2 RATIO    = 1: 12.7419          W/FCO2 gm.hr./mol=     59.4684
RE(superficial)= 143.26                RE(particle)     =     6.73
INITIAL TEMPERATURE PROFILE:-
REACTOR  :      270.00     274.00     271.00     267.00 C
WALL     :      274.00     277.00     275.00     274.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.3059
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
    8.6138    86.6619     1.3770      0.0547       0.4839       2.8087

$$$$$$$$$$      CONV.OF H2:    74.08 %     CONV.OF CO2:    81.45 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     286.00     302.00     299.00 C
WALL       :     275.00     285.00     295.00     297.00 C
PEAK TEMP.:      302.00 C          EXIT TEMP:     299.00 C
```

APPENDIX D

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF STEADY STATE METHANATION OF CO IN ADIABATIC REACTOR

```
C                   COMPUTER PROGRAM (CO.FOR)
C   FOR STEADY STATE METHANATION OF CO IN THE FIXED BED REACTOR
C  *  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C  *  THIS PROGRAM CALCULATES THE PRODUCT COMPOSITIONS AND TABULATES *
C  *  THE RESULTS BY TAKING THE INITIAL CONDITIONS OF OPERATION AND  *
C  *  THE GAS CHROMATOGRAPH PEAK AREAS FOR THE PRODUCTS               *
C  *  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C   ********************************************************
C   * NT           NUMBER OF RUNS                              *
C   * FRUN         RUN NUMBER                                  *
C   * NP           NUMBER OF PEAKS IN PORAPAK COLUMN           *
C   * NC           NUMBER OF PEAKS IN MOLECULAR SIEVE          *
C   * JP           NUMBER OF COMPOUNDS ANALYZED                *
C   * JPK          TOTAL NUMBER OF COMPOUNDS PRESENT           *
C   ********************************************************
C   * RSP          RESPONSE FACTOR IN PORAPAK COLUMN           *
C   * RSC          RESPONSE FACTOR IN MOLECULAR SIEVE COLUMN   *
C   * HYDCON       HYDROGEN CONVERSION                         *
C   * PCNT         MOL PERCENT OF PRODUCT GASES                *
C   * PR           FLOW RATE OF WATER FREE COMPOUND            *
C   ********************************************************

C   * *****************************************************
C   * CWT     WT. OF CATALYST,GM.                            *
C   * FD      DIAMETER OF REACTOR,CM.                        *
C   * FBD     BULK DENSITY OF CATALYST PELLET,GM/CC.         *
C   * FDP     DIAMETER OF CATALYST PELLETS,CM.               *
C   * FN2P    MOL PERCENT N2 IN FEED                         *
C   * TPK     PEAK TEMPERATURE OF REACTOR                    *
C   * TEX     EXIT TEMPERATURE OF REACTOR                    *
C   *******************************************************
C   * TNH     INITIAL TEMPERATURE PROFILE OF REACTOR         *
C   * TNHW    INITIAL TEMPERATURE PROFILE OF REACTOR WALL    *
C   * RT      FINAL TEMPERATURE PROFILE OF REACTOR           *
C   * WT      FINAL TEMPERATURE PROFILE OF REACTOR WALL      *
C   * *****************************************************

      DIMENSION RSP(6),RSC(6),RPN(6),PR(6)
      DIMENSION PRA(6),PRH(6),PRW(6),CPH(6),CHW(6),CHA(6)
      DIMENSION PRAM(6),CHAM(6),CHAP(6),PCNT(6)

      OPEN(UNIT=1,FILE = 'CODATA',STATUS = 'UNKNOWN')
      OPEN(UNIT=3,FILE = 'COOUT',STATUS = 'UNKNOWN')

      READ(1,*)NP,NC,JP,JPK,NT
      READ(1,*)(RSP(I),I=1,NP)
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)TC1,PC1,FM1,ZC1,FMUE1
      READ(1,*)TC2,PC2,FM2,ZC2,FMUE2
      READ(1,*)TC3,PC3,FM3,ZC3,FMUE3
      READ(1,*)FD,FBD,CWT,FDP

      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)

200   FORMAT(/,'EXPERIMENTAL RESULTS OF METHENATION OF CO IN A FIXED BED
     + REACTOR',/,25x,'Steady state')
201   FORMAT('---------------------------------------------------------
     +------')
```

```
204    FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'8.23 gm',///,'DILUTION
     + RATIO, CATALYST:INERT',5X,':',3X,'Undiluted',///,'CATALYST SIZE',
     +22X,':',3X,'25-40 mesh.',///,'INERT SIZE',25X,':',3X,'25-40 mesh.'
     +,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (ZFCL)')
205    FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'8.0 cm.',///,'LENGT
     +H OF INERT BED BEFORE CATALYST:',3X,'13.5 cm.',///,'LENGTH OF INER
     +T BED AFTER CATALYST :',3X,'22.0 cm.',///,'BULK DENSITY OF CATALYS
     +T',11X,':',3X,'0.7565 gm./c.c.')
210    FORMAT(//,'BULK DENSITY OF INERT',14X,':',3X,'1.821 gm./c.c.',///,
     +'OD OF REACTOR',22X,':',3X,'17.00 mm.',///,'ID OF REACTOR',22X,':'
     +,3X,'12.00 mm.',///,'THERMO COUPLE LOCATIONS FROM INLET :',3X,'0.0
     + cm. 3.0 cm. 6.0 cm. 8.0 cm.',/////////////////////)
140    FORMAT('>>>>>>>>>>>>>>>        RUN NUMBER:',1X,F6.1,5X,'<<<<<<<<<<<<
     +<<<')
220    FORMAT(/,'**********    INLET CONDITION:-')
207    FORMAT('TEMPRATURE:',F8.2,1X,'K',12X,'PRESSURE:',F8.2,1X,'mm.')
251    FORMAT(10X,'FLOW RATE,lit/hr.',6X,'FLOW RATE,mol/hr.',9X,'mol%')
224    FORMAT('H2',8X,F10.2,12X,F10.3,12X,F10.2)
212    FORMAT('N2',8X,F10.2,12X,F10.3,12X,F10.2)
214    FORMAT('CO',8X,F10.2,12X,F10.3,12X,F10.2)
213    FORMAT('TOTAL',5X,F10.2,12X,F10.3,12X,F10.2)
246    FORMAT(/,'SPACE VELOCITY,lit.gas/lit.cat.hr.                   =',E1
     +0.4,/,'CO:H2 RATIO     = 1:',F8.4,8X,'W/FCO gm.hr./mol=',F10.4)
234    FORMAT('RE(superficial)=',F7.2,12X,'RE(particle)     =',F8.2)
226    FORMAT('INITIAL TEMPERATURE PROFILE:-')
227    FORMAT('REACTOR :',4F10.2,1X,'C')
228    FORMAT('WALL    :',4F10.2,1X,'C')
215    FORMAT(/,'!!!!!!!!!!       EXIT CONDITION:-')
293    FORMAT('GAS FLOW RATE, mol/hr. :',F8.4)
222    FORMAT('GAS COMPOSITION (mol %):-')
223    FORMAT(6X,'H2',9X,'N2',9X,'CH4',9X,'CO',9X,'CO2',9X,'H2O')
100    FORMAT(F10.4,1X,F10.4,1X,F10.4,1X,F10.4,2X,F10.4, 2X,F10.4)
105    FORMAT(/,'$$$$$$$$$$      ','CONV.OF H2:',F8.2,1X,'%',5X,'CONV.OF C
     +O:',F8.2,1X,'%')
261    FORMAT(/,'TEMPERATURE PROFILE:-')
97     FORMAT('REACTOR    :',4F10.2,1X,'C')
260    FORMAT('WALL       :',4F10.2,1X,'C')
221    FORMAT('PEAK TEMP.:',F10.2,1X,'C',8X,'EXIT TEMP:',F10.2,1X,'C',/)

       DO 75 LPN=1,NT

       READ(1,*)FRUN
       READ(1,*)T,P,FY1,FY2,FY3
       READ(1,*)TNH1,TNH2,TNH3,TNH4
       READ(1,*)TNHW1,TNHW2,TNHW3,TNHW4
       READ(1,*)(PRH(I),PRW(I),PRA(I),I=1,NP)
       READ(1,*)(CPH(I),CHW(I),CHA(I),I=1,NC)
       READ(1,*)TPK,TEX
       READ(1,*)RT1,RT2,RT3,RT4
       READ(1,*)WT1,WT2,WT3,WT4

C **   CALCULATE INLET CONDITIONS ***********************************
C      HERE COMPONENT NO. 1=N2, 2=H2, 3=CO

       FA=0.785*FD**2.0
       FW1=FY1/22.4
       FW2=FY2/22.4
       FW3=FY3/22.4
       FY4=FY1+FY2+FY3
       FW4=FW1+FW2+FW3
       FN2P=FW1*100.0/FW4
       FH2P=FW2*100.0/FW4
```

```
      FCOP=FW3*100.0/FW4
      Y1=FW1/FW4
      Y2=FW2/FW4
      Y3=FW3/FW4
      AMW=Y1*FM1+Y2*FM2+Y3*FM3
      FTL=FN2P+FH2P+FCOP
      RCH=FH2P/FCOP
      RH2N=FH2P/FN2P
      RCON=FCOP/FN2P
      WRCO=CWT/FW3
      VO=FY4*T/273.0
      V=CWT/(FBD*1000.0)
      U=VO*1000.0/(3600.0*FA)
      RO=AMW*P/(82.05*760.0*T)
      ST=V/VO
      SV=1.0/ST

C   * CALCULATE VISCOSITIES OF PURE COMPONENTS BY LUCUS METHODS  *

      TR1=T/TC1
      FJITA1=0.176*(TC1/((FM1**3.0)*(PC1**4.0)))**(1.0/6.0)
      FJ1=1.0/FJITA1
      FMUER1=52.46*(FMUE1**2.0)*PC1/TC1**2.0
      FP=1.0
      FE1=(0.807*(TR1**0.618)-0.357*EXP(-0.449*TR1)+0.34*EXP(-4.058*TR1)
     ++0.018)*FP*FJ1
      TR2=T/TC2
      FJITA2=0.176*(TC2/((FM2**3.0)*(PC2**4.0)))**(1.0/6.0)
      FJ2=1.0/FJITA2
      FMUER2=52.46*(FMUE2**2.0)*PC2/TC2**2.0
      Q=0.76
      FOQ2=1.22*(Q**0.15)*(1.0+0.00385*((TR2-12.0)**2.0)**(1.0/FM2)+1.0)
      FE2=(0.807*(TR2**0.618)-0.357*EXP(-0.449*TR2)+0.34*EXP(-4.058*TR2)
     ++0.018)*FP*FOQ2*FJ2
      TR3=T/TC3
      FJITA3=0.176*(TC3/((FM3**3.0)*(PC3**4.0)))**(1.0/6.0)
      FJ3=1.0/FJITA3
      FMUER3=52.46*(FMUE3**2.0)*PC3/TC3**2.0
      FE3=(0.807*(TR3**0.618)-0.357*EXP(-0.449*TR3)+0.34*EXP(-4.058*TR3)
     ++0.018)*FP*FJ3

C  ** CALCULATE MIXTURE VISCOSITY BY WILKE'S METHODS ******************

      F12=(1.0+((FE1/FE2)**0.5)*(FM2/FM1)**0.25)**2.0/(8.0*(1.0+FM1/FM2)
     +)**0.5
      F13=(1.0+(FE1/FE3)**0.5*(FM3/FM1)**0.25)**2.0/(8.0*(1.0+FM1/FM3))*
     +*0.5
      F21=FE2*FM1*F12/(FE1*FM2)
      F23=(1.0+(FE2/FE3)**0.5*(FM3/FM2)**0.25)**2.0/(8.0*(1.0+FM2/FM3))*
     +*0.5
      F31=FE3*FM1*F13/(FE1*FM3)
      F32=FE3*FM2*F23/(FE2*FM3)
      F1=Y1*FE1/(Y1+Y2*F12+Y3*F13)
      F2=Y2*FE2/(Y1*F21+Y2+Y3*F23)
      F3=Y3*FE3/(Y1*F31+Y2*F32+Y3)
      FT=F1+F2+F3
      FTT=FT*1.0E-06
      FRE1=FD*U*RO/FTT
      FRE2=FDP*U*RO/FTT

C  ** CALCULATE EXIT COMPOSITION *************************************
```

```
C     HERE COMPONENT NO. 1=H2, 2=N2, 3=CH4, 4=CO, 5=CO2, 6=H2O
C  ** PRAM = MOL PERSENT IN PORAPAK COLUMN

      PRAS=0.0
      DO 10 I=1,NP
      PRAM(I)=PRH(I)*PRW(I)*PRA(I)*RSP(I)
      PRAS=PRAS+PRAM(I)
10    CONTINUE
      DO 11 I=1,NP
11    PRAM(I)=PRAM(I)/(PRAS)*100.0

C   * * CHAM = MOL PERCENT IN MOLECULAR SIEVE COLUMN * * * * * * * * * *

      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CPH(I)*CHW(I)*CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
13    CHAP(I)=CHAM(I)/(CHAS)*100.0

C     ****************************************************************
C     FIND MOL PERCENT IN EXIT GAS FOR MOLECULAR SIEVE COLUMN. PEAK 1 IN
C     PORAPAK COLUMN STANDS FOR ALL THE PEAKS IN MOLECULAR SIEVE COLUMN.
C     THERE ARE ONLY TWO PEAKS IN PORAPAK COLUMN. THE SECOND PEAK IS
C     COMPONENT NUMBER JP (CARBON DIOXIDE).
C     ****************************************************************

      TCNT=0.0
      DO 14 I=1,NC
      PCNT(I)=CHAP(I)*PRAM(1)/100.0
      TCNT=TCNT+PCNT(I)
14    CONTINUE
      PCNT(JP)=PRAM(NP)
      FR=FW1/PCNT(2)*100.0
      DO 21 I=1,JP
21    PR(I)=FR*PCNT(I)/100.0

C        FR=FLOW RAT OF WATER FREE PRODUCT  , PR=FLOW RATE OF WATER FREE
C        COMPOUNDS . THE AMOUNT OF WATER FORMED IS FOUND OUT BY MATERIAL
C        BALANCE CALCULATIONS
C     ****************************************************************

      R1=PR(3)
      R2=PR(5)
      TCOR=R1+R2
      TH2R=3.0*R1-R2
      TH2OP=R1-R2
      PR(6)=TH2OP
      PTOT=FR+PR(6)
      DO 23 I=1,JPK
      PCNT(I)=PR(I)/(PTOT)*100.0
23    CONTINUE

C     ****************************************************************
C                  PTOT=TOTAL FLOW RATE OF PRODUCT
C     THE CALCULATION FOR PRODUCT GAS COMPOSITION HAS BEEN COMPLETED
C              RPN => MOL COMPONENT/MOL N2 IN PRODUCT
C     ****************************************************************

      DO 26 I=1,JPK
      RPN(I)=PCNT(I)/PCNT(2)
```

```
26    CONTINUE
      COCON=(RCON-RPN(4))/(RCON)*100.0
      HYDCON=(RH2N-RPN(1))/(RH2N)*100.0

      WRITE(3,140)FRUN
      WRITE(3,220)
      WRITE(3,207)T,P
      WRITE(3,251)
      WRITE(3,224)FY2,FW2,FH2P
      WRITE(3,212)FY1,FW1,FN2P
      WRITE(3,214)FY3,FW3,FCOP
      WRITE(3,213)FY4,FW4,FTL
      WRITE(3,246)SV,RCH,WRCO
      WRITE(3,234)FRE1,FRE2
      WRITE(3,226)
      WRITE(3,227)TNH1,TNH2,TNH3,TNH4
      WRITE(3,228)TNHW1,TNHW2,TNHW3,TNHW4
      WRITE(3,215)
      WRITE(3,293)PTOT
      WRITE(3,222)
      WRITE(3,223)
      WRITE(3,100)(PCNT(I),I=1,JPK)
      WRITE(3,105)HYDCON,COCON
      WRITE(3,261)
      WRITE(3,97)RT1,RT2,RT3,RT4
      WRITE(3,260)WT1,WT2,WT3,WT4
      WRITE(3,221)TPK,TEX

75    CONTINUE
      STOP
      END
```

```
2 4 5 6 22
1 .8
36 1 1 1.13
126.2 33.9 28.0 0.29 0.0
33.2 13 2 0.303 0
132.9 35 28 0.295 0.1
1.2 0.7565 8.23 0.0564
3001
543 760 107 39.5 0.88
270 265 250 247
276 275 269 264
11037052 1 1
0 1 1
27432 1 1
5078366 1 1
18972 1 1
0 1 1
273 250
270 273 257 250
280 281 274 268
3002
543 760 107 39.5 1.64
270 265 250 247
276 275 269 264
11307198 1 1
0 1 1
23948 1 1
5210762 1 1
60630 1 1
0 1 1
289 255
270 289 274 255
280 287 280 272
3003
543 760 107 39.5 2.32
270 265 250 247
276 275 269 264
11630727 1 1
0 1 1
23249 1 1
5205372 1 1
100492 1 1
0 1 1
299 267
270 299 298 267
280 295 289 279
3004
523 760 107 39.5 2.32
250 248 231 226
260 258 252 248
11642555 1 1
1977 1 1
20953 1 1
5314303 1 1
93358 1 1
866 1 1
280 259
250 263 280 259
260 268 275 269
3005
523 760 107 39.5 1.64
250 248 231 226
```

```
260 258 252 248
11233394 1 1
0 1 1
25598 1 1
5175252 1 1
56834 1 1
0 1 1
258 246
250 254 258 246
260 265 264 257
3006
523 760 107 39.5 0.88
250 248 231 226
260 258 252 248
11032916 1 1
0 1 1
27454 1 1
5153900 1 1
23598 1 1
0 1 1
251 233
250 251 239 233
260 261 255 249
3007
508 760 107 39.5 1.64
235 229 215 214
244 241 235 231
11276293 1 1
912 1 1
25006 1 1
5241544 1 1
32582 1 1
18427 1 1
235 226
235 234 228 226
243 243 243 239
3008
513 760 107 39.5 0.88
240 235 223 218
244 241 236 232
13712404 1 1
0 1 1
30720 1 1
6496602 1 1
30771 1 1
0 1 1
245 220
240 245 232 220
246 247 242 235
3009
513 760 107 39.5 1.64
240 235 223 218
244 241 236 232
13983931 1 1
1720 1 1
29963 1 1
6543376 1 1
71088 1 1
3520 1 1
250 236
240 250 249 236
249 253 255 251
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3010
513 760 107 39.5 2.32
240 235 223 218
244 241 236 232
14138033 1 1
5990 1 1
28307 1 1
6555823 1 1
83092 1 1
30602 1 1
244 242
240 244 243 242
250 253 256 254
3011
513 760 85.5 39.5 1.64
240 235 223 218
244 241 236 232
12576622 1 1
1000 1 1
45846 1 1
6033888 1 1
82738 1 1
618 1 1
246 233
240 246 245 233
250 253 252 245
3012
513 760 66 39.5 1.64
240 235 223 218
244 241 236 232
11691146 1 1
2396 1 1
63138 1 1
5523876 1 1
103492 1 1
655 1 1
246 227
240 246 243 227
250 254 250 241
3018
513 760 107 68 1.64
240 235 223 218
244 241 236 232
10110554 1 1
689 1 1
64008 1 1
4550649 1 1
56503 1 1
769 1 1
246 233
240 246 245 233
247 250 251 246
3019
513 760 107 39.5 0.88
240 235 223 218
244 241 236 232
11610168 1 1
0 1 1
31932 1 1
5412661 1 1
26898 1 1
0 1 1
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240 222
240 240 229 222
247 248 243 237
3024.1
543 760 107 39.5 2.45
270 265 250 247
276 275 269 264
12393348 1 1
11798 1 1
24799 1 1
5655342 1 1
115636 1 1
140 1 1
292 273
270 288 292 273
283 293 294 286
3024.2
543 760 107 39.5 2.45
270 265 250 247
276 275 269 264
12393348 1 1
11798 1 1
24528 1 1
5652949 1 1
114315 1 1
46 1 1
292 273
270 288 292 273
282 293 294 286
3039
483 760 107 39.5 0.88
210 206 186 186
216 213 209 204
19852712 1 1
0 1 1
37319 1 1
9208511 1 1
19185 1 1
12029 1 1
210 191
210 209 191 191
217 215 212 208
3040
483 760 107 39.5 1.64
210 206 186 186
216 213 209 204
18583438 1 1
2882 1 1
51609 1 1
8663573 1 1
24934 1 1
75867 1 1
211 190
210 211 191 190
218 215 212 209
3041
483 760 107 39.5 2.32
210 206 186 186
216 213 209 204
18782438  1 1
6780 1 1
64676 1 1
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8696818 1 1
27936 1 1
141744 1 1
210 188
210 208 188 188
217 218 216 211
3042
497 760 107 39.5 2.32
224 224 202 202
235 233 225 223
18876782 1 1
6257 1 1
49102 1 1
8764522 1 1
35562 1 1
139820 1 1
228 206
224 228 209 206
235 233 230 226
3043
497 760 107 39.5 1.64
224 224 202 202
235 233 225 223
18817808 1 1
3580 1 1
65763 1 1
8733847 1 1
37924 1 1
73168 1 1
224 206
224 224 206 206
232 231 228 224
3044
497 760 107 39.5 0.88
224 224 202 202
235 233 225 223
18623688 1 1
0 1 1
50127 1 1
8823812 1 1
33543 1 1
660 1 1
228 207
224 228 210 207
236 235 232 227
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EXPERIMENTAL RESULTS OF METHENATION OF CO IN A FIXED BED REACTOR

Steady state

WEIGHT OF CATALYST : 8.23 gm

DILUTION RATIO, CATALYST:INERT : Undiluted

CATALYST SIZE : 25-40 mesh.

INERT SIZE : 25-40 mesh.

CATALYST TYPE : Ni on Alumina (ZFCL)

LENGTH OF CATALYST BED : 8.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 13.5 cm.

LENGTH OF INERT BED AFTER CATALYST : 22.0 cm.

BULK DENSITY OF CATALYST : 0.7565 gm./c.c.

BULK DENSITY OF INERT : 1.821 gm./c.c.

OD OF REACTOR : 17.00 mm.

ID OF REACTOR : 12.00 mm.

THERMO COUPLE LOCATIONS FROM INLET : 0.0 cm. 3.0 cm. 6.0 cm. 8.0 cm

```
>>>>>>>>>>>>>>>      RUN NUMBER: 3001.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.             mol%
H2               39.50                1.763                     26.80
N2              107.00                4.777                     72.60
CO                0.88                0.039                      0.60
TOTAL           147.38                6.579                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2695E+05
CO:H2 RATIO     = 1: 44.8864        W/FCO gm.hr./mol=  209.4909
RE(superficial)= 143.16             RE(particle)     =    6.73
INITIAL TEMPERATURE PROFILE:-
REACTOR :     270.00     265.00     250.00     247.00 C
WALL    :     276.00     275.00     269.00     264.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7414
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   16.1791    83.1992     0.3108      0.0000       0.0000       0.3108

$$$$$$$$$$     CONV.OF H2:    47.32 %     CONV.OF CO:   100.00 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     273.00     257.00     250.00 C
WALL       :     280.00     281.00     274.00     268.00 C
PEAK TEMP.:      273.00 C          EXIT TEMP:     250.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 3002.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.             mol%
H2               39.50                1.763                     26.66
N2              107.00                4.777                     72.23
CO                1.64                0.073                      1.11
TOTAL           148.14                6.613                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2708E+05
CO:H2 RATIO     = 1: 24.0854        W/FCO gm.hr./mol=  112.4098
RE(superficial)= 144.19             RE(particle)     =    6.78
INITIAL TEMPERATURE PROFILE:-
REACTOR :     270.00     265.00     250.00     247.00 C
WALL    :     276.00     275.00     269.00     264.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6783
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   13.9184    84.1239     0.9788      0.0000       0.0000       0.9788

$$$$$$$$$$     CONV.OF H2:    55.18 %     CONV.OF CO:   100.00 %

TEMPERATURE PROFILE:-
REACTOR    :     270.00     289.00     274.00     255.00 C
WALL       :     280.00     287.00     280.00     272.00 C
PEAK TEMP.:      289.00 C          EXIT TEMP:     255.00 C
```

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>>>>>>>>>>>>>>>       RUN NUMBER: 3003.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol%
H2              39.50                    1.763                  26.54
N2             107.00                    4.777                  71.90
CO               2.32                    0.104                   1.56
TOTAL          148.82                    6.644                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2721E+05
CO:H2 RATIO     = 1: 17.0259        W/FCO gm.hr./mol=    79.4621
RE(superficial)= 145.11             RE(particle)     =    6.82
INITIAL TEMPERATURE PROFILE:-
REACTOR :     270.00     265.00     250.00     247.00 C
WALL    :     276.00     275.00     269.00     264.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7293
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO           CO2          H2O
   13.4058    83.3751     1.6096      0.0000       0.0000       1.6096

$$$$$$$$$$     CONV.OF H2:   56.44 %     CONV.OF CO:  100.00 %

TEMPERATURE PROFILE:-
REACTOR     :     270.00     299.00     298.00     267.00 C
WALL        :     280.00     295.00     289.00     279.00 C
PEAK TEMP.:       299.00 C          EXIT TEMP:     267.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3004.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol%
H2              39.50                    1.763                  26.54
N2             107.00                    4.777                  71.90
CO               2.32                    0.104                   1.56
TOTAL          148.82                    6.644                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2621E+05
CO:H2 RATIO     = 1: 17.0259        W/FCO gm.hr./mol=    79.4621
RE(superficial)= 148.86             RE(particle)     =    7.00
INITIAL TEMPERATURE PROFILE:-
REACTOR :     250.00     248.00     231.00     226.00 C
WALL    :     260.00     258.00     252.00     248.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6235
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO           CO2          H2O
   12.0568    84.9431     1.4922      0.0156       0.0134       1.4788

$$$$$$$$$$     CONV.OF H2:   61.55 %     CONV.OF CO:   99.15 %

TEMPERATURE PROFILE:-
REACTOR     :     250.00     263.00     280.00     259.00 C
WALL        :     260.00     268.00     275.00     269.00 C
PEAK TEMP.:       280.00 C          EXIT TEMP:     259.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 3005.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol%
H2             39.50                     1.763                    26.66
N2            107.00                     4.777                    72.23
CO              1.64                     0.073                     1.11
TOTAL         148.14                     6.613                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2609E+05
CO:H2 RATIO     = 1: 24.0854           W/FCO gm.hr./mol=  112.4098
RE(superficial)= 147.92                RE(particle)     =    6.95
INITIAL TEMPERATURE PROFILE:-
REACTOR :      250.00     248.00     231.00     226.00 C
WALL    :      260.00     258.00     252.00     248.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7323
GAS COMPOSITION (mol %):-
      H2           N2           CH4          CO           CO2           H2O
   14.8384     83.3314      0.9151      0.0000       0.0000        0.9151

$$$$$$$$$$      CONV.OF H2:    51.76 %      CONV.OF CO:   100.00 %

TEMPERATURE PROFILE:-
REACTOR    :      250.00     254.00     258.00     246.00 C
WALL       :      260.00     265.00     264.00     257.00 C
PEAK TEMP.:       258.00 C         EXIT TEMP:      246.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 3006.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol%
H2             39.50                     1.763                    26.80
N2            107.00                     4.777                    72.60
CO              0.88                     0.039                     0.60
TOTAL         147.38                     6.579                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2595E+05
CO:H2 RATIO     = 1: 44.3864           W/FCO gm.hr./mol=  209.4909
RE(superficial)= 146.86                RE(particle)     =    6.90
INITIAL TEMPERATURE PROFILE:-
REACTOR :      250.00     248.00     231.00     226.00 C
WALL    :      260.00     258.00     252.00     248.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7366
GAS COMPOSITION (mol %):-
      H2           N2           CH4          CO           CO2           H2O
   15.9682     83.2692      0.3813      0.0000       0.0000        0.3813

$$$$$$$$$$      CONV.OF H2:    48.05 %      CONV.OF CO:   100.00 %

TEMPERATURE PROFILE:-
REACTOR    :      250.00     251.00     239.00     233.00 C
WALL       :      260.00     261.00     255.00     249.00 C
PEAK TEMP.:       251.00 C         EXIT TEMP:      233.00 C
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>>>>>>>>>>>>>>>         RUN NUMBER: 3007.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  508.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.             mol%
H2             39.50                      1.763                     26.66
N2            107.00                      4.777                     72.23
CO              1.64                      0.073                      1.11
TOTAL         148.14                      6.613                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2534E+05
CO:H2 RATIO     = 1: 24.0854            W/FCO gm.hr./mol=   112.4098
RE(superficial)= 150.89                 RE(particle)    =     7.09
INITIAL TEMPERATURE PROFILE:-
REACTOR :     235.00     229.00     215.00     214.00 C
WALL    :     244.00     241.00     235.00     231.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6755
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   14.4549     84.1644     0.5232      0.3344      0.0064       0.5167

$$$$$$$$$$      CONV.OF H2:    53.48 %      CONV.OF CO:    74.08 %

TEMPERATURE PROFILE:-
REACTOR     :     235.00     234.00     228.00     226.00 C
WALL        :     243.00     243.00     243.00     239.00 C
PEAK TEMP.:       235.00 C          EXIT TEMP:     226.00 C

>>>>>>>>>>>>>>>         RUN NUMBER: 3008.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.             mol%
H2             39.50                      1.763                     26.80
N2            107.00                      4.777                     72.60
CO              0.88                      0.039                      0.60
TOTAL         147.38                      6.579                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2546E+05
CO:H2 RATIO     = 1: 44.8864            W/FCO gm.hr./mol=   209.4909
RE(superficial)= 148.80                 RE(particle)    =     6.99
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6352
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   14.4299     84.7671     0.4015      0.0000      0.0000       0.4015

$$$$$$$$$$      CONV.OF H2:    53.89 %      CONV.OF CO:   100.00 %

TEMPERATURE PROFILE:-
REACTOR     :     240.00     245.00     232.00     220.00 C
WALL        :     246.00     247.00     242.00     235.00 C
PEAK TEMP.:       245.00 C          EXIT TEMP:     220.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 3009.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.              mol%
H2              39.50                    1.763                       26.66
N2             107.00                    4.777                       72.23
CO               1.64                    0.073                        1.11
TOTAL          148.14                    6.613                      100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2559E+05
CO:H2 RATIO     = 1: 24.0854          W/FCO gm.hr./mol=   112.4098
RE(superficial)= 149.88               RE(particle)      =     7.04
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6709
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  13.8857     84.2329     0.9151      0.0512       0.0097       0.9054

$$$$$$$$$$     CONV.OF H2:    55.34 %      CONV.OF CO:    96.03 %

TEMPERATURE PROFILE:-
REACTOR    :     240.00     250.00     249.00     236.00 C
WALL       :     249.00     253.00     255.00     251.00 C
PEAK TEMP.:      250.00 C          EXIT TEMP:     236.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3010.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.              mol%
H2              39.50                    1.763                       26.54
N2             107.00                    4.777                       71.90
CO               2.32                    0.104                        1.56
TOTAL          148.82                    6.644                      100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2571E+05
CO:H2 RATIO     = 1: 17.0259          W/FCO gm.hr./mol=    79.4621
RE(superficial)= 150.84               RE(particle)      =     7.09
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.6656
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  13.1057     84.3123     1.0686      0.4447       0.0335       1.0351

$$$$$$$$$$     CONV.OF H2:    57.89 %      CONV.OF CO:    75.67 %

TEMPERATURE PROFILE:-
REACTOR    :     240.00     244.00     243.00     242.00 C
WALL       :     250.00     253.00     256.00     254.00 C
PEAK TEMP.:      244.00 C          EXIT TEMP:     242.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 3011.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.              mol%
H2             39.50                     1.763                      31.19
N2             85.50                     3.817                      67.51
CO              1.64                     0.073                       1.30
TOTAL         126.64                     5.654                     100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2187E+05
CO:H2 RATIO     = 1: 24.0854           W/FCO gm.hr./mol=  112.4098
RE(superficial)= 120.16                RE(particle)     =    5.65
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  4.9661
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   21.0235    76.8597     1.0539     0.0089       0.0063       1.0476

$$$$$$$$$$     CONV.OF H2:    40.79 %     CONV.OF CO:    99.40 %

TEMPERATURE PROFILE:-
REACTOR    :     240.00     246.00     245.00     233.00 C
WALL       :     250.00     253.00     252.00     245.00 C
PEAK TEMP.:      246.00 C         EXIT TEMP:      233.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3012.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.              mol%
H2             39.50                     1.763                      36.87
N2             66.00                     2.946                      61.60
CO              1.64                     0.073                       1.53
TOTAL         107.14                     4.783                     100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.1851E+05
CO:H2 RATIO     = 1: 24.0854           W/FCO gm.hr./mol=  112.4098
RE(superficial)=  93.31                RE(particle)     =    4.39
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  4.2696
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   28.3959    69.0090     1.2929     0.0092       0.0162       1.2767

$$$$$$$$$$     CONV.OF H2:    31.25 %     CONV.OF CO:    99.46 %

TEMPERATURE PROFILE:-
REACTOR    :     240.00     246.00     243.00     227.00 C
WALL       :     250.00     254.00     250.00     241.00 C
PEAK TEMP.:      246.00 C         EXIT TEMP:      227.00 C
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>>>>>>>>>>>>>>>       RUN NUMBER: 3018.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol%
H2              68.00                    3.036                  38.50
N2             107.00                    4.777                  60.58
CO               1.64                    0.073                   0.93
TOTAL          176.64                    7.886                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                        =0.3051E+05
CO:H2 RATIO     = 1: 41.4634         W/FCO gm.hr./mol=  112.4098
RE(superficial)= 149.89              RE(particle)     =     7.04
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  7.3151
GAS COMPOSITION (mol %):-
     H2           N2          CH4          CO          CO2          H2O
   33.0657     65.3002      0.8108      0.0125      0.0054       0.8054

$$$$$$$$$$      CONV.OF H2:    20.32 %      CONV.OF CO:    98.75 %

TEMPERATURE PROFILE:-
REACTOR    :      240.00     246.00     245.00     233.00 C
WALL       :      247.00     250.00     251.00     246.00 C
PEAK TEMP.:       246.00 C          EXIT TEMP:     233.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3019.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol%
H2              39.50                    1.763                  26.80
N2             107.00                    4.777                  72.60
CO               0.88                    0.039                   0.60
TOTAL          147.38                    6.579                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                        =0.2546E+05
CO:H2 RATIO     = 1: 44.8864         W/FCO gm.hr./mol=  209.4909
RE(superficial)= 148.80              RE(particle)     =     6.99
INITIAL TEMPERATURE PROFILE:-
REACTOR :     240.00     235.00     223.00     218.00 C
WALL    :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.8388
GAS COMPOSITION (mol %):-
     H2           N2          CH4          CO          CO2          H2O
   17.3753     81.8116      0.4066      0.0000      0.0000       0.4066

$$$$$$$$$$      CONV.OF H2:    42.47 %      CONV.OF CO:   100.00 %

TEMPERATURE PROFILE:-
REACTOR    :      240.00     240.00     229.00     222.00 C
WALL       :      247.00     248.00     243.00     237.00 C
PEAK TEMP.:       240.00 C          EXIT TEMP:     222.00 C
```

```
>>>>>>>>>>>>>>>       RUN NUMBER: 3024.1     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol%
H2             39.50                     1.763                  26.52
N2            107.00                     4.777                  71.84
CO              2.45                     0.109                   1.64
TOTAL         148.95                     6.650                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2723E+05
CO:H2 RATIO     = 1: 16.1224           W/FCO gm.hr./mol=   75.2457
RE(superficial)= 145.29                RE(particle)     =    6.83
INITIAL TEMPERATURE PROFILE:-
REACTOR :     270.00     265.00     250.00     247.00 C
WALL    :     276.00     275.00     269.00     264.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7263
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   13.1685    83.4178     1.7057      0.0023       0.0749       1.6308

$$$$$$$$$$       CONV.OF H2:    57.24 %      CONV.OF CO:    99.88 %

TEMPERATURE PROFILE:-
REACTOR     :     270.00     288.00     292.00     273.00 C
WALL        :     283.00     293.00     294.00     286.00 C
PEAK TEMP.:       292.00 C          EXIT TEMP:     273.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3024.2     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  543.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol%
H2             39.50                     1.763                  26.52
N2            107.00                     4.777                  71.84
CO              2.45                     0.109                   1.64
TOTAL         148.95                     6.650                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2723E+05
CO:H2 RATIO     = 1: 16.1224           W/FCO gm.hr./mol=   75.2457
RE(superficial)= 145.29                RE(particle)     =    6.83
INITIAL TEMPERATURE PROFILE:-
REACTOR :     270.00     265.00     250.00     247.00 C
WALL    :     276.00     275.00     269.00     264.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7162
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   13.0533    83.5662     1.6899      0.0008       0.0749       1.6150

$$$$$$$$$$       CONV.OF H2:    57.69 %      CONV.OF CO:    99.96 %

TEMPERATURE PROFILE:-
REACTOR     :     270.00     288.00     292.00     273.00 C
WALL        :     282.00     293.00     294.00     286.00 C
PEAK TEMP.:       292.00 C          EXIT TEMP:     273.00 C
```

```
>>>>>>>>>>>>>>>       RUN NUMBER: 3039.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  483.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.             mol%
H2              39.50                     1.763                    26.80
N2             107.00                     4.777                    72.60
CO               0.88                     0.039                     0.60
TOTAL          147.38                     6.579                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2397E+05
CO:H2 RATIO     = 1: 44.8864          W/FCO gm.hr./mol=   209.4909
RE(superficial)= 155.10               RE(particle)      =     7.29
INITIAL TEMPERATURE PROFILE:-
REACTOR :     210.00     206.00     186.00     186.00 C
WALL    :     216.00     213.00     209.00     204.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.5007
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   12.6696    86.8403     0.1809      0.1282      0.0000       0.1809

$$$$$$$$$$      CONV.OF H2:    60.48 %      CONV.OF CO:    82.05 %

TEMPERATURE PROFILE:-
REACTOR    :      210.00     209.00     191.00     191.00 C
WALL       :      217.00     215.00     212.00     208.00 C
PEAK TEMP.:       210.00 C          EXIT TEMP:     191.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3040.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  483.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.             mol%
H2              39.50                     1.763                    26.66
N2             107.00                     4.777                    72.23
CO               1.64                     0.073                     1.11
TOTAL          148.14                     6.613                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2409E+05
CO:H2 RATIO     = 1: 24.0854          W/FCO gm.hr./mol=   112.4098
RE(superficial)= 156.22               RE(particle)      =     7.34
INITIAL TEMPERATURE PROFILE:-
REACTOR :     210.00     206.00     186.00     186.00 C
WALL    :     216.00     213.00     209.00     204.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.8759
GAS COMPOSITION (mol %):-
      H2          N2          CH4          CO          CO2          H2O
   17.4337    81.2939     0.2340      0.8044      0.0124       0.2216

$$$$$$$$$$      CONV.OF H2:    41.91 %      CONV.OF CO:    35.44 %

TEMPERATURE PROFILE:-
REACTOR    :      210.00     211.00     191.00     190.00 C
WALL       :      218.00     215.00     212.00     209.00 C
PEAK TEMP.:       211.00 C          EXIT TEMP:     190.00 C
```

```
>>>>>>>>>>>>>>>       RUN NUMBER: 3041.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  483.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol%
H2             39.50                      1.763                   26.54
N2            107.00                      4.777                   71.90
CO              2.32                      0.104                    1.56
TOTAL         148.82                      6.644                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                            =0.2420E+05
CO:H2 RATIO     = 1: 17.0259         W/FCO gm.hr./mol=    79.4621
RE(superficial)= 157.22              RE(particle)     =     7.39
INITIAL TEMPERATURE PROFILE:-
REACTOR :     210.00     206.00     186.00     186.00 C
WALL    :     216.00     213.00     209.00     204.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.1743
GAS COMPOSITION (mol %):-
     H2           N2          CH4           CO          CO2          H2O
   20.7125    77.3656      0.2485      1.4249       0.0288       0.2197

$$$$$$$$$$      CONV.OF H2:    27.48 %      CONV.OF CO:    15.06 %

TEMPERATURE PROFILE:-
REACTOR     :      210.00     208.00     188.00     188.00 C
WALL        :      217.00     218.00     216.00     211.00 C
PEAK TEMP.:        210.00 C         EXIT TEMP:      188.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3042.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  497.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol%
H2             39.50                      1.763                   26.54
N2            107.00                      4.777                   71.90
CO              2.32                      0.104                    1.56
TOTAL         148.82                      6.644                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                            =0.2490E+05
CO:H2 RATIO     = 1: 17.0259         W/FCO gm.hr./mol=    79.4621
RE(superficial)= 154.16              RE(particle)     =     7.25
INITIAL TEMPERATURE PROFILE:-
REACTOR :     224.00     224.00     202.00     202.00 C
WALL    :     235.00     233.00     225.00     223.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.8651
GAS COMPOSITION (mol %):-
     H2           N2          CH4           CO          CO2          H2O
   16.4262    81.4447      0.3305      1.4682       0.0264       0.3040

$$$$$$$$$$      CONV.OF H2:    45.37 %      CONV.OF CO:    16.86 %

TEMPERATURE PROFILE:-
REACTOR     :      224.00     228.00     209.00     206.00 C
WALL        :      235.00     233.00     230.00     226.00 C
PEAK TEMP.:        228.00 C         EXIT TEMP:      206.00 C
```

```
>>>>>>>>>>>>>>>        RUN NUMBER: 3043.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  497.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.               mol%
H2            39.50                       1.763                     26.66
N2           107.00                       4.777                     72.23
CO             1.64                       0.073                      1.11
TOTAL        148.14                       6.613                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2479E+05
CO:H2 RATIO     = 1: 24.0854          W/FCO gm.hr./mol=  112.4098
RE(superficial)= 153.17               RE(particle)     =     7.20
INITIAL TEMPERATURE PROFILE:-
REACTOR :      224.00      224.00      202.00      202.00 C
WALL    :      235.00      233.00      225.00      223.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.1583
GAS COMPOSITION (mol %):-
     H2           N2          CH4          CO           CO2           H2O
   21.0258     77.5663     0.3368      0.7343       0.0152       0.3216

$$$$$$$$$$      CONV.OF H2:    26.57 %      CONV.OF CO:    38.24 %

TEMPERATURE PROFILE:-
REACTOR    :      224.00     224.00     206.00     206.00 C
WALL       :      232.00     231.00     228.00     224.00 C
PEAK TEMP.:       224.00 C           EXIT TEMP:    206.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 3044.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  497.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.               mol%
H2            39.50                       1.763                     26.80
N2           107.00                       4.777                     72.60
CO             0.88                       0.039                      0.60
TOTAL        147.38                       6.579                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2466E+05
CO:H2 RATIO     = 1: 44.8864          W/FCO gm.hr./mol=  209.4909
RE(superficial)= 152.07               RE(particle)     =     7.15
INITIAL TEMPERATURE PROFILE:-
REACTOR :      224.00      224.00      202.00      202.00 C
WALL    :      235.00      233.00      225.00      223.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7904
GAS COMPOSITION (mol %):-
     H2           N2          CH4          CO           CO2           H2O
   16.8711     82.4947     0.3136      0.0070       0.0000       0.3136

$$$$$$$$$$      CONV.OF H2:    44.60 %      CONV.OF CO:    98.97 %

TEMPERATURE PROFILE:-
REACTOR    :      224.00     228.00     210.00     207.00 C
WALL       :      236.00     235.00     232.00     227.00 C
PEAK TEMP.:       228.00 C           EXIT TEMP:    207.00 C
```

APPENDIX E

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF STEADY STATE METHANATION OF MIXTURE OF CO AND CO_2 IN ADIABATIC REACTOR.

```
C                 COMPUTER PROGRAM (MX.FOR) FOR
C      STEADY STATE METHANATION OF  THE MIXURE OF CO & CO2 IN THE
C                          FIXED BED REACTOR
C  *  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C  *  THIS PROGRAM CALCULATES THE PRODUCT COMPOSITIONS AND TABULATES *
C  *  THE RESULTS BY TAKING THE INITIAL CONDITIONS OF OPERATION AND  *
C  *  THE GAS CHROMATOGRAPH PEAK AREAS FOR THE PRODUCTS               *
C   * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C   *********************************************************
C   * N          NUMBER OF COMPONENTS IN THE FEED           *
C   * NT         NUMBER OF RUNS                             *
C   * FRUN       RUN NUMBER                                 *
C   * NP         NUMBER OF PEAKS IN PORAPAK COLUMN          *
C   * NC         NUMBER OF PEAKS IN MOLECULAR SIEVE         *
C   * JP         NUMBER OF COMPOUNDS ANALYZED               *
C   * JPK        TOTAL NUMBER OF COMPOUNDS PRESENT          *
C   *********************************************************
C   * RSP        RESPONSE FACTOR IN PORAPAK COLUMN          *
C   * RSC        RESPONSE FACTOR IN MOLECULAR SIEVE COLUMN  *
C   * HYDCON     HYDROGEN CONVERSION                        *
C   * COCON      CARBON MONOXIDE CONVERSION                 *
C   * CO2CON     CARBON DIOXIDE COVERSION                   *
C   * PCNT       MOL PERCENT OF PRODUCT GASES               *
C   * ******************************************************
C   * CWT     WT. OF CATALYST                              *
C   * FD      DIAMETER OF REACTOR,CM.                      *
C   * FBD     BULK DENSITY OF CATALYST PELLET,GM/CC.       *
C   * FDP     DIAMETER OF CATALYST PELLETS,CM.             *
C   * FN2P    MOL PERCENT N2 IN FEED                       *
C   * TPK     PEAK TEMPERATURE OF REACTOR                  *
C   * TEX     EXIT TEMPERATURE OF REACTOR                  *
C   ********************************************************
C   * TNH     INITIAL TEMPERATURE PROFILE OF REACTOR       *
C   * TNHW    INITIAL TEMPERATURE PROFILE OF REACTOR WALL  *
C   * RT      FINAL TEMPERATURE PROFILE OF REACTOR         *
C   * WT      FINAL TEMPERATURE PROFILE OF REACTOR WALL    *
C   * ******************************************************

      DIMENSION RSP(6),RSC(6),RPN(6),PR(6)
      DIMENSION PRA(6),PRH(6),PRW(6),CPH(6),CHW(6),CHA(6)
      DIMENSION PRAM(6),CHAM(6),CHAP(6),PCNT(6)
      DIMENSION TR(6),TC(6),PC(6),FM(6),ZC(6),FMU(6),FMUR(6),FPD1(6)
      DIMENSION FPD2(6),FPD(6),ET(6),FQ1(6),FQ(6),EM(6),F(6,6),Y(6)
      DIMENSION X(6),XY(6,6),E(6),FY(6),FW(6),FMP(6),FMW(6)

      OPEN(UNIT=1,FILE = 'XC12',STATUS = 'UNKNOWN')
      OPEN(UNIT=3,FILE = 'XCOUT',STATUS = 'UNKNOWN')

      READ(1,*)NP,NC,JP,JPK,N,NT
      READ(1,*)(RSP(I),I=1,NP)
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)(TC(I),PC(I),FM(I),ZC(I),FMU(I),I=1,N)
      READ(1,*)FD,FBD,CWT,FDP

      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)

200   FORMAT('EXPERIMENTAL RESULT OF METHENATION OF CO & CO2 IN A FIXED
     ?BED REACTOR',/,26x,'Steady stae')
```

```
201   FORMAT('----------------------------------------------------------
     ?-----------')
204   FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'8.23 gm',///,'DILUTION
     ? RATIO, CATALYST:INERT',5X,':',3X,'Undiluted',///,'CATALYST SIZE',
     ?22X,':',3X,'25-40 mesh.',///,'INERT SIZE',25X,':',3X,'25-40 mesh.'
     ?,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (ZFCL)')
205   FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'8.0 cm.',///,'LENGT
     ?H OF INERT BED BEFORE CATALYST:',3X,'13.5 cm.',///,'LENGTH OF INER
     ?T BED AFTER CATALYST :',3X,'22.0 cm.',///,'BULK DENSITY OF CATALYS
     ?T',11X,':',3X,'0.7565 gm./c.c.')
210   FORMAT(//,'BULK DENSITY OF INERT',14X,':',3X,'1.821 gm./c.c.',///,
     ?'OD OF REACTOR',22X,':',3X,'17.00 mm.',///,'ID OF REACTOR',22X,':'
     ?,3X,'12.00 mm.',///,'THERMO COUPLE LOCATIONS FROM INLET :',3X,'0.0
     ? cm. 3.0 cm. 6.0 cm. 8.0 cm.',///////////////////)
140   FORMAT('>>>>>>>>>>>>>>>      RUN NUMBER:',1X,F6.1,5X,'<<<<<<<<<<<<
     ?<<<')
220   FORMAT(/,'**********   INLET CONDITION:-')
207   FORMAT('TEMPRATURE:',F8.2,1X,'K',12X,'PRESSURE:',F8.2,1X,'mm.')
251   FORMAT(10X,'FLOW RATE,lit/hr.',6X,'FLOW RATE,mol/hr.',8X,'mol%')
224   FORMAT('H2',8X,F10.2,12X,F10.3,12X,F10.2)
212   FORMAT('N2',8X,F10.2,12X,F10.3,12X,F10.2)
217   FORMAT('CO',8X,F10.2,12X,F10.3,12X,F10.2)
214   FORMAT('CO2',7X,F10.2,12X,F10.3,12X,F10.2)
213   FORMAT('TOTAL',5X,F10.2,12X,F10.3,12X,F10.2)
246   FORMAT(/,'SPACE VELOCITY,lit.gas/lit.cat.hr.                 =',E1
     ?0.4,/,'CO:H2 RATIO    = 1:',F8.4,7X,'W/FCO gm.hr./mol.=',F10.4,/,'
     ?CO2:H2 RATIO   = 1:',F8.4,7X,'W/FCO2 gm.hr./mol=',F10.4)
234   FORMAT('RE(superficial)=',F7.2,11X,'RE(particle)     =',F8.2)
226   FORMAT('INITIAL TEMPERATURE PROFILE:-')
227   FORMAT('REACTOR:',4F10.2,1X,'C')
228   FORMAT('WALL   :',4F10.2,1X,'C')
215   FORMAT(/,'!!!!!!!!!!     EXIT CONDITION:-')
293   FORMAT('GAS FLOW RATE, mol/hr. :',F8.4)
222   FORMAT('GAS COMPOSITION (mol %):-')
223   FORMAT(6X,'H2',9X,'N2',9X,'CH4',9X,'CO',9X,'CO2',9X,'H2O')
100   FORMAT(F10.4,1X,F10.4,1X,F10.4,1X,F10.4,2X,F10.4, 2X,F10.4)
105   FORMAT(/,'$$$$ ','CONV.OF H2:',F6.2,1X,'% ,',2X,'CONV.OF CO2:',F6.
     ?2,1X,'% ,',2X,'CONV. OF CO:',F6.2,1X,'%' )
261   FORMAT('TEMPERATURE PROFILE:-')
97    FORMAT('REACTOR   :',4F10.2,1X,'C')
260   FORMAT('WALL      :',4F10.2,1X,'C')
221   FORMAT('PEAK TEMP.:',F10.2,1X,'C',8X,'EXIT TEMP:',F10.2,1X,'C',/)

      DO 75 LPN=1,NT

      READ(1,*)FRUN
      READ(1,*)T,P,(FY(I),I=1,N)
      READ(1,*)TNH1,TNH2,TNH3,TNH4
      READ(1,*)TNHW1,TNHW2,TNHW3,TNHW4
      READ(1,*)(PRH(I),PRW(I),PRA(I),I=1,NP)
      READ(1,*)(CPH(I),CHW(I),CHA(I),I=1,NC)
      READ(1,*)TPK,TEX
      READ(1,*)RT1,RT2,RT3,RT4
      READ(1,*)WT1,WT2,WT3,WT4

C **  CALCULATE INLET COMPOSITIONS ************************************
C     HERE COMPONENT NO. 1=H2,2=N2,3=CO,4=CO2

      FA=0.785*FD**2.0
      X1=100.0
      X2=22.4
      FWT=0.0
```

```
      FYT=0.0
      DO 8 I=1,N
      FW(I)=FY(I)/X2
      FWT=FWT+FW(I)
      FYT=FYT+FY(I)
8     CONTINUE
      FTP=0.0
      AMW=0.0
      DO 9 I=1,N
      Y(I)=FW(I)/FWT
      FMP(I)=Y(I)*X1
      FTP=FTP+FMP(I)
      FMW(I)=Y(I)*FM(I)
      AMW=AMW+FMW(I)
9     CONTINUE
      RHCO=FMP(1)/FMP(3)
      RHCO2=FMP(1)/FMP(4)
      RH2N=FMP(1)/FMP(2)
      RCON=FMP(3)/FMP(2)
      RCO2N=FMP(4)/FMP(2)
      WFCO=CWT/FW(3)
      WFCO2=CWT/FW(4)
      VO=FYT*T/273.0
      V=CWT/(FBD*1000.0)
      U=VO*1000.0/(3600.0*FA)
      RO=AMW*P/(82.05*760.0*T)
      ST=V/VO
      SV=1.0/ST

C   * CALCULATE VISCOSITIES OF PURE COMPONENTS BY LUCUS METHODS   *

      DO 25 I=1,N
      TR(I)=T/TC(I)
      FMUR(I)=52.46*(FMU(I)**2.0)*PC(I)/(TC(I)**2.0)
      FPD1(I)=0.96+0.1*(TR(I)-0.7)
      FPD2(I)=1.0+30.55*((0.292-ZC(I))**2)
      IF(FMUR(I)-0.075)2001,22,22
22    IF(FPD1(I)-0.0)32,33,33
33    FPD(I)=FPD2(I)*FPD1(I)
      GO TO 25
32    FPD(I)=FPD2(I)*(-FPD1(I))
      GO TO 25
2001  IF(FMUR(I)-0.022)2003.24,24
24    FPD(I)=FPD2(I)
      GO TO 25
2003  FPD(I)=1.0
25    CONTINUE

C     CALCULATE MIXURE VISCOSITY BY WILKE'S METHOD  *

      Q=0.76
      DO 301 I=1,N
      FQ1(I)=1.0+0.00385*(((TR(I)-12.0)**2)**(1.0/FM(I)))
      IF(I-1)27,28,27
28    IF(TR(I)-12.0)29,30,30
30    FQ1(I)=1.0+0.00385*(((TR(I)-12.0)**2)**(1.0/FM(I)))
      FQ(I)=1.22*(Q**0.15)*(FQ1(I)+1.0)
      GO TO 31
29    FQ(I)=1.22*(Q**0.15)*(FQ1(I)-1.0)
      GO TO 31
27    FQ(I)=1.0
31    ET(I)=0.176*((TC(I)/((FM(I)**3.0)*(PC(I)**4.0)))**(1.0/6.0))
```

```
      EM(I)=((0.807*TR(I)**0.618-0.357*EXP(-0.449*TR(I))+0.340*EXP(
     ?-4.058*TR(I))+0.018)*FPD(I)*FQ(I))/ET(I)
301   CONTINUE
      DO 110 I=1,N
      DO 120 J=1,N
      F(I,J)=((1.0+((EM(I)/EM(J))**0.5)*((FM(J)/FM(I))**0.25))**2.0)/((
     ?8.0*(1.0+FM(I)/FM(J)))**0.5)
120   CONTINUE
110   CONTINUE

      EMT=0.0
      DO 180 I=1,N
      X(I)=Y(I)*EM(I)
      YX=0.0
      DO 208 J=1,N
      XY(I,J)=Y(J)*F(I,J)
      YX=YX+XY(I,J)
208   CONTINUE
      E(I)=X(I)/YX
      EMT=EMT+E(I)
180   CONTINUE
      EMTT=EMT*1.0E-06
      FRE1=FD*U*RO/EMTT
      FRE2=FDP*U*RO/EMTT

C  ** CALCULATE EXIT COMPOSITIONS **************************************
C     HERE COMPONENT NO. 1=H2, 2=N2, 3=CH4, 4=CO, 5=CO2, 6=H2O
C  ** PRAM = MOL PERCENT IN PORAPAK COLUMN

      PRAS=0.0
      DO 10 I=1,NP
      PRAM(I)=PRH(I)*PRW(I)*PRA(I)*RSP(I)
      PRAS=PRAS+PRAM(I)
10    CONTINUE
      DO 11 I=1,NP
11    PRAM(I)=PRAM(I)/(PRAS)*100.0

C   * * CHAM = MOL PERCENT IN MOLECULAR SIEVE COLUMN * * * * * * * * * *

      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CPH(I)*CHW(I)*CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
13    CHAP(I)=CHAM(I)/(CHAS)*100.0
C     ******************************************************************
C     FIND MOL PERCENT IN EXIT GAS FOR MOLECULAR SIEVE COLUMN. PEAK 1 IN
C     PORAPAK COLUMN STANDS FOR ALL THE PEAKS IN MOLECULAR SIEVE COLUMN.
C     ******************************************************************
C     THERE ARE ONLY TWO PEAKS IN PORAPAK COLUMN. THE SECOND PEAK IS
C     COMPONENT NUMBER JP (CARBON DIOXIDE).
C     ******************************************************************

      TCNT=0.0
      DO 14 I=1,NC
      PCNT(I)=CHAP(I)*PRAM(1)/100.0
      TCNT=TCNT+PCNT(I)
14    CONTINUE
      PCNT(JP)=PRAM(NP)
      FR=FW(2)/PCNT(2)*100.0
      DO 21 I=1,JP
```

```
21    PR(I)=FR*PCNT(I)/100.0

C  ******* FR=FLOW RAT OF WATER FREE PRODUCT ***************************
C  ******* PR=FLOW RATE OF WATER FREE COMPOUNDS **********************
C     THE AMOUNT OF WATER FORMED IS FOUND OUT BY MATERIAL BALANCE
C     CALCULATIONS
C     *******************************************************************

      R1=FW(3)-PR(4)
      R2=FW(4)-PR(5)
      TCOR=R1
      TCO2R=R2
      TH2R=3.0*R1+4.0*R2
      TH2OP=R1+2.0*R2
      PR(6)=TH2OP
      PTOT=FR+PR(6)
C   *******  PTOT=TOTAL FLOW RATE OF PRODUCT ***************************

      DO 23 I=1,JPK
      PCNT(I)=PR(I)/(PTOT)*100.0
23    CONTINUE

C     *******************************************************************
C     THE CALCULATION FOR PRODUCT GAS COMPOSITION HAS BEEN COMPLETED
C     ******  RPN => MOL COMPONENT/MOL N2 IN PRODUCT *******************
      DO 26 I=1,JPK
      RPN(I)=PCNT(I)/PCNT(2)
26    CONTINUE
      COCON=(RCON-RPN(4))/RCON*X1
      CO2CON=(RCO2N-RPN(5))/(RCO2N)*X1
      HYDCON=(RH2N-RPN(1))/RH2N*X1

      WRITE(3,140)FRUN
      WRITE(3,220)
      WRITE(3,207)T,P
      WRITE(3,251)
      WRITE(3,224)FY(1),FW(1),FMP(1)
      WRITE(3,212)FY(2),FW(2),FMP(2)
      WRITE(3,217)FY(3),FW(3),FMP(3)
      WRITE(3,214)FY(4),FW(4),FMP(4)
      WRITE(3,213)FYT,FWT,FTP
      WRITE(3,246)SV,RHCO,WFCO,RHCO2,WFCO2
      WRITE(3,234)FRE1,FRE2
      WRITE(3,226)
      WRITE(3,227)TNH1,TNH2,TNH3,TNH4
      WRITE(3,228)TNHW1,TNHW2,TNHW3,TNHW4
      WRITE(3,215)
      WRITE(3,293)PTOT
      WRITE(3,222)
      WRITE(3,223)
      WRITE(3,100)(PCNT(I),I=1,JPK)
      WRITE(3,105)HYDCON,CO2CON,COCON
      WRITE(3,261)
      WRITE(3,97)RT1,RT2,RT3,RT4
      WRITE(3,260)WT1,WT2,WT3,WT4
      WRITE(3,221)TPK,TEX
75    CONTINUE
      STOP
      END
```

```
2    4    5    6    4   18
 1.0      0.8
36.0      1.0       1.0       1.13
 33.2     13.0       2.0      0.303     0.0
126.2     33.9      28.0      0.290     0.0
132.9     35.0      28.0      0.295     0.1
304.1     73.8      44.0      0.274     0.0
1.2       0.7565    8.23      0.0564
3027.0
533.00    760.00    39.50     107.00    0.88      1.05
260.00    256.00    236.00    233.00
268.00    265.00    260.00    255.00
15054616.00    1.00           1.00
28285.00       1.00           1.00
33518.00       1.00           1.00
6890824.00     1.00           1.00
82573.00       1.00           1.00
284.00         1.00           1.00
273.00    248.00
260.00    273.00    261.00    248.00
268.00    273.00    272.00    265.00
3028.0
533.00    760.00    39.50     107.00    0.88      1.80
260.00    256.00    236.00    233.00
268.00    265.00    260.00    255.00
15116250.0     1.00           1.00
53057.00       1.00           1.00
34723.00       1.00           1.00
6914281.00     1.00           1.00
101732.00      1.00           1.00
659.00         1.00           1.00
278.00    254.00
260.00    278.00    272.00    254.00
272.00    278.00    277.00    271.00
3029.0
533.00    760.00    39.50     107.00    0.88      2.45
260.00    256.00    236.00    233.00
268.00    265.00    260.00    255.00
15525030.00    1.00           1.00
98830.00       1.00           1.00
27578.00       1.00           1.00
7159188.00     1.00           1.00
129236.00      1.00           1.00
1305.00        1.00           1.00
276.00    249.00
260.00    274.00    276.00    259.00
268.00    276.00    276.00    271.00
3030.0
523.00    760.00    39.50     107.00    0.88      2.45
250.00    246.00    230.00    225.00
256.00    254.00    249.00    244.00
14742257.00    1.00           1.00
187752.00      1.00           1.00
36603.00       1.00           1.00
6866477.00     1.00           1.00
79995.00       1.00           1.00
1191.00        1.00           1.00
258.00    244.00
250.00    258.00    255.00    244.00
257.00    262.00    261.00    256.00
3031.0
523.00    760.00    39.50     107.00    0.88      1.80
```

```
250.00      246.00      230.00      225.00
256.00      254.00      249.00      244.00
15032985.00      1.00               1.00
115140.00        1.00               1.00
33885.00         1.00               1.00
6993698.00       1.00               1.00
86047.00         1.00               1.00
900.00           1.00               1.00
264.00      244.00
250.00      264.00      261.00      244.00
262.00      267.00      267.00      262.00
3032.0
523.00      760.00       39.50      107.00      0.88       1.05
250.00      246.00      230.00      225.00
256.00      254.00      249.00      244.00
14722190.00      1.00               1.00
65937.00         1.00               1.00
52046.00         1.00               1.00
6880116.00       1.00               1.00
67856.00         1.00               1.00
459.00           1.00               1.00
260.00      239.00
250.00      260.00      250.00      239.00
257.00      262.00      261.00      256.00
3033.0
523.00      760.00       39.50       85.50      0.88       1.80
250.00      246.00      230.00      225.00
256.00      254.00      249.00      244.00
13876356.00      1.00               1.00
108295.00        1.00               1.00
46254.00         1.00               1.00
6572773.00       1.00               1.00
115627.00        1.00               1.00
746.00           1.00               1.00
266.00      242.00
250.00      266.00      260.00      242.00
262.00      269.00      267.00      260.00
3034.0
523.00      760.00       39.50       66.00      0.88       1.80
250.00      246.00      230.00      225.00
256.00      254.00      249.00      244.00
12445143.00      1.00               1.00
137358.00        1.00               1.00
66791.00         1.00               1.00
5905803.00       1.00               1.00
155584.00        1.00               1.00
595.00           1.00               1.00
264.00      239.00
250.00      264.00      258.00      239.00
259.00      266.00      263.00      253.00
3035.0
523.00      760.00       68.00      107.00      0.88       1.80
250.00      246.00      230.00      225.00
256.00      254.00      249.00      244.00
12247821.00      1.00               1.00
108640.00        1.00               1.00
82024.0          1.00               1.00
5787240.00       1.00               1.00
72962.00         1.00               1.00
1361.00          1.00               1.00
257.00      244.00
250.00      257.00      247.00      244.00
```

```
260.00    264.00    265.00    261.00
3036.0
513.00    760.00     39.50    107.00    0.88      1.80
240.00    235.00    223.00    218.00
244.00    241.00    236.00    232.00
14552572.00    1.00           1.00
196829.00      1.00           1.00
39129.00       1.00           1.00
6869486.00     1.00           1.00
56803.00       1.00           1.00
2534.00        1.00           1.00
244.00    232.00
240.00    244.00    234.00    232.00
251.00    252.00    252.00    248.00
3037.0
513.00    760.00     39.50    107.00    0.88      2.45
240.00    235.00    223.00    218.00
244.00    241.00    236.00    232.00
14577424.00    1.00           1.00
248443.00      1.00           1.00
39327.00       1.00           1.00
6870929.00     1.00           1.00
58302.00       1.00           1.00
3434.00        1.00           1.00
243.00    233.00
240.00    243.00    234.00    233.00
249.00    252.00    252.00    248.00
3038.0
513.00    760.00     39.50    107.00    0.88      1.05
240.00    235.00    223.00    218.00
244.00    241.00    236.00    232.00
14607662.00    1.00           1.00
105428.00      1.00           1.00
40603.00       1.00           1.00
6899750.00     1.00           1.00
51889.00       1.00           1.00
1059.00        1.00           1.00
242.00    231.00
240.00    242.00    232.00    231.00
250.00    252.00    251.00    247.00
3045.00
543.00    760.00     39.50    107.00    0.88      1.80
270.00    263.00    243.00    245.00
276.00    275.00    271.00    266.00
14230248.00    1.00           1.00
22968.00       1.00           1.00
25771.00       1.00           1.00
6415962.00     1.00           1.00
106227.00      1.00           1.00
383.00         1.00           1.00
285.00    271.00
270.00    285.00    282.00    271.00
284.00    292.00    292.00    287.00
3046.1
553.00    760.00    39.50     107.00    0.88      1.80
280.00    273.00    258.00    255.00
285.00    284.00    279.00    275.00
14322710.00    1.00           1.00
8091.00        1.00           1.00
25685.00       1.00           1.00
6471210.00     1.00           1.00
115133.00      1.00           1.00
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178.00         1.00           1.00
297.00    280.00
280.00    297.00    295.00    280.00
292.00    302.00    302.00    294.00
3046.2
553.00    760.00    39.50     107.00     0.88      1.80
280.00    273.00    258.00    255.00
285.00    284.00    279.00    275.00
14322710.00    1.00           1.00
8091.00        1.00           1.00
24996.00       1.00           1.00
6546581.00     1.00           1.00
114847.00      1.00           1.00
123.00         1.00           1.00
297.00    280.00
280.00    297.00    295.00    280.00
292.00    302.00    302.00    294.00
3047.0
497.00    760.00     39.50    107.00     0.88      1.80
224.00    221.00    200.00    201.00
235.00    232.00    226.00    222.00
13712510.00    1.00           1.00
160078.00      1.00           1.00
32475.00       1.00           1.00
6385322.00     1.00           1.00
20429.00       1.00           1.00
19977.00       1.00           1.00
224.00    206.00
224.00    223.00    207.00    206.00
233.00    232.00    228.00    225.00
3048.0
497.00    760.00     39.50    107.00     0.88      1.05
224.00    221.00    200.00    201.00
235.00    232.00    226.00    222.00
13556622.00    1.00           1.00
102118.00      1.00           1.00
34494.00       1.00           1.00
6319322.00     1.00           1.00
21037.00       1.00           1.00
8668.00        1.00           1.00
225.00    206.00
224.00    225.00    207.00    206.00
232.00    231.00    228.00    225.00
3049.0
497.00    760.00     39.50    107.00     0.88      2.45
224.00    221.00    200.00    201.00
235.00    232.00    226.00    222.00
13522104.00    1.00           1.00
235570.00      1.00           1.00
33454.00       1.00           1.00
6322204.00     1.00           1.00
17464.00       1.00           1.00
27865.00       1.00           1.00
225.00    205.00
224.00    225.00    207.00    205.00
233.00    232.00    228.00    224.00
```

EXPERIMENTAL RESULT OF METHENATION OF CO & CO2 IN A FIXED BED REACTOR

Steadv stae

WEIGHT OF CATALYST : 8.23 gm

DILUTION RATIO, CATALYST:INERT : Undiluted

CATALYST SIZE : 25-40 mesh.

INERT SIZE : 25-40 mesh.

CATALYST TYPE : Ni on Alumina (ZFCL)

LENGTH OF CATALYST BED : 8.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 13.5 cm.

LENGTH OF INERT BED AFTER CATALYST : 22.0 cm.

BULK DENSITY OF CATALYST : 0.7565 gm./c.c.

BULK DENSITY OF INERT : 1.821 gm./c.c.

OD OF REACTOR : 17.00 mm.

ID OF REACTOR : 12.00 mm.

THERMO COUPLE LOCATIONS FROM INLET : 0.0 cm. 3.0 cm. 6.0 cm. 8.0 cm.

```
>>>>>>>>>>>>>>>        RUN NUMBER: 3027.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  533.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol%
H2             39.50                     1.763                    26.61
N2            107.00                     4.777                    72.09
CO              0.88                     0.039                     0.59
CO2             1.05                     0.047                     0.71
TOTAL         148.43                     6.626                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2664E+05
CO:H2 RATIO     = 1: 44.8864          W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO    = 1: 37.6190          W/FCO2 gm.hr./mol=  175.5733
RE(superficial)= 147.25               RE(particle)     =     6.92
INITIAL TEMPERATURE PROFILE:-
REACTOR:     260.00     256.00     236.00     233.00 C
WALL   :     268.00     265.00     260.00     255.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7950
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
   14.4342    82.4295     0.9878      0.0038       0.1471       1.9977

$$$$ CONV.OF H2: 52.57 % ,  CONV.OF CO2: 81.82 % ,  CONV. OF CO: 99.43
TEMPERATURE PROFILE:-
REACTOR    :     260.00     273.00     261.00     248.00 C
WALL       :     268.00     273.00     272.00     265.00 C
PEAK TEMP.:      273.00 C         EXIT TEMP:      248.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 3028.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  533.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.            mol%
H2             39.50                     1.763                    26.48
N2            107.00                     4.777                    71.73
CO              0.88                     0.039                     0.59
CO2             1.80                     0.080                     1.21
TOTAL         149.18                     6.660                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2677E+05
CO:H2 RATIO     = 1: 44.8864          W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO    = 1: 21.9444          W/FCO2 gm.hr./mol=  102.4178
RE(superficial)= 148.88               RE(particle)     =     7.00
INITIAL TEMPERATURE PROFILE:-
REACTOR:     260.00     256.00     236.00     233.00 C
WALL   :     268.00     265.00     260.00     255.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.8946
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
   14.6505    81.0363     1.1923      0.0087       0.2721       2.8401

$$$$ CONV.OF H2: 51.03 % ,  CONV.OF CO2: 80.04 % ,  CONV. OF CO: 98.69
TEMPERATURE PROFILE:-
REACTOR    :     260.00     278.00     272.00     254.00 C
WALL       :     272.00     278.00     277.00     271.00 C
PEAK TEMP.:      278.00 C         EXIT TEMP:      254.00 C
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>>>>>>>>>>>>>>>      RUN NUMBER: 3029.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  533.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.           mol%
H2               39.50                    1.763                    26.36
N2              107.00                    4.777                    71.41
CO                0.88                    0.039                     0.59
CO2               2.45                    0.109                     1.64
TOTAL           149.83                    6.689                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2689E+05
CO:H2 RATIO      = 1: 44.8864          W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO     = 1: 16.1224          W/FCO2 gm.hr./mol=   75.2457
RE(superficial)= 150.29                RE(particle)     =    7.06
INITIAL TEMPERATURE PROFILE:-
REACTOR:      260.00     256.00     236.00     233.00 C
WALL    :     268.00     265.00     260.00     255.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.7553
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
   11.5098    82.9976     1.4983      0.0171      0.4890      3.4883

$$$$ CONV.OF H2: 62.43 % ,  CONV.OF CO2: 74.27 % ,   CONV. OF CO: 97.50
TEMPERATURE PROFILE:-
REACTOR    :      260.00     274.00     276.00     259.00 C
WALL       :      268.00     276.00     276.00     271.00 C
PEAK TEMP.:       276.00 C          EXIT TEMP:     249.00 C

>>>>>>>>>>>>>>>      RUN NUMBER: 3030.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                 PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.           mol%
H2               39.50                    1.763                    26.36
N2              107.00                    4.777                    71.41
CO                0.88                    0.039                     0.59
CO2               2.45                    0.109                     1.64
TOTAL           149.83                    6.689                   100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2638E+05
CO:H2 RATIO      = 1: 44.8864          W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO     = 1: 16.1224          W/FCO2 gm.hr./mol=   75.2457
RE(superficial)= 152.25                RE(particle)     =    7.16
INITIAL TEMPERATURE PROFILE:-
REACTOR:      250.00     246.00     230.00     225.00 C
WALL    :     256.00     254.00     249.00     244.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.9486
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
   15.4102    80.3014     0.9355      0.0157      0.9848      2.3523

$$$$ CONV.OF H2: 48.02 % ,  CONV.OF CO2: 46.44 % ,   CONV. OF CO: 97.62
TEMPERATURE PROFILE:-
REACTOR    :      250.00     258.00     255.00     244.00 C
WALL       :      257.00     262.00     261.00     256.00 C
PEAK TEMP.:       258.00 C          EXIT TEMP:     244.00 C
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>>>>>>>>>>>>>>>        RUN NUMBER: 3031.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.        mol%
H2             39.50                    1.763                26.48
N2            107.00                    4.777                71.73
CO              0.88                    0.039                 0.59
CO2             1.80                    0.080                 1.21
TOTAL         149.18                    6.660               100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.2627E+05
CO:H2 RATIO     = 1: 44.8864        W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO    = 1: 21.9444        W/FCO2 gm.hr./mol=   102.4178
RE(superficial)= 150.82             RE(particle)     =     7.09
INITIAL TEMPERATURE PROFILE:-
REACTOR:      250.00     246.00     230.00     225.00 C
WALL   :      256.00     254.00     249.00     244.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.8340
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  14.2815     81.8784     1.0074      0.0119       0.5954       2.2254

$$$$ CONV.OF H2: 52.75 % ,  CONV.OF CO2: 56.77 % ,  CONV. OF CO: 98.23
TEMPERATURE PROFILE:-
REACTOR    :     250.00     264.00     261.00     244.00 C
WALL       :     262.00     267.00     267.00     262.00 C
PEAK TEMP.:      264.00 C          EXIT TEMP:     244.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 3032.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K               PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.        mol%
H2             39.50                    1.763                26.61
N2            107.00                    4.777                72.09
CO              0.88                    0.039                 0.59
CO2             1.05                    0.047                 0.71
TOTAL         148.43                    6.626               100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.2614E+05
CO:H2 RATIO     = 1: 44.8864        W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO    = 1: 37.6190        W/FCO2 gm.hr./mol=   175.5733
RE(superficial)= 149.17             RE(particle)     =     7.01
INITIAL TEMPERATURE PROFILE:-
REACTOR:      250.00     246.00     230.00     225.00 C
WALL   :      256.00     254.00     249.00     244.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  6.2358
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  20.8610     76.6021     0.7555      0.0058       0.3519       1.4238

$$$$ CONV.OF H2: 26.23 % ,  CONV.OF CO2: 53.18 % ,  CONV. OF CO: 99.08
TEMPERATURE PROFILE:-
REACTOR    :     250.00     260.00     250.00     239.00 C
WALL       :     257.00     262.00     261.00     256.00 C
PEAK TEMP.:      260.00 C          EXIT TEMP:     239.00 C
```

```
>>>>>>>>>>>>>>>       RUN NUMBER: 3033.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol%
H2             39.50                     1.763                   30.94
N2             85.50                     3.817                   66.96
CO              0.88                     0.039                    0.69
CO2             1.80                     0.080                    1.41
TOTAL         127.68                     5.700                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2248E+05
CO:H2 RATIO     = 1: 44.8864         W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO    = 1: 21.9444         W/FCO2 gm.hr./mol=  102.4178
RE(superficial)= 121.47              RE(particle)      =    5.71
INITIAL TEMPERATURE PROFILE:-
REACTOR:     250.00     246.00     230.00     225.00 C
WALL   :     256.00     254.00     249.00     244.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.0208
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  19.2596    76.0229     1.3374     0.0098       0.6033       2.7671

$$$$ CONV.OF H2: 45.16 % ,  CONV.OF CO2: 62.31 % ,  CONV. OF CO: 98.75
TEMPERATURE PROFILE:-
REACTOR    :     250.00     266.00     260.00     242.00 C
WALL       :     262.00     269.00     267.00     260.00 C
PEAK TEMP.:      266.00 C         EXIT TEMP:      242.00 C

>>>>>>>>>>>>>>>       RUN NUMBER: 3034.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.           mol%
H2             39.50                     1.763                   36.51
N2             66.00                     2.946                   61.01
CO              0.88                     0.039                    0.81
CO2             1.80                     0.080                    1.66
TOTAL         108.18                     4.829                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1905E+05
CO:H2 RATIO     = 1: 44.8864         W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO    = 1: 21.9444         W/FCO2 gm.hr./mol=  102.4178
RE(superficial)=  94.95              RE(particle)      =    4.46
INITIAL TEMPERATURE PROFILE:-
REACTOR:     250.00     246.00     230.00     225.00 C
WALL   :     256.00     254.00     249.00     244.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  4.3864
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  27.3485    67.1726     1.7696     0.0076       0.8503       2.8514

$$$$ CONV.OF H2: 31.97 % ,  CONV.OF CO2: 53.59 % ,  CONV. OF CO: 99.15
TEMPERATURE PROFILE:-
REACTOR    :     250.00     264.00     258.00     239.00 C
WALL       :     259.00     266.00     263.00     253.00 C
PEAK TEMP.:      264.00 C         EXIT TEMP:      239.00 C
```

```
>>>>>>>>>>>>>>>        RUN NUMBER: 3035.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  523.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol%
H2             68.00                     3.036                   38.27
N2            107.00                     4.777                   60.22
CO              0.88                     0.039                    0.50
CO2             1.80                     0.080                    1.01
TOTAL         177.68                     7.932                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.3129E+05
CO:H2 RATIO     = 1: 77.2727        W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO    = 1: 37.7778        W/FCO2 gm.hr./mol=   102.4178
RE(superficial)= 150.78             RE(particle)     =     7.09
INITIAL TEMPERATURE PROFILE:-
REACTOR:      250.00      246.00      230.00      225.00 C
WALL    :     256.00      254.00      249.00      244.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   7.4227
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  32.8358     64.3540     0.8113      0.0171      0.6955      1.2862

$$$$ CONV.OF H2: 19.71 % ,   CONV.OF CO2: 35.75 % ,   CONV. OF CO: 96.77
TEMPERATURE PROFILE:-
REACTOR     :      250.00      257.00      247.00      244.00 C
WALL        :      260.00      264.00      265.00      261.00 C
PEAK TEMP.:        257.00 C          EXIT TEMP:        244.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 3036.0     <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol%
H2             39.50                     1.763                   26.48
N2            107.00                     4.777                   71.73
CO              0.88                     0.039                    0.59
CO2             1.80                     0.080                    1.21
TOTAL         149.18                     6.660                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2577E+05
CO:H2 RATIO     = 1: 44.8864        W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO    = 1: 21.9444        W/FCO2 gm.hr./mol=   102.4178
RE(superficial)= 152.83             RE(particle)     =     7.18
INITIAL TEMPERATURE PROFILE:-
REACTOR:      240.00      235.00      223.00      218.00 C
WALL    :     244.00      241.00      236.00      232.00 C

!!!!!!!!!!      EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.9331
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  16.5095     80.5112     0.6657      0.0336      1.0574      1.2227

$$$$ CONV.OF H2: 44.45 % ,   CONV.OF CO2: 21.93 % ,   CONV. OF CO: 94.93
TEMPERATURE PROFILE:-
REACTOR     :      240.00      244.00      234.00      232.00 C
WALL        :      251.00      252.00      252.00      248.00 C
PEAK TEMP.:        244.00 C          EXIT TEMP:        232.00 C
```

```
>>>>>>>>>>>>>>>        RUN NUMBER: 3037.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol%
H2              39.50                     1.763                 26.36
N2             107.00                     4.777                 71.41
CO               0.88                     0.039                  0.59
CO2              2.45                     0.109                  1.64
TOTAL          149.83                     6.689                100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.2588E+05
CO:H2 RATIO      = 1: 44.8864         W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO     = 1: 16.1224         W/FCO2 gm.hr./mol=   75.2457
RE(superficial)= 154.29               RE(particle)     =    7.25
INITIAL TEMPERATURE PROFILE:-
REACTOR:     240.00     235.00     223.00     218.00 C
WALL   :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.9805
GAS COMPOSITION (mol %):-
      H2         N2         CH4          CO          CO2          H2O
   16.4580    79.8729    0.6777      0.0451      1.3233       1.6230

$$$$ CONV.OF H2: 44.18 % ,  CONV.OF CO2: 27.65 % ,  CONV. OF CO: 93.13
TEMPERATURE PROFILE:-
REACTOR    :     240.00     243.00     234.00     233.00 C
WALL       :     249.00     252.00     252.00     248.00 C
PEAK TEMP.:      243.00 C          EXIT TEMP:     233.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 3038.0      <<<<<<<<<<<<<<<

**********   INLET CONDITION:-
TEMPRATURE:  513.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.          FLOW RATE,mol/hr.          mol%
H2              39.50                     1.763                 26.61
N2             107.00                     4.777                 72.09
CO               0.88                     0.039                  0.59
CO2              1.05                     0.047                  0.71
TOTAL          148.43                     6.626                100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.2564E+05
CO:H2 RATIO      = 1: 44.8864         W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO     = 1: 37.6190         W/FCO2 gm.hr./mol=  175.5733
RE(superficial)= 151.15               RE(particle)     =    7.10
INITIAL TEMPERATURE PROFILE:-
REACTOR:     240.00     235.00     223.00     218.00 C
WALL   :     244.00     241.00     236.00     232.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.9241
GAS COMPOSITION (mol %):-
      H2         N2         CH4          CO          CO2          H2O
   17.0822    80.6335    0.6064      0.0140      0.5678       1.0961

$$$$ CONV.OF H2: 42.61 % ,  CONV.OF CO2: 28.24 % ,  CONV. OF CO: 97.8
TEMPERATURE PROFILE:-
REACTOR    :     240.00     242.00     232.00     231.00 C
WALL       :     250.00     252.00     251.00     247.00 C
PEAK TEMP.:      242.00 C          EXIT TEMP:     231.00 C
```

```
>>>>>>>>>>>>>>>        RUN NUMBER: 3045.0      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   543.00 K                PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.               mol%
H2             39.50                      1.763                        26.48
N2            107.00                      4.777                        71.73
CO              0.88                      0.039                         0.59
CO2             1.80                      0.080                         1.21
TOTAL         149.18                      6.660                       100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2727E+05
CO:H2 RATIO      = 1: 44.8864          W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO     = 1: 21.9444          W/FCO2 gm.hr./mol=   102.4178
RE(superficial)= 147.00                RE(particle)      =     6.91
INITIAL TEMPERATURE PROFILE:-
REACTOR:      270.00      263.00      243.00      245.00 C
WALL    :     276.00      275.00      271.00      266.00 C

!!!!!!!!!!        EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.7394
GAS COMPOSITION (mol %):-
      H2           N2            CH4            CO            CO2            H2O
   12.0348     83.2274      1.3780       0.0056        0.1248         3.2295

$$$$ CONV.OF H2: 60.83 % ,   CONV.OF CO2: 91.09 % ,   CONV. OF CO: 99.1
TEMPERATURE PROFILE:-
REACTOR     :      270.00      285.00      282.00      271.00 C
WALL        :      284.00      292.00      292.00      287.00 C
PEAK TEMP.:        285.00 C          EXIT TEMP:        271.00 C

>>>>>>>>>>>>>>>        RUN NUMBER: 3046.1      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   553.00 K                PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.               mol%
H2             39.50                      1.763                        26.48
N2            107.00                      4.777                        71.73
CO              0.88                      0.039                         0.59
CO2             1.80                      0.080                         1.21
TOTAL         149.18                      6.660                       100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2778E+05
CO:H2 RATIO      = 1: 44.8864          W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO     = 1: 21.9444          W/FCO2 gm.hr./mol=   102.4178
RE(superficial)= 145.19                RE(particle)      =     6.82
INITIAL TEMPERATURE PROFILE:-
REACTOR:      280.00      273.00      258.00      255.00 C
WALL    :     285.00      284.00      279.00      275.00 C

!!!!!!!!!!        EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.7418
GAS COMPOSITION (mol %):-
      H2           N2            CH4            CO            CO2            H2O
   11.8873     83.1930      1.4801       0.0026        0.0436         3.3934

$$$$ CONV.OF H2: 61.29 % ,   CONV.OF CO2: 96.88 % ,   CONV. OF CO: 99.6
TEMPERATURE PROFILE:-
REACTOR     :      280.00      297.00      295.00      280.00 C
WALL        :      292.00      302.00      302.00      294.00 C
PEAK TEMP.:        297.00 C          EXIT TEMP:        280.00 C
```

```
>>>>>>>>>>>>>>>          RUN NUMBER: 3046.2      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   553.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.        mol%
H2              39.50                     1.763                26.48
N2             107.00                     4.777                71.73
CO               0.88                     0.039                 0.59
CO2              1.80                     0.080                 1.21
TOTAL          149.18                     6.660               100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.2778E+05
CO:H2 RATIO     = 1: 44.8864          W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO    = 1: 21.9444          W/FCO2 gm.hr./mol=  102.4178
RE(superficial)= 145.19               RE(particle)     =    6.82
INITIAL TEMPERATURE PROFILE:-
REACTOR:     280.00     273.00     258.00     255.00 C
WALL    :    285.00     284.00     279.00     275.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.7147
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  11.4895     83.5880      1.4664      0.0018      0.0436       3.4107

$$$$ CONV.OF H2: 62.77 % ,  CONV.OF CO2: 96.90 % ,  CONV. OF CO: 99.7
TEMPERATURE PROFILE:-
REACTOR   :     280.00     297.00     295.00     280.00 C
WALL      :     292.00     302.00     302.00     294.00 C
PEAK TEMP.:     297.00 C        EXIT TEMP:       280.00 C

>>>>>>>>>>>>>>>          RUN NUMBER: 3047.0      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   497.00 K                PRESSURE:  760.00 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.        mol%
H2              39.50                     1.763                26.48
N2             107.00                     4.777                71.73
CO               0.88                     0.039                 0.59
CO2              1.80                     0.080                 1.21
TOTAL          149.18                     6.660               100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.2496E+05
CO:H2 RATIO     = 1: 44.8864          W/FCO gm.hr./mol.=  209.4909
CO2:H2 RATIO    = 1: 21.9444          W/FCO2 gm.hr./mol=  102.4178
RE(superficial)= 156.21               RE(particle)     =    7.34
INITIAL TEMPERATURE PROFILE:-
REACTOR:     224.00     221.00     200.00     201.00 C
WALL    :    235.00     232.00     226.00     222.00 C

!!!!!!!!!!     EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :  5.8136
GAS COMPOSITION (mol %):-
     H2          N2          CH4          CO          CO2          H2O
  15.0439     82.1660      0.2629      0.2905      0.9130       1.3237

$$$$ CONV.OF H2: 50.40 % ,  CONV.OF CO2: 33.95 % ,  CONV. OF CO: 57.
TEMPERATURE PROFILE:-
REACTOR   :     224.00     223.00     207.00     206.00 C
WALL      :     233.00     232.00     228.00     225.00 C
PEAK TEMP.:     224.00 C        EXIT TEMP:       206.00 C
```

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>>>>>>>>>>>>>>>          RUN NUMBER: 3048.0      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   497.00 K                    PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.               FLOW RATE,mol/hr.          mol%
H2               39.50                        1.763                  26.61
N2              107.00                        4.777                  72.09
CO                0.88                        0.039                   0.59
CO2               1.05                        0.047                   0.71
TOTAL           148.43                        6.626                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2484E+05
CO:H2 RATIO      = 1: 44.8864            W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO     = 1: 37.6190            W/FCO2 gm.hr./mol=   175.5733
RE(superficial)= 154.48                  RE(particle)      =     7.26
INITIAL TEMPERATURE PROFILE:-
REACTOR:      224.00       221.00      200.00      201.00 C
WALL    :     235.00       232.00      226.00      222.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.8298
GAS COMPOSITION (mol %):-
      H2           N2          CH4          CO           CO2          H2O
   16.1012      81.9373      0.2728      0.1270       0.5932       0.9686

$$$$ CONV.OF H2: 46.77 % ,  CONV.OF CO2: 26.22 % ,  CONV. OF CO: 81.1
TEMPERATURE PROFILE:-
REACTOR    :       224.00      225.00      207.00      206.00 C
WALL       :       232.00      231.00      228.00      225.00 C
PEAK TEMP.:        225.00 C          EXIT TEMP:        206.00 C

>>>>>>>>>>>>>>>          RUN NUMBER: 3049.0      <<<<<<<<<<<<<<<

**********    INLET CONDITION:-
TEMPRATURE:   497.00 K                    PRESSURE:   760.00 mm.
          FLOW RATE,lit/hr.               FLOW RATE,mol/hr.          mol%
H2               39.50                        1.763                  26.36
N2              107.00                        4.777                  71.41
CO                0.88                        0.039                   0.59
CO2               2.45                        0.109                   1.64
TOTAL           149.83                        6.689                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2507E+05
CO:H2 RATIO      = 1: 44.8864            W/FCO gm.hr./mol.=   209.4909
CO2:H2 RATIO     = 1: 16.1224            W/FCO2 gm.hr./mol=    75.2457
RE(superficial)= 157.70                  RE(particle)      =     7.41
INITIAL TEMPERATURE PROFILE:-
REACTOR:      224.00       221.00      200.00      201.00 C
WALL    :     235.00       232.00      226.00      222.00 C

!!!!!!!!!!       EXIT CONDITION:-
GAS FLOW RATE, mol/hr. :   5.8782
GAS COMPOSITION (mol %):-
      H2           N2          CH4          CO           CO2          H2O
   15.4801      81.2628      0.2245      0.4047       1.3571       1.2709

$$$$ CONV.OF H2: 48.40 % ,  CONV.OF CO2: 27.07 % ,  CONV. OF CO: 39.
TEMPERATURE PROFILE:-
REACTOR    :       224.00      225.00      207.00      205.00 C
WALL       :       233.00      232.00      228.00      224.00 C
PEAK TEMP.:        225.00 C          EXIT TEMP:        205.00 C
```

APPENDIX F

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF UNSTEADY STATE METHANATION OF CO_2 IN ADIABATIC REACTOR

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C                          COMPUTER PROGRAM (USCO2.FOR)
C      OF UNSTEADY STATE CO2 METHANATION IN THE FIXED  BED REACTOR.

C      This program calculates the product composition and tabulates
C      the results by taking the initial conditions of operation and
C      the Gas chromatograph peak areas for products.

C      * NT      Number of Runs
C      * NRUN    Integer Run Number
C      * FRUN    Floating Run Number
C      * NA,NB   Number of subruns
C      * NC      Number of peaks in Molecular sieve column
C      * RSC     Response factor in Molecular  ''    ''
C      * FY      Flow rate , lit/hr.
C      * FD      Diameter of reactor, cm.
C      * FBD     Bulk density of catalyst pellet, gm/cc.
C      * CWT     Catalyst weight, gm.
C      * TR      Reactor temperature, C.
C      * TW      Wall temperature, C.
C      * WFCO2   Ratio of catalyst wt. and CO2 flow rate,gm.hr/lit.
C      * RHCO2   Ratio of H2 and CO2.
C      * SV      Space velocity, hr-1
C      * FWT     Total molar flow rate, mol/hr.
C      * FCO2P   Mol % CO2
C      * FH2P    Mol % H2
C      * FN2P    Mol % N2

       DIMENSION RSC(4),CHA(4),CHAM(4),CHAP(4),TR(4),TW(4)

       OPEN(UNIT=1,FILE='USCO2DAT',STATUS='UNKNOWN')
       OPEN(UNIT=3,FILE='USCO2OUT',STATUS='UNKNOWN')

       READ(1,*)NC,NT,NA,NB
       READ(1,*)(RSC(I),I=1,NC)
       READ(1,*)FD,FBD,CWT

       WRITE(3,200)
       WRITE(3,201)
       WRITE(3,204)
       WRITE(3,205)
       WRITE(3,210)

       DO 75 LPN=1,NT

       READ(1,*)NRUN
       READ(1,*)T,P,FY1,FY2,FY3,FY4

       WRITE(3,140)NRUN
       WRITE(3,141)
       WRITE(3,220)
       WRITE(3,230)

       X1=100.0
       X2=22.4
       FW1=FY1/X2
       FW2=FY2/X2
       FW3=FY3/X2
       FW4=FY4/X2
       FWT1=FW1+FW2+FW3
       FCO2=FW3*X1/FWT1
       FWT=FW1+FW2+FW4
```

```
      FH2P=FW1*X1/FWT
      FN2P=FW2*X1/FWT
      FCO2P=FW4*X1/FWT
      RHCO2=FH2P/FCO2P
      WFCO2=CWT/FW4
      FYT=FY1+FY2+FY4
      VO=FYT*T/273.0
      V=CWT/(FBD*1000.0)
      ST=V/VO
      SV=1.0/ST

      WRITE(3,207)T,P
      WRITE(3,208)FWT
      WRITE(3,194)FW1,FW2,FW3,FW4
      WRITE(3,219)FCO2,FCO2P,FH2P,FN2P
      WRITE(3,246)RHCO2,WFCO2,SV
      WRITE(3,94)
      WRITE(3,95)
      WRITE(3,211)
      WRITE(3,212)

      DO 76 LNA=1,NA
      READ(1,*)FRUN,TIME
      READ(1,*)(CHA(I),I=1,NC)
      CHAS=0.0
C     CHAM=MOL % IN MOLECULER SIEVE COLUMN

      DO 12 I=1,NC
      CHAM(I)=CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE

      DO 13 I=1,NC
      CHAP(I)=CHAM(I)/CHAS*X1
13    CONTINUE
      WRITE(3,213)FRUN,TIME,(CHAP(I),I=1,NC)
76    CONTINUE

C     TEMPERATURE PROFILES AT DIFFERENT TIMES
      WRITE(3,96)
      WRITE(3,97)

      DO 77 LNB=1,NB
      READ(1,*)TIME,(TR(I),I=1,NC)
      READ(1,*)(TW(I),I=1,NC)
      WRITE(3,7)TIME,(TR(I),I=1,NC)
      WRITE(3,8)(TW(I),I=1,NC)
77    CONTINUE
      WRITE(3,9)

75    CONTINUE

200   FORMAT('EXPERIMENTAL RESULT OF METHANATION OF CO2 IN A FIXED BED R
     ?EACTOR',/,25x,'Unsteady state')
201   FORMAT('----------------------------------------------------------
     ?------')
204   FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X.'8.23 gm',///,'DILUTION
     ? RATIO, CATALYST:INERT',5X.':',3x,'Undiluted',///,'CATALYST SIZE',
     ?22X,':',3X,'25-40 mesh.',///.'INERT SIZE',25X,':',3X,'25-40 Mesh.'
     ?,///,'CATALYST TYPE',22X,':'.3X,'Ni on Alumina (ZFCL)')
205   FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'8.0 cm.',///,'LENGT
```

```
     ?H OF INERT BED BEFORE CATALYST:',3X,'13.5 cm.',///,'LENGTH OF INER
     ?T BED AFTER CATALYST :',3X,'22.0 cm.',///,'BULK DENSITY OF CATALYS
     ?T',11X,':',3X,'0.7565 gm./cc.')
210   FORMAT(//,'BULK DENSITY OF INERT',14X,':',3X,'1.821 gm./cc.',///,'
     ?OD OF REACTOR',22X,':',3X,'17.00 mm.',///,'ID OF REACTOR',22X,':',
     ?3X,'12.00 mm.',///,'THERMOCOUPLE LOCATIONS FROM INLET  :',3X,'0.0
     ?cm. 3.0 cm. 6.0 cm. 8.0 cm.',////////////////)
140   FORMAT(///////,'RUN NUMBER:',1x,I5)
141   FORMAT('****************')
220   FORMAT(/,'INLET CONDITION:')
230   FORMAT('----------------')
207   FORMAT('TEMPERATURE:',F6.1,1X,'K',9X,'PRESSURE:',F6.1,1X,'mm.')
208   FORMAT(/,'TOTAL GAS FLOW RATE, mol./hr.:',F6.2)
194   FORMAT(/,'GAS FLOW RATE,mols./hr.:-  H2:',F8.4,4X,'N2:',F8.4,/,26X
     ?,'CO2:',F8.4,4X,'to',1X,F8.4)
219   FORMAT(/,12X,'STEP CHANGE:- CO2:',F6.2,6X,'to',1X,F6.2,4X,'mol %',
     ?/,27X,'H2:',F6.2,6X,'N2:',F6.2,4X,'mol %')
246   FORMAT(/,'CO2:H2 RATIO= 1:',F6.2,5X,'W/FCO2,gm.hr./mol.=',F6.2,/,'
     ?SPACE VELOCITY,lit.gas/lit.cat.hr.=',F10.2)
94    FORMAT(/,'EXIT CONDITION:-')
95    FORMAT('----------------')
211   FORMAT('COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
     ?')
212   FORMAT('RUN NO.',5X,'TIME(min)',5X,'H2',10X,'N2',9X,'CH4',8X,'CO
     ?')
213   FORMAT(F6.1,8X,F4.1,5X,F7.3,5X,F7.3,4X,F7.3,4X,F7.3)
96    FORMAT(/,'TEMPERATURE PROFILES AT DIFFERENT TIMES:-')
97    FORMAT('TIME(min)',15X,'T E M P E R A T U R E  in deg.C')
7     FORMAT(2X,F4.1,5X,'REACTOR:',4F10.1)
8     FORMAT(11X,'WALL    :',4F10.1)
9     FORMAT(///////)

      STOP
      END
```

```
 4 5 7 7
 36.0 1.0 1.0 1.13
 1.2 0.7565 8.23
 2033
 543.0 760.0 39.5 103.0 3.1 1.25
 2033.0 0.0
 3853.0 723639.0 8618.0 0.0
 2033.1 1.0
 2257.0 743147.0 7291.0 0.0
 2033.2 6.0
 2887.0 745684.0 3536.0 0.0
 2033.3 9.0
 4829.0 682403.0 3433.0 0.0
 2033.4 13.0
 4844.0 687774.0 3206.0 0.0
 2033.5 17.0
 4837.0 684097.0 3761.0 0.0
 2033.6 21.0
 4799.0 683249.0 3308.0 0.0
 0.0 270.0 285.0 301.0 298.0
     274.0 283.0 292.0 295.0
 1.0 271.0 284.0 294.0 291.0
     275.0 283.0 291.0 291.0
 3.0 270.0 282.0 291.0 287.0
     274.0 282.0 288.0 289.0
 5.0 270.0 282.0 291.0 285.0
     275.0 283.0 288.0 288.0
 9.0 270.0 282.0 289.0 283.0
     274.0 281.0 285.0 285.0
18.0 270.0 281.0 288.0 282.0
     273.0 280.0 284.0 283.0
30.0 270.0 281.0 287.0 281.0
     273.0 280.0 283.0 283.0
 2034
543.0 760.0 39.5 103.0 1.25 3.10
2034.0 0.0
4633.0 685225.0 3294.0 0.0
2034.1 1.0
4650.0 688450.0 3172.0 0.0
2034.2 5.0
3830.0 696251.0 6508.0 0.0
2034.3 9.0
3849.0 702704.0 7008.0 0.0
2034.4 13.0
3847.0 706485.0 7206.0 0.0
2034.5 17.0
3809.0 705659.0 6869.0 0.0
2034.6 21.0
3841.0 701122.0 7027.0 0.0
0.0 270.0 281.0 287.0 281.0
    273.0 280.0 283.0 283.0
1.0 270.0 283.0 295.0 288.0
    274.0 281.0 287.0 287.0
3.0 270.0 284.0 297.0 292.0
    276.0 284.0 290.0 291.0
5.0 270.0 284.0 299.0 294.0
    272.0 282.0 290.0 292.0
8.0 270.0 284.0 299.0 296.0
    273.0 283.0 291.0 293.0
14.0 270.0 284.0 299.0 297.0
     274.0 284.0 292.0 294.0
30.0 270.0 285.0 300.0 297.0
```

```
     273.0 283.0 292.0 294.0
2035
543.0 760.0 39.5 103.0 0.0 1.93
2035.0 0.0
55851.0 6467260.0 0.0 0.0
2035.1 1.0
52514.0 6352087.0 0.0 0.0
2035.2 5.0
47238.0 6511103.0 44410.0 0.0
2035.3 10.0
43272.0 6450909.0 50467.0 0.0
2035.4 18.0
40545.0 6470698.0 51243.0 0.0
2035.5 64.0
34519.0 6515490.0 60713.0 0.0
2035.6 64.0
34519.0 6515490.0 60713.0 0.0
0.0 270.0 275.0 271.0 267.0
    274.0 276.0 275.0 274.0
1.0 270.0 277.0 276.0 269.0
    272.0 276.0 276.0 274.0
2.0 270.0 278.0 281.0 272.0
    274.0 279.0 279.0 276.0
3.0 270.0 281.0 286.0 277.0
    274.0 280.0 282.0 279.0
6.0 270.0 282.0 291.0 281.0
    274.0 281.0 285.0 284.0
10.0 270.0 283.0 293.0 287.0
     275.0 283.0 288.0 288.0
55.0 270.0 284.0 295.0 287.0
     275.0 283.0 288.0 288.0
2036
543.0 760.0 39.5 103.0 1.93 0.00001
2036.1 1.0
30374.0 6529533.0 69638.0 0.0
2036.2 5.0
41056.0 6356891.0 1054.0 0.0
2036.3 11.0
41191.0 6437345.0 873.0 0.0
2036.4 15.0
40459.0 6403566.0 895.0 0.0
2036.5 21.0
39220.0 6805064.0 775.0 0.0
2036.6 31.0
40436.0 6097133.0 787.0 0.0
2036.6 31.0
40436.0 6097133.0 787.0 0.0
0.0 270.0 284.0 294.0 287.0
    275.0 283.0 288.0 288.0
1.0 271.0 280.0 280.0 278.0
    273.0 278.0 282.0 282.0
3.0 270.0 276.0 275.0 272.0
    273.0 277.0 278.0 278.0
6.0 270.0 275.0 273.0 269.0
    272.0 275.0 276.0 275.0
8.0 270.0 275.0 272.0 268.0
    273.0 276.0 275.0 274.0
13.0 270.0 275.0 271.0 266.0
     273.0 275.0 274.0 273.0
56.0 270.0 275.0 271.0 266.0
     274.0 276.0 275.0 273.0
2037
```

```
543.0 760.0 39.5 103.0 0.0 3.1
2037.0 0.0
35489.0 6097133.0 787.0 0.0
2037.1 2.0
39230.0 5969567.0 58614.0 0.0
2037.2 6.0
34350.0 6008972.0 87751.0 0.0
2037.3 10.0
33246.0 6079522.0 97880.0 0.0
2037.4 22.0
30847.0 6061366.0 101640.0 0.0
2037.5 25.0
32817.0 6111494.0 108904.0 0.0
2037.6 28.0
32414.0 6243038.0 107274.0 0.0
0.0 270.0 275.0 271.0 266.0
    274.0 276.0 275.0 273.0
1.0 270.0 281.0 288.0 277.0
    274.0 280.0 281.0 279.0
3.0 270.0 283.0 294.0 285.0
    273.0 281.0 285.0 285.0
7.0 270.0 285.0 299.0 293.0
    275.0 285.0 292.0 292.0
12.0 270.0 286.0 303.0 298.0
     276.0 287.0 295.0 297.0
18.0 270.0 286.0 303.0 300.0
     274.0 285.0 295.0 298.0
48.0 270.0 286.0 305.0 302.0
     275.0 287.0 297.0 300.0
```

EXPERIMENTAL RESULT OF METHANATION OF CO2 IN A FIXED BED REACTOR
Unsteady state

WEIGHT OF CATALYST : 8.23 gm

DILUTION RATIO, CATALYST:INERT : Undiluted

CATALYST SIZE : 25-40 mesh.

INERT SIZE : 25-40 Mesh.

CATALYST TYPE : Ni on Alumina (ZFCL)

LENGTH OF CATALYST BED : 8.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 13.5 cm.

LENGTH OF INERT BED AFTER CATALYST : 22.0 cm.

BULK DENSITY OF CATALYST : 0.7565 gm./cc.

BULK DENSITY OF INERT : 1.821 gm./cc.

OD OF REACTOR : 17.00 mm.

ID OF REACTOR : 12.00 mm.

THERMOCOUPLE LOCATIONS FROM INLET : 0.0 cm. 3.0 cm. 6.0 cm. 8.0 cm

```
RUN NUMBER:  2033
*****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.42

GAS FLOW RATE,mols./hr.:-  H2:  1.7634    N2:  4.5982
                          CO2:  0.1384    to   0.0558

            STEP CHANGE:- CO2:  2.13      to   0.87    mol %
                           H2: 27.48      N2: 71.65    mol %

CO2:H2 RATIO= 1: 31.60     W/FCO2,gm.hr./mol.=147.48
SPACE VELOCITY,lit.gas/lit.cat.hr.=  26281.74

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)     H2         N2         CH4        CO
2033.0        0.0       15.926     83.085      0.989      0.000
2033.1        1.0        9.770     89.354      0.877      0.000
2033.2        6.0       12.182     87.403      0.414      0.000
2033.3        9.0       20.222     79.379      0.399      0.000
2033.4       13.0       20.152     79.478      0.370      0.000
2033.5       17.0       20.201     79.363      0.436      0.000
2033.6       21.0       20.105     79.510      0.385      0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      270.0      285.0      301.0      298.0
           WALL   :      274.0      283.0      292.0      295.0
   1.0     REACTOR:      271.0      284.0      294.0      291.0
           WALL   :      275.0      283.0      291.0      291.0
   3.0     REACTOR:      270.0      282.0      291.0      287.0
           WALL   :      274.0      282.0      288.0      289.0
   5.0     REACTOR:      270.0      282.0      291.0      285.0
           WALL   :      275.0      283.0      288.0      288.0
   9.0     REACTOR:      270.0      282.0      289.0      283.0
           WALL   :      274.0      281.0      285.0      285.0
  18.0     REACTOR:      270.0      281.0      288.0      282.0
           WALL   :      273.0      280.0      284.0      283.0
  30.0     REACTOR:      270.0      281.0      287.0      281.0
           WALL   :      273.0      280.0      283.0      283.0
```

```
RUN NUMBER:  2034
****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K           PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.50

GAS FLOW RATE,mols./hr.:-  H2:  1.7634     N2:  4.5982
                          CO2:  0.0558     to   0.1384

         STEP CHANGE:- CO2:  0.87       to   2.13    mol %
                        H2: 27.13       N2: 70.74    mol %

CO2:H2 RATIO= 1: 12.74     W/FCO2,gm.hr./mol.= 59.47
SPACE VELOCITY,lit.gas/lit.cat.hr.=  26619.98

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)     H2          N2          CH4         CO
2034.0          0.0      19.500      80.115      0.385       0.000
2034.1          1.0      19.487      80.143      0.369       0.000
2034.2          5.0      16.402      82.824      0.774       0.000
2034.3          9.0      16.335      82.839      0.826       0.000
2034.4         13.0      16.251      82.903      0.846       0.000
2034.5         17.0      16.139      83.053      0.808       0.000
2034.6         21.0      16.336      82.833      0.830       0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      270.0       281.0       287.0       281.0
           WALL   :      273.0       280.0       283.0       283.0
   1.0     REACTOR:      270.0       283.0       295.0       288.0
           WALL   :      274.0       281.0       287.0       287.0
   3.0     REACTOR:      270.0       284.0       297.0       292.0
           WALL   :      276.0       284.0       290.0       291.0
   5.0     REACTOR:      270.0       284.0       299.0       294.0
           WALL   :      272.0       282.0       290.0       292.0
   8.0     REACTOR:      270.0       284.0       299.0       296.0
           WALL   :      273.0       283.0       291.0       293.0
  14.0     REACTOR:      270.0       284.0       299.0       297.0
           WALL   :      274.0       284.0       292.0       294.0
  30.0     REACTOR:      270.0       285.0       300.0       297.0
           WALL   :      273.0       283.0       292.0       294.0
```

```
RUN NUMBER:  2035
****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K           PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.45

GAS FLOW RATE,mols./hr.:-  H2:  1.7634    N2:  4.5982
                          CO2:  0.0000    to   0.0862

         STEP CHANGE:- CO2:  0.00        to    1.34    mol %
                        H2: 27.35        N2:  71.31    mol %

CO2:H2 RATIO= 1: 20.47     W/FCO2,gm.hr./mol.= 95.52
SPACE VELOCITY,lit.gas/lit.cat.hr.=  26406.07

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)      H2          N2          CH4         CO
2035.0         0.0       23.716      76.284       0.000       0.000
2035.1         1.0       22.936      77.064       0.000       0.000
2035.2         5.0       20.598      78.864       0.538       0.000
2035.3        10.0       19.329      80.044       0.626       0.000
2035.4        18.0       18.287      81.071       0.642       0.000
2035.5        64.0       15.893      83.330       0.776       0.000
2035.6        64.0       15.893      83.330       0.776       0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      270.0       275.0       271.0       267.0
           WALL    :     274.0       276.0       275.0       274.0
   1.0     REACTOR:      270.0       277.0       276.0       269.0
           WALL    :     272.0       276.0       276.0       274.0
   2.0     REACTOR:      270.0       278.0       281.0       272.0
           WALL    :     274.0       279.0       279.0       276.0
   3.0     REACTOR:      270.0       281.0       286.0       277.0
           WALL    :     274.0       280.0       282.0       279.0
   6.0     REACTOR:      270.0       282.0       291.0       281.0
           WALL    :     274.0       281.0       285.0       284.0
  10.0     REACTOR:      270.0       283.0       293.0       287.0
           WALL    :     275.0       283.0       288.0       288.0
  55.0     REACTOR:      270.0       284.0       295.0       287.0
           WALL    :     275.0       283.0       288.0       288.0
```

```
RUN NUMBER:  2036
****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.36

GAS FLOW RATE,mols./hr.:-  H2:  1.7634     N2:  4.5982
                          CO2:  0.0862     to   0.0000

           STEP CHANGE:- CO2:  1.34       to   0.00    mol %
                          H2: 27.72       N2: 72.28    mol %

CO2:H2 RATIO= 1:******      W/FCO2,gm.hr./mol.=******
SPACE VELOCITY,lit.gas/lit.cat.hr.=  26053.21

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)      H2          N2          CH4         CO
2036.1          1.0       14.214      84.880      0.905       0.000
2036.2          5.0       18.862      81.125      0.013       0.000
2036.3         11.0       18.721      81.268      0.011       0.000
2036.4         15.0       18.529      81.460      0.011       0.000
2036.5         21.0       17.181      82.809      0.009       0.000
2036.6         31.0       19.272      80.718      0.010       0.000
2036.6         31.0       19.272      80.718      0.010       0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 T E M P E R A T U R E  in deg.C
   0.0     REACTOR:       270.0       284.0       294.0       287.0
           WALL    :      275.0       283.0       288.0       288.0
   1.0     REACTOR:       271.0       280.0       280.0       278.0
           WALL    :      273.0       278.0       282.0       282.0
   3.0     REACTOR:       270.0       276.0       275.0       272.0
           WALL    :      273.0       277.0       278.0       278.0
   6.0     REACTOR:       270.0       275.0       273.0       269.0
           WALL    :      272.0       275.0       276.0       275.0
   8.0     REACTOR:       270.0       275.0       272.0       268.0
           WALL    :      273.0       276.0       275.0       274.0
  13.0     REACTOR:       270.0       275.0       271.0       266.0
           WALL    :      273.0       275.0       274.0       273.0
  56.0     REACTOR:       270.0       275.0       271.0       266.0
           WALL    :      274.0       276.0       275.0       273.0
```

```
RUN NUMBER:  2037
****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.50

GAS FLOW RATE,mols./hr.:-  H2:  1.7634     N2:  4.5982
                          CO2:  0.0000     to   0.1384

            STEP CHANGE:- CO2:  0.00       to   2.13     mol %
                           H2: 27.13       N2: 70.74     mol %

CO2:H2 RATIO= 1: 12.74     W/FCO2.gm.hr./mol.= 59.47
SPACE VELOCITY,lit.gas/lit.cat.hr.=  26619.98

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)      H2          N2          CH4          CO
2037.0        0.0        17.322      82.667      0.011        0.000
2037.1        2.0        18.981      80.231      0.788        0.000
2037.2        6.0        16.863      81.941      1.197        0.000
2037.3       10.0        16.230      82.442      1.327        0.000
2037.4       22.0        15.268      83.335      1.397        0.000
2037.5       25.0        15.961      82.568      1.471        0.000
2037.6       28.0        15.523      83.050      1.427        0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 T E M P E R A T U R E  in deg.C
   0.0      REACTOR:      270.0      275.0      271.0      266.0
            WALL   :      274.0      276.0      275.0      273.0
   1.0      REACTOR:      270.0      281.0      288.0      277.0
            WALL   :      274.0      280.0      281.0      279.0
   3.0      REACTOR:      270.0      283.0      294.0      285.0
            WALL   :      273.0      281.0      285.0      285.0
   7.0      REACTOR:      270.0      285.0      299.0      293.0
            WALL   :      275.0      285.0      292.0      292.0
  12.0      REACTOR:      270.0      286.0      303.0      298.0
            WALL   :      276.0      287.0      295.0      297.0
  18.0      REACTOR:      270.0      286.0      303.0      300.0
            WALL   :      274.0      285.0      295.0      298.0
  48.0      REACTOR:      270.0      286.0      305.0      302.0
            WALL   :      275.0      287.0      297.0      300.0
```

APPENDIX G

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF UNSTEADY STATE METHANATION OF CO IN ADIABATIC REACTOR

```
C                    COMPUTER PROGRAM (USCO.FOR)
C     OF UNSTEADY STATE CO METHANATION IN THE FIXED  BED REACTOR.

C     This program calculates the product composition and tabulates
C     the results by taking the initial conditions of operation and
C     the Gas chromatograph peak areas for products.

C     * NT      Number of Runs
C     * NRUN    Integer Run Number
C     * FRUN    Floating Run Number
C     * NA,NB   Number of subruns
C     * NC      Number of peaks in Molecular sieve column
C     * RSC     Response factor in Molecular   ''     ''
C     * FY      Flow rate , lit/hr.
C     * FD      Diameter of reactor, cm.
C     * FBD     Bulk density of catalyst pellet, gm/cc.
C     * CWT     Catalyst weight, gm.
C     * TR      Reactor temperature, C.
C     * TW      Wall temperature, C.
C     * WFCO    Ratio of catalyst wt. and CO flow rate,gm.hr/lit.
C     * RHCO    Ratio of H2 and CO.
C     * SV      Space velocity, hr-1
C     * FWT     Total molar flow rate, mol/hr.
C     * FCOP    Mol % CO
C     * FH2P    Mol % H2
C     * FN2P    Mol % N2

      DIMENSION RSC(4),CHA(4),CHAM(4),CHAP(4),TR(4),TW(4)

      OPEN(UNIT=1,FILE='USCODAT',STATUS='UNKNOWN')
      OPEN(UNIT=3,FILE='USCOOUT',STATUS='UNKNOWN')

      READ(1,*)NC,NT,NA,NB
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)FD,FBD,CWT
      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)
      DO 75 LPN=1,NT
      READ(1,*)NRUN
      READ(1,*)T,P,FY1,FY2,FY3,FY4
      WRITE(3,140)NRUN
      WRITE(3,141)
      WRITE(3,220)
      WRITE(3,230)
      X1=100.0
      X2=22.4
      FW1=FY1/X2
      FW2=FY2/X2
      FW3=FY3/X2
      FW4=FY4/X2
      FWT1=FW1+FW2+FW3
      FWT=FW1+FW2+FW4
      FH2P=FW1*X1/FWT

C &&&&& FOR STEP CHANGE CO &&&&&&&&&&&&&&&&&&&&&&&&&

C *** FY1=H2,FY2=N2,FY3=CO(Previous),FY4=CO(Changed)
C *** DATA FILE NAME IS USCODAT
```

```
C *** OUT FILE NAME IS USCOOUT
C *** when step changed N2 is used then this block
C *** will be within C command
C *** WRITE(3,219)FCO,FCOP,FH2P,FN2P
C ** In 194, 219 FORMAT N2 will be interchanged by CO

      FCO=FW3*X1/FWT1
      FN2P=FW2*X1/FWT
      FCOP=FW4*X1/FWT
      WFCO=CWT/FW4

C &&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&

C ##### FOR STEP CHANGE N2 ########################

C *** FY1=H2,FY2=CO,FY3=N2(Previous),FY4=N2(Changed)
C *** DATA FILE NAME IS UCONDAT
C *** OUT FILE NAME IS UCONOUT
C *** when step changed CO is used then this block
C *** will be within C command
C *** WRITE(3,219)FN2,FN2P,FH2P,FCOP
C **In 194, 219 FORMAT CO will be interchanged by N2

C     FN2=FW3*X1/FWT1
C     FN2P=FW4*X1/FWT
C     FCOP=FW2*X1/FWT
C     WFCO=CWT/FW2

C ################################

      RHCO=FH2P/FCOP
      FYT=FY1+FY2+FY4
      VO=FYT*T/273.0
      V=CWT/(FBD*1000.0)
      ST=V/VO
      SV=1.0/ST
      WRITE(3,207)T,P
      WRITE(3,208)FWT
      WRITE(3,194)FW1,FW2,FW3,FW4

      WRITE(3,219)FCO,FCOP,FH2P,FN2P

      WRITE(3,246)RHCO,WFCO,SV
      WRITE(3,94)
      WRITE(3,95)
      WRITE(3,211)
      WRITE(3,212)
      DO 76 LNA=1,NA
      READ(1,*)FRUN,TIME

C READ GAS CROMATOGRAPH DATA
C CHAM=MOL % IN MOLECULER SIEVE COLUMN

      READ(1,*)(CHA(I),I=1,NC)
      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
      CHAP(I)=CHAM(I)/CHAS*X1
```

```
13     CONTINUE
       WRITE(3,213)FRUN,TIME,(CHAP(I),I=1,NC)
76     CONTINUE

C TEMPERATURE PROFILES AT DIFFERENT TIMES

       WRITE(3,96)
       WRITE(3,97)
       DO 77 LNB=1,NB
       READ(1,*)TIME,(TR(I),I=1,NC)
       READ(1,*)(TW(I),I=1,NC)
       WRITE(3,7)TIME,(TR(I),I=1,NC)
       WRITE(3,8)(TW(I),I=1,NC)
77     CONTINUE
       WRITE(3,9)
75     CONTINUE

200     FORMAT('EXPERIMENTAL RESULT OF METHANATION OF CO IN A FIXED BED RE
     ?ACTOR',/,25x,'Unsteady state ')
201     FORMAT('----------------------------------------------------------
     ?-----')
204     FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'8.23 gm',///,'DILUTION
     ? RATIO, CATALYST:INERT',5X,':',3x,'Undiluted',///,'CATALYST SIZE',
     ?22X,':',3X,'25-40 mesh.',///,'INERT SIZE',25X,':',3X,'25-40 Mesh.'
     ?,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (ZFCL)')
205     FORMAT(//,'LENGTH OF CATALYST BED',13X.':',3X,'8.0 cm.',///,'LENGT
     ?H OF INERT BED BEFORE CATALYST:',3X,'13.5 cm.',///,'LENGTH OF INER
     ?T BED AFTER CATALYST :',3X,'22.0 cm.',///,'BULK DENSITY OF CATALYS
     ?T',11X,':',3X,'0.7565 gm./cc.')
210     FORMAT(//,'BULK DENSITY OF INERT',14X,':',3X,'1.821 gm./cc.',///,'
     ?OD OF REACTOR',22X,':',3X,'17.00 mm.',///,'ID OF REACTOR',22X,':',
     ?3X,'12.00 mm.',///,'THERMOCOUPLE LOCATIONS FROM INLET  :',3X,'0.0
     ?cm. 3.0 cm. 6.0 cm. 8.0 cm.',/////////////////)
140     FORMAT(///////,'RUN NUMBER:',1x,I5)
141     FORMAT('*****************')
220     FORMAT(/,'INLET CONDITION:')
230     FORMAT('----------------')
207     FORMAT('TEMPERATURE:',F6.1.1X,'K',9X,'PRESSURE:'.F6.1,1X,'mm.')
208     FORMAT(/,'TOTAL GAS FLOW RATE, mol./hr.:',F6.2)
194     FORMAT(/,'GAS FLOW RATE,mols./hr.:-  H2:',F8.4,4X,'N2:',F8.4,/,27X
     ?,'CO:',F8.4,4X,'to',1X,F8.4)
219     FORMAT(/,12X,'STEP CHANGE:-  CO:',F6.2,6X,'to'.1X,F6.2,4X,'mol %',
     ?/,27X,'H2:',F6.2,6X,'N2:',F6.2,4X,'mol %')
246     FORMAT(/,'CO:H2 RATIO=  1:',F6.2,5X,'W/FCO ,gm.hr./mol.=',F6.2,/,'
     ?SPACE VELOCITY,lit.gas/lit.cat.hr.=',F10.2)
94      FORMAT(/,'EXIT CONDITION:-')
95      FORMAT('----------------')
211     FORMAT('COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
     ?')
212     FORMAT('RUN NO.',5X,'TIME(min)',5X,'H2',10X,'N2',9X,'CH4',8X,'CO
     ?')
213     FORMAT(F6.1,8X,F4.1,5X,F7.3,5X.F7.3,4X,F7.3,4X,F7.3)
96      FORMAT(/,'TEMPERATURE PROFILES AT DIFFERENT TIMES:-')
97      FORMAT('TIME(min)',15X,'T E M P E R A T U R E  in deg.C')
7       FORMAT(2X,F4.1,5X,'REACTOR:',4F10.1)
8       FORMAT(11X,'WALL    :',4F10.1)
9       FORMAT(///////)

        STOP
        END
```

```
4 3 3 5
36.0 1.0 1.0 1.13
1.2 0.7565 8.23
3013
513.0 760.0 39.5 107.0 0.0 1.50
3013.0 2.0
37387.0 5351043.0 40085.0 84.0
3013.1 2.0
37387.0 5351043.0 40085.0 84.0
3013.2 6.0
36228.0 5409723.0 39978.0 58.0
0.0 240.0 240.0 225.0 212.0
    245.0 242.0 237.0 232.0
1.0 240.0 244.0 236.0 218.0
    246.0 246.0 242.0 236.0
3.0 240.0 247.0 242.0 224.0
    248.0 250.0 247.0 241.0
5.0 240.0 248.0 244.0 225.0
    246.0 249.0 248.0 242.0
14.0 240.0 249.0 245.0 226.0
     246.0 249.0 247.0 243.0
3014
513.0 760.0 39.5 107.0 1.5 2.15
3014.1 1.0
38226.0 5393256.0 36881.0 56.0
3014.2 5.0
34811.0 5432402.0 83704.0 33.0
3014.3 9.0
34822.0 5422306.0 82958.0 17.0
0.0 240.0 249.0 245.0 226.0
    248.0 250.0 249.0 243.0
1.0 240.0 248.0 248.0 234.0
    246.0 248.0 250.0 246.0
4.0 240.0 247.0 245.0 235.0
    249.0 252.0 252.0 249.0
9.0 240.0 249.0 251.0 238.0
    243.0 246.0 250.0 251.0
14.0 241.0 250.0 251.0 237.0
     244.0 247.0 251.0 249.0
3015
513.0 760.0 39.5 107.0 2.15 1.8
3015.1 1.0
34696.0 5456436.0 77243.0 0.0
3015.2 5.0
33643.0 5437358.0 103569.0 0.0
3015.3 9.0
32054.0 5444613.0 82418.0 0.0
0.0 241.0 248.0 248.0 236.0
    244.0 246.0 250.0 248.0
2.0 240.0 248.0 246.0 233.0
    248.0 251.0 251.0 248.0
5.0 241.0 249.0 250.0 235.0
    245.0 248.0 251.0 248.0
14.0 240.0 249.0 248.0 235.0
     246.0 250.0 252.0 249.0
16.0 240.0 249.0 248.0 235.0
     248.0 251.0 253.0 251.0
```

```
4 2 3 5
36.0 1.0 1.0 1.13
1.2 0.7565 8.23
3016
513.0 760.0 39.5 1.64 107.0 85.5
3016.1 1.0
37173.0 5372754.0 52835.0 0.0
3016.2 5.0
47605.0 5072331.0 59634.0 0.0
3016.3 9.0
47648.0 5026992.0 59450.0 0.0
0.0 240.0 247.0 246.0 233.0
    246.0 250.0 251.0 247.0
3.0 240.0 249.0 251.0 229.0
    244.0 247.0 249.0 245.0
6.0 240.0 248.0 249.0 228.0
    244.0 247.0 248.0 243.0
8.0 240.0 249.0 249.0 228.0
    244.0 248.0 248.0 243.0
9.0 240.0 249.0 249.0 229.0
    247.0 250.0 250.0 244.0
3017
513.0 760.0 39.5 1.64 85.5 66.0
3017.0 1.0
31872.0 4775254.0 52303.0 0.0
3017.2 5.0
36770.0 5085042.0 54141.0 0.0
3017.3 9.0
54920.0 4656268.0 66959.0 0.0
0.0 240.0 247.0 243.0 225.0
    245.0 248.0 245.0 238.0
1.0 240.0 246.0 240.0 222.0
    244.0 246.0 243.0 235.0
5.0 240.0 246.0 238.0 221.0
    243.0 245.0 241.0 233.0
9.0 240.0 244.0 237.0 220.0
    242.0 244.0 240.0 232.0
13.0 240.0 244.0 237.0 219.0
     244.0 245.0 240.0 232.0
```

EXPERIMENTAL RESULT OF METHANATION OF CO IN A FIXED BED REACTOR
Unsteady state

WEIGHT OF CATALYST : 8.23 gm

DILUTION RATIO, CATALYST:INERT : Undiluted

CATALYST SIZE : 25-40 mesh.

INERT SIZE : 25-40 Mesh.

CATALYST TYPE : Ni on Alumina (ZFCL)

LENGTH OF CATALYST BED : 8.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 13.5 cm.

LENGTH OF INERT BED AFTER CATALYST : 22.0 cm.

BULK DENSITY OF CATALYST : 0.7565 gm./cc.

BULK DENSITY OF INERT : 1.821 gm./cc.

OD OF REACTOR : 17.00 mm.

ID OF REACTOR : 12.00 mm.

THERMOCOUPLE LOCATIONS FROM INLET : 0.0 cm. 3.0 cm. 6.0 cm. 8.0 cm

```
RUN NUMBER:  3013
*****************

INLET CONDITION:
----------------
TEMPERATURE: 513.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.61

GAS FLOW RATE,mols./hr.:-  H2:  1.7634    N2:  4.7768
                           CO:  0.0000    to   0.0670

            STEP CHANGE:-  CO:  0.00      to   1.01     mol %
                           H2: 26.69      N2: 72.30     mol %

CO:H2 RATIO=  1: 26.33     W/FCO ,gm.hr./mol.=122.90
SPACE VELOCITY,lit.gas/lit.cat.hr.=  25563.81

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)     H2          N2          CH4         CO
3013.0         2.0      19.978      79.426       0.595      0.001
3013.1         2.0      19.978      79.426       0.595      0.001
3013.2         6.0      19.310      80.097       0.592      0.001

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)               T E M P E R A T U R E  in deg.C
   0.0     REACTOR:     240.0      240.0      225.0      212.0
           WALL   :     245.0      242.0      237.0      232.0
   1.0     REACTOR:     240.0      244.0      236.0      218.0
           WALL   :     246.0      246.0      242.0      236.0
   3.0     REACTOR:     240.0      247.0      242.0      224.0
           WALL   :     248.0      250.0      247.0      241.0
   5.0     REACTOR:     240.0      248.0      244.0      225.0
           WALL   :     246.0      249.0      248.0      242.0
  14.0     REACTOR:     240.0      249.0      245.0      226.0
           WALL   :     246.0      249.0      247.0      243.0
```

```
RUN NUMBER:  3014
*****************

INLET CONDITION:
----------------
TEMPERATURE: 513.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.64

GAS FLOW RATE,mols./hr.:-  H2:  1.7634     N2:  4.7768
                           CO:  0.0670     to   0.0960

            STEP CHANGE:-  CO:  1.01       to    1.45    mol %
                           H2: 26.57       N2: 71.98     mol %

CO:H2 RATIO=  1: 18.37     W/FCO ,gm.hr./mol.= 85.75
SPACE VELOCITY,lit.gas/lit.cat.hr.=  25676.08

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)      H2           N2          CH4           CO
3014.1          1.0       20.218       79.239       0.542        0.001
3014.2          5.0       18.513       80.250       1.237        0.001
3014.3          9.0       18.547       80.225       1.227        0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 T E M P E R A T U R E  in deg.C
  0.0      REACTOR:       240.0       249.0       245.0       226.0
           WALL   :       248.0       250.0       249.0       243.0
  1.0      REACTOR:       240.0       248.0       248.0       234.0
           WALL   :       246.0       248.0       250.0       246.0
  4.0      REACTOR:       240.0       247.0       245.0       235.0
           WALL   :       249.0       252.0       252.0       249.0
  9.0      REACTOR:       240.0       249.0       251.0       238.0
           WALL   :       243.0       246.0       250.0       251.0
 14.0      REACTOR:       241.0       250.0       251.0       237.0
           WALL   :       244.0       247.0       251.0       249.0
```

```
RUN NUMBER:  3015
*****************

INLET CONDITION:
----------------
TEMPERATURE: 513.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  6.62

GAS FLOW RATE,mols./hr.:-  H2:  1.7634     N2:  4.7768
                           CO:  0.0960     to   0.0804

            STEP CHANGE:-  CO:  1.45       to   1.21     mol %
                           H2: 26.64       N2: 72.15     mol %

CO:H2 RATIO=  1: 21.94     W/FCO ,gm.hr./mol.=102.42
SPACE VELOCITY,lit.gas/lit.cat.hr.=  25615.63

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)      H2          N2          CH4         CO
3015.1          1.0       18.415      80.446       1.139       0.000
3015.2          5.0       17.937      80.529       1.534       0.000
3015.3          9.0       17.272      81.494       1.234       0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 TEMPERATURE  in deg.C
  0.0       REACTOR:      241.0      248.0      248.0      236.0
            WALL   :      244.0      246.0      250.0      248.0
  2.0       REACTOR:      240.0      248.0      246.0      233.0
            WALL   :      248.0      251.0      251.0      248.0
  5.0       REACTOR:      241.0      249.0      250.0      235.0
            WALL   :      245.0      248.0      251.0      248.0
 14.0       REACTOR:      240.0      249.0      248.0      235.0
            WALL   :      246.0      250.0      252.0      249.0
 16.0       REACTOR:      240.0      249.0      248.0      235.0
            WALL   :      248.0      251.0      253.0      251.0
```

```
RUN NUMBER:  3016
*****************

INLET CONDITION:
----------------
TEMPERATURE: 513.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  5.65

GAS FLOW RATE,mols./hr.:-  H2:  1.7634    CO:  0.0732
                           N2:  4.7768    to   3.8170

            STEP CHANGE:-  N2: 72.23      to  67.51    mol %
                           H2: 31.19      CO:  1.30    mol %

CO:H2 RATIO=  1: 24.09     W/FCO ,gm.hr./mol.=112.41
SPACE VELOCITY,lit.gas/lit.cat.hr.=  21874.33

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)     H2          N2          CH4        CO
3016.1          1.0      19.785      79.434      0.781      0.000
3016.2          5.0      25.034      74.095      0.871      0.000
3016.3          9.0      25.219      73.907      0.874      0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      240.0       247.0       246.0       233.0
           WALL   :      246.0       250.0       251.0       247.0
   3.0     REACTOR:      240.0       249.0       251.0       229.0
           WALL   :      244.0       247.0       249.0       245.0
   6.0     REACTOR:      240.0       248.0       249.0       228.0
           WALL   :      244.0       247.0       248.0       243.0
   8.0     REACTOR:      240.0       249.0       249.0       228.0
           WALL   :      244.0       248.0       248.0       243.0
   9.0     REACTOR:      240.0       249.0       249.0       229.0
           WALL   :      247.0       250.0       250.0       244.0
```

```
RUN NUMBER:  3017
*****************

INLET CONDITION:
----------------
TEMPERATURE: 513.0 K          PRESSURE: 760.0 mm.

TOTAL GAS FLOW RATE, mol./hr.:  4.78

GAS FLOW RATE,mols./hr.:-  H2:  1.7634    CO:  0.0732
                           N2:  3.8170    to   2.9464

            STEP CHANGE:-  N2: 67.51      to  61.60    mol %
                           H2: 36.87      CO:  1.53    mol %

CO:H2 RATIO=  1: 24.09     W/FCO ,gm.hr./mol.=112.41
SPACE VELOCITY,lit.gas/lit.cat.hr.=  18506.13

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)      H2          N2          CH4          CO
3017.0         1.0       19.203      79.921      0.875       0.000
3017.2         5.0       20.482      78.680      0.838       0.000
3017.3         9.0       29.508      69.493      0.999       0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      240.0       247.0       243.0       225.0
           WALL    :     245.0       248.0       245.0       238.0
   1.0     REACTOR:      240.0       246.0       240.0       222.0
           WALL    :     244.0       246.0       243.0       235.0
   5.0     REACTOR:      240.0       246.0       238.0       221.0
           WALL    :     243.0       245.0       241.0       233.0
   9.0     REACTOR:      240.0       244.0       237.0       220.0
           WALL    :     242.0       244.0       240.0       232.0
  13.0     REACTOR:      240.0       244.0       237.0       219.0
           WALL    :     244.0       245.0       240.0       232.0
```

APPENDIX H

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF UNSTEADY STATE METHANATION OF MIXTURE OF CO AND CO_2 IN ADIABATIC REACTOR

```
C     COMPUTER PROGRAM (USCO12.FOR) OF UNSTEADY STATE METHANATION
C     OF THE MIXURE OF CO & CO2 IN THE FIXED BED REACTOR.

C     This program calculates the product composition and tabulates
C     the results by taking the initial conditions of operation and
C     the Gas chromatograph peak areas for products.In this case CO
C     flow rate is constant allover,only CO2 folw rate is changed.

C     * NT      Number of Runs
C     * NRUN    Integer Run Number
C     * FRUN    Floating Run Number
C     * NA,NB   Number of subruns
C     * NC      Number of peaks in Molecular sieve column
C     * RSC     Response factor in Molecular  ''     ''
C     * FY      Flow rate , lit/hr.
C     * FD      Diameter of reactor, cm.
C     * FBD     Bulk density of catalyst pellet, gm/cc.
C     * CWT     Catalyst weight, gm.
C     * TR      Reactor temperature, C.
C     * TW      Wall temperature, C.
C     * WFCO    Ratio of catalyst wt. and CO flow rate,gm.hr/lit.
C     * WFCO2   Ratio of catalyst wt. and CO2 flow rate,gm.hr/lit.
C     * RHCO    Ratio of H2 and CO.
C     * RHCO2   Ratio of H2 and CO2.
C     * SV      Space velocity, hr-1
C     * FWT     Total molar flow rate, mol/hr.
C     * FCOP    Mol % CO
C     * FCO2P   Mol % CO2
C     * FH2P    Mol % H2
C     * FN2P    Mol % N2

      DIMENSION RSC(4),CHA(4),CHAM(4),CHAP(4),TR(4),TW(4)

      OPEN(UNIT=1,FILE='USN12DAT',STATUS='UNKNOWN')
      OPEN(UNIT=3,FILE='USN12OUT',STATUS='UNKNOWN')

      READ(1,*)NC,NT,NA,NB
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)FD,FBD,CWT
      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)

      DO 75 LPN=1,NT

      READ(1,*)NRUN
      READ(1,*)T,P,FY1,FY2,FY3,FY4,FY5
      WRITE(3,140)NRUN
      WRITE(3,141)
      WRITE(3,220)
      WRITE(3,230)

      X1=100.0
      X2=22.4
      FW1=FY1/X2
      FW2=FY2/X2
      FW3=FY3/X2
      FW4=FY4/X2
      FW5=FY5/X2
```

```
      FWT1=FW1+FW2+FW3+FW4
      FWT=FW1+FW2+FW3+FW5
      FH2P=FW1*X1/FWT

C $$$$$ FOR STEP CHANGE CO2 $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

C *** FY1=H2,FY2=N2,FY3=CO,FY4=CO2(Previous),FY5=CO2(Changed)
C *** DATA FILE NAME IS USCO12DAT
C *** OUT FILE NAME IS USCO12OUT
C *** when step change N2 is used then this block will be -
C *** within C command
C *** WRITE(3,219)FCO2,FCO2P,FH2P,FN2P,FCOP
C 194, 219 FORMAT will be adjusted as N2 will be interchanged by CO2

C       FCO2=FW4*X1/FWT1
C       FN2P=FW2*X1/FWT
C       FCOP=FW3*X1/FWT
C       FCO2P=FW5*X1/FWT
C       WFCO=CWT/FW3
C       WFCO2=CWT/FW5

C $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

C #### FOR STEP CHANGE N2 ##################################

C *** FY1=H2,FY2=CO,FY3=CO2,FY4=N2(Previous),FY5=N2(Changed)
C *** DATA FILE NAME IS USN12DAT
C *** OUT FILE NAME IS USN12OUT
C *** when step change CO2 is used then this block will be -
C *** within C command
C *** WRITE(3,219)FN2,FN2P,FH2P,FCO2P,FCOP
C 219 FORMAT will be adjusted CO2 will be interchanged by N2

      FN2=FW4*X1/FWT1
      FN2P=FW5*X1/FWT
      FCOP=FW2*X1/FWT
      FCO2P=FW3*X1/FWT
      WFCO=CWT/FW2
      WFCO2=CWT/FW3

C ######################################

      RHCO=FH2P/FCOP
      RHCO2=FH2P/FCO2P
      FYT=FY1+FY2+FY3+FY5
      VO=FYT*T/273.0
      V=CWT/(FBD*1000.0)
      ST=V/VO
      SV=1.0/ST
      WRITE(3,207)T,P
      WRITE(3,194)FW1,FW2,FW3,FW4,FW5
      WRITE(3,208)FWT
      WRITE(3,219)FN2,FN2P,FH2P,FCO2P,FCOP
      WRITE(3,246)RHCO,RHCO2,WFCO,WFCO2,SV
      WRITE(3,94)
      WRITE(3,95)
      WRITE(3,211)
      WRITE(3.212)

      DO 76 LNA=1,NA
```

```
      READ(1,*)FRUN,TIME
      READ(1,*)(CHA(I),I=1,NC)

C     CHAM=MOL % IN MOLECULER SIEVE COLUMN
      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
      CHAP(I)=CHAM(I)/CHAS*X1
13    CONTINUE
      WRITE(3,213)FRUN,TIME,(CHAP(I),I=1,NC)
76    CONTINUE

C     TEMPERATURE PROFILES AT DIFFERENT TIMES
      WRITE(3,96)
      WRITE(3,97)
      DO 77 LNB=1,NB
      READ(1,*)TIME,(TR(I),I=1,NC)
      READ(1,*)(TW(I),I=1,NC)
      WRITE(3,7)TIME,(TR(I),I=1,NC)
      WRITE(3,8)(TW(I),I=1,NC)
77    CONTINUE
      WRITE(3,9)
75    CONTINUE

200    FORMAT('EXPERIMENTAL RESULT OF METHANATION OF CO & CO2 IN A FIXED
      ?BED REACTOR',/,26x,'Unsteady state')
201    FORMAT('---------------------------------------------------------
      ?-----------')
204    FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'8.23 gm',///,'DILUTION
      ? RATIO, CATALYST:INERT',5X,':',3x,'Undiluted',///,'CATALYST SIZE',
      ?22X,':',3X,'25-40 mesh.',///,'INERT SIZE',25X,':',3X,'25-40 Mesh.'
      ?,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (ZFCL)')
205    FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'8.0 cm.',///,'LENGT
      ?H OF INERT BED BEFORE CATALYST:',3X,'13.5 cm.',///,'LENGTH OF INER
      ?T BED AFTER CATALYST :',3X,'22.0 cm.',///,'BULK DENSITY OF CATALYS
      ?T',11X,':',3X,'0.7565 gm./cc.')
210    FORMAT(//,'BULK DENSITY OF INERT',14X,':',3X,'1.821 gm./cc.',///,'
      ?OD OF REACTOR',22X,':',3X,'17.00 mm.',///,'ID OF REACTOR',22X,':',
      ?3X,'12.00 mm.',///,'THERMOCOUPLE LOCATIONS FROM INLET  :',3X,'0.0
      ?cm. 3.0 cm. 6.0 cm. 8.0 cm.',/////////////////)

140    FORMAT(///////,'RUN NUMBER:',1x,I5)
141    FORMAT('*****************')
220    FORMAT(/,'INLET CONDITION:')
230    FORMAT('----------------')
207    FORMAT('TEMPERATURE:',F6.1,1X,'K',9X,'PRESSURE:',F6.1,1X,'mm.')
208    FORMAT(/,'TOTAL GAS FLOW RATE, mols./hr.:',F6.2)
194    FORMAT(/,'GAS FLOW RATE,mols./hr.: H2:',F8.4,4X,'CO:',F8.4,4X,'CO2
      ?:',F8.4,/,25X,'N2:',F8.4,4X,'to',1X,F8.4)
219    FORMAT(/,'STEP CHANGE:-  N2:-',F6.2,4X,'To',2X,F6.2,3X,'mol%',/,15
      ?X,'H2:',F6.2,4X,'CO2:',F6.2,4X,'CO:',F6.2,2X,'mol %')
246    FORMAT(/,'CO:H2 RATIO=1:',F7.2,15X,'CO2:H2 RATIO=1:',F7.2,/,'W/FCO
      ?,gm.hr./mol.=',F7.2,11X,'W/FCO2,gm.hr./mol.=',F7.2,/,'SPACE VELOCI
      ?TY,lit.gas/lit.cat.hr.=',F10.2)
94     FORMAT(/,'EXIT CONDITION:-')
95     FORMAT('----------------')
211    FORMAT('COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
      ?')
```

```
212   FORMAT('RUN NO.',5X,'TIME(min)',5X,'H2',10X,'N2',9X,'CH4',8X,'CO
     2')
213   FORMAT(F6.1,8X,F4.1,5X,F7.3,5X,F7.3,4X,F7.3,4X,F7.3)
96    FORMAT(/,'TEMPERATURE PROFILES AT DIFFERENT TIMES:-')
97    FORMAT('TIME(min)',15X,'T E M P E R A T U R E  in deg.C')
7     FORMAT(2X,F4.1,5X,'REACTOR:',4F10.1)
8     FORMAT(11X,'WALL    :',4F10.1)
9     FORMAT(///////)
      STOP
      END
```

```
4 2 3 5
36.0 1.0 1.0 1.13
1.2 0.7565 8.23
3020
512.0 760.0 39.5 107.0 0.88 0.0 1.3
3020.1 1.0
31566.0 5426954.0 26147.0 0.0
3020.2 5.0
29968.0 5483048.0 40312.0 375.0
3020.3 9.0
29247.0 5458694.0 41292.0 346.0
0.0 239.0 240.0 229.0 222.0
    247.0 248.0 243.0 237.0
1.0 239.0 240.0 231.0 223.0
    247.0 248.0 243.0 237.0
4.0 239.0 240.0 234.0 227.0
    244.0 245.0 244.0 239.0
10.0 239.0 241.0 235.0 227.0
     244.0 247.0 245.0 240.0
27.0 239.0 243.0 237.0 230.0
     246.0 248.0 247.0 242.0
3021
512.0 760.0 39.5 107.0 0.88 1.3 2.5
3021.1 1.0
29514.0 5488455.0 41307.0 350.0
3021.2 5.0
28442.0 54819660.0 47320.0 2273.0
3021.3 9.0
26736.0 5503702.0 46192.0 2066.0
0.0 239.0 244.0 237.0 229.0
    246.0 248.0 247.0 242.0
1.0 239.0 243.0 239.0 231.0
    244.0 246.0 246.0 242.0
6.0 239.0 245.0 239.0 232.0
    245.0 248.0 248.0 244.0
10.0 239.0 244.0 240.0 233.0
     244.0 246.0 248.0 244.0
37.0 239.0 248.0 243.0 233.0
     249.0 253.0 255.0 251.0
```

```
4 4 3 5
36.0 1.0 1.0 1.13
1.2 0.7565 8.23
3022
512.0 760.0 39.5 0.88 2.5 107.0 85.5
3022.1 1.0
28180.0 5465030.0 54777.0 959.0
3022.2 5.0
41896.0 5055202.0 78160.0 1227.0
3022.3 9.0
62077.0 5025431.0 81212.0 1132.0
0.0 239.0 248.0 243.0 233.0
    249.0 253.0 255.0 251.0
3.0 239.0 248.0 248.0 235.0
    249.0 253.0 255.0 250.0
7.0 239.0 247.0 248.0 235.0
    251.0 254.0 255.0 250.0
10.0 239.0 246.0 247.0 235.0
     250.0 253.0 255.0 250.0
35.0 239.0 246.0 247.0 237.0
     251.0 256.0 257.0 250.0
3023
512.0 760.0 39.5 0.88 2.5 85.5 66.0
3023.1 1.0
41303.0 5045308.0 79495.0 1549.0
3023.2 5.0
58291.0 4538482.0 116168.0 1168.0
3023.3 9.0
52766.0 4699557.0 109812.0 836.0
0.0 239.0 247.0 248.0 236.0
    249.0 254.0 255.0 250.0
4.0 239.0 248.0 255.0 236.0
    249.0 255.0 256.0 249.0
6.0 239.0 249.0 255.0 237.0
    251.0 257.0 258.0 251.0
12.0 239.0 246.0 253.0 235.0
     248.0 253.0 256.0 248.0
46.0 239.0 246.0 252.0 235.0
     251.0 255.0 256.0 249.0
3025
543.0 760.0 39.5 0.88 2.5 107.0 85.5
3025.1 1.0
24166.0 5697241.0 111585.0 253.0
3025.2 5.0
31013.0 5428067.0 147185.0 180.0
3025.3 9.0
31467.0 5429616.0 146538.0 94.0
0.0 270.0 288.0 292.0 293.0
    280.0 290.0 292.0 285.0
1.0 270.0 291.0 292.0 269.0
    280.0 291.0 291.0 283.0
4.0 270.0 292.0 292.0 268.0
    281.0 293.0 291.0 281.0
7.0 270.0 292.0 292.0 267.0
    281.0 293.0 290.0 281.0
35.0 270.0 292.0 293.0 268.0
     281.0 293.0 290.0 279.0
3026
543.0 760.0 39.5 0.88 2.5 85.5 66.0
3026.1 1.0
30683.0 5380906.0 144109.0 178.0
3026.2 5.0
```

```
44829.0 4920251.0 167462.0 0.0
3026.3 9.0
45785.0 4976709.0 168466.0 0.0
0.0 270.0 292.0 293.0 268.0
    281.0 292.0 290.0 279.0
3.0 270.0 294.0 278.0 257.0
    279.0 289.0 282.0 271.0
9.0 270.0 293.0 276.0 254.0
    279.0 288.0 279.0 267.0
16.0 270.0 293.0 276.0 253.0
     279.0 289.0 279.0 267.0
28.0 270.0 295.0 277.0 253.0
     280.0 290.0 279.0 267.0
```

EXPERIMENTAL RESULT OF METHANATION OF CO & CO2 IN FIXED BED REACTOR
Unsteady state

WEIGHT OF CATALYST : 8.23 gm

DILUTION RATIO, CATALYST:INERT : Undiluted

CATALYST SIZE : 25-40 mesh.

INERT SIZE : 25-40 Mesh.

CATALYST TYPE : Ni on Alumina (ZFCL)

LENGTH OF CATALYST BED : 8.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 13.5 cm.

LENGTH OF INERT BED AFTER CATALYST : 22.0 cm.

BULK DENSITY OF CATALYST : 0.7565 gm./cc.

BULK DENSITY OF INERT : 1.821 gm./cc.

OD OF REACTOR : 17.00 mm.

ID OF REACTOR : 12.00 mm.

THERMOCOUPLE LOCATIONS FROM INLET : 0.0 cm. 3.0 cm. 6.0 cm. 8.0 cm

```
RUN NUMBER:  3020
*****************

INLET CONDITION:
-----------------
TEMPERATURE: 512.0 K           PRESSURE: 760.0 mm.

GAS FLOW RATE,mols./hr.: H2:  1.7634     N2:  4.7768    CO:  0.0393
                        CO2:  0.0000     to   0.0580

TOTAL GAS FLOW RATE, mols./hr.:  6.64

STEP CHANGE:- CO2:-  0.00   To    0.87   mol%
               H2: 26.57    N2: 71.97    CO:  0.59  mol %

CO:H2 RATIO=1:  44.89                 CO2:H2 RATIO=1:  30.38
W/FCO,gm.hr./mol.= 209.49             W/FCO2,gm.hr./mol.= 141.81
SPACE VELOCITY,lit.gas/lit.cat.hr.=  25631.21

EXIT CONDITION:-
-----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)     H2         N2          CH4        CO
3020.1         1.0      17.245     82.358       0.397      0.000
3020.2         5.0      16.340     83.043       0.611      0.006
3020.3         9.0      16.067     83.297       0.630      0.006

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)               T E M P E R A T U R E  in deg.C
   0.0     REACTOR:     239.0      240.0      229.0      222.0
           WALL   :     247.0      248.0      243.0      237.0
   1.0     REACTOR:     239.0      240.0      231.0      223.0
           WALL   :     247.0      248.0      243.0      237.0
   4.0     REACTOR:     239.0      240.0      234.0      227.0
           WALL   :     244.0      245.0      244.0      239.0
  10.0     REACTOR:     239.0      241.0      235.0      227.0
           WALL   :     244.0      247.0      245.0      240.0
  27.0     REACTOR:     239.0      243.0      237.0      230.0
           WALL   :     246.0      248.0      247.0      242.0
```

```
RUN NUMBER:  3021
****************

INLET CONDITION:
----------------
TEMPERATURE: 512.0 K          PRESSURE: 760.0 mm.

GAS FLOW RATE,mols./hr.: H2:  1.7634     N2:  4.7768    CO:  0.0393
                        CO2:  0.0580     to   0.1116

TOTAL GAS FLOW RATE, mols./hr.:  6.69

STEP CHANGE:- CO2:-  0.87    To     1.67    mol%
               H2: 26.35    N2: 71.39    CO:   0.59   mol %

CO:H2 RATIO=1:  44.89                CO2:H2 RATIO=1:  15.80
W/FCO,gm.hr./mol.= 209.49            W/FCO2,gm.hr./mol.=  73.74
SPACE VELOCITY,lit.gas/lit.cat.hr.=  25838.07

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)     H2          N2          CH4         CO
3021.1          1.0      16.116      83.251       0.627       0.006
3021.2          5.0       1.832      98.079       0.085       0.005
3021.3          9.0      14.774      84.481       0.709       0.036

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      239.0       244.0       237.0       229.0
           WALL    :     246.0       248.0       247.0       242.0
   1.0     REACTOR:      239.0       243.0       239.0       231.0
           WALL    :     244.0       246.0       246.0       242.0
   6.0     REACTOR:      239.0       245.0       239.0       232.0
           WALL    :     245.0       248.0       248.0       244.0
  10.0     REACTOR:      239.0       244.0       240.0       233.0
           WALL    :     244.0       246.0       248.0       244.0
  37.0     REACTOR:      239.0       248.0       243.0       233.0
           WALL    :     249.0       253.0       255.0       251.0
```

```
RUN NUMBER:  3022
*****************

INLET CONDITION:
-----------------
TEMPERATURE: 512.0 K           PRESSURE: 760.0 mm.

GAS FLOW RATE,mols./hr.: H2:  1.7634    CO:  0.0393    CO2:  0.1116
                         N2:  4.7768    to   3.8170

TOTAL GAS FLOW RATE, mols./hr.:  5.73

STEP CHANGE:-  N2:- 71.39    To   66.60   mol%
               H2: 30.77    CO2:  1.95    CO:  0.69  mol %

CO:H2 RATIO=1:  44.89                CO2:H2 RATIO=1:  15.80
W/FCO,gm.hr./mol.= 209.49            W/FCO2,gm.hr./mol.=  73.74
SPACE VELOCITY,lit.gas/lit.cat.hr.=  22131.65

EXIT CONDITION:-
-----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.     TIME(min)     H2          N2          CH4          CO
3022.1         1.0      15.523      83.622       0.838        0.017
3022.2         5.0      22.704      76.098       1.177        0.021
3022.3         9.0      30.435      68.441       1.106        0.017

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      239.0      248.0      243.0      233.0
           WALL   :      249.0      253.0      255.0      251.0
   3.0     REACTOR:      239.0      248.0      248.0      235.0
           WALL   :      249.0      253.0      255.0      250.0
   7.0     REACTOR:      239.0      247.0      248.0      235.0
           WALL   :      251.0      254.0      255.0      250.0
  10.0     REACTOR:      239.0      246.0      247.0      235.0
           WALL   :      250.0      253.0      255.0      250.0
  35.0     REACTOR:      239.0      246.0      247.0      237.0
           WALL   :      251.0      256.0      257.0      250.0
```

```
RUN NUMBER:  3023
*****************

INLET CONDITION:
----------------
TEMPERATURE: 512.0 K          PRESSURE: 760.0 mm.

GAS FLOW RATE,mols./hr.: H2:   1.7634     CO:   0.0393     CO2:   0.1116
                         N2:   3.8170     to    2.9464

TOTAL GAS FLOW RATE, mols./hr.:  4.86

STEP CHANGE:-  N2:- 66.60    To    60.62    mol%
               H2: 36.28    CO2:   2.30    CO:   0.81   mol %

CO:H2 RATIO=1:  44.89                   CO2:H2 RATIO=1:  15.80
W/FCO,gm.hr./mol.= 209.49               W/FCO2,gm.hr./mol.=  73.74
SPACE VELOCITY,lit.gas/lit.cat.hr.=  18770.01

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)      H2          N2          CH4         CO
3023.1          1.0       22.483      76.288       1.202       0.026
3023.2          5.0       31.068      67.193       1.720       0.020
3023.3          9.0       28.310      70.039       1.637       0.014

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 T E M P E R A T U R E  in deg.C
  0.0      REACTOR:       239.0       247.0       248.0       236.0
           WALL   :       249.0       254.0       255.0       250.0
  4.0      REACTOR:       239.0       248.0       255.0       236.0
           WALL   :       249.0       255.0       256.0       249.0
  6.0      REACTOR:       239.0       249.0       255.0       237.0
           WALL   :       251.0       257.0       258.0       251.0
 12.0      REACTOR:       239.0       246.0       253.0       235.0
           WALL   :       248.0       253.0       256.0       248.0
 46.0      REACTOR:       239.0       246.0       252.0       235.0
           WALL   :       251.0       255.0       256.0       249.0
```

```
RUN NUMBER:  3025
*****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K          PRESSURE: 760.0 mm.

GAS FLOW RATE,mols./hr.: H2:  1.7634    CO:  0.0393    CO2:  0.1116
                         N2:  4.7768    to   3.8170

TOTAL GAS FLOW RATE, mols./hr.:  5.73

STEP CHANGE:-  N2:- 71.39    To    66.60   mol%
               H2: 30.77    CO2:  1.95    CO:  0.69   mol %

CO:H2 RATIO=1:  44.89               CO2:H2 RATIO=1:  15.80
W/FCO,gm.hr./mol.= 209.49           W/FCO2,gm.hr./mol.=  73.74
SPACE VELOCITY,lit.gas/lit.cat.hr.=  23471.65

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)     H2          N2          CH4         CO
3025.1          1.0      13.025      85.300       1.671       0.004
3025.2          5.0      16.684      81.114       2.199       0.003
3025.3          9.0      16.885      80.929       2.184       0.002

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                T E M P E R A T U R E  in deg.C
   0.0     REACTOR:      270.0      288.0      292.0      293.0
           WALL    :     280.0      290.0      292.0      285.0
   1.0     REACTOR:      270.0      291.0      292.0      269.0
           WALL    :     280.0      291.0      291.0      283.0
   4.0     REACTOR:      270.0      292.0      292.0      268.0
           WALL    :     281.0      293.0      291.0      281.0
   7.0     REACTOR:      270.0      292.0      292.0      267.0
           WALL    :     281.0      293.0      290.0      281.0
  35.0     REACTOR:      270.0      292.0      293.0      268.0
           WALL    :     281.0      293.0      290.0      279.0
```

```
RUN NUMBER:  3026
****************

INLET CONDITION:
----------------
TEMPERATURE: 543.0 K          PRESSURE: 760.0 mm.

GAS FLOW RATE,mols./hr.: H2:  1.7634    CO:  0.0393    CO2:  0.1116
                         N2:  3.8170    to   2.9464

TOTAL GAS FLOW RATE, mols./hr.:  4.86

STEP CHANGE:-  N2:- 66.60    To    60.62    mol%
               H2: 36.28    CO2:  2.30     CO:  0.81   mol %

CO:H2 RATIO=1:  44.89                 CO2:H2 RATIO=1:  15.80
W/FCO,gm.hr./mol.= 209.49             W/FCO2,gm.hr./mol.=  73.74
SPACE VELOCITY,lit.gas/lit.cat.hr.=  19906.48

EXIT CONDITION:-
----------------
COMPOSITION OF EXIT GASES (mol %) ON H2O & CO2 FREE BASIS:
RUN NO.      TIME(min)      H2          N2          CH4         CO
3026.1          1.0       16.661      81.162       2.174       0.003
3026.2          5.0       24.082      73.420       2.499       0.000
3026.3          9.0       24.263      73.258       2.480       0.000

TEMPERATURE PROFILES AT DIFFERENT TIMES:-
TIME(min)                 T E M P E R A T U R E  in deg.C
   0.0     REACTOR:       270.0       292.0       293.0       268.0
           WALL    :      281.0       292.0       290.0       279.0
   3.0     REACTOR:       270.0       294.0       278.0       257.0
           WALL    :      279.0       289.0       282.0       271.0
   9.0     REACTOR:       270.0       293.0       276.0       254.0
           WALL    :      279.0       288.0       279.0       267.0
  16.0     REACTOR:       270.0       293.0       276.0       253.0
           WALL    :      279.0       289.0       279.0       267.0
  28.0     REACTOR:       270.0       295.0       277.0       253.0
           WALL    :      280.0       290.0       279.0       267.0
```

APPENDIX I

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF ISOTHERMAL METHANATION OF CO_2 IN ISOTHERMAL REACTOR

```
C                     COMPUTER PROGRAM (ITCO2.FOR) FOR
C     STEADY STATE METHANATION OF CARBON DIOXIDE IN A FIXED BED REACTOR
C            ISOTHERMAL REACTOR IMMERSED IN A FLUIDIZED SAND BATH
C     This program calculates the product compositions and tabulates the
C     results by taking the initial conditions of operation and the GAS
C     CROMATOGRAPH peak areas for the products.

C     *NT       Number of runs
C     *FRUN     Run number
C     *NP       Number of peaks in porapak column
C     *NC       Number peaks in molecular sieve column
C     *JP       Number compound analyzed
C     *JPK      Total number of compounds
C     *RSP      Response factor in porapak column
C     *RSC      Response factor in molecular sieve column
C     *HYDCON   H2 conversion
C     *CO2CON    CO2 conversion
C     *PCNT     Mol % of product gases
C     *PR       Flow rate of water free compound
C     *CWT      Catalyst weight,gm.
C     *FD       Diameter of reactor,cm.
C     *FBD      Bulk density of catalyst pellet,gm/cc.
C     *FDP      Diameter of catalyst pellets,cm.
C     *FN2P     Mol % N2 in feed
C     *FH2P       "    H2    "
C     *FCO2P      "    CO2   "
C     *RT      Reactor temperature profile
C     *FY      Flow rate in feed,lit/hr.
C     *SV      Space velocity

      DIMENSION RSP(6),RPN(6),PRA(6),PRAM(6),PCNT(6),PR(6),TC(6),PC(6)
      DIMENSION RSC(4),CHA(4),CHAM(4),CHAP(4),TR(4),FM(6),ZC(6),FMP(6)
      DIMENSION FMU(6),FMUR(6),FPD1(6),FPD2(6),FPD(6),ET(6),FQ1(6),FQ(6)
      DIMENSION EM(6),F(6,6),Y(6),X(6),XY(6,6),E(6),FY(6),FW(6),FMW(6)

      OPEN(UNIT=1,FILE='ITCO2DAT',STATUS='UNKNOWN')
      OPEN(UNIT=3,FILE='ITCO2OUT',STATUS='UNKNOWN')

      READ(1,*)NC,NP,JP,JPK,N,NT
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)(RSP(I),I=1,NP)
      READ(1,*)(TC(I),PC(I),FM(I),ZC(I),FMU(I),I=1,N)
      READ(1,*)FD,FBD,CWT,FDP

      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)

      DO 75 LPN=1,NT

      READ(1,*)FRUN
      READ(1,*)T,P,(FY(I),I=1,N)
      READ(1,*)(CHA(I),I=1,NC)
      READ(1,*)(PRA(I),I=1,NP)
      READ(1,*)RT1,RT2,RT3

C     CALCULATE INLET COMPOSITIONS ******************
C     Here Component No. 1=H2,2=N2,3=CO2
```

```
      FA=0.785*FD**2.0
      X1=100.0
      X2=22.4
      FWT=0.0
      FYT=0.0
      DO 8 I=1,N
      FW(I)=FY(I)/X2
      FWT=FWT+FW(I)
      FYT=FYT+FY(I)
8     CONTINUE
      FTP=0.0
      AMW=0.0

      DO 9 I=1,N
      Y(I)=FW(I)/FWT
      FMP(I)=Y(I)*X1
      FTP=FTP+FMP(I)
      FMW(I)=Y(I)*FM(I)
      AMW=AMW+FMW(I)
9     CONTINUE
      RHCO2=FMP(1)/FMP(3)
      RH2N=FMP(1)/FMP(2)
      RCO2N=FMP(3)/FMP(2)
      WFCO2=CWT/FW(3)
      VO=FYT*T/273.0
      V=CWT/(FBD*1000.0)
      U=VO*1000.0/(3600.0*FA)
      RO=AMW*P/(82.05*760.0*T)
      ST=V/VO
      SV=1.0/ST

C     CALCULATE VISCOSITIES OF PURE COMPONENTS BY LUCAS METHOD

      DO 25 I=1,N
      TR(I)=T/TC(I)
      FMUR(I)=52.46*(FMU(I)**2.0)*PC(I)/(TC(I)**2.0)
      FPD1(I)=0.96+0.1*(TR(I)-0.7)
      FPD2(I)=1.0+30.55*((0.292-ZC(I))**2)
      IF(FMUR(I)-0.075)239,22,22
22    IF(FPD1(I)-0.0)32,33,33
33    FPD(I)=FPD2(I)*FPD1(I)
      GO TO 25
32    FPD(I)=FPD2(I)*(-FPD1(I))
      GO TO 25
239   IF(FMUR(I)-0.022)241,24,24
24    FPD(I)=FPD2(I)
      GO TO 25
241   FPD(I)=1.0
25    CONTINUE

C **  CALCULATE MIXURE VISCOSITY BY WILKE'S METHOD *****************

      Q=0.76
      DO 301 I=1,N
      FQ1(I)=1.0+0.00385*(((TR(I)-12.0)**2)**(1.0/FM(I)))
      IF(I-1)27,28,27
28    IF(TR(I)-12.0)29,30,30
30    FQ1(I)=1.0+0.00385*(((TR(I)-12.0)**2)**(1.0/FM(I)))
      FQ(I)=1.22*(Q**0.15)*(FQ1(I)+1.0)
      GO TO 31
29    FQ(I)=1.22*(Q**0.15)*(FQ1(I)-1.0)
```

```
      GO TO 31
27    FQ(I)=1.0
31    ET(I)=0.176*((TC(I)/((FM(I)**3.0)*(PC(I)**4.0)))**(1.0/6.0))
      EM(I)=((0.807*TR(I)**0.618-0.357*EXP(-0.449*TR(I))+0.340*EXP(-4.05
     +8*TR(I))+0.018)*FPD(I)*FQ(I))/ET(I)
301   CONTINUE

      DO 110 I=1,N
      DO 120 J=1,N
      F(I,J)=((1.0+((EM(I)/EM(J))**0.5)*((FM(J)/FM(I))**0.25))**2.0)/((
     +8.0*(1.0+FM(I)/FM(J)))**0.5)
120   CONTINUE
110   CONTINUE

      EMT=0.0
      DO 180 I=1,N
      X(I)=Y(I)*EM(I)
      YX=0.0
      DO 208 J=1,N
      XY(I,J)=Y(J)*F(I,J)
      YX=YX+XY(I,J)
208   CONTINUE
      E(I)=X(I)/YX
      EMT=EMT+E(I)
180   CONTINUE
      EMTT=EMT*1.0E-06
      FRE1=FD*U*RO/EMTT
      FRE2=FDP*U*RO/EMTT

C $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C     CALCULATE EXIT COMPOSITION
C     Here component no. 1=H2, 2=N2, 3=CH4, 4=CO, 5=CO2, 6=H2O
C     CHAM=MOL % IN MOLECULER SIEVE COLUMN

      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
      CHAP(I)=CHAM(I)/CHAS*X1
13    CONTINUE

C PRAM= mol % in PORAPAK column **************

      PRAS=0.0
      DO 10 I=1,NP
      PRAM(I)=PRA(I)*RSP(I)
      PRAS=PRAS+PRAM(I)
10    CONTINUE
      DO 11 I=1,NP
      PRAM(I)=PRAM(I)/PRAS*X1
11    CONTINUE

C Find mol % in exit gas for molecular sieve column. Peak 1 in porapak
C column stands for all the peaks in molecular sieve column.
C There are only two peaks in porapak column,second peak is component
C no. JP (CO2)

      TCNT=0.0
      DO 14 I=1,NC
```

```
      PCNT(I)=CHAP(I)*PRAM(1)/X1
      TCNT=TCNT+PCNT(I)
 14   CONTINUE
      PCNT(JP)=PRAM(NP)
      FR=FW(2)/PCNT(2)*X1

C FR= Flow rate of H2O free product ******************
C PR=Flow rate of H2O free compounds ***************

      DO 21 I=1,JP
      PR(I)=FR*PCNT(I)/X1
 21   CONTINUE

C Amount of H2O formed is found out by material balance calculations

      R1=PR(3)
      R2=PR(4)
      TCO2R=R1+R2
      TH2R=4.0*R1+R2
      TH2OP=2.0*R1+R2
      PR(6)=TH2OP
      PTOT=FR+PR(6)
      DO 23 I=1,JPK
      PCNT(I)=PR(I)/PTOT*X1
 23   CONTINUE

C PTOT=Total flow rate of product *************
C Calculation for product gas composition has been completed
C RPN=> Mol component/Mol N2 in component

      DO 26 I=1,JPK
      RPN(I)=PCNT(I)/PCNT(2)
 26   CONTINUE
      CO2CON=(RCO2N-RPN(5))/RCO2N*X1
      HYDCON=(RH2N-RPN(1))/RH2N*X1

      WRITE(3,140)FRUN
      WRITE(3,141)
      WRITE(3,220)
      WRITE(3,230)
      WRITE(3,207)T,P
      WRITE(3,251)
      WRITE(3,224)FY(1),FW(1),FMP(1)
      WRITE(3,212)FY(2),FW(2),FMP(2)
      WRITE(3,217)FY(3),FW(3),FMP(3)
      WRITE(3,216)
      WRITE(3,213)FYT,FWT,FTP
      WRITE(3,246)SV,RHCO2,WFCO2
      WRITE(3,234)FRE1,FRE2
      WRITE(3,215)
      WRITE(3,229)
      WRITE(3,293)PTOT
      WRITE(3,222)
      WRITE(3,223)
      WRITE(3,100)(PCNT(I),I=1,JPK)
      WRITE(3,105)HYDCON,CO2CON
      WRITE(3,261)
      WRITE(3,97)RT1,RT2,RT3
 75   CONTINUE

 200  FORMAT('EXPERIMENTAL RESULT OF METHANATION OF CO2 IN A FIXED BED R
```

```
     +EACTOR',/,6X,'ISOTHERMAL REACTOR IMMERSED IN A FLUIDIZED SAND BATH
     +')
201   FORMAT('---------------------------------------------------------
     +-----')
204   FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'0.94 gm',///,'DILUTION
     + RATIO, CATALYST:INERT',5X,':',3X,'1:8',///,'CATALYST SIZE',22X,':
     +',3X,'25-40 mesh',///,'INERT SIZE',25X,':',3X,'25-40 & 40-65 mesh'
     +,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (UFFL)')
205   FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'5.0 cm.',///,'LENGT
     +H OF INERT BED BEFORE CATALYST:',3X,'5.9 cm.',///,'LENGTH OF INERT
     + BED AFTER CATALYST :',3X,'4.0 cm.',///,'BULK DENSITY OF CATALYST'
     +,11X,':',3X,'0.6815 gm/cc.')
210   FORMAT(//,'BULK DENSITY OF INERT',14X,':',3x,'1.831 gm/cc.',///,'O
     +D OF REACTOR',22X,':',3X,'12.9 mm.',///,'ID OF REACTOR',22X,':',3X
     +,'10.5 mm.',///,'THERMOCOUPLE LOCATIONS FROM INLET  :',3X,'0.0 cm.
     + 2.5 cm. 5.0 cm.',////////////////////)
140   FORMAT(//,'RUN NUMBER:',1x,F6.1)
141   FORMAT('******************')
220   FORMAT('INLET CONDITION:')
230   FORMAT('----------------')
207   FORMAT('TEMPERATURE:',F6.1,1X,'K',11X,'PRESSURE:',F6.1,1X,'mm.')
251   FORMAT(10X,'FLOW RATE,lit/hr.',4X,'FLOW RATE,mol/hr.',9X,'mol %')
224   FORMAT('H2',7X,F10.2,12X,F10.4,10X,F10.2)
212   FORMAT('N2',7X,F10.2,12X,F10.4,10X,F10.2)
217   FORMAT('CO2',6X,F10.2,12X,F10.4,10X,F10.2)
216   FORMAT('-----',7X,'----------',12X,'---------',11X,'---------')
213   FORMAT('TOTAL',4X,F10.2,12X,F10.4,10X,F10.2)
246   FORMAT(/,'SPACE VELOCITY,lit.gas/lit.cat.hr.',19x,'=',E10.4,/,'CO2
     +:H2 RATIO   =  1:',F7.2,8X,'W/FCO2, gm.hr/mol.=',F7.2)
234   FORMAT('RE(Superficial)=',F7.2,12X,'RE(Particle)       =',F7.2)
215   FORMAT(/,'EXIT CONDITION:-')
229   FORMAT('----------------')
293   FORMAT('GAS FLOW RATE,mols/hr.',11X,':',F8.2)
222   FORMAT('COMPOSITION OF EXIT GASES (mol %):')
223   FORMAT(5X,'H2',9X,'N2',9X,'CH4',9X,'CO',9X,'CO2',9X,'H2O')
100   FORMAT(F10.4,1X,F10.4,1X,F10.4,1X,F10.4,2X,F10.4,2X,F10.4)
105   FORMAT(/,'******* CONV. OF H2 :',F8.2,1X,'%',4X,'******* CONV. OF
     +CO2 :',F8.2,1X,'%')
261   FORMAT(/,'TEMPERATURE PROFILE:-')
97    FORMAT('REACTOR:',3F10.1,1X,'C',/)

      STOP
      END
```

```
4 2 5 6 3 34
36.0 1.0 1.0 1.13
1.0 0.8
33.2 13.0 2.0 0.303 0.0
126.2 33.9 28.0 0.29 0.0
304.1 73.8 44.0 0.274 0.0
1.05 0.6815 0.94 0.0564
5001.1
536.0 760.0 17.0 92.0 0.88
1965.0 1636163.0 3584.0 145.0
3698077.0 19308.0
263.0 254.0 253.0
5001.2
535.0 760.0 17.0 92.0 0.88
2093.0 1642180.0 3356.0 129.0
3692258.0 18772.0
262.0 253.0 252.0
5002.1
531.0 760.0 39.5 126.6 1.34
22329.0 6009081.0 7500.0 548.0
13552097.0 87601.0
258.0 249.0 246.0
5002.2
531.0 760.0 39.5 126.6 1.34
26936.0 6093086.0 7435.0 574.0
13319384.0 109624.0
258.0 250.0 247.0
5003.1
531.0 760.0 68.0 135.5 1.64
47553.0 5049684.0 6418.0 0.0
11667333.0 111867.0
258.0 251.0 249.0
5003.2
531.0 760.0 68.0 135.5 1.64
47307.0 4374315.0 7086.0 0.0
11416029.0 112201.0
257.0 250.0 248.0
5004.1
532.0 760.0 17.0 52.5 0.88
18936.0 5672320.0 28121.0 0.0
12922097.0 162784.0
259.0 255.0 254.0
5004.2
530.0 760.0 17.0 52.5 0.88
22624.0 5590977.0 27069.0 0.0
12803098.0 162443.0
257.0 253.0 252.0
5005.1
524.0 760.0 39.5 66.0 1.34
90564.0 561313724.0 16401.0 0.0
11578350.0 159179.0
251.0 245.0 242.0
5005.2
523.0 760.0 39.5 66.0 1.34
92225.0 5479287.0 12167.0 0.0
11445116.0 137137.0
250.0 245.0 244.0
5006.0
533.0 760.0 39.5 90.0 1.64
79797.0 6184863.0 23348.0 0.0
```

```
13467273.0 91212.0
261.0 251.0 250.0
5007.1
528.0 760.0 17.0 37.1 0.88
59112.0 6007228.0 42784.0 0.0
13038952.0 118549.0
255.0 251.0 250.0
5007.2
529.0 760.0 17.0 37.1 0.88
76683.0 5962481.0 39578.0 0.0
12963473.0 131963.0
256.0 249.0 250.0
5008.1
531.0 760.0 39.5 42.9 1.34
131905.0 4407682.0 41796.0 0.0
8952299.0 144013.0
258.0 255.0 262.0
5008.2
533.0 760.0 39.5 42.9 1.34
132796.0 4495906.0 40084.0 0.0
11033392.0 174162.0
260.0 255.0 254.0
5009.1
534.0 760.0 39.5 61.4 1.64
96093.0 5329830.0 27350.0 0.0
11033489.0 172438.0
261.0 254.0 252.0
5009.2
531.0 760.0 39.5 61.4 1.64
96858.0 5264550.0 24603.0 0.0
11033492.0 174162.0
258.0 252.0 250.0
5010.0
522.0 760.0 17.0 92.0 0.88
28722.0 8080356.0 10925.0 557.0
18468592.0 38811.0
249.0 242.0 239.0
5011.1
517.0 760.0 39.5 126.6 1.34
38066.0 7394077.0 5250.0 0.0
16308897.0 49747.0
244.0 237.0 236.0
5011.2
517.0 760.0 39.5 126.6 1.34
37875.0 7356368.0 4882.0 0.0
16280342.0 49468.0
244.0 236.0 235.0
5012.1
522.0 760.0 68.0 135.5 1.64
83201.0 6292175.0 7052.0 0.0
13234220.0 64132.0
249.0 243.0 241.0
5012.2
522.0 760.0 68.0 135.5 1.64
91269.0 6265539.0 8074.0 0.0
13170831.0 70235.0
248.0 245.0 243.0
5013.1
520.0 760.0 17.0 52.5 0.88
41009.0 7324236.0 24631.0 129.0
15935347.0 105248.0
247.0 243.0 241.0
```

```
5013.2
514.0 760.0 17.0 52.5 0.88
41070.0 7043601.0 17878.0 0.0
15496196.0 88579.0
241.0 238.0 237.0
5014.1
513.0 760.0 39.5 66.0 1.34
96191.0 5688067.0 11746.0 0.0
11734881.0 121246.0
240.0 238.0 237.0
5014.2
513.0 760.0 39.5 66.0 1.34
96815.0 5667350.0 15101.0 0.0
11678415.0 122377.0
240.0 238.0 238.0
5015.1
520.0 760.0 39.5 90.0 1.64
62975.0 6500005.0 13209.0 3983.0
14241380.0 127540.0
247.0 241.0 240.0
5015.2
515.0 760.0 39.5 90.0 1.64
62740.0 6576348.0 10271.0 726.0
14185555.0 125721.0
242.0 238.0 238.0
5016.1
517.0 760.0 17.0 37.1 0.88
55899.0 6401652.0 35060.0 0.0
14012364.0 121368.0
244.0 241.0 241.0
5016.2
517.0 760.0 17.0 37.1 0.88
54398.0 6412805.0 31079.0 0.0
13996259.0 123579.0
244.0 241.0 241.0
5017.1
517.0 760.0 39.5 42.9 1.34
139454.0 5022734.0 29765.0 1908.0
10043454.0 169912.0
244.0 241.0 241.0
5017.2
515.0 760.0 39.5 42.9 1.34
137483.0 5099600.0 24431.0 760.0
10152929.0 175141.0
242.0 240.0 240.0
5018.1
516.0 760.0 39.5 61.4 1.64
94950.0 5575108.0 17803.0 188.0
11561844.0 142532.0
243.0 239.0 239.0
5018.2
516.0 760.0 39.5 61.4 1.64
92297.0 5609741.0 23438.0 0.0
11557973.0 137769.0
243.0 240.0 240.0
```

EXPERIMENTAL RESULT OF METHANATION OF CO2 IN A FIXED BED REACTOR ISOTHERMAL REACTOR IMMERSED IN A FLUIDIZED SAND BATH

WEIGHT OF CATALYST : 0.94 gm

DILUTION RATIO, CATALYST:INERT : 1:8

CATALYST SIZE : 25-40 mesh

INERT SIZE : 25-40 & 40-65 mesh

CATALYST TYPE : Ni on Alumina (UFFL)

LENGTH OF CATALYST BED : 5.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 5.9 cm.

LENGTH OF INERT BED AFTER CATALYST : 4.0 cm.

BULK DENSITY OF CATALYST : 0.6815 gm/cc.

BULK DENSITY OF INERT : 1.831 gm/cc.

OD OF REACTOR : 12.9 mm.

ID OF REACTOR : 10.5 mm.

THERMOCOUPLE LOCATIONS FROM INLET : 0.0 cm. 2.5 cm. 5.0 cm.

```
RUN NUMBER: 5001.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 536.0 K                PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.              mol %
H2            17.00                     0.7589                     15.47
N2            92.00                     4.1071                     83.73
CO2            0.88                     0.0393                      0.80
-----      ----------               ---------                  ---------
TOTAL        109.88                     4.9054                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                            =0.1564E+06
CO2:H2 RATIO    =  1:  19.32            W/FCO2, gm.hr/mol.=  23.93
RE(Superficial)= 143.40                 RE(Particle)       =   7.70

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :    4.33
COMPOSITION OF EXIT GASES (mol %):
     H2         N2          CH4         CO          CO2         H2O
  4.1006     94.8430     0.2078      0.0095      0.4142      0.4250

******* CONV. OF H2 :   76.60 %    ******* CONV. OF CO2 :   54.34 %

TEMPERATURE PROFILE:-
REACTOR:      263.0      254.0      253.0 C


RUN NUMBER: 5001.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 535.0 K                PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.              mol %
H2            17.00                     0.7589                     15.47
N2            92.00                     4.1071                     83.73
CO2            0.88                     0.0393                      0.80
-----      ----------               ---------                  ---------
TOTAL        109.88                     4.9054                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                            =0.1561E+06
CO2:H2 RATIO    =  1:  19.32            W/FCO2, gm.hr/mol.=  23.93
RE(Superficial)= 143.58                 RE(Particle)       =   7.71

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :    4.34
COMPOSITION OF EXIT GASES (mol %):
     H2         N2          CH4         CO          CO2         H2O
  4.3431     94.6563     0.1934      0.0084      0.4035      0.3953

******* CONV. OF H2 :   75.17 %    ******* CONV. OF CO2 :   55.44 %

TEMPERATURE PROFILE:-
REACTOR:      262.0      253.0      252.0 C
```

```
RUN NUMBER: 5002.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 531.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2            39.50                 1.7634                  23.59
N2           126.60                 5.6518                  75.61
CO2            1.34                 0.0598                   0.80
-----      ----------           ---------              ---------
TOTAL        167.44                 7.4750                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                     =0.2361E+06
CO2:H2 RATIO     =   1:   29.48     W/FCO2, gm.hr/mol.=  15.71
RE(Superficial)= 198.37             RE(Particle)      =  10.66

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :    6.46
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4         CO          CO2          H2O
  11.6975     87.4438     0.1091      0.0090      0.5133       0.2273

******* CONV. OF H2 :    57.13 %     ******* CONV. OF CO2 :    44.54 %

TEMPERATURE PROFILE:-
REACTOR:       258.0      249.0      246.0 C


RUN NUMBER: 5002.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 531.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2            39.50                 1.7634                  23.59
N2           126.60                 5.6518                  75.61
CO2            1.34                 0.0598                   0.80
-----      ----------           ---------              ---------
TOTAL        167.44                 7.4750                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                     =0.2361E+06
CO2:H2 RATIO     =   1:   29.48     W/FCO2, gm.hr/mol.=  15.71
RE(Superficial)= 198.37             RE(Particle)      =  10.66

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :    6.62
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4         CO          CO2          H2O
  13.5946     85.4218     0.1042      0.0091      0.6527       0.2176

******* CONV. OF H2 :    48.99 %     ******* CONV. OF CO2 :    27.81 %

TEMPERATURE PROFILE:-
REACTOR:       258.0      250.0      247.0 C
```

```
RUN NUMBER: 5003.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 531.0 K                PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol %
H2            68.00                     3.0357                   33.15
N2           135.50                     6.0491                   66.05
CO2            1.64                     0.0732                    0.80
-----      ----------               ----------               ----------
TOTAL        205.14                     9.1580                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                              =0.2893E+06
CO2:H2 RATIO    =   1:   41.46          W/FCO2, gm.hr/mol.=   12.84
RE(Superficial)= 212.53                 RE(Particle)      =   11.42

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                     :      8.19
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4           CO           CO2          H2O
   25.0544     73.9040      0.0939       0.0000       0.7598       0.1879

******* CONV. OF H2 :    32.45 %     ******* CONV. OF CO2 :    15.06 %

TEMPERATURE PROFILE:-
REACTOR:       258.0      251.0      249.0 C
```

```
RUN NUMBER: 5003.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 531.0 K                PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.            mol %
H2            68.00                     3.0357                   33.15
N2           135.50                     6.0491                   66.05
CO2            1.64                     0.0732                    0.80
-----      ----------               ----------               ----------
TOTAL        205.14                     9.1580                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                              =0.2893E+06
CO2:H2 RATIO    =   1:   41.46          W/FCO2, gm.hr/mol.=   12.84
RE(Superficial)= 212.53                 RE(Particle)      =   11.42

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                     :      8.50
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4           CO           CO2          H2O
   27.7078     71.1680      0.1153       0.0000       0.7783       0.2306

******* CONV. OF H2 :    22.42 %     ******* CONV. OF CO2 :     9.64 %

TEMPERATURE PROFILE:-
REACTOR:       257.0      250.0      248.0 C
```

```
RUN NUMBER: 5004.1
*****************
INLET CONDITION:
----------------
TEMPERATURE: 532.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2           17.00                  0.7589                   24.15
N2           52.50                  2.3438                   74.60
CO2           0.88                  0.0393                    1.25
-----      ----------             ---------                ---------
TOTAL        70.38                  3.1420                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.9943E+05
CO2:H2 RATIO    =  1:  19.32        W/FCO2, gm.hr/mol.=   23.93
RE(Superficial)=  82.95             RE(Particle)        =    4.46

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                    :    2.69
COMPOSITION OF EXIT GASES (mol %):
     H2           N2           CH4          CO           CO2          H2O
  10.4833      87.2303      0.4325       0.0000       0.9891       0.8649

******* CONV. OF H2 :   62.89 %    ******* CONV. OF CO2 :   32.35 %

TEMPERATURE PROFILE:-
REACTOR:      259.0      255.0      254.0 C



RUN NUMBER: 5004.2
*****************
INLET CONDITION:
----------------
TEMPERATURE: 530.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2           17.00                  0.7589                   24.15
N2           52.50                  2.3438                   74.60
CO2           0.88                  0.0393                    1.25
-----      ----------             ---------                ---------
TOTAL        70.38                  3.1420                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.9906E+05
CO2:H2 RATIO    =  1:  19.32        W/FCO2, gm.hr/mol.=   23.93
RE(Superficial)=  83.16             RE(Particle)        =    4.47

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                    :    2.75
COMPOSITION OF EXIT GASES (mol %):
     H2           N2           CH4          CO           CO2          H2O
  12.4309      85.3332      0.4131       0.0000       0.9965       0.8263

******* CONV. OF H2 :   55.01 %    ******* CONV. OF CO2 :   30.33 %

TEMPERATURE PROFILE:-
REACTOR:      257.0      253.0      252.0 C
```

```
RUN NUMBER: 5005.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 524.0 K                  PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2            39.50                       1.7634                     36.97
N2            66.00                       2.9464                     61.77
CO2            1.34                       0.0598                      1.25
-----       ----------               ----------                 ---------
TOTAL        106.84                       4.7696                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                              =0.1487E+06
CO2:H2 RATIO    =   1:   29.48            W/FCO2, gm.hr/mol.=   15.71
RE(Superficial)= 105.84                   RE(Particle)       =    5.69

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :     3.00
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
   0.5711     98.3324     0.0029      0.0000       1.0878       0.0057

******* CONV. OF H2 :    99.03 %     ******* CONV. OF CO2 :    45.51 %

TEMPERATURE PROFILE:-
REACTOR:      251.0       245.0       242.0 C



RUN NUMBER: 5005.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 523.0 K                  PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2            39.50                       1.7634                     36.97
N2            66.00                       2.9464                     61.77
CO2            1.34                       0.0598                      1.25
-----       ----------               ----------                 ---------
TOTAL        106.84                       4.7696                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                              =0.1484E+06
CO2:H2 RATIO    =   1:   29.48            W/FCO2, gm.hr/mol.=   15.71
RE(Superficial)= 105.98                   RE(Particle)       =    5.69

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :     4.80
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  37.2194     61.4245     0.1364      0.0000       0.9469       0.2728

******* CONV. OF H2 :    -1.25 %     ******* CONV. OF CO2 :    24.07 %

TEMPERATURE PROFILE:-
REACTOR:      250.0       245.0       244.0 C
```

```
RUN NUMBER: 5006.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 533.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.            mol %
H2             39.50                  1.7634                   30.12
N2             90.00                  4.0179                   68.63
CO2             1.64                  0.0732                    1.25
-----        ----------            ---------              ---------
TOTAL         131.14                  5.8545                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1856E+06
CO2:H2 RATIO    =   1:  24.09         W/FCO2, gm.hr/mol.=  12.84
RE(Superficial)= 142.18               RE(Particle)       =   7.64

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :     5.96
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO           CO2          H2O
  31.3038     67.3967      0.2544      0.0000       0.5362       0.5088

******* CONV. OF H2 :    -5.83 %    ******* CONV. OF CO2 :    56.34 %

TEMPERATURE PROFILE:-
REACTOR:      261.0      251.0      250.0 C



RUN NUMBER: 5007.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 528.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.            mol %
H2             17.00                  0.7589                   30.92
N2             37.10                  1.6563                   67.48
CO2             0.88                  0.0393                    1.60
-----        ----------            ---------              ---------
TOTAL          54.98                  2.4545                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.7709E+05
CO2:H2 RATIO    =   1:  19.32         W/FCO2, gm.hr/mol.=  23.93
RE(Superficial)=  59.49               RE(Particle)       =   3.20

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :     2.29
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO           CO2          H2O
  25.5678     72.1754      0.5140      0.0000       0.7147       1.0281

******* CONV. OF H2 :    22.69 %    ******* CONV. OF CO2 :    58.25 %

TEMPERATURE PROFILE:-
REACTOR:      255.0      251.0      250.0 C
```

```
RUN NUMBER: 5007.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 529.0 K                PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.           mol %
H2             17.00                    0.7589                  30.92
N2             37.10                    1.6563                  67.48
CO2             0.88                    0.0393                   1.60
-----       ----------              ---------              ---------
TOTAL          54.98                    2.4545                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.7724E+05
CO2:H2 RATIO     =   1:   19.32         W/FCO2, gm.hr/mol.=   23.93
RE(Superficial)=   59.41                RE(Particle)      =    3.19

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                :     2.48
COMPOSITION OF EXIT GASES (mol %):
     H2           N2           CH4           CO           CO2           H2O
   30.9720     66.8952      0.4440       0.0000       0.8006        0.8881

******* CONV. OF H2 :   -1.04 %     ******* CONV. OF CO2 :    49.54 %

TEMPERATURE PROFILE:-
REACTOR:       256.0      249.0      250.0 C



RUN NUMBER: 5008.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 531.0 K                PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.         FLOW RATE,mol/hr.           mol %
H2             39.50                    1.7634                  47.17
N2             42.90                    1.9152                  51.23
CO2             1.34                    0.0598                   1.60
-----       ----------              ---------              ---------
TOTAL          83.74                    3.7384                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.1181E+06
CO2:H2 RATIO     =   1:   29.48         W/FCO2, gm.hr/mol.=   15.71
RE(Superficial)=   69.64                RE(Particle)      =    3.74

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                :     4.08
COMPOSITION OF EXIT GASES (mol %):
     H2           N2           CH4           CO           CO2           H2O
   50.5167     46.8901      0.4446       0.0000       1.2593        0.8893

******* CONV. OF H2 :  -17.01 %     ******* CONV. OF CO2 :    14.02 %

TEMPERATURE PROFILE:-
REACTOR:       258.0      255.0      262.0 C
```

```
RUN NUMBER: 5008.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 533.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.            mol %
H2              39.50                 1.7634                   47.17
N2              42.90                 1.9152                   51.23
CO2              1.34                 0.0598                    1.60
-----        ----------           ----------               ---------
TOTAL           83.74                 3.7384                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1185E+06
CO2:H2 RATIO    =   1:  29.48     W/FCO2, gm.hr/mol.=   15.71
RE(Superficial)=   69.46          RE(Particle)       =    3.73

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :    4.05
COMPOSITION OF EXIT GASES (mol %):
    H2           N2          CH4          CO          CO2          H2O
  50.2462     47.2534      0.4213      0.0000      1.2365       0.8426

******* CONV. OF H2 :  -15.49 %    ******* CONV. OF CO2 :    16.22 %

TEMPERATURE PROFILE:-
REACTOR:       260.0      255.0      254.0 C



RUN NUMBER: 5009.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 534.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.            mol %
H2              39.50                 1.7634                   38.52
N2              61.40                 2.7411                   59.88
CO2              1.64                 0.0732                    1.60
-----        ----------           ----------               ---------
TOTAL          102.54                 4.5777                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1454E+06
CO2:H2 RATIO    =   1:  24.09     W/FCO2, gm.hr/mol.=   12.84
RE(Superficial)=   98.19          RE(Particle)       =    5.27

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :    4.62
COMPOSITION OF EXIT GASES (mol %):
    H2           N2          CH4          CO          CO2          H2O
  38.5165     59.3426      0.3045      0.0000      1.2273       0.6090

******* CONV. OF H2 :    -0.89 %    ******* CONV. OF CO2 :    22.57 %

TEMPERATURE PROFILE:-
REACTOR:       261.0      254.0      252.0 C
```

```
RUN NUMBER: 5009.2
*****************
INLEFT CONDITION:
----------------
TEMPERATURE: 531.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.            mol %
H2            39.50                   1.7634                   38.52
N2            61.40                   2.7411                   59.88
CO2            1.64                   0.0732                    1.60
-----       ----------            ---------               ---------
TOTAL        102.54                   4.5777                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1446E+06
CO2:H2 RATIO    =  1:  24.09          W/FCO2, gm.hr/mol.=  12.84
RE(Superficial)=  98.57               RE(Particle)      =   5.29

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                :     4.65
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4         CO          CO2          H2O
   39.0204     58.9135     0.2753      0.0000      1.2402       0.5506

******* CONV. OF H2 :   -2.96 %    ******* CONV. OF CO2 :     21.19 %

TEMPERATURE PROFILE:-
REACTOR:      258.0      252.0      250.0 C



RUN NUMBER: 5010.0
*****************
INLET CONDITION:
----------------
TEMPERATURE: 522.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.            mol %
H2            17.00                   0.7589                   15.47
N2            92.00                   4.1071                   83.73
CO2            0.88                   0.0393                    0.80
-----       ----------            ---------               ---------
TOTAL        109.88                   4.9054                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1523E+06
CO2:H2 RATIO    =  1:  19.32          W/FCO2, gm.hr/mol.=  23.93
RE(Superficial)= 146.02               RE(Particle)      =   7.84

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                :     4.66
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4         CO          CO2          H2O
   11.2835     88.1777     0.1192      0.0069      0.1674       0.2453

******* CONV. OF H2 :    30.75 %    ******* CONV. OF CO2 :     80.15 %

TEMPERATURE PROFILE:-
REACTOR:      249.0      242.0      239.0 C
```

```
RUN NUMBER: 5011.1
******************
INLEX CONDITION:
----------------
TEMPERATURE: 517.0 K               PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.        FLOW RATE,mol/hr.           mol %
H2              39.50                  1.7634                  23.59
N2             126.60                  5.6518                  75.61
CO2              1.34                  0.0598                   0.80
-----        ----------            ---------               ---------
TOTAL          167.44                  7.4750                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2299E+06
CO2:H2 RATIO    =   1:  29.48          W/FCO2, gm.hr/mol.=   15.71
RE(Superficial)= 202.03                RE(Particle)      =   10.85

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     6.73
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO           CO2          H2O
   15.5696     84.0083     0.0596       0.0000       0.2431       0.1193

******* CONV. OF H2 :    40.60 %     ******* CONV. OF CO2 :    72.66 %

TEMPERATURE PROFILE:-
REACTOR:      244.0      237.0      236.0 C



RUN NUMBER: 5011.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 517.0 K               PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.        FLOW RATE,mol/hr.           mol %
H2              39.50                  1.7634                  23.59
N2             126.60                  5.6518                  75.61
CO2              1.34                  0.0598                   0.80
-----        ----------            ---------               ---------
TOTAL          167.44                  7.4750                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.2299E+06
CO2:H2 RATIO    =   1:  29.48          W/FCO2, gm.hr/mol.=   15.71
RE(Superficial)= 202.03                RE(Particle)      =   10.85

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     6.73
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO           CO2          H2O
   15.5727     84.0178     0.0558       0.0000       0.2422       0.1115

******* CONV. OF H2 :    40.59 %     ******* CONV. OF CO2 :    72.76 %

TEMPERATURE PROFILE:-
REACTOR:      244.0      236.0      235.0 C
```

```
RUN NUMBER: 5012.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 522.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.           mol %
H2             68.00                  3.0357                  33.15
N2            135.50                  6.0491                  66.05
CO2             1.64                  0.0732                   0.80
-----        ----------           ---------                ---------
TOTAL         205.14                  9.1580                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2844E+06
CO2:H2 RATIO     =   1:   41.46       W/FCO2, gm.hr/mol.=   12.84
RE(Superficial)= 215.02               RE(Particle)      =   11.55

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                       :     8.98
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO           CO2          H2O
   32.0531     67.3349     0.0755      0.0000       0.3856       0.1509

******* CONV. OF H2 :     5.14 %    ******* CONV. OF CO2 :     52.69 %

TEMPERATURE PROFILE:-
REACTOR:      249.0      243.0      241.0 C



RUN NUMBER: 5012.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 522.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.           mol %
H2             68.00                  3.0357                  33.15
N2            135.50                  6.0491                  66.05
CO2             1.64                  0.0732                   0.80
-----        ----------           ---------                ---------
TOTAL         205.14                  9.1580                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2844E+06
CO2:H2 RATIO     =   1:   41.46       W/FCO2, gm.hr/mol.=   12.84
RE(Superficial)= 215.02               RE(Particle)      =   11.55

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                       :     9.28
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO           CO2          H2O
   34.1681     65.1559     0.0840      0.0000       0.4241       0.1679

******* CONV. OF H2 :    -4.50 %    ******* CONV. OF CO2 :     46.22 %

TEMPERATURE PROFILE:-
REACTOR:      248.0      245.0      243.0 C
```

```
RUN NUMBER: 5013.1
*****************
INLET CONDITION:
----------------
TEMPERATURE: 520.0 K             PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.      FLOW RATE,mol/hr.            mol %
H2             17.00                 0.7589                   24.15
N2             52.50                 2.3438                   74.60
CO2             0.88                 0.0393                    1.25
-----        ----------          ---------               ---------
TOTAL          70.38                 3.1420                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.9719E+05
CO2:H2 RATIO     =   1:   19.32      W/FCO2, gm.hr/mol.=   23.93
RE(Superficial)=   84.26             RE(Particle)      =    4.53

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                    :     2.85
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  16.5482     82.0976     0.2761      0.0016      0.5227       0.5538

******* CONV. OF H2 :    37.75 %     ******* CONV. OF CO2 :     62.02 %

TEMPERATURE PROFILE:-
REACTOR:      247.0      243.0      241.0 C



RUN NUMBER: 5013.2
*****************
INLET CONDITION:
----------------
TEMPERATURE: 514.0 K             PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.      FLOW RATE,mol/hr.            mol %
H2             17.00                 0.7589                   24.15
N2             52.50                 2.3438                   74.60
CO2             0.88                 0.0393                    1.25
-----        ----------          ---------               ---------
TOTAL          70.38                 3.1420                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.9607E+05
CO2:H2 RATIO     =   1:   19.32      W/FCO2, gm.hr/mol.=   23.93
RE(Superficial)=   84.93             RE(Particle)      =    4.56

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                    :     2.87
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  17.1625     81.7616     0.2075      0.0000      0.4533       0.4151

******* CONV. OF H2 :    35.17 %     ******* CONV. OF CO2 :     66.92 %

TEMPERATURE PROFILE:-
REACTOR:      241.0      238.0      237.0 C
```

```
RUN NUMBER: 5014.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 513.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2            39.50                 1.7634                   36.97
N2            66.00                 2.9464                   61.77
CO2            1.34                 0.0598                    1.25
-----       ----------          ----------               ---------
TOTAL        106.84                 4.7696                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                        =0.1456E+06
CO2:H2 RATIO    =  1:  29.48        W/FCO2, gm.hr/mol.=  15.71
RE(Superficial)= 107.39             RE(Particle)      =   5.77

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.              :     4.80
COMPOSITION OF EXIT GASES (mol %):
    H2           N2          CH4          CO          CO2          H2O
  37.3883     61.4135      0.1268      0.0000      0.8177      0.2536

******* CONV. OF H2 :   -1.72 %    ******* CONV. OF CO2 :   34.42 %

TEMPERATURE PROFILE:-
REACTOR:      240.0      238.0      237.0 C



RUN NUMBER: 5014.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 513.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2            39.50                 1.7634                   36.97
N2            66.00                 2.9464                   61.77
CO2            1.34                 0.0598                    1.25
-----       ----------          ----------               ---------
TOTAL        106.84                 4.7696                  100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                        =0.1456E+06
CO2:H2 RATIO    =  1:  29.48        W/FCO2, gm.hr/mol.=  15.71
RE(Superficial)= 107.39             RE(Particle)      =   5.77

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.              :     4.82
COMPOSITION OF EXIT GASES (mol %):
    H2           N2          CH4          CO          CO2          H2O
  37.5784     61.1045      0.1628      0.0000      0.8286      0.3256

******* CONV. OF H2 :   -2.76 %    ******* CONV. OF CO2 :   33.21 %

TEMPERATURE PROFILE:-
REACTOR:      240.0      238.0      238.0 C
```

```
RUN NUMBER: 5015.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 520.0 K               PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.        FLOW RATE,mol/hr.          mol %
H2            39.50                    1.7634                 30.12
N2            90.00                    4.0179                 68.63
CO2            1.64                    0.0732                  1.25
-----       ----------             ---------             ---------
TOTAL        131.14                    5.8545                100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1811E+06
CO2:H2 RATIO    =  1:  24.09       W/FCO2, gm.hr/mol.=  12.84
RE(Superficial)= 144.60            RE(Particle)      =   7.77

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                 :     5.49
COMPOSITION OF EXIT GASES (mol %):
    H2          N2          CH4          CO           CO2          H2O
  25.5342    73.2092     0.1488      0.0507       0.7089       0.3482

******* CONV. OF H2 :   20.53 %    ******* CONV. OF CO2 :   46.86 %

TEMPERATURE PROFILE:-
REACTOR:      247.0      241.0      240.0 C



RUN NUMBER: 5015.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 515.0 K               PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.        FLOW RATE,mol/hr.          mol %
H2            39.50                    1.7634                 30.12
N2            90.00                    4.0179                 68.63
CO2            1.64                    0.0732                  1.25
-----       ----------             ---------             ---------
TOTAL        131.14                    5.8545                100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1794E+06
CO2:H2 RATIO    =  1:  24.09       W/FCO2, gm.hr/mol.=  12.84
RE(Superficial)= 145.57            RE(Particle)      =   7.82

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                 :     5.46
COMPOSITION OF EXIT GASES (mol %):
    H2          N2          CH4          CO           CO2          H2O
  25.2923    73.6420     0.1150      0.0092       0.7023       0.2392

******* CONV. OF H2 :   21.75 %    ******* CONV. OF CO2 :   47.66 %

TEMPERATURE PROFILE:-
REACTOR:      242.0      238.0      238.0 C
```

```
RUN NUMBER: 5016.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 517.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.         mol %
H2            17.00                 0.7589                30.92
N2            37.10                 1.6563                67.48
CO2            0.88                 0.0393                 1.60
-----       ----------          ---------             ---------
TOTAL         54.98                 2.4545               100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                      =0.7549E+05
CO2:H2 RATIO    =  1:  19.32        W/FCO2, gm.hr/mol.=  23.93
RE(Superficial)=  60.36             RE(Particle)      =    3.24

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     2.22
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  23.4603     74.6310      0.4087      0.0000      0.6825      0.8175

******* CONV. OF H2 :    31.40 %    ******* CONV. OF CO2 :    61.44 %

TEMPERATURE PROFILE:-
REACTOR:      244.0      241.0      241.0 C



RUN NUMBER: 5016.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 517.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.         mol %
H2            17.00                 0.7589                30.92
N2            37.10                 1.6563                67.48
CO2            0.88                 0.0393                 1.60
-----       ----------          ---------             ---------
TOTAL         54.98                 2.4545               100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                      =0.7549E+05
CO2:H2 RATIO    =  1:  19.32        W/FCO2, gm.hr/mol.=  23.93
RE(Superficial)=  60.36             RE(Particle)      =    3.24

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     2.20
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  22.9750     75.2348      0.3646      0.0000      0.6963      0.7292

******* CONV. OF H2 :    33.36 %    ******* CONV. OF CO2 :    60.98 %

TEMPERATURE PROFILE:-
REACTOR:      244.0      241.0      241.0 C
```

```
RUN NUMBER: 5017.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 517.0 K              PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.      FLOW RATE,mol/hr.          mol %
H2              39.50                1.7634                  47.17
N2              42.90                1.9152                  51.23
CO2              1.34                0.0598                   1.60
-----         ----------          ---------              ---------
TOTAL           83.74                3.7384                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1150E+06
CO2:H2 RATIO    =  1:  29.48          W/FCO2, gm.hr/mol.=  15.71
RE(Superficial)=  70.92               RE(Particle)      =   3.81

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :    3.92
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
   48.8691    48.8924     0.2897      0.0210      1.3273       0.6005

******* CONV. OF H2 :   -8.56 %    ******* CONV. OF CO2 :    13.09 %

TEMPERATURE PROFILE:-
REACTOR:      244.0      241.0      241.0 C



RUN NUMBER: 5017.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 515.0 K              PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.      FLOW RATE,mol/hr.          mol %
H2              39.50                1.7634                  47.17
N2              42.90                1.9152                  51.23
CO2              1.34                0.0598                   1.60
-----         ----------          ---------              ---------
TOTAL           83.74                3.7384                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1145E+06
CO2:H2 RATIO    =  1:  29.48          W/FCO2, gm.hr/mol.=  15.71
RE(Superficial)=  71.11               RE(Particle)      =   3.82

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :    3.85
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
   48.2254    49.6890     0.2380      0.0084      1.3546       0.4845

******* CONV. OF H2 :   -5.41 %    ******* CONV. OF CO2 :    12.72 %

TEMPERATURE PROFILE:-
REACTOR:      242.0      240.0      240.0 C
```

```
RUN NUMBER: 5018.1
******************
INLET CONDITION:
----------------
TEMPERATURE: 516.0 K             PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.      FLOW RATE,mol/hr.           mol %
H2            39.50                  1.7634                  38.52
N2            61.40                  2.7411                  59.88
CO2            1.64                  0.0732                   1.60
-----     ----------             ---------              ---------
TOTAL        102.54                  4.5777                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1405E+06
CO2:H2 RATIO    =  1:  24.09         W/FCO2, gm.hr/mol.=  12.84
RE(Superficial)= 100.52              RE(Particle)      =   5.40

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.              :     4.49
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
   37.4146     61.0234     0.1949     0.0023      0.9728      0.3921

******* CONV. OF H2 :     4.70 %    ******* CONV. OF CO2 :   40.32 %

TEMPERATURE PROFILE:-
REACTOR:      243.0      239.0      239.0 C



RUN NUMBER: 5018.2
******************
INLET CONDITION:
----------------
TEMPERATURE: 516.0 K             PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.      FLOW RATE,mol/hr.           mol %
H2            39.50                  1.7634                  38.52
N2            61.40                  2.7411                  59.88
CO2            1.64                  0.0732                   1.60
-----     ----------             ---------              ---------
TOTAL        102.54                  4.5777                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                       =0.1405E+06
CO2:H2 RATIO    =  1:  24.09         W/FCO2, gm.hr/mol.=  12.84
RE(Superficial)= 100.52              RE(Particle)      =   5.40

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.              :     4.44
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
   36.5607     61.7259     0.2579     0.0000      0.9397      0.5158

******* CONV. OF H2 :     7.93 %    ******* CONV. OF CO2 :   43.00 %

TEMPERATURE PROFILE:-
REACTOR:      243.0      240.0      240.0 C
```

APPENDIX J

COMPUTER PROGRAM, DATA AND EXPERIMENTAL RESULTS OF ISOTHERMAL METHANATION OF CO IN ISOTHERMAL REACTOR

```
C                   COMPUTER PROGRAM (ITCO.FOR) FOR
C     STEADY STATE METHANATION OF CARBON MONOXIDE IN A FIXED BED REACTOR
C            ISOTHERMAL REACTOR IMMERSED IN A FLUIDIZED SAND BATH
C     This program calculates the product compositions and tabulates the
C     results by taking the initial conditions of operation and the GAS
C     CROMATOGRAPH peak areas for the products.

C     *NT         Number of runs
C     *FRUN       Run number
C     *NP         Number of peaks in porapak column
C     *NC         Number peaks in molecular sieve column
C     *JP         Number compound analyzed
C     *JPK        Total number of compounds
C     *RSP        Response factor in porapak column
C     *RSC        Response factor in molecular sieve column
C     *HYDCON     H2 conversion
C     *COCON      CO conversion
C     *PCNT       Mol % of product gases
C     *PR         Flow rate of water free compound
C     *CWT        Catalyst weight,gm.
C     *FD         Diameter of reactor,cm.
C     *FBD        Bulk density of catalyst pellet,gm/cc.
C     *FDP        Diameter of catalyst pellets,cm.
C     *FN2P       Mol % N2 in feed
C     *FH2P         "    H2   "
C     *FCOP         "    CO   "
C     *RT        Reactor temperature profile
C     *FY        Flow rate in feed,lit/hr.
C     *SV        Space velocity

      DIMENSION RSP(6),RPN(6),PRA(6),PRAM(6),PCNT(6),PR(6),TC(6),PC(6)
      DIMENSION RSC(4),CHA(4),CHAM(4),CHAP(4),TR(4),FM(6),ZC(6)
      DIMENSION FMU(6),FMUR(6),FPD1(6),FPD2(6),FPD(6),ET(6),FQ1(6),FQ(6)
      DIMENSION EM(6),F(6,6),Y(6),X(6),XY(6,6),E(6),FY(6),FW(6)
      DIMENSION FMP(6),FMW(6)

      OPEN(UNIT=1,FILE='ITCODAT',STATUS='UNKNOWN')
      OPEN(UNIT=3,FILE='ITCOOUT',STATUS='UNKNOWN')

      READ(1,*)NC,NP,JP,JPK,N,NT
      READ(1,*)(RSC(I),I=1,NC)
      READ(1,*)(RSP(I),I=1,NP)
      READ(1,*)(TC(I),PC(I),FM(I),ZC(I),FMU(I),I=1,N)
      READ(1,*)FD,FBD,CWT,FDP

      WRITE(3,200)
      WRITE(3,201)
      WRITE(3,204)
      WRITE(3,205)
      WRITE(3,210)

      DO 75 LPN=1,NT

      READ(1,*)FRUN
      READ(1,*)T,P,(FY(I),I=1,N)
      READ(1,*)(CHA(I),I=1,NC)
      READ(1,*)(PRA(I),I=1,NP)
      READ(1,*)RT1,RT2,RT3
```

```
C     CALCULATE INLET COMPOSITIONS*******************************
C     Here Component No. 1=H2,2=N2,3=CO

      FA=0.785*FD**2.0
      X1=100.0
      X2=22.4
      FWT=0.0
      FYT=0.0
      DO 8 I=1,N
      FW(I)=FY(I)/X2
      FWT=FWT+FW(I)
      FYT=FYT+FY(I)
8     CONTINUE
      FTP=0.0
      AMW=0.0

      DO 9 I=1,N
      Y(I)=FW(I)/FWT
      FMP(I)=Y(I)*X1
      FTP=FTP+FMP(I)
      FMW(I)=Y(I)*FM(I)
      AMW=AMW+FMW(I)
9     CONTINUE
      RHCO=FMP(1)/FMP(3)
      RH2N=FMP(1)/FMP(2)
      RCON=FMP(3)/FMP(2)
      WFCO=CWT/FW(3)
      VO=FYT*T/273.0
      V=CWT/(FBD*1000.0)
      U=VO*1000.0/(3600.0*FA)
      RO=AMW*P/(82.05*760.0*T)
      ST=V/VO
      SV=1.0/ST

C     * CALCULATE VISCOSITIES OF PURE COMPONENTS BY LUCAS METHOD *

      DO 25 I=1,N
      TR(I)=T/TC(I)
      FMUR(I)=52.46*(FMU(I)**2.0)*PC(I)/(TC(I)**2.0)
      FPD1(I)=0.96+0.1*(TR(I)-0.7)
      FPD2(I)=1.0+30.55*((0.292-ZC(I))**2)
      IF(FMUR(I)-0.075)239,22,22
22    IF(FPD1(I)-0.0)32,33,33
33    FPD(I)=FPD2(I)*FPD1(I)
      GO TO 25
32    FPD(I)=FPD2(I)*(-FPD1(I))
      GO TO 25
239   IF(FMUR(I)-0.022)241,24,24
24    FPD(I)=FPD2(I)
      GO TO 25
241   FPD(I)=1.0
25    CONTINUE

C **  CALCULATE MIXURE VISCOSITY BY WILKE'S METHOD ******************

      Q=0.76
      DO 301 I=1,N
      FQ1(I)=1.0+0.00385*(((TR(I)-12.0)**2)**(1.0/FM(I)))
      IF(I-1)27,28,27
28    IF(TR(I)-12.0)29,30,30
30    FQ1(I)=1.0+0.00385*(((TR(I)-12.0)**2)**(1.0/FM(I)))
```

```
      FQ(I)=1.22*(Q**0.15)*(FQ1(I)+1.0)
      GO TO 31
29    FQ(I)=1.22*(Q**0.15)*(FQ1(I)-1.0)
      GO TO 31
27    FQ(I)=1.0
31    ET(I)=0.176*((TC(I)/((FM(I)**3.0)*(PC(I)**4.0)))**(1.0/6.0))
      EM(I)=((0.807*TR(I)**0.618-0.357*EXP(-0.449*TR(I))+0.340*EXP(-4.05
     +8*TR(I))+0.018)*FPD(I)*FQ(I))/ET(I)
301   CONTINUE

      DO 110 I=1,N
      DO 120 J=1,N
      F(I,J)=((1.0+((EM(I)/EM(J))**0.5)*((FM(J)/FM(I))**0.25))**2.0)/((
     +8.0*(1.0+FM(I)/FM(J)))**0.5)
120   CONTINUE
110   CONTINUE

      EMT=0.0
      DO 180 I=1,N
      X(I)=Y(I)*EM(I)
      YX=0.0
      DO 208 J=1,N
      XY(I,J)=Y(J)*F(I,J)
      YX=YX+XY(I,J)
208   CONTINUE
      E(I)=X(I)/YX
      EMT=EMT+E(I)
180   CONTINUE
      EMTT=EMT*1.0E-06
      FRE1=FD*U*RO/EMTT
      FRE2=FDP*U*RO/EMTT

C     $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
C     CALCULATE EXIT COMPOSITION
C     Here component no. 1=H2, 2=N2, 3=CH4, 4=CO, 5=CO2, 6=H2O
C     CHAM=MOL % IN MOLECULER SIEVE COLUMN

      CHAS=0.0
      DO 12 I=1,NC
      CHAM(I)=CHA(I)*RSC(I)
      CHAS=CHAS+CHAM(I)
12    CONTINUE
      DO 13 I=1,NC
      CHAP(I)=CHAM(I)/CHAS*X1
13    CONTINUE

C PRAM= mol % in PORAPAK column **************

      PRAS=0.0
      DO 10 I=1,NP
      PRAM(I)=PRA(I)*RSP(I)
      PRAS=PRAS+PRAM(I)
10    CONTINUE
      DO 11 I=1,NP
      PRAM(I)=PRAM(I)/PRAS*X1
11    CONTINUE

C Find mol % in exit gas for molecular sieve column. Peak 1 in porapak
C column stands for all the peaks in molecular sieve column.
C There are only two peaks in porapak column,second peak is component
C no. JP (CO2)
```

```
      TCNT=0.0
      DO 14 I=1,NC
      PCNT(I)=CHAP(I)*PRAM(1)/X1
      TCNT=TCNT+PCNT(I)
14    CONTINUE
      PCNT(JP)=PRAM(NP)
      FR=FW(2)/PCNT(2)*X1

C FR= Flow rate of H2O free product ******************
C PR=Flow rate of H2O free compounds ****************

      DO 21 I=1,JP
      PR(I)=FR*PCNT(I)/X1
21    CONTINUE

C Amount of H2O formed is found out by material balance calculations

      R1=PR(3)
      R2=PR(5)
      TCOR=R1+R2
      TH2R=3.0*R1-R2
      TH2OP=R1-R2
      PR(6)=TH2OP
      PTOT=FR+PR(6)
      DO 23 I=1,JPK
      PCNT(I)=PR(I)/PTOT*X1
23    CONTINUE

C                PTOT=Total flow rate of product
C     Calculation for product gas composition has been completed
C     RPN=> Mol component/Mol N2 in component

      DO 26 I=1,JPK
      RPN(I)=PCNT(I)/PCNT(2)
26    CONTINUE

      COCON=(RCON-RPN(4))/RCON*X1
      HYDCON=(RH2N-RPN(1))/RH2N*X1

      WRITE(3,140)FRUN
      WRITE(3,141)
      WRITE(3,220)
      WRITE(3,230)
      WRITE(3,207)T,P
      WRITE(3,251)
      WRITE(3,224)FY(1),FW(1),FMP(1)
      WRITE(3,212)FY(2),FW(2),FMP(2)
      WRITE(3,217)FY(3),FW(3),FMP(3)
      WRITE(3,216)
      WRITE(3,213)FYT,FWT,FTP
      WRITE(3,246)SV,RHCO,WFCO
      WRITE(3,234)FRE1,FRE2
      WRITE(3,215)
      WRITE(3,229)
      WRITE(3,293)PTOT
      WRITE(3,222)
      WRITE(3,223)
      WRITE(3,100)(PCNT(I),I=1,JPK)
      WRITE(3,105)HYDCON,COCON
      WRITE(3,261)
```

```
      WRITE(3,97)RT1,RT2,RT3
75    CONTINUE
200    FORMAT('EXPERIMENTAL RESULT OF METHANATION OF CO IN A FIXED BED RE
     +ACTOR',/,6X,'ISOTHERMAL REACTOR IMMERGED IN A FLUIDIZED SAND BATH'
     +)
201    FORMAT('-------------------------------------------------------
     +-----')
204    FORMAT(///,'WEIGHT OF CATALYST',17X,':',3X,'0.94 gm',///,'DILUTION
     + RATIO, CATALYST:INERT',5X,':',3X,'1:8',///,'CATALYST SIZE',22X,':
     +',3X,'25-40 mesh',///,'INERT SIZE',25X,':',3X,'25-40 & 40-65 mesh'
     +,///,'CATALYST TYPE',22X,':',3X,'Ni on Alumina (UFFL)')
205    FORMAT(//,'LENGTH OF CATALYST BED',13X,':',3X,'5.0 cm.',///,'LENGT
     +H OF INERT BED BEFORE CATALYST:',3X,'5.9 cm.',///,'LENGTH OF INERT
     + BED AFTER CATALYST :',3X,'4.0 cm.',///,'BULK DENSITY OF CATALYST'
     +,11X,':',3X,'0.6815 gm/cc.')
210    FORMAT(//,'BULK DENSITY OF INERT',14X,':',3x,'1.831 gm/cc.',///,'O
     +D OF REACTOR',22X,':',3X,'12.9 mm.',///,'ID OF REACTOR',22X,':',3X
     +,'10.5 mm.',///,'THERMOCOUPLE LOCATIONS FROM INLET  :',3X,'0.0 cm.
     + 2.5 cm. 5.0 cm.',/////////////////////)
140    FORMAT(//,'RUN NUMBER:',1x,F6.1)
141    FORMAT('*****************')
220    FORMAT('INLET CONDITION:')
230    FORMAT('----------------')
207    FORMAT('TEMPERATURE:',F6.1,1X,'K',11X,'PRESSURE:',F6.1,1X,'mm.')
251    FORMAT(10X,'FLOW RATE,lit/hr.',4X,'FLOW RATE,mol/hr.',9X,'mol %')
224    FORMAT('H2',7X,F10.2,12X,F10.4,10X,F10.2)
212    FORMAT('N2',7X,F10.2,12X,F10.4,10X,F10.2)
217    FORMAT('CO',7X,F10.2,12X,F10.4,10X,F10.2)
216    FORMAT('-----',7X,'----------',12X,'---------',11X,'---------')
213    FORMAT('TOTAL',4X,F10.2,12X,F10.4,10X,F10.2)
246    FORMAT(/,'SPACE VELOCITY,lit.gas/lit.cat.hr.',19x,'=',E10.4,/,'CO:
     +H2 RATIO    =  1:',F7.2,8X,'W/FCO, gm.hr./mol.=',F7.2)
234    FORMAT('RE(Superficial)=',F7.2,12X,'RE(Particle)      =',F7.2)
215    FORMAT(/,'EXIT CONDITION:-')
229    FORMAT('----------------')
293    FORMAT('GAS FLOW RATE,mols/hr.',11X,':',F8.2)
222    FORMAT('COMPOSITION OF EXIT GASES (mol %):')
223    FORMAT(5X,'H2',9X,'N2',9X,'CH4',9X,'CO',9X,'CO2',9X,'H2O')
100    FORMAT(F10.4,1X,F10.4,1X,F10.4,1X,F10.4,2X,F10.4,2X,F10.4)
105    FORMAT(/,'******* CONV. OF H2 :',F8.2,1X,'%',4X,'******* CONV. OF
     +CO :',F8.2,1X,'%')
261    FORMAT(/,'TEMPERATURE PROFILE:-')
97     FORMAT('REACTOR:',3F10.1,1X,'C',/)
       STOP
       END
```

```
4 2 5 6 3 18
36.0 1.0 1.0 1.13
1.0 0.8
33.2 13.0 2.0 0.303 0.0
126.2 33.9 28.0 0.29 0.0
132.9 35.0 28.0 0.295 0.1
1.05 0.6815 0.94 0.0564
4001.0
493.0 760.0 17.0 53.0 0.88
24677.0 5910688.0 3327.0 45596.0
12859960.0 5748.0
220.0 208.0 207.0
4002.0
493.0 760.0 39.5 91.0 1.64
41368.0 5395727.0 2705.0 72200.0
11603388.0 6104.0
220.0 208.0 204.0
4003.0
495.0 760.0 68.0 117.5 2.32
58537.0 4850082.0 1981.0 68813.0
10491769.0 694.0
222.0 222.0 221.0
4004.0
493.0 760.0 17.0 92.0 0.88
8641.0 6594038.0 628.0 31018.0
14912772.0 200.0
220.0 220.0 219.0
4005.0
493.0 760.0 17.0 37.1 0.88
41906.0 5306050.0 1573.0 92168.0
11374605.0 3352.0
220.0 220.0 219.0
4006.0
494.0 760.0 39.5 42.9 1.34
94528.0 4031866.0 2646.0 86047.0
8920124.0 2103.0
221.0 220.0 220.0
4007.0
492.0 760.0 39.5 126.6 1.34
24487.0 5953400.0 1108.0 56561.0
13164865.0 100.0
219.0 219.0 218.0
4008.0
493.0 760.0 68.0 135.5 1.64
53450.0 5091742.0 1812.0 57613.0
11468524.0 100.0
220.0 220.0 219.0
4009.0
495.0 760.0 39.5 61.4 1.64
66224.0 4574651.0 4258.0 94108.0
9830136.0 2410.0
221.0 211.0 210.0
4010.0
512.0 760.0 17.0 92.0 0.88
8209.0 6463925.0 4441.0 8325.0
14505232.0 1313.0
239.0 220.0 217.0
4011.0
512.0 760.0 39.5 126.6 1.34
24235.0 5896728.0 2228.0 46353.0
```

```
12882506.0 3162.0
239.0 219.0 214.0
4012.0
513.0 760.0 68.0 135.5 1.64
47604.0 5142658.0 2975.0 52755.0
10862932.0 3004.0
240.0 223.0 218.0
4013.0
511.0 760.0 68.0 117.5 2.32
58043.0 4789048.0 2704.0 94890.0
10315822.0 3409.0
238.0 222.0 217.0
4014.0
507.0 760.0 39.5 91.0 1.64
41337.0 5176492.0 4776.0 76418.0
10985941.0 1074.0
234.0 228.0 226.0
4015.0
505.0 760.0 17.0 53.0 0.88
19880.0 5626222.0 6733.0 69988.0
12278192.0 1159.0
232.0 227.0 226.0
4016.0
505.0 760.0 17.0 37.1 0.88
40587.0 5191267.0 11587.0 90709.0
11098669.0 1260.0
232.0 229.0 228.0
4017.0
505.0 760.0 39.5 42.9 1.34
94478.0 3921914.0 9379.0 93926.0
8593731.0 938.0
232.0 228.0 226.0
4018.0
506.0 760.0 39.5 61.4 1.64
69556.0 4539260.0 6232.0 112720.0
9684725.0 1089.0
233.0 228.0 226.0
4019.1
518.0 760.0 17.0 92.0 0.88
12118.0 7789306.0 29008.0 1180.0
17910966.0 0.0
245.0 240.0 239.0
4019.2
517.0 760.0 17.0 92.0 0.88
12411.0 7782326.0 28310.0 0.0
17923904.0 0.0
244.0 239.0 238.0
4019.3
521.0 760.0 17.0 92.0 0.88
12622.0 7762556.0 26591.0 0.0
17844932.0 0.0
248.0 243.0 243.0
4020.1
516.0 760.0 39.5 42.9 1.34
123077.0 4728359.0 127555.0 0.0
9633150.0 0.0
243.0 242.0 242.0
4020.2
516.0 760.0 39.5 42.9 1.34
122318.0 4725007.0 120406.0 0.0
9646678.0 0.0
```

```
243.0 241.0 240.0
4021.1
515.0 760.0 39.5 61.4 1.64
92000.0 5457346.0 135664.0 0.0
11479101.0 0.0
242.0 239.0 238.0
4021.2
515.0 760.0 39.5 61.4 1.64
91709.0 5457857.0 136913.0 0.0
11494906.0 0.0
242.0 239.0 238.0
```

EXPERIMENTAL RESULT OF METHANATION OF CO IN A FIXED BED REACTOR ISOTHERMAL REACTOR IMMERGED IN A FLUIDIZED SAND BATH

WEIGHT OF CATALYST : 0.94 gm

DILUTION RATIO, CATALYST:INERT : 1:8

CATALYST SIZE : 25-40 mesh

INERT SIZE : 25-40 & 40-65 mesh

CATALYST TYPE : Ni on Alumina (UFFL)

LENGTH OF CATALYST BED : 5.0 cm.

LENGTH OF INERT BED BEFORE CATALYST: 5.9 cm.

LENGTH OF INERT BED AFTER CATALYST : 4.0 cm.

BULK DENSITY OF CATALYST : 0.6815 gm/cc.

BULK DENSITY OF INERT : 1.831 gm/cc.

OD OF REACTOR : 12.9 mm.

ID OF REACTOR : 10.5 mm.

THERMOCOUPLE LOCATIONS FROM INLET : 0.0 cm. 2.5 cm. 5.0 cm.

```
RUN NUMBER: 4001.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 493.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.           mol %
H2            17.00                 0.7589                  23.98
N2            53.00                 2.3661                  74.77
CO             0.88                 0.0393                   1.24
-----       ----------            ---------               ---------
TOTAL         70.88                 3.1643                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.9280E+05
CO:H2 RATIO      =   1:   19.32     W/FCO, gm.hr./mol.=   23.93
RE(Superficial)=   87.36            RE(Particle)      =    4.69

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :     2.74
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4          CO          CO2          H2O
  12.9552      86.1964      0.0485      0.7514       0.0357       0.0128

******* CONV. OF H2 :    53.14 %     ******* CONV. OF CO :    47.50 %

TEMPERATURE PROFILE:-
REACTOR:       220.0       208.0       207.0 C
```

```
RUN NUMBER: 4002.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 493.0 K            PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.     FLOW RATE,mol/hr.           mol %
H2            39.50                 1.7634                  29.89
N2            91.00                 4.0625                  68.87
CO             1.64                 0.0732                   1.24
-----       ----------            ---------               ---------
TOTAL        132.14                 5.8991                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1730E+06
CO:H2 RATIO      =   1:   24.09     W/FCO, gm.hr./mol.=   12.84
RE(Superficial)= 150.04             RE(Particle)      =    8.06

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :     5.25
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4          CO          CO2          H2O
  21.3605      77.3917      0.0388      1.1702       0.0421      -0.0033

******* CONV. OF H2 :    36.41 %     ******* CONV. OF CO :    16.10 %

TEMPERATURE PROFILE:-
REACTOR:       220.0       208.0       204.0 C
```

```
RUN NUMBER: 4003.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 495.0 K                PRESSURE: 760.0 mm.
              FLOW RATE,lit/hr.     FLOW RATE,mol/hr.          mol %
H2               68.00                  3.0357                  36.20
N2              117.50                  5.2455                  62.56
CO                2.32                  0.1036                   1.24
-----          ----------           ---------                ---------
TOTAL           187.82                  8.3848                 100.00

                                                        =0.2469E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO      =  1:  29.31          W/FCO, gm.hr./mol.=   9.08
RE(Superficial)= 193.54                RE(Particle)      =  10.40

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :    7.61
COMPOSITION OF EXIT GASES (mol %):
    H2          N2          CH4          CO          CO2          H2O
  29.9374     68.9017      0.0281      1.1047      0.0053       0.0229

******* CONV. OF H2 :   24.92 %     ******* CONV. OF CO :    18.80 %

TEMPERATURE PROFILE:-
REACTOR:      222.0       222.0       221.0 C


RUN NUMBER: 4004.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 493.0 K                PRESSURE: 760.0 mm.
              FLOW RATE,lit/hr.     FLOW RATE,mol/hr.          mol %
H2               17.00                  0.7589                  15.47
N2               92.00                  4.1071                  83.73
CO                0.88                  0.0393                   0.80
-----          ----------           ---------                ---------
TOTAL           109.88                  4.9054                 100.00

                                                        =0.1439E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO      =  1:  19.32          W/FCO, gm.hr./mol.=  23.93
RE(Superficial)= 151.00                RE(Particle)      =   8.11

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :    4.32
COMPOSITION OF EXIT GASES (mol %):
    H2          N2          CH4          CO          CO2          H2O
   4.4814     94.9955      0.0090      0.5049      0.0011       0.0080

******* CONV. OF H2 :   74.47 %     ******* CONV. OF CO :    44.43 %

TEMPERATURE PROFILE:-
REACTOR:      220.0       220.0       219.0 C
```

```
RUN NUMBER: 4005.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 493.0 K                  PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2             17.00                     0.7589                     30.92
N2             37.10                     1.6563                     67.48
CO              0.88                     0.0393                      1.60
-----         ----------              ---------                 ---------
TOTAL          54.98                     2.4545                    100.00

                                                               =0.7198E+05
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO     =  1:  19.32          W/FCO, gm.hr./mol.=   23.93
RE(Superficial)=  61.51               RE(Particle)      =    3.30

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     2.16
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  21.7946     76.6553      0.0227      1.5046      0.0236      -0.0008

******* CONV. OF H2 :   37.95 %    ******* CONV. OF CO :   17.25 %

TEMPERATURE PROFILE:-
REACTOR:       220.0      220.0      219.0 C


RUN NUMBER: 4006.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 494.0 K                  PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.           FLOW RATE,mol/hr.              mol %
H2             39.50                     1.7634                     47.17
N2             42.90                     1.9152                     51.23
CO              1.34                     0.0598                      1.60
-----         ----------              ---------                 ---------
TOTAL          83.74                     3.7384                    100.00

                                                               =0.1099E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO     =  1:  29.48          W/FCO, gm.hr./mol.=   15.71
RE(Superficial)=  71.92               RE(Particle)      =    3.86

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     3.58
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  45.1483     53.4915      0.0351      1.2900      0.0189       0.0163

******* CONV. OF H2 :    8.33 %    ******* CONV. OF CO :   22.79 %

TEMPERATURE PROFILE:-
REACTOR:       221.0      220.0      220.0 C
```

```
RUN NUMBER: 4007.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 492.0 K             PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2               39.50               1.7634                  23.59
N2              126.60               5.6518                  75.61
CO                1.34               0.0598                   0.80
-----          ----------          ----------              ----------
TOTAL           167.44               7.4750                 100.00

                                                         =0.2188E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO     =  1:  29.48       W/FCO, gm.hr./mol.=  15.71
RE(Superficial)= 207.72            RE(Particle)       =  11.16

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     6.55
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4          CO          CO2          H2O
   12.7739     86.2679      0.0161       0.9261      0.0006       0.0154

******* CONV. OF H2 :    52.54 %     ******* CONV. OF CO :    -1.43 %

TEMPERATURE PROFILE:-
REACTOR:       219.0      219.0      218.0 C


RUN NUMBER: 4008.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 493.0 K             PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.     FLOW RATE,mol/hr.            mol %
H2               68.00               3.0357                  33.15
N2              135.50               6.0491                  66.05
CO                1.64               0.0732                   0.80
-----          ----------          ----------              ----------
TOTAL           205.14               9.1580                 100.00

                                                         =0.2686E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO     =  1:  41.46       W/FCO, gm.hr./mol.=  12.84
RE(Superficial)= 222.05            RE(Particle)       =  11.93

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                  :     8.42
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4          CO          CO2          H2O
   27.1601     71.8699      0.0256       0.9189      0.0007       0.0249

******* CONV. OF H2 :    24.70 %     ******* CONV. OF CO :    -5.64 %

TEMPERATURE PROFILE:-
REACTOR:       220.0      220.0      219.0 C


RUN NUMBER: 4009.0
```

```
******************
INLET CONDITION:
----------------
TEMPERATURE: 495.0 K               PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.       FLOW RATE,mol/hr.             mol %
H2             39.50                   1.7634                     38.52
N2             61.40                   2.7411                     59.88
CO              1.64                   0.0732                      1.60
-----        ----------             ---------                 ---------
TOTAL         102.54                   4.5777                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.1348E+06
CO:H2 RATIO     =  1:  24.09           W/FCO, gm.hr./mol.=   12.84
RE(Superficial)= 101.88                RE(Particle)      =    5.47

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                     :      4.24
COMPOSITION OF EXIT GASES (mol %):
    H2          N2           CH4          CO            CO2           H2O
  33.7038     64.6724      0.0602       1.5034        0.0196        0.0406

******* CONV. OF H2 :    18.99 %      ******* CONV. OF CO :    12.97 %

TEMPERATURE PROFILE:-
REACTOR:        221.0       211.0       210.0 C


RUN NUMBER: 4010.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 512.0 K               PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.       FLOW RATE,mol/hr.             mol %
H2             17.00                   0.7589                     15.47
N2             92.00                   4.1071                     83.73
CO              0.88                   0.0393                      0.80
-----        ----------             ---------                 ---------
TOTAL         109.88                   4.9054                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.1494E+06
CO:H2 RATIO     =  1:  19.32           W/FCO, gm.hr./mol.=   23.93
RE(Superficial)= 147.13                RE(Particle)      =    7.90

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                     :      4.31
COMPOSITION OF EXIT GASES (mol %):
    H2          N2           CH4          CO            CO2           H2O
  4.3602      95.3699      0.0655       0.1388        0.0072        0.0583

******* CONV. OF H2 :    75.26 %      ******* CONV. OF CO :    84.79 %

TEMPERATURE PROFILE:-
REACTOR:        239.0       220.0       217.0 C


RUN NUMBER: 4011.0
******************
```

```
INLET CONDITION:
-----------------
TEMPERATURE: 512.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.              mol %
H2             39.50                  1.7634                     23.59
N2            126.60                  5.6518                     75.61
CO              1.34                  0.0598                      0.80
-----        ----------          ----------                  ---------
TOTAL         167.44                  7.4750                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2277E+06
CO:H2 RATIO      =   1:   29.48       W/FCO, gm.hr./mol.=   15.71
RE(Superficial)= 202.11               RE(Particle)       =   10.86

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                 :      6.54
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4         CO          CO2         H2O
  12.7814     86.3860      0.0326     0.7673       0.0196      0.0130

******* CONV. OF H2 :    52.58 %     ******* CONV. OF CO :    16.08 %

TEMPERATURE PROFILE:-
REACTOR:       239.0       219.0       214.0 C



RUN NUMBER: 4012.0
******************
INLET CONDITION:
-----------------
TEMPERATURE: 513.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.              mol %
H2             68.00                  3.0357                     33.15
N2            135.50                  6.0491                     66.05
CO              1.64                  0.0732                      0.80
-----        ----------          ----------                  ---------
TOTAL         205.14                  9.1580                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                          =0.2795E+06
CO:H2 RATIO      =   1:   41.46       W/FCO, gm.hr./mol.=   12.84
RE(Superficial)= 216.08               RE(Particle)       =   11.61

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                 :      8.14
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4         CO          CO2         H2O
  24.7581     74.2948      0.0430     0.8612       0.0221      0.0209

******* CONV. OF H2 :    33.60 %     ******* CONV. OF CO :     4.23 %

TEMPERATURE PROFILE:-
REACTOR:       240.0       223.0       218.0 C
```

```
RUN NUMBER: 4013.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 511.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.              mol %
H2             68.00                  3.0357                     36.20
N2            117.50                  5.2455                     62.56
CO              2.32                  0.1036                      1.24
-----      ----------            ---------                 ---------
TOTAL         187.82                  8.3848                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.2549E+06
CO:H2 RATIO     =  1:   29.31        W/FCO, gm.hr./mol.=     9.08
RE(Superficial)= 189.37              RE(Particle)       =    10.17

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :      7.66
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  29.8881     68.5008      0.0387      1.5337       0.0264       0.0123

******* CONV. OF H2 :    24.61 %     ******* CONV. OF CO :   -13.40 %

TEMPERATURE PROFILE:-
REACTOR:        238.0        222.0       217.0 C


RUN NUMBER: 4014.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 507.0 K              PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.       FLOW RATE,mol/hr.              mol %
H2             39.50                  1.7634                     29.89
N2             91.00                  4.0625                     68.87
CO              1.64                  0.0732                      1.24
-----      ----------            ---------                 ---------
TOTAL         132.14                  5.8991                    100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                         =0.1779E+06
CO:H2 RATIO     =  1:   24.09        W/FCO, gm.hr./mol.=    12.84
RE(Superficial)= 147.18              RE(Particle)       =     7.91

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                   :      5.31
COMPOSITION OF EXIT GASES (mol %):
     H2          N2          CH4          CO          CO2          H2O
  22.0121     76.5693      0.0706      1.2773       0.0078       0.0628

******* CONV. OF H2 :    33.77 %     ******* CONV. OF CO :     7.44 %

TEMPERATURE PROFILE:-
REACTOR:        234.0        228.0       226.0 C
```

```
RUN NUMBER: 4015.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 505.0 K               PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.        FLOW RATE,mol/hr.            mol %
H2              17.00                  0.7589                  23.98
N2              53.00                  2.3661                  74.77
CO               0.88                  0.0393                   1.24
-----         ----------             ---------               ---------
TOTAL           70.88                  3.1643                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.9506E+05
CO:H2 RATIO      =   1:   19.32        W/FCO, gm.hr./mol.=   23.93
RE(Superficial)=   85.93               RE(Particle)       =    4.62

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                    :     2.71
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4          CO           CO2          H2O
   11.1226     87.4390      0.1046      1.2291       0.0075       0.0971

******* CONV. OF H2 :    60.34 %     ******* CONV. OF CO :    15.34 %

TEMPERATURE PROFILE:-
REACTOR:       232.0      227.0      226.0 C


RUN NUMBER: 4016.0
******************
INLET CONDITION:
----------------
TEMPERATURE: 505.0 K               PRESSURE: 760.0 mm.
          FLOW RATE,lit/hr.        FLOW RATE,mol/hr.            mol %
H2              17.00                  0.7589                  30.92
N2              37.10                  1.6563                  67.48
CO               0.88                  0.0393                   1.60
-----         ----------             ---------               ---------
TOTAL           54.98                  2.4545                 100.00

SPACE VELOCITY,lit.gas/lit.cat.hr.                           =0.7373E+05
CO:H2 RATIO      =   1:   19.32        W/FCO, gm.hr./mol.=   23.93
RE(Superficial)=   60.51               RE(Particle)       =    3.25

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                    :     2.16
COMPOSITION OF EXIT GASES (mol %):
     H2           N2          CH4          CO           CO2          H2O
   21.5567     76.5891      0.1709      1.5122       0.0091       0.1619

******* CONV. OF H2 :    38.58 %     ******* CONV. OF CO :    16.76 %

TEMPERATURE PROFILE:-
REACTOR:       232.0      229.0      228.0 C
```

```
RUN NUMBER: 4017.0
*****************
INLET CONDITION:
----------------
TEMPERATURE: 505.0 K                PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.        FLOW RATE,mol/hr.           mol %
H2             39.50                    1.7634                 47.17
N2             42.90                    1.9152                 51.23
CO              1.34                    0.0598                  1.60
-----        ----------             ---------              ---------
TOTAL          83.74                    3.7384                100.00

                                                          =0.1123E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO     =  1:  29.48        W/FCO, gm.hr./mol.=    15.71
RE(Superficial)=   70.85            RE(Particle)       =     3.81

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                 :      3.64
COMPOSITION OF EXIT GASES (mol %):
    H2          N2          CH4          CO          CO2          H2O
  45.6660     52.6572     0.1259       1.4250      0.0087       0.1172

******* CONV. OF H2 :     5.81 %     ******* CONV. OF CO :    13.36 %

TEMPERATURE PROFILE:-
REACTOR:        232.0        228.0        226.0 C
```

```
RUN NUMBER: 4018.0
*****************
INLET CONDITION:
----------------
TEMPERATURE: 506.0 K                PRESSURE: 760.0 mm.
           FLOW RATE,lit/hr.        FLOW RATE,mol/hr.           mol %
H2             39.50                    1.7634                 38.52
N2             61.40                    2.7411                 59.88
CO              1.64                    0.0732                  1.60
-----        ----------             ---------              ---------
TOTAL         102.54                    4.5777                100.00

                                                          =0.1378E+06
SPACE VELOCITY,lit.gas/lit.cat.hr.
CO:H2 RATIO     =  1:  24.09        W/FCO, gm.hr./mol.=    12.84
RE(Superficial)= 100.36             RE(Particle)       =     5.39

EXIT CONDITION:-
----------------
GAS FLOW RATE,mols/hr.                 :      4.34
COMPOSITION OF EXIT GASES (mol %):
    H2          N2          CH4          CO          CO2          H2O
  34.8598     63.1935     0.0868       1.7732      0.0090       0.0778

******* CONV. OF H2 :    14.25 %     ******* CONV. OF CO :    -5.06 %

TEMPERATURE PROFILE:-
REACTOR:        233.0        228.0        226.0 C
```