ANALYSIS AND SIMULATION OF AMMONIA SYNTHESIS REACTOR

A DISSERTATION
submitted in partial fulfilment
of
the requirements for the award of the Degree
of
MASTER OF ENGINEERING
in
CHEMICAL ENGINEERING
(EQUIPMENT AND PLANT DESIGN)

By

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CERTIFICATE

CERTIFIED that the thesis entitled 'ANALYSIS AND SIMULATION OF AMMONIA SYNTHESIS REACTOR' which is being submitted by Sri Sudhindra Nath Sinha in partial fulfilment of the requirements for the award of the Degree of MASTER OF ENGINEERING IN CHEMICAL ENGINEERING (Equipment and Plant Design) of the University of Roorkee, is a record of candidate's own work carried out by him under the supervision and guidance of the undersigned. The matter embodied in this thesis has not been submitted for the award of any other degree or diploma.

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CHAPTER - I

INTRODUCTION

The growing need for fertiliser nitrogen to meet the demand of food grains for the rapidly increasing population gave a considerable fillip to the development of large size ammonia synthesis reactor to reduce capital and operating costs. The first ammonia reactor having a capacity of 30 Tons/day went on stream in Germany in 1913 and since then reactor size increased rapidly reaching upto 900 Tons/day in 1965 and upto 2000 Ton/day in 1975. As a consequence of the large size of ammonia reactor now in operation, the use of computer to control the operation has now become essential, when a computer is used for control, it is necessary to develop a mathematical model to realistically describe the performance of the reactor for feed forward and feed back control as well as off-line and on-line optimisation.

Ammonia is produced by catalytic reaction of hydrogen and nitrogen in the mole ratio of approximately 3:1 at elevated pressures (100 to 1000 kg/cm^2) and temperatures (400 to 650 ^{o}C). Single pass conversion from multibed reactors varies from 12 to 35 percent using doubly promoted iron catalyst. Since the reaction is exothermic reversible, it is essential to carryout the reaction in various types of autothermic reactors with external heat exchange and quench type cooling and/or internal heat exchange in view of the critical behaviour, of ammonia synthesis reactor its analysis and simulation is most important.

Van Heerden and Baddour and co-workers have presented the stability analysis of simplified single bed models. In a more recent study Shah has used a two bed adiabatic reactor model with cold shot cooling and external heat exchanger capacity. The nonidealities in rate equation and energy balance equation have also been accounted by him..

In this study a more general model for ammonia synthesis reactor is chosen for analysis and simulation. ICI type quench converter with three catalyst bed, bottom heat exchange and internal heat exchange capacity and with provisions for introducing quench gas at the inlet of each catalyst bed is chosen as the model. Reaction rate, heat capacity and heat of reactions relationships used in the present model are the same as used by Shah. The coupled non-linear mass and energy balance equations are solved numerically using Milne's predictor corrector method.

The simulated model is solved for a total of 72 set of operating conditions for adiabatic reactor operation to study the effect of changes in the first bed inlet temperatures T_{10} of 598, 648 and 698 $^{\circ}K$, cold shot fraction distribution at second and third bed as 0, 0; 0·20, 0; 0, 0·15 and 0·2, 0·15, space velocities of $9{\cdot}0 \times 10^3$, $13{\cdot}5 \times 10^3$ and $18{\cdot}0 \times 10^3$ $Nm^3/(hr)(m^3)$, cold shot temperatures of 413 $^{\circ}K$ and equal to first bed inlet temperature and feed composition of H_2, N_2, NH_3, CH_4 and A as 64·5, 21·5, 2·0, 10·0 and 2·0 and also as 60·75, 20·25, 4·0, 12·0 and 3·0 respectively.

The results of simulation for ammonia synthesis reactor indicate that the net ammonia production rate is quite sensitive to the operating parameters, such as, first bed inlet temperature, space velocity, cold shot temperature and distribution, concentration of ammonia and inerts in synthesis gas feed and pressure, and design parameters, such as, cold shot location and internal and external heat exchange capacities. The ammonia production rate can be improved substantially by proper control of operating and design conditions based on the results on simulation model.

CHAPTER - II

LITERATURE REVIEW

To study the behaviour of 'Autothermic Processes'. Van Heerden^1 in 1953 considered the ammonia synthesis reactor as an example and presented its simplified simulated model. His reactor consists of a cylindrical catalyst vessel with large number of countercurrent tubes inside. The cold nitrogen-hydrogen mixture enters the column at the bottom, flows upward through the heat exchanger tubes and downward through the catalyst bed, and leaves at the bottom. To facilitate the formulation of the problem, following assumptions have been made.

1. There is no temperature difference between the catalyst granules and the interstitial gas.
2. The temperature in the catalyst bed is constant in any cross-section of the converter.
3. As a consequence of the second assumption, the rate of heat exchange between ascending and descending currents of gas is represented by an overall heat transfer coefficient, U, which is constant through out the reactor.
4. The heat capacity of gas is independent of temperature and conversion.
5. The reactor is operated adiabatically and the

temperature rise of reacting gas corresponding to the adiabatic formation of 1% of ammonia is constant and equals 15°C.

6. The reaction velocity constant satisfies the Temkin and Pyzhev[1] rate equation.
7. The numerical data used are as follows:

Height of converter, L, meter	12
Diameter of converter, meter	0·7
Pressure, atm	300
N_2 to H_2 ratio	1 to 3
Inlet NH_3%	1·5
Inlet temperature, °C	50
Linear gas velocity in empty vessel, meter/sec.	0·16

8. There is no pressure drop

Starting from the above assumptions, he has written material and energy balance differential equations and suggested a method to solve them by making use of stepwise integration. As stated in the paper results of calculations are also in quantitative agreement with practice.

Temperature distribution in the considered reactor shows that following the path of gas stream, the temperature rises gradually inside the heat exchanger tubes. In the upper part of the catalyst bed where the heat of reaction exceeds the heat removed by the cooling tubes, the temperature rises and passes through a maximum value. In the lower part of the converter the reaction rate decreases gradually, so that the bottom section mainly serves as a heat exchanger. It indicates that a separate heat exchanger may be used to heat feed gases from the sensible heat of product gases and thus length of reactor may be reduced effectively. This concept, suggested by Van Heerden[1] has later been utilized by other workers.

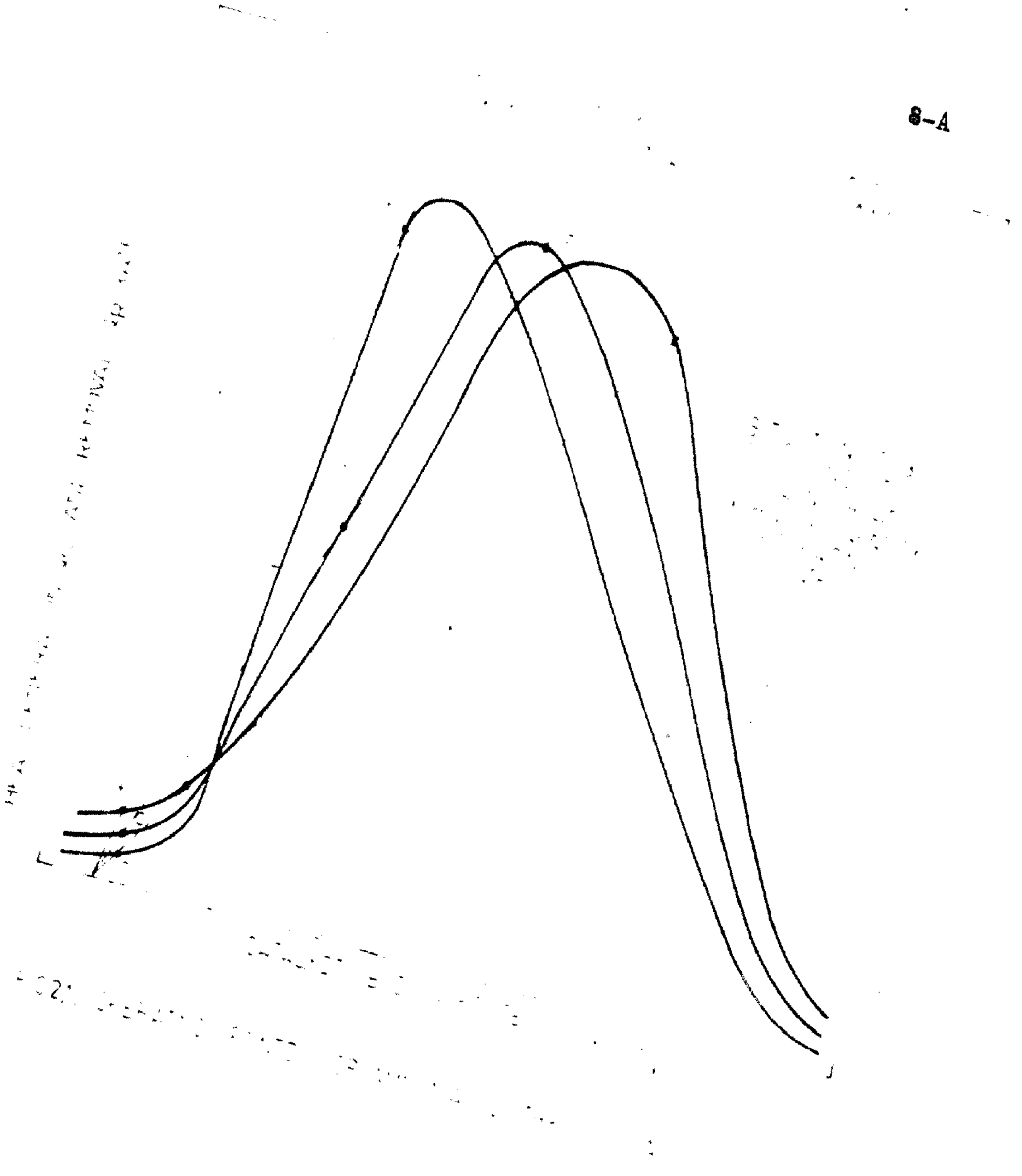
He found that for steady state operation of reactor it is essential that the rate of reaction heat generation must be equal to the rate of heat removal by the coolant, if any, and the total sensible heat gain of reactants and products. On account of sigmoid shape of the heat generation curve when only one intersection occurs with heat removal rate curve, the possibility of its occurrence either at low or high degree of conversion is more in comparison to intermediate value. However, in certain cases heat removal curve intersects the heat

three points. Van Heerden concluded that the upper and lower intersection points are stable but the intermediate intersection point is inherently unstable. He concluded that for stable operation of an autothermal reactor the slope of heat removal rate curve must be greater than the heat generation rate curve at the point of intersection. Thus, on a positive deviation from the intersection temperature, heat removal rate is more than the heat generation rate and the reaction temperature will return to the steady state temperature; similarily, a negative deviation will cause more heat to be generated than removed so that the temperature will rise to the steady state value.

Van Heerden[1] found that reactor stability decreases when heat transfer coefficient or catalyst activity decreases or feed rate increases.

The effect of operating parameters, such as feed rate, reactant concentration and coolant temperature and design parameters, such as, heat exchange capacity on reactor operation and stability is discussed by Saraf[10]. At certain critical values of these variables reaction is said to be 'ignited' and 'quenched' and in between ignition and quenching conditions reactor operation shows hysterisis. For exothermic reversible reactions, operation at low temperature results in low conversion due to the limitation of reaction rate and operation at high temperatures also gives low conversion due to the equilibrium limitations. It is clear from the above discussion that there is a definite range of these parameters for stable operation of an autothermic reactor such as ammonia synthesis reactor at high conversion conditions. Van Heerden[1] and Baddour et al[4,5] indicate that the desirable stable point for maximum ammonia conversion is in the vicinity of quenching or blow-out point-as shown in Fig.2·1.

To investigate the steady state behaviour of Ammonia synthesis reactor (Haber-Besch type), Like Van Heerden[1], Annable[2], Bentler and Roberts[2] have derived one dimensional models allowing for temperature and composition variations in one direction only. Even though their results approximated experimental results, none of them have investigated the effect of operating and design variables on the production, stability and temperature profiles in the reactor. Kjaer[2] has considered the variations of temperature in both the longitudal and radial directions. His mathematical model consists



of three partial differential equations which have been solved by hand computation using a double step integration technique. The agreement of the computed production rate and average bed temperatures with plant data was found to be very good. However, the Kjaer model could not explain the radial temperature gradient reported by Slack, Allgood and Maune[3] Kjaer[2] has given a qualitative explanation of this discrepancy based on the location of the various thermocouple wells with respect to the cooling tubes in catalyst bed.

In order to study the effect of operating and design variables on the optimum feed temperature, the stability of the reactor and the temperature profiles in the reactor, Baddour et al[4] have also developed a simple one-dimensional model of T.V.A. ammonia synthesis reactor (Tennesse Valley Authority reactor) which approximates within 15 to 20 percent the temperature profiles and the ammonia production rates of an industrial reactor.

Like Van Heerden[1] and others, they have also neglected the temperature and concentration gradients in radial direction. The temperature of the gas flowing through the catalyst at each location has been assumed equal to the temperature of catalyst particle. Same Temkin and Pyzhev[2]'s reaction rate expression is used. It has also been assumed that heat capacity of gas is independent of temperature and the effect of pressure on enthalpy is negligible. Heat of reaction is assumed to be constant. The pressure was kept constant and the hydrogen to nitrogen ratio was equal to 3. Range of parameters studied has been given in following table:

Table

	Lower Limit	Standard	Upper Limit
Space velocity, (hr^{-1})	9,000	13,800	18,000
Ammonia mole fraction in the feed.	0·01	0·05	0·1
Inert mole fraction in the feed	0·0	0·08	0·15
Catalyst activity	0·4	1·0	1·0
Total heat conductance, US Cal/(Sec)(K)	30,000	55,000	80,000

With their above described simplified model, Baddour et al[4,5] have studied the effect of design and operating parameters on reactor stability, ammonia production rate and catalyst bed temperature profile. It has been shown that an increase in space velocity increases ammonia production rate but decreases reactor stability and requires that the converter be operated at a higher temperature level. Any increase in ammonia or inert content of the feed gas has been found to decrease both production rate and stability but not to affect the average temperature of the bed. The use of a less active catalyst has been shown to decrease both production rate and stability and to necessiate operation at a higher temperature level. The heat transfer coefficient per unit volume of catalyst has been found to have a small effect on the production rate and the average bed temperature but a marked influence on stability, a high coefficient increasing stability and lowering the inlet temperature of the reactor. The optimum temperature profiles have been found to be relatively insensitive to operating parameter variation, the use of a high coefficient of heat transfer increases local overheating of the catalyst.

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In 1967 Shah[2] has made another attempt to simulate ammonia synthesis reactor. His reactor consists of catalyst beds and an external heat exchanger. The feed is divided in to several parts; one portion goes to the heat exchanger and the others are divided in to several 'cold shots' for mixing with the gases between consecutive catalyst beds. He has also made certain simplifying assumptions in the model development to obtain the differential equations in manageable form. Some of the assumptions are similar to those used by Van Heerden[1]. However, Unlike Van Heerden[1] and other workers[4,5] he has considered the non-ideal behaviour of the gases not only in the reaction rate expressions but also in the energy balance equation, where the specific heat and heat of reaction are functions of temperature and pressure since these non-idealities have marked influence on performance of reactor.

If we have a look on Temkin and Pyzhev[1] rate expression for ammonia synthesis, used by previous workers, it have two serious short comings. Firstly it has been found to be less accurate with varying temperature and pressure secondly the rate becomes infinite at zero ammonia concentration. Due to this reason Shah has used modified Temkin and Pyzhev[2] rate expression.

Shah[2] has considered the dependency of physical properties like heat of reaction and heat capacity etc. of constituent reaction mixture on temperature and pressure. These relationships have been described in the later chapters. From the literature available, it is clear that relationships presented by Shah[2] are quite close to reality. Shah[2] has taken the polynomial form of relationship for variation of heat capacity with temperature as suggested by Houghen and Watson[6]. To take into account the pressure effect on heat capacity, he assumes that coefficients of the polynomial varies linearly with pressure in the probable operation range (200-600 atm) of ammonia synthesis reactor. Shah[2] has observed that there is no appreciable effect of pressure on heat capacities of H_2, N_2, CH_4, and A While heat capacity of ammonia changes significantly with pressure. Expressions for heat of reaction used by Shah[2], which takes into account effect of both temperature and pressure have also been described, elsewhere in this thesis.

For pressure drop within the reactor following linear relationship is used by Shah[2] since the values are small.

$$p = p_0 - \omega Z$$

where ω ---- coefficient

Z ---- distance in flow direction within catalyst bed.

For solving coupled differential equations Shah[2] has used Milne Predictor corrector integration subroutine which chooses its own step size ΔZ, subject to the limitation of absolute error or relative error specified.

Shah[2] has found that effect of change in N_2/H_2 ratio is not significant on production of NH_3. The effect of increase in inerts was found to decrease the stability of reactor operation significantly whereas NH_3 production decreased slightly. Increase in NH_3 initially present in feed decreased production and stability of reactor, The increase in cold shot fraction resulted in decrease in stability of reactor.

Shah found that as the inlet temperature of the gas entering first bed increases the yield of NH_3 first shows an increase and later a decrease. Increase in total pressure of the feed is shown to increase the yield. Effect of space velocity, catalyst activity, NH_3 and inerts content in feed on NH_3 yield was also found to be same as discussed by Baddour et al[4].

PHYSICAL PROPERTIES

Most of the workers including Van Heerden[1] and Baddour[4,5] have taken the physical properties heat of reaction and heat capacity etc. of constituents of reaction mixture as constants. But in fact these depend on pressure and temperature. Shah[2] was more realistic and considered this dependency in order to obtain better simulated model. From the literature available, it is clear that relationships presented by Shah[2] are quite close to reality. Shah[2] has taken the polynomial form of relationship for variation of heat capacity with temperature as suggested by Houghen and Watson[6]. To take in to account the pressure effect on heat capacity, he assumed that coefficients of the polynomial varies linearly with pressure in the probable operation range (200-600 atm) of ammonia synthesis reactor. Shah[2] has observed that there is no appreciable effect of pressure on heat capacities of H_2, N_2, CH_4 and A while heat capacity of ammonia changes significantly with pressure.

The relationships, used by Shah[2], are applicable in the temperature range of 500-900°K and are given in the Appendix-C.

CHAPTER - III

REACTOR MODELLING AND DESIGN RELATIONSHIPS

Formulation of reactor model consists of mass, energy and momentum balance equations for each of the reactor section. For simulation purpose only the steady state behaviour is considered and it is assumed that the variation in operating parameters is so slow that the corresponding change in reactor operation can be regarded as succession of pseudo-steady states and that there are no gross perturbations which would deliberately push the steady conversion to another steady state value. Shah[2] has discussed the validity and utility of such steady state analysis for off-line as well as on-line control and optimization.

Fig.3·1 shows a simplified flow diagram of a typical three bed quench type high capacity ammonia synthesis reactor with interval and external heat exchange capacities. The feed is divided into four parts; one fraction goes to bottom heat exchanger and the remaining feed gases are divided into three cold shots for mixing with the gases entering different catalyst beds.

The rigourous model precisely defining the heterogeneous ammonia synthesis reaction may be written in the form of momentum, mass and energy

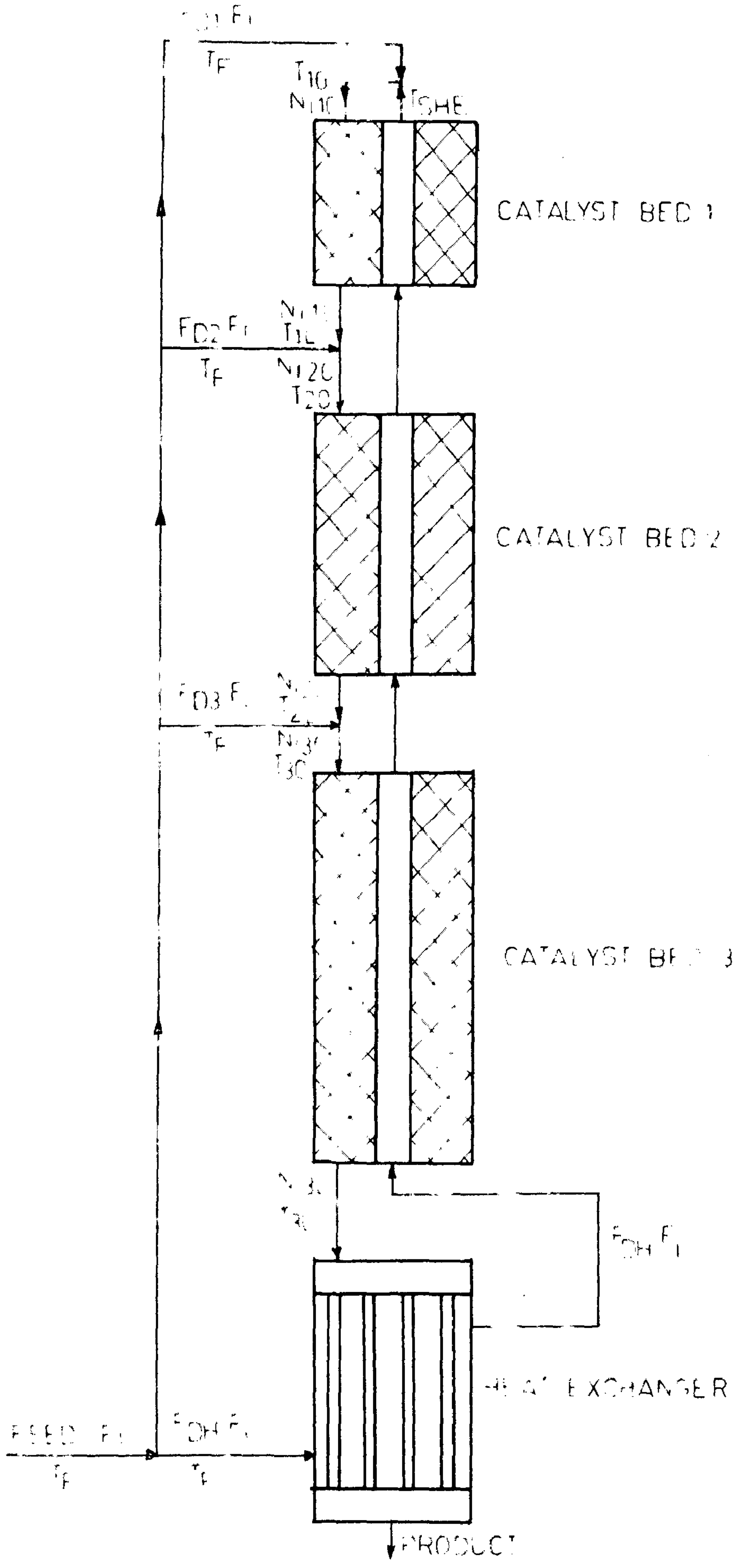


FIG. [illegible] SIMPLIFIED FLOW DIAGRAM OF THREE BED QUENCH TYPE AMMONIA SYNTHESIS REACTOR WITH INTERNAL AND EXTERNAL HEAT EXCHANGE CAPACITY balance in three dimensional space and time. However, such a system generating a set of non-linear and coupled partial differential equations will be very difficult to solve even on the fastest available new-generation computer. These difficulties inherent in solution are enhanced for auto-thermal reactor operation with external and/or internal heat exchange between the reaction mixture and feed due to the convergence problem. Therefore,a rigorous approach is unpractical and recourse must be had to more approximate 'engineering' approach so as to predict reactor exit conditions and stability of operation with reasonable accuracy for simulation purpose. This necessitates certain simplifying assumptions to be made for the solution of the differential equations.

ASSUMPTIONS

For obtaining mass, energy and momentum balance equations in manageable form, the following simplifying assumptions are made and their usefulness and limitations are discussed subsequently:

1. Reactor is operating at steady state.
2. There is no radial velocity, temperature and concentration gradients across the bed.
3. Pressure drop varies linearly and the effect of cold slot is accounted by assuming that the

coefficient of pressure drop varies with 1·8 power to the fraction of total feed entering in a bed.

4. Heat exchange capacity, that is the product of heat transfer coefficient and heat transfer area per unit catalyst bed volume, does not vary with axial position in catalyst beds.
5. Intraparticle and gas-solid interphase heat and mass transfer limitations are absent.
6. Cold shot enters the reactor at temperature T_F and at a pressure equal to the pressure in the reactor at the point of entry.

VALIDITY OF ASSUMPTIONS:

The reactor is assumed to operate at steady state in normal conditions except during the start-up and shut-down when the operation is at unsteady state.

For shut down and start-up periods, unsteady state conditions should be taken into account for a realistic analysis of the reactor operation. The radial velocity, temperature and concentration gradients across the bed are assumed to be insignificant and their effect minimal as compared to the axial gradients. The pressure drop across the bed is very small as compared to the pressure of the gas at any point in the bed. Therefore, the assumption of linear variation of pressure drop is justified. In case where cold shot is added to the feed to a bed, it increases the pressure drop across the bed. With the assumption of linear variation of pressure drop across the bed, the effect of cold shot is taken into account by assuming that the coefficient of pressure drop **varies by 1·8 power of** the fraction of total feed entering into **a** bed. Though in ammonia synthesis reactor, the temperature varies across the bed, and thereby the overall heat transfer coefficient varies, however, the variation over the bed length is very small and for all practical purposes, it may be assumed to be constant throughout the bed-length. Since the effectiveness factor for the catalyst pellets used is approximately 1·0, and in any case, this can be determined for the reactor catalyst, the assumption of absence of intraparticle and interphase heat and mass transfer resistances is justified. In the reactor, cold shot enters the reactor at feed temperature T_F and Feed pressure P_F. However, for simplicity in the analysis, it is assumed that it enters at a pressure equal to the pressure in the reactor at the point of entry.

With the above assumptions and their justification, the mass momentum and heat balances equation can be written for the reaction.

$$\frac{3}{2} H_2 + \frac{1}{2} N_2 \rightleftharpoons NH_3 \qquad \ldots (3.1)$$

over the differential reactor section of catalyst volume dvj in bed j.

MASS BALANCE

The mass balance for hydrogen (subscript 1) is given by,

$$F_1 \, dx_{1j} = - r_1 \, dv_j \qquad \ldots (3.2)$$

ENERGY BALANCE

The energy balance equation is obtained by equating the heat of reaction to the sum of sensible heat gain of the reacting gas and the heat transferred to the synthesis gas in the internal preheating section to give,

$$-\Delta H_{R_1} (-r_1) \, dv_j = \left(\sum_{i=1}^{5} Nij \, Cp_i \right) d \, T_j + (UA)_j \, (T_j - T_{sj}) \, dv_j \qquad \ldots (3.3)$$

where F_1 is the total moles of hydrogen fed to the reactor, N_i is moles of component i, T is the gas temperature in the catalyst bed and T_s is the gas temperature in the internal preheating section (UA) is the heat exchange capacity per unit catalyst bed volume and can be used without any loss of generality. Subscript i designates components (1- hydrogen, 2- nitrogen, 3- ammonia, 4- methane and 5- argon)

$$N_{ijo} = F_i \left(F_{DH} + \sum_{j=1}^{j} F_{Dj}\right) + \alpha_i F_1 X_{1jo} \quad ; \qquad \ldots(3\cdot5)$$

$i = 1,2, \ldots, 5$ and $j = 1,2,3$ and at the exit (subscript L) ...

$$N_{ijL} = F_i \left(F_{DH} + \sum_{j=1}^{j} F_{Dj}\right) + \alpha_i F_1 X_{1jL} \quad ;$$

$$i = 1,2, \ldots, 5 \text{ and } j = 1,2,3 \qquad \ldots(3\cdot6)$$

Energy Balance Equations

At the Entry of Bed 1 (after mixing of coldshot) ...

$$\left(\sum_{i=1}^{5} N_{i10}\, Cp_i\right) T_{10} = F_{DH} \left(\sum_{i=1}^{5} F_i\, Cp_i\right) T_{SHE} + F_{D1} \left(\sum_{i=1}^{5} F_i\, Cp_i\right) T_F \qquad \ldots(3\cdot7)$$

At the Entry of Bed 2 and 3 (after mixing of coldshot)

$$\left(\sum_{i=1}^{5} N_{ijo}\, Cp_i\right) T_{jo} = \left(\sum_{i=1}^{5} N_{i(j-1)L}\, Cp_i\right) T_{(j-1)L} + F_{Dj} \left(\sum_{i=1}^{5} F_i\, Cp_i\right) T_F, \quad j = 2,3 \qquad \ldots(3\cdot8)$$

where N_{ij} is the flow rate of component i, T_{SHE} is the temperature of the preheated feed gases after passing through the external and internal preheating sections. Subscripts 0 and L designate inlet and exit of the bed respectively. Coefficient α_i is proportional to stoichiometric coefficient for component i and have values: $\alpha_1 = -1$, $\alpha_2 = -\frac{1}{3}$, $\alpha_3 = \frac{2}{3}$ and $\alpha_4 = \alpha_5 = 0$.

In the external heat exchanger (subscript H) no chemical reaction occurs and it is simply a counter-current heat exchanger to preheat only F_{DH} fraction of the total cold feed gases by all the gases leaving the last reactor bed. The energy balance for the feed gas gives

$$F_{DH}\left(\sum_{i=1}^{5} F_i \, Cp_i\right) d\,T_{SH} = -\,(UA)_H\,(T_H - T_{SH})\,d\,V_H \quad \ldots (3\cdot 9)$$

and for the product gas

$$\left(\sum_{i=1}^{5} N_{i3L} \, Cp_i\right) d\,T_H = -\,(UA)_H\,(T_H - T_{SH})\,d\,V_H \quad \ldots (3\cdot 10)$$

where T_{SH} is the gas temperature in the preheating side, T_H is the product gases temperature, $(UA)_H$ is the heat exchange capacity per unit volume V_H of the external heat exchanger and N_{i3L} is the moles of component i leaving third catalyst bed and entering the external heat exchanger.

Equations 3·2 to 3·10 constitute the necessary relationships for the simulation model for the reactor. The relationships for heat capacities, heat of reaction and reaction rate necessary for the solution of the simulation model are given in Append. Table C·1 Eqn. C·1 to C·10. Moles of component i at any point in bed j, N_{ij}, can be easily obtained from Eqn(3·5) by omitting subscript 0 and total moles, N_{Tj}, are obtained by

$$N_{Tj} = \sum_{i=1}^{5} N_{ij} \qquad \ldots(3\cdot11)$$

In the reaction rate Eqn. C·7 , catalyst activity factor f and total pressure p are also used. Zayarni[2] has reported changes in catalyst activity by as much as 20% as the reaction mixture passes from top to bottom of the catalyst bed. Factor f can be assigned any numerical value to account for catalyst deactivation and can also be made to vary with position in the catalyst bed.

As the synthesis gas flows through the heat exchanger and catalyst beds the pressure changes and a suitable expression to estimate the pressure drop within the reactor is essential. Precise calculations can be carried out to obtain the pressure drop flow of gases through the heat exchanger and the packed beds. However, for the purpose of simulation model, since the pressure drop across the converter rarely exceeds 10 kg/cm^2 or approximately 5 percent of the pressure at reactor inlet, p is expressed in a linear form and pressure drop dP_j for flow of gas in bed j is calculated by

$$- dP_j = \omega_N \left\{ \frac{\sum_{i=1}^{5} N_{ijo}}{\sum_{i=1}^{5} F_{iN}} \right\}^{1\cdot 8} dV_j \qquad \ldots (3\cdot 12)$$

where subscript N corresponds to a reference (normal) value, and ω is a coefficient for pressure drop. It is further assumed that the pressure drop in bed j varies as 1·8 power of the total molar flow rate at the entry of the bed j. Similar expressions can be written for pressure drop in external heat exchanger and preheating section of the catalyst bed if necessary.

A reasonable value for the total pressure drop across the reactor is assumed and this is distributed in a realistic manner for external and internal preheating sections, catalyst beds and product gas cooling in external heat exchanger. For preheating sections, an average pressure value, average of inlet and outlet pressures is used, since the change in pressure is extremely small and its effect on specific heat values will not be significant. For catalyst beds linear pressure drop function is assumed in each bed to account for the effect of pressure change on reaction rate, equilibrium constant and specific heats. A linear pressure drop function is assumed for product gas cooling in external heat exchanger also.

CHAPTER - IV

COMPUTATION TECHNIQUE AND COMPUTER PROGRAM FEATURES

4.1 COMPUTATION TECHNIQUE

The differential equations obtained in Chapter III by writing material and Energy balance for reactor to describe its performance are highly non-linear and coupled. Since analytical integration is not possible, it is better to solve them by numerical methods. In numerical integration a small step size is chosen and calculations are performed step by step. Accuracy of computation depends upon magnitude of step size.

Computation technique followed has been shown in block diagram 4·1. Step wise procedure is as follows:

Step 1: Assume any arbitrary temperature T_{SHE} of the feed gas coming from the internal preheater(i.e. tube side of catalyst bed) at the inlet of first bed for starting otherwise follow convergence policy given at the end of this algorithm. If cold shot is added then go to step 2 otherwise go to step 3.

Step 2: Determine the temperature of resultant stream by trial and error since heat

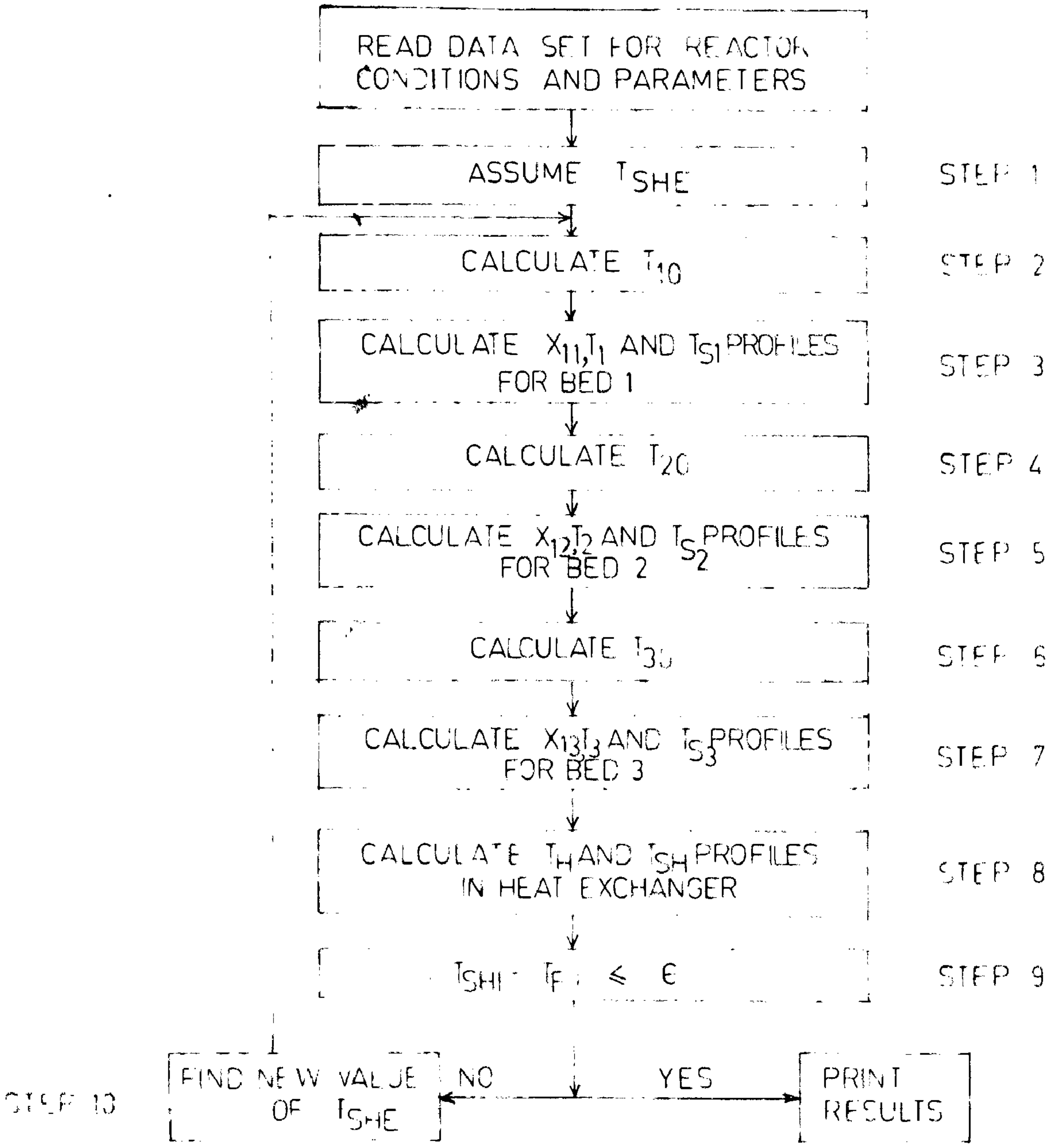


FIG.4.1. BLOCK DIAGRAM FOR COMPUTER CALCULATION PROCEDURE

capacity of the mixture is not known. Molal flow rate is obtained by simple material balance.

Step 3: Carry out the numerical integration step by step in forward direction upto the end of first bed. So the conditions there are known.

If cold shot is added to second bed also then go to step 4 otherwise go to step 5

Step 4: Determine the temperature and molal flow rate of resultant stream as discussed in step 2.

Step 5: Carry out the numerical integration for second bed up to its exit.

If cold shot is added to the inlet of third bed also then go to step 6 otherwise to step 7.

Step 6: Determine the molar flow rate and temperature of resultant stream.

Step 7: Carry out numerical integration for the third bed up to its exit.

Step 8: Carry out numerical integration for

External heat exchanger upto its exit.

Step 9: The temperature of feed gases is known for a assumed temperature at first bed inlet. If thus obtained feed gas temperature matches within a certain tolerance with its original value then assumed temperature is the correct temperature and print results otherwise go to step 10

Step 10: Decide new T_{SHE} and go to step 2.

4.1.1 CONVERGENCE POLICY

Let us explain it by taking an example. Suppose for an assumed value (= 700°K) of temperature (T) of inlet gases to first bed, ΔT_F(= +200K) is the difference of calculated temperature of feed gases to external preheater and cold shot.(feed fr.) temp.

Again an arbitrary value of T is assumed depending upon magnitude of step size, supplied by the input data say 680°K. Corresponding to this T new value of ΔT_F, $\Delta T'_F$ is obtained. Now there may be three possibilities.

(i) $\Delta T'_F$ is less than ΔT_F. Again there may be two possible cases.

(a) $\Delta T'_F = + 100°K$. It indicates that T may be further reduced. Let for a new T, 660, instead of decreasing, ΔT_F starts increasing again. Say + 150. This indicates the parabolic nature of the function ΔT_F in this region. Results of our computations show that ΔT_F is a mutiprabolic function of T. In such a situation, two searches are made in order to check whether there exists zero value or not. Otherwise a jump is made from this region towards lower ΔT_F.

(b) $\Delta T_F' = -100^{\circ}K$. It means solution should exist in between 680 and 700°K. A new value of T, say 690 is assumed and computation is made in the similar fashion.

(ii) $\Delta T_F'$ is more than ΔT_F. Say 300°K. It indicates that with decrease in T, ΔT_F is increasing. So higher value of T i.e. 720 should be selected for further computation.

(iii) $\Delta T_F'$ may be very close to ΔT_F. It indicates that solution does not exist here and a jump from this point is necessary. Direction of jump is decided whether $\Delta T_F'$ is less than ΔT_F or more than ΔT_F. Magnitude of jump has been taken as eight times the step size.

This magnitude may be changed, if desired, based on nature of the problem.

During computation it has been observed in some iterations that temperature of the bed at some point becomes negative for a certain value of T. This creates problem in computation due to presence of logarithmic terms in rate expression. In such a situation a fresh value of T is assumed to proceed further.

4.1.2 NUMERICAL INTEGRATION METHOD

For integration of non-linear and coupled differential equation, Milne-Predictor and corrector method[7] is used. This method has also been used by Shah[8]. He has found it to be stable and convergence is fast at each step. Error in computation is less as compared to Fourth order Runge Kutta method[9].

This method involves in generating first four points by following predictor and corrector steps[8].

First Point: This point is the inlet to first bed where by assuming the temperature, T_{SHE} all informations are available so that derivative values may be calculated by making use of material and energy balance equations.

Second Point:

Predictor step: Predictor step involves making first guess of second point values with the help of derivative values (Slope) **calcutted at first point.** Since in our problem there are three differential equations to be solved simultaneously with three variables viz. conversion, bed temperature and preheater side temperature, so above principle is extended to all the three.

$$y_2=y_1+hy_1', \quad y_1'=f(y_1,x_1)$$

Corrector step:

Once a guess of second point is available from predictor step then derivative values at this second point may be determined from material and energy balance equations . These values are utilised further to get more refined values of second point variables.

$$y_2 = y_1 + \frac{1}{2} h (y_2' + y_1')$$

In present problem following form of differential equations exists.

$$X' = \frac{dX}{dV} = f(X, T, P)$$

$$T' = \frac{dT}{dV} = f(X, T, P)$$

$$T_s' = \frac{dT_s}{dV} = f(T, T_s)$$

At first point in inlet to reactor $X(1)$, $T(1)$, $T_s(1)$

and P(1) are known because we have already assumed inlet bed temperature and pressure drop on preheater side. Thus from predictor step, the second point values are given by

$$\left.\begin{aligned} X(2) &= X(1) + H\cdot X'(1) \\ T(2) &= T(1) + H\cdot T'(1) \\ T_s(2) &= T_s(1) + H\cdot T_s'(1) \end{aligned}\right\vert$$

where H is a suitable small step size chosen for differential volume of catalyst which will be occupied between point 2 and 1 of the reactor.

From these values at second point derivative values at second point are calculated and corrector step is applied again to generate new values of X, T, T_s at point 2 which are more accurate.

Corrector Step:

$$X(2) = X(1) + \frac{H}{2}\left(X'(2) + X'(1)\right)$$

$$T(2) = T(1) + \frac{H}{2}\left(T'(2) + T'(1)\right)$$

$$T_s(2) = T_s'(1) + \frac{H}{2}\left(T_s'(2) + T_s'(1)\right)$$

These new values of variables are now compared again with previous values, obtained by predictor step. If these are within a required tolerance limit, then the new values are taken as correct otherwise the procedure of corrector step with the new values is repeated until new and old values are found to be within the required tolerance limit. The new values are stored for the calculation of third point.

Third Point:

For third point as discussed earlier, similar predictor and corrector steps are applied as stated below:

Predictor Step:

$$y_3 = y_2 + (1/2)h\ (3\ y_2' - y_1')$$

Corrector Step:

$$y_3 = y_2 + (1/12)h\ (5\ y_3' + 8\ y_2' - y_1')$$

These are stable methods and expected to give variable values within reasonable tolerance even if the corrector step is applied once or at the maximum twice only.

Fourth Point:

Predictor Step:

$$y_4 = y_3 + (1/12)h\ (23\ y_3' - 16\ y_2' + 5\ y_1')$$

Corrector Step:

$$y_4 = y_3 + (1/24)h\ (9\ y_4' + 19\ y_3' - 5\ y_2' + y_1')$$

After generating above four points, the Milne predictor-corrector[7] step is applied to generate remaining points as it is more stable and gives fast convergence. It is also expected to give accurate value in only single application of corrected step.

Predictor Step:

$$y_5 = y_1 + (4/3)h\ (2\ y_2' - y_3' + 2\ y_4')$$

Corrector Step:

$$y_5 = y_3 + (h/3)(y_3' + 4\ y_4' + y_5')$$

As described earlier the corrector step is repeated until the new values reach within a specified tolerance limit.

In our programme we have used for generation of sixth point onwards a modifier step in between predictor corrector making use of the magnitude of error at previous point between values from predictor and corrector steps. Thus this error is added in the value obtained from predictor step to guess in advance values which are utilised for finding derivative values to be used in corrector step. For example if for fifth point the value of conversion at predictor step is 0·001 and corrector step is 0·001005. Thus the error is 0·000005 and if tolerance is 0·00001 then corrector step value is within tolerance. Based on this value if Predictor step for sixth point gives 0·0015. Then for finding derivative values at sixth point for use in corrector step instead of 0·oo15 variable value the modifier step is utilised making use of error at fifth point i.e. ·0·000005. Thus derivative value is found at 0·001505 instead of 0·0015 which has been found to give fast convergence at corrector step.

In our calculations tolerance limits for conversion and temperature are 5×10^{-5} and 5×10^{-3} respectively. Provision has also been made in the computer program to change these tolerance limits, if so desired.

4.2 COMPUTER PROGRAM FEATURES

A computer program to simulate ammonia synthesis reactor has been written in FORTRAN-IV and executed on IBM360/Model 44 system of Delhi University computer centre. As usual it consists of a main program followed by various subroutines. Main program consists of three sections viz. READ DATA, convergence policy and PRINT RESULTS. Numerous comment cards have been inserted in main program and subroutines to make them more understandable. Computer program is given in appendix A.

4.2.1 DETAILS OF INPUT DATA

Following variables should be supplied to the computer program as data in the required format.

1) W11------ Initial guess for first bed inlet temp. in °K (say 700) for first iteration

C2 ---- Step size for second iteration in ^{o}K, say 20

C3 ---- Step size for next jump to search for another possible solution, say 80 then the next trial will begin at 620 for searching next solution, in K

C4 ---- Tolerance allowed in calculated values of feed temp.and mixture temperature, say 0·1, in K

C51 ---- Fractional pressure drop in shell side and internal preheater tube side for feed gas, say 0·03 of total feed pressure based on some reference feed rate

C611 ---- Pressure drop per unit volume of catalyst, say 10^{-7} based on a given reactor geometry, catalyst packing and for some reference gas rate, in atm/cm^3.

C621 ---- Pressure drop per unit volume of tube side in heat exchanger, say 10^{-7} based on a given tube size and roughness and for some reference gas rate, in atm/cm^3.

VW ---- Tolerance allowed in calculated

values of variables at each point in numerical integration by predictor corrector step. Say in our case tolerances in **fr. conversion and** temp are 5 x 10^{-5} and 5 x 10^{-3}K respectively.

H1,H2,H3, and H4 ---- Step sizes of volumes for catalyst beds 1, 2, 3 and heat exchanger respectively for numerical integration. These are to be chosen such that the bed is divided in a number of points (100 or 200), say 9 x 10^4, 18 x 10^4, 36 x 10^4 and 20 x 10^4 respectively. Where catalyst bed volumes and heat exchanger volume are 9 x 10^6, 18 x 10^6, 36 x 10^6 and 20 x 10^6 respectively, all in cm^3.

C71,C72,C73, and C74 ---- Various values for control of storage for only such points which are desired to be printed e.g., if these have values equal to 10 for bed divided in 100 points then prints will be available for 11th, 21st, 31st etc. points with a spacing of desired beds , say 2. This means first bed results will not be printed and print will start from 2nd bed onwards.

K8 --- Bed spacing in print output, say 1

FF --- Ratio of total feed rate to the feed rate at its normal (reference) value.

PF(I),TF(I) --- feed pressure (atmosphere) and feed temperature (^{o}K) for run No.I, say 160 and 413 respectively.

F11(I),F22(I),F33(I),F44(I) and F55(I) --- Total molar flow rates of hydrogen, nitrogen, ammonia, mithane and Argon in feed gas for run No.I, say 4540, 1510, 141, 705 and 141 respectively, in gm moles/sec.

FD22(I),FD33(I) and FD44(I) --- fraction of total feed entering as coldshot to second, third and first catalyst bed inlets for run No.I, say 0·20, 0·15 and 0·10 respectively, dimensionless.

Z11(I),Z22(I),Z33(I) and HLL(I) --- The volume of catalyst in first, second and third beds and total volume of heat exchanger for run No.I, say 9 x 10^6, 18 x 10^6, 36 x 10^6 and 20 x 10^6 respectively, in cm^3.

UAR(I) AND UAH(I) --- Heat transfer capacities per unit volume of total catalyst and heat exchanger total volume for run No.I, say $3x10^{-4}$ and $25x10^{-4}$ respectively, in $\frac{Cal}{(sec)(K)(cm^3)}$

10 and in addition for first four points. If they are set at 1 then at all the 100 points prints will come.

F --- Catalyst activity decay factor say 0·7 i.e. 70% of the activity of a new catalyst for which rate equation coefficient is applicable

M5 --- No. of sets of runs (operating and design conditions) to be computed on computer, say 3

M8 --- No. of iterations after which the search in one region for a solution is terminated, say 10

IJ1, IJ2, IJ3 and IJ4 ---- Date, month, year and run No. respectively e.g. say 15, 10, 1977 and 51 respectively.

J5 --- No. of solutions to be searched for any sets of conditions or run, say 2(maximum 3).

M12 --- No. of points to be printed in output for any bed, say 14.

K5 --- No. of beds for which prints are desired, say 4

M15 --- The first point from which print is to be started, say 1

M16 --- Spacing to be maintained in printout by skipping the point not desired, say 1

K7 --- This is control to obtain the print for

CHAPTER - V

RESULTS AND DISCUSSION

With the help of simulated model, the effect of changes in the first bed inlet temperature coldshot fraction added to second and third bed, space velocity, temperature of coldshot and fractional content of inerts in the synthesis gas on the performance of ammonia synthesis reactor are analyzed. Eventhough, the simulated model is general enough to study the effect of internal and external heat exchange capacities on the reactor performance, but due to the convergence problem these effects could not be analyzed in detail and only the results of adiabatic reactor operation are presented. The operating and design variables and their ranges are given in Table 5·1 and the summary of computed results is presented in Tables 5·2 to 5·7. The details of temperature and conversion profiles in the reactor for some of the important situations are given in Table B.1 to B.25, Appendix B, and are presented in Figures 5·1 to 5·7. The operation and design parameter values given in Table 5·1 are based on the values normally used in ammonia synthesis plant having a quench convertor of approximately 800 tons/day of ammonia capacity[2,11].

5.1 Effect of First Bed Inlet Temperature T_{10}

At a space velocity of $9\cdot0\times10^3$ $Nm^3/(hr)(m^3$ catalyst)

TABLE 5·1: RANGE OF VARIABLES STUDIED

Feed Rate, Nm^3/hr	$5·675x10^5$	$3·513x10^5$	$11·350x10^5$	
1st Bed **inlet temperature**, T_{10}, ^oK	593	643	693	
1st bed inlet pressure, ATM	160			
Cold shot distribution				
2nd bed inlet, F_{D2}	0·00	0·00	0·20	0·20
3rd bed inlet, F_{D3}	0·00	0·15	0·00	0·15
Cold shot temperature, K	413	T_{10}		
Feed compositions (mole %)				
H_2	64·5	60·75		
N_2	21·5	20·25		
NH_3	2·0	4·00		
CH_4	10·0	12·00		
A	2·0	3·0		
Catalyst volume, m^3	63			
Catalyst activity factor	0·70			
Catalyst distribution, m^3				
1st bed	9			
2nd bed	18			
3rd bed	36			

Feed comp.(Mole %): H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0

Feed Pressure=160 ATM; catalyst volume=63 m^3, Activity=70%

S. No	Space vol. hr^{-1}	Coldshot distribution* 2nd bed	Coldshot distribution* 3rd bed	Temp., K 1st bed inlet	Temp., K Cold shot	Reactor Exi Temp, K	Reactor Exi Mole NH_3	ressure op in ed, ATM	NH_3 Prod. Tons/day	Remarks** Catalyst vol, m^3	Remarks** Bed Temp, K
1.	9·0x10^3	0·00	0·00	598·0	-	617·9	2·96	5·65	95·8		
2.		0·00	0·15	598·0	598·0	618·3	2·97	5·03	97·3		
3.		0·00	0·15	598·0	413·0	583·7	2·62	5·03	61·8		
4.		0·20	0·00	598·0	598·0	618·3	2·97	5·38	97·3		
5.		0·20	0·00	598·0	413·0	569·3	2·35	5·39	35·1		
6.		0·20	0·15	598·0	598·0	613·6	2·99	4·80	92·6		
7.		0·20	0·15	598·0	413·0	539·6	2·24	4·81	23·8		
8.	13·5x10^3	0·00	0·00	598·0	-	609·9	2·58	11·73	86·5		
9.		0·00	0·15	598·0	598·0	610·3	1·34	10·45	89·0		
10.		0·00	0·15	598·0	413·0	579·0	2·38	10·45	57·6		
11.		0·20	0·00	598·0	598·0	610·3	2·60	11·18	89·1		
12.		0·20	0·00	598·0	413·0	566·7	2·22	11·19	33·2		
13.		0·20	0·15	598·0	598·0	610·7	2·61	9·97	91·4		
14.		0·20	0·15	598·0	413·0	537·9	2·16	9·99	23·0		
15.	18·0x10^3	0·00	0·00	598·0	-	606·1	2·39	19·71	78·3		
16.		0·00	0·15	598·0	598·0	606·5	2·41	17·56	82·2		
17.		0·00	0·15	598·0	413·0	576·6	2·27	17·56	53·8		
18.		0·20	0·00	598·0	598·0	606·5	2·41	18·77	82·4		
19.		0·20	0·00	598·0	413·0	565·4	2·16	18·79	31·3		
20.		0·20	0·15	598·0	598·0	606·9	2·43	16·75	85·9		
21.		0·20	0·15	598·0	413·0	537·0	2·11	16·77	22·1		

NOTE:- Space velocity is in Nm^3 of total synthesis gas per hour per m^3 of catalyst volume.

*Coldshot distribution is given as fraction of total feed.

**Showing reactor position and bed temperature at which conversion reaches max. value.

TABLE NO.5·3: SUMMARY OF COMPUTED RESULTS
Feed composition(Mole %): H_2=64·5,N_2=21·5,NH_3=2·0,CH_4=10·0,A=2·0
Feed Pressure=160 ATM;catalyst volume=63 m^3, Activity=70%

S. No.	Space vel. hr^{-1}	Coldshot distribution*		Temp., K		Reactor Exit		Pressure drop in bed,ATM	NH_3 Prod. Tons/day	Remarks**	
		2nd bed	3rd bed	1st bed inlet	Cold shot	Temp.,K	Mole % NH_3			Catalyst Bed vol.m^3	Temp,K
1.	9·0x10^3	0·00	0·00	648·0	648·0	795·6	9·00	5·54	663·0		
2.		0·00	0·15	648·0	648·0	800·4	9·23	4·92	684·2		
3.		0·00	0·15	648·0	413·0	695·6	5·92	4·92	373·5		
4.		0·20	0·00	648·0	648·0	798·4	9·13	5·28	675·1		
5.		0·20	0·00	648·0	413·0	639·9	3·78	5·33	172·8		
6.		0·20	0·15	648·0	648·0	803·0	9·56	4·69	695·1		
7.		0·20	0·15	648·0	413·0	591·6	3·14	4·76	112·0		
8.	13·5x10^3	0·00	0·00	648·0	-	717·7	5·28	11·61	482·2		
9.		0·00	0·15	648·0	648·0	721·1	5·44	10·52	505·2		
10.		0·00	0·15	648·0	413·0	656·2	4·01	10·32	293·0		
11.		0·20	0·00	648·0	648·0	720·6	5·51	11·04	501·6		
12.		0·20	0·00	648·0	413·0	623·8	3·04	11·12	156·8		
13.		0·20	0·15	648·0	648·0	723·6	5·56	9·84	522·6		
14.		0·20	0·15	648·0	413·0	582·7	2·70	9·92	105·3		
15.	18·0x10^3	0·00	0·00	648·0	-	690·7	4·00	19·56	397·5		
16.		0·00	0·15	648·0	648·0	693·5	4·13	17·41	422·4		
17.		0·00	0·15	648·0	413·0	641·9	3·32	17·41	262·5		
18.		0·20	0·00	648·0	648·0	693·4	4·13	18·62	422·7		
19.		0·20	0·00	648·0	413·0	618·0	2·72	18·70	143·6		
20.		0·20	0·15	648·0	648·0	696·0	4·25	16·59	445·5		
21.		0·20	0·15	648·0	413·0	578·7	2·50	16·69	99·5		

NOTE:- Space velocity is in Nm^3 of total synthesis gas per hour per m^3 of catalyst volume.

* Coldshot distribution is given as fraction of total feed.

** Showing reactor position and bed temperature at which conversion reaches max. volume.

TABLE NO. 5·4: SUMMARY OF COMPUTED RESULTS
Feed composition (Mole %): $H_2=64\cdot5, N_2=21\cdot5, NH_3=2\cdot0, CH_4=10\cdot0, A=2\cdot0$
Feed Pressure=160 ATM, catalyst volume=63 m^3, Activity=70%

S. No.	Space vel. hr^{-1}	Coldshot distribution*		Temp., K		Reactor Exit		Pressure drop in bed, ATM	NH_3 Prod. Tons/day	Remarks**	
		2nd bed	3rd bed	1st bed inlet	Cold shot	Temp, K	Mole % NH_3			Catalyst vol, m^3	Bed Temp, K
1.	$9\cdot0\times10^3$	0·00	0·00	698·0	-	836·4	8·33	5·28	603·7	34·2	837·6
2.		0·00	0·15	698·0	698·0	838·1	8·35	4·71	605·1	41·4	838·6
3.		0·00	0·15	698·0	413·0	822·4	9·46	4·71	704·0	52·2	822·7
4.		0·20	0·00	698·0	698·0	837·2	8·37	5·01	606·9	30·6	833·3
5.		0·20	0·00	698·0	413·0	814·5	10·05	5·10	756·0		
6.		0·20	0·15	698·0	698·0	838·9	8·37	4·48	607·5	41·4	839·3
7.		0·20	0·15	698·0	413·0	762·7	9·74	4·52	728·0		
8.	$13\cdot5\times10^3$	0·00	0·00	698·0	-	832·1	8·13	11·15	878·5	48·6	833·0
9.		0·00	0·15	698·0	698·0	834·1	8·18	9·88	885·8	45·0	835·0
10.		0·00	0·15	698·0	413·0	817·8	9·31	9·88	1037·0		
11.		0·20	0·00	698·0	698·0	833·7	8·21	10·57	888·8	45·0	834·7
12.		0·20	0·00	698·0	413·0	754·3	7·19	10·85	750·0		
13.		0·20	0·15	698·0	698·0	835·6	8·25	9·38	894·4	45·0	836·5
14.		0·20	0·15	698·0	413·0	667·3	5·11	9·67	458·0		
15.	$18\cdot0\times10^3$	0·00	0·00	698·0	-	825·1	7·81	19·06	1113·5		
16.		0·00	0·15	698·0	698·0	828·4	7·96	16·87	1140·5	59·4	828·6
17.		0·00	0·15	698·0	413·0	794·1	8·31	16·87	1207·0		
18.		0·20	0·00	698·0	698·0	828·4	7·96	18·08	1140·9	59·4	828·5
19.		0·20	0·00	698·0	413·0	708·6	5·02	18·40	594·0		
20.		0·20	0·15	698·0	698·0	831·1	8·08	16·02	1162·3	55·8	831·4
21.		0·20	0·15	698·0	413·0	643·7	3·97	16·40	391·0		

NOTE:- Space velocity is in Nm^3 of total synthesis gas per hour per m^3 of catalyst volume.

* Coldshot distribution is given as fraction of total feed.

**Showing reactor position and bed temperature at which conversion reaches max. value.

TABLE NO.5·5: SUMMARY OF COMPUTED RESULTS
Feed composition (Mole %): H_2=60·75, N_2=20·25, NH_3=4·00, CH_4=12·00, A=3·00
Feed Pressure=160 ATM; catalyst volume=63 m^3, Activity=70%

S. No.	Space vel. hr^{-1}	Coldshot distribution*		Temp, K		Reactor Exit		Pressure drop in bed, ATM	NH_3 Prod. Tons/day	Remarks**	
		2nd bed	3rd bed	1st bed inlet	Cold shot	Temp, K	Mole % NH_3			Catalyst vol. m^3	Bed Temp, K
1.	9·0x10^3	0·00	0·00	598·0	-	606·0	4·41	5·66	40·3		
2.		0·00	0·15	598·0	598·0	606·1	4·41	5·05	40·9		
3.		0·00	0·15	598·0	413·0	576·3	4·26	5·05	26·2		
4.		0·20	0·00	598·0	598·0	606·1	4·41	5·39	40·9		
5.		0·20	0·00	598·0	413·0	565·0	4·15	5·40	15·0		
6.		0·20	0·15	598·0	598·0	606·2	4·42	4·81	41·5		
7.		0·20	0·15	598·0	413·0	536·8	4·10	4·82	10·2		
8.	13·5x10^3	0·00	0·00	598·0	-	602·9	4·25	11·75	37·0		
9.		0·00	0·15	598.0	598·0	603·0	4·25	10·47	38·0		
10.		0·00	0·15	598·0	413·0	574·4	4·17	10·47	24·7		
11.		0·20	0·00	598·0	598·0	603·0	4·25	11·20	38·0		
12.		0·20	0·00	598·0	413·0	564·0	4·10	11·20	14·2		
13.		0·20	0·15	598·0	598·0	603·1	4·26	9·99	39·0		
14.		0·20	0·15	598·0	413·0	536·1	4·07	10·00	9·9		
15.	18·0x10^3	0·00	0·00	598·0	-	601·3	4·17	19·73	33·6		
16.		0·00	0·15	598·0	598·0	601·5	4·13	17·58	35·3		
17.		0·00	0·15	598·0	413·0	573·4	4·12	17·58	23·1		
18.		0·20	0·00	598·0	598·0	601·5	4·18	18·79	35·3		
19.		0·20	0·00	598·0	413·0	563·4	4·07	18·80	13·4		
20.		0·20	0·15	598·0	598·0	601·6	4·19	16·78	36·8		
21.		0·20	0·15	598·0	413·0	535·7	4·05	16·78	9·5		

NOTE:- Space velocity is in Nm^3 of total synthesis gas per hour per m^3 of catalyst volume.

*Coldshot distribution is given as fraction of total feed.

**Showing reactor position and bed temperature at which conversion reaches max. value.

Feed composition (Mole %): H_2=60·75, N_2=20·25, NH_3=4·00, CH_4=12·00, A=3·00

Feed Pressure=160 ATM, catalyst volume=63 m^3, Activity=70%

S. No	Space vel. hr^{-1}	Coldshot distri-* bution		Temp., K		Reactor Exit		Pressure drop in bed, ATM	NH_3 Prod. Tons/day	Remarks**	
		2nd bed	3rd bed	1st bed inlet	Cold shot	Temp, K	Mole % NH_3			Catalyst vol. m^3	Bed Temp, K
1.	9·0x10^3	0·00	0·00	648·0	-	696·8	6·41	5·62	239·3		
2.		0·00	0·15	648·0	648·0	698·2	6·48	5·00	239·5		
3.		0·00	0·15	648·0	413·0	643·1	5·44	5·00	144·0		
4.		0·20	0·00	648·0	648·0	697·8	6·46	5·35	239·2		
5.		0·20	0·00	648·0	413·0	617·9	4·74	5·37	74·2		
6.		0·20	0·15	648·0	648·0	699·2	6·53	4·77	245·9		
7.		0·20	0·15	648·0	413·0	578·1	4·48	4·80	49·0		
8.	13·5x10^3	0·00	0·00	648·0	-	674·5	5·31	11·70	192·8		
9.		0·00	0·15	648·0	648·0	675·6	5·35	10·42	200·2		
10.		0·00	0·15	648·0	413·0	631·2	4·83	10·42	123·1		
11.		0·20	0·00	648·0	648·0	675·5	5·35	11·14	199·6		
12.		0·20	0·00	648·0	413·0	612·2	4·45	11·17	66·6		
13.		0·20	0·15	648·0	648·0	676·4	5·40	9·94	206·3		
14.		0·20	0·15	648·0	413·0	574·7	4·30	9·97	45·1		
15.	18·0x10^3	0·00	0·00	648·0	-	655·2	4·85	19·67	167·5		
16.		0·00	0·15	648·0	648·0	666·2	4·90	17·52	177·0		
17.		0·00	0·15	648·0	413·0	625·9	4·57	17·52	112·0		
18.		0·20	0·00	648·0	648·0	666·2	4·90	18·73	177·1		
19.		0·20	0·00	648·0	413·0	609·5	4·31	18·77	61·7		
20.		0·20	0·15	648·0	648·0	667·1	4·94	16·71	185·7		
21.		0·20	0·15	648·0	413·0	573·0	4·22	16·75	42·9		

NOTE:- Space velocity is in Nm^3 of total synthesis gas per hour per m^3 of catalyst volume.

*Coldshot distribution is given as fraction of total feed.

**Showing reactor position and bed temperature at which conversion reaches max.value.

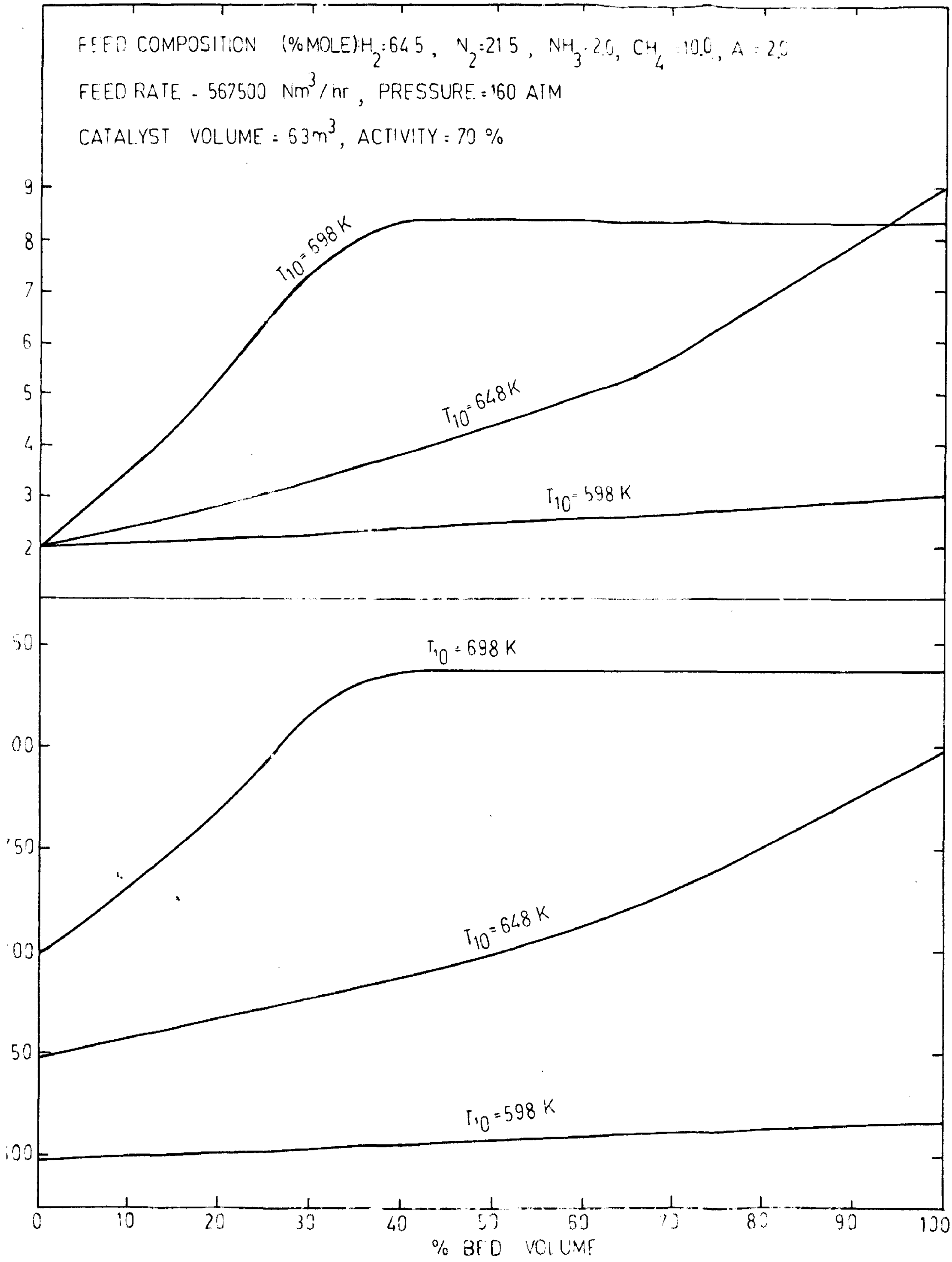
TABLE NO.5·7: SUMMARY OF COMPUTED RESULTS
Feed composition (Mole %): H_2=60·75,N_2=20·25,NH_3=4·00,CH_4=12·00,A=3·00
Feed Pressure=160 ATM; catalyst volume=63 m^3, Activity=70%

S. No.	Space vel. hr^{-1}	Coldshot distribution*		Temp., K		Reactor Exit		Pressure drop in bed, ATM	NH_3 Prod. Tons/day	Remarks**	
		2nd bed	3rd bed	1st bed inlet	Cold shot	Temp.,K	Mole % NH_3			Catalyst vol.m^3	Bed Temp,K
1.	9·0x10^3	0·00	0·00	698·0	-	812·9	9·53	5·45	521·5	55·8	813·0
2.		0·00	0·15	698·0	698·0	813·8	9·55	4·83	523·8	55·8	814·0
3.		0·00	0·15	698·0	413·0	796·5	10·67	4·83	623·5		
4.		0·20	0·00	698·0	698·0	813·6	9·56	5·18	524·7	55·8	813·8
5.		0·20	0·00	698·0	413·0	720·6	7·74	5·28	359·0		
6.		0·20	0·15	698·0	698·0	814·4	9·58	4·59	526·5	55·8	814·6
7.		0·20	0·15	698·0	413·0	647·5	6·21	4·71	215·0		
8.	13·5x10^3	0·00	0·00	698·0	-	802·9	9·04	11·50	716·8		
9.		0·00	0·15	698·0	698·0	805·9	9·19	10·21	736·2		
10.		0·00	0·15	698·0	413·0	743·2	8·12	10·21	591·0		
11.		0·20	0·00	698·0	698·0	805·5	9·17	10·93	734·1		
12.		0·20	0·00	698·0	413·0	683·9	5·91	11·06	280·0		
13.		0·20	0·15	698·0	698·0	808·1	9·28	9·72	750·5		
14.		0·20	0·15	698·0	413·0	628·0	5·23	9·86	180·7		
15.	18·0x10^3	0·00	0·00	698·0	-	772·4	7·57	19·45	685·2		
16.		0·00	0·15	698·0	698·0	778·1	7·84	17·28	736·3		
17.		0·00	0·15	698·0	413·0	709·2	6·47	17·28	479·0		
18.		0·20	0·00	698·0	698·0	777·6	7·82	18·49	732·1		
19.		0·20	0·00	698·0	413·0	670·3	5·24	18·63	244·0		
20.		0·20	0·15	698·0	698·0	783·0	8·08	16·46	779·5		
21.		0·20	0·15	698·0	413·0	620·2	4·84	16·63	165·0		

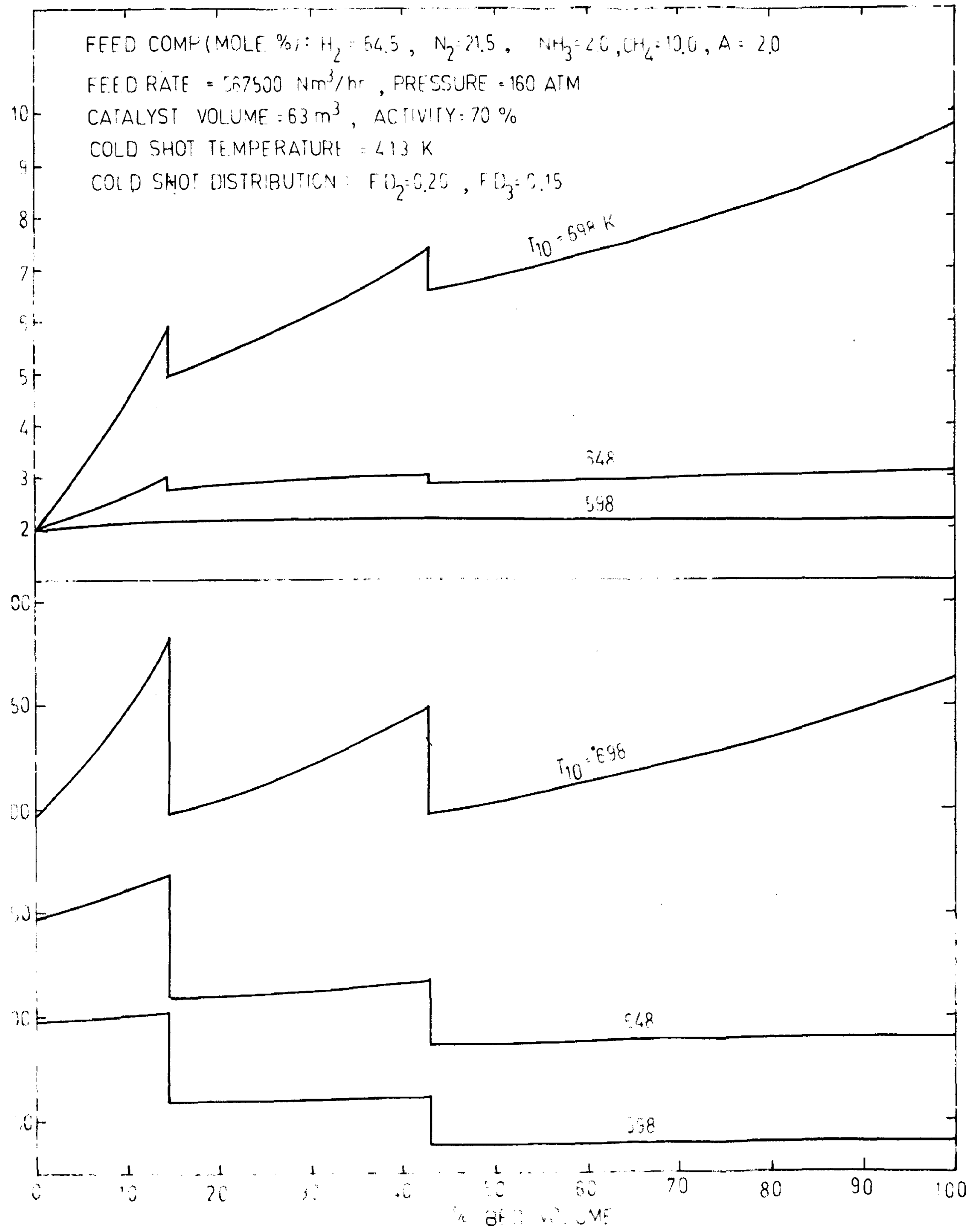
NOTE:- Space velocity is in Nm^3 of total synthesis gas per hour per m^3 of catalyst volume.

*Coldshot distribution is given as fraction of total feed..

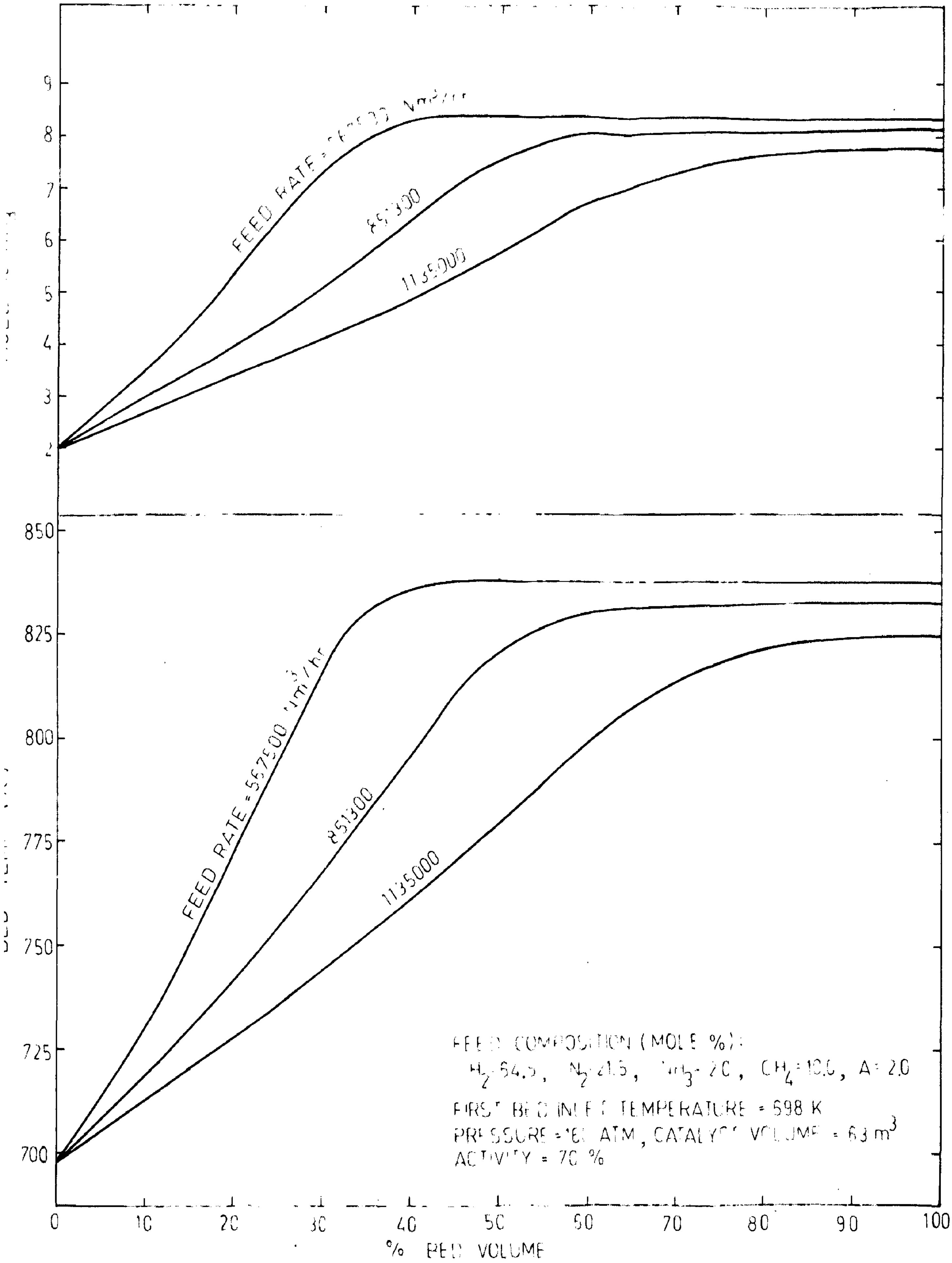
**Showing reactor position and bed temperature at which conversion reaches max. value.



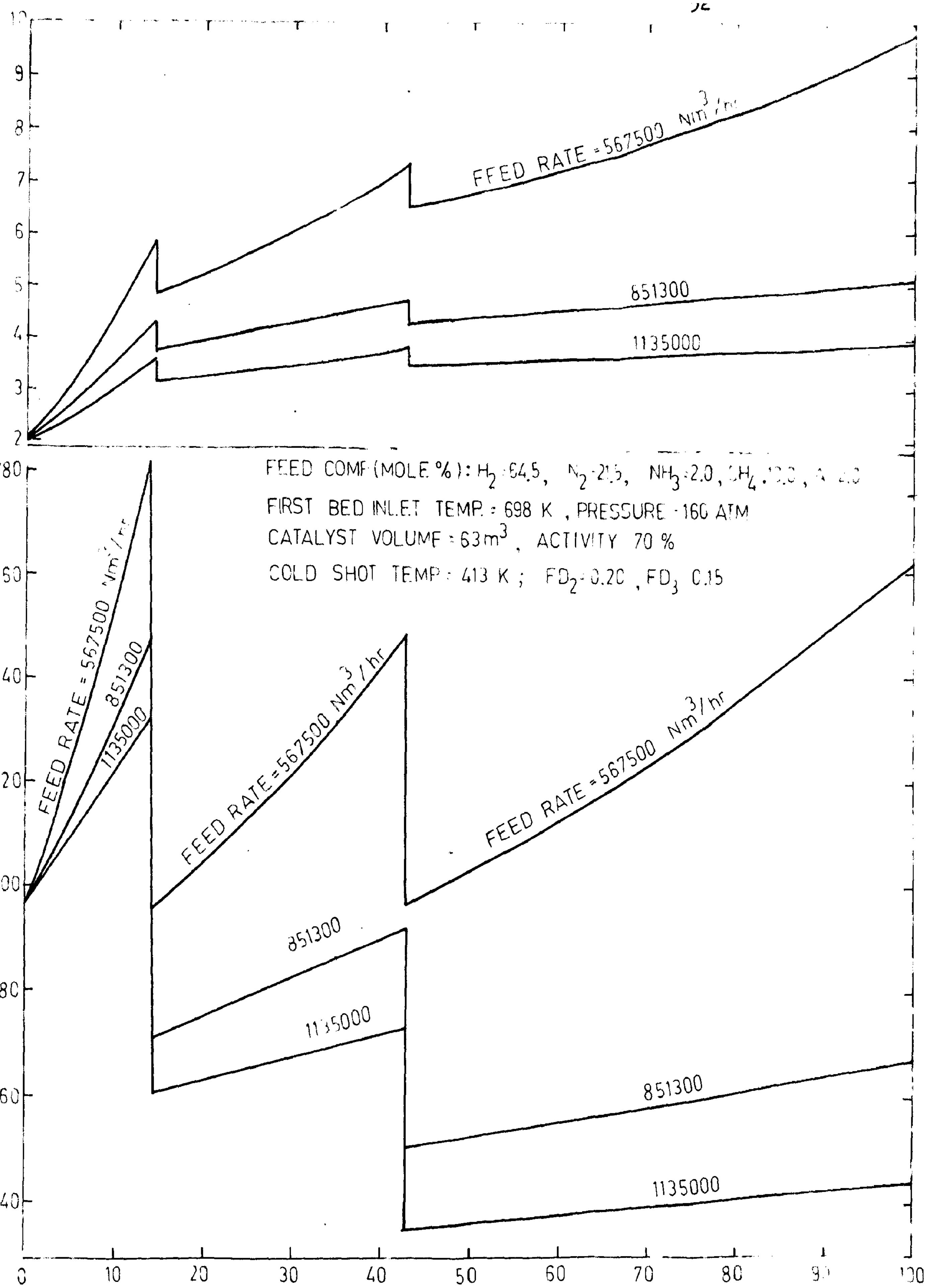
5.1 EFFECT OF FIRST BED INLET TEMPERATURE T_{10} ON CONVERSION AND BED TEMPERATURE WITHOUT COLD SHOT COOLING



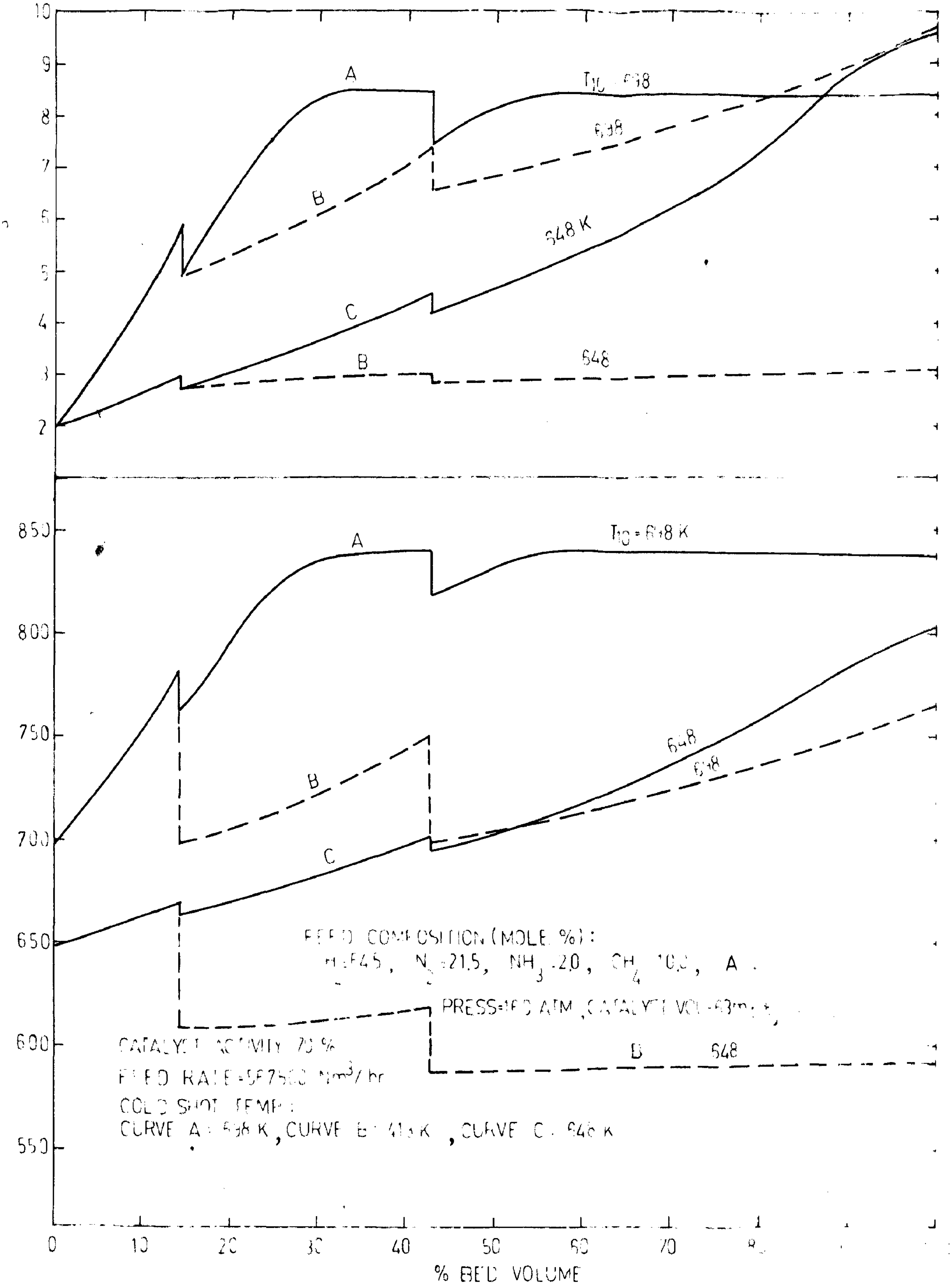
2 EFFECT OF FIRST BED INLET TEMPERATURE ON CONVERSION AND BED TEMPERATURE WITH COLD SHOT COOLING



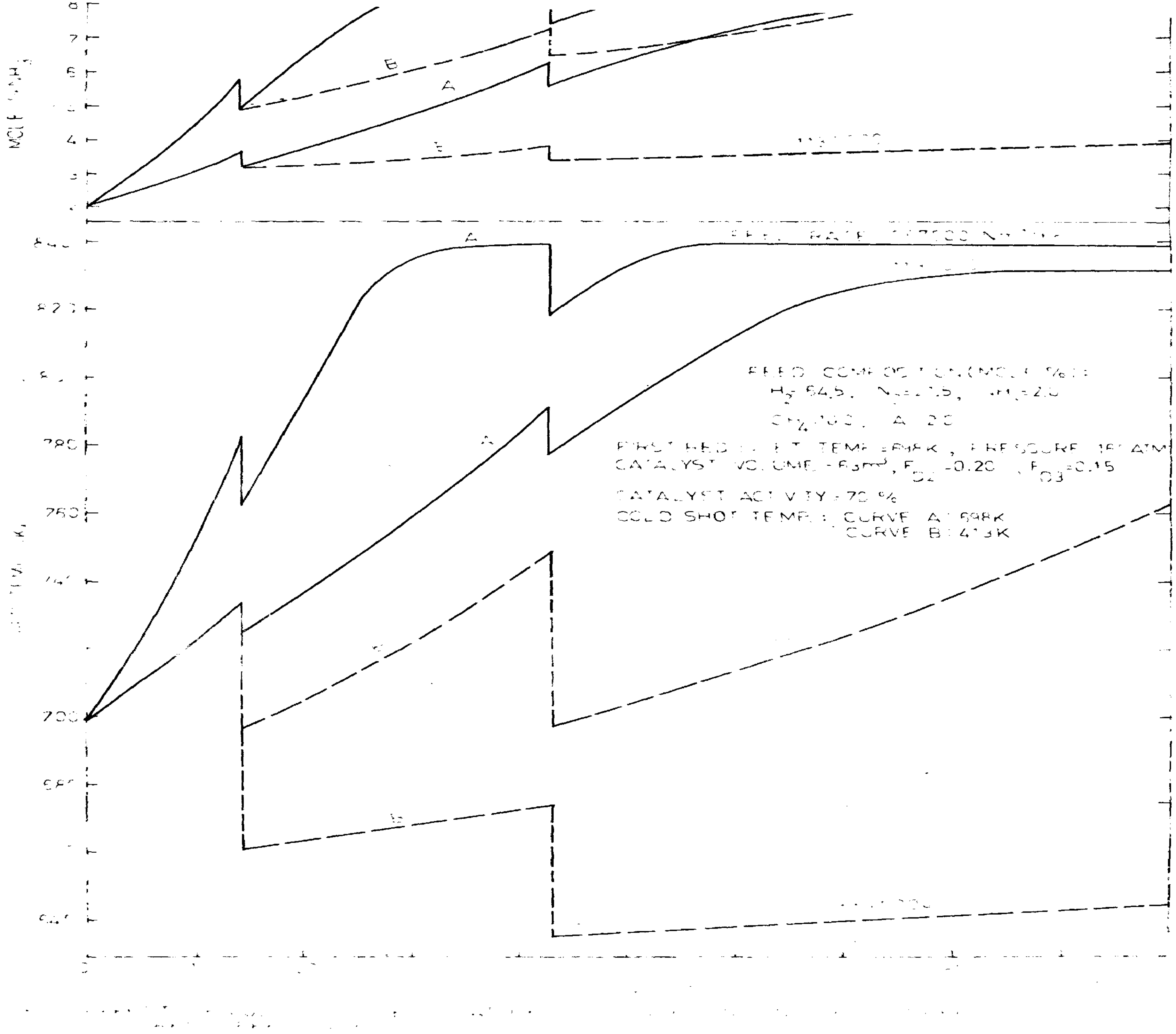
5.3 EFFECT OF FEED RATE ON CONVERSION AND BED TEMPERATURE WITHOUT COLD SHOT COOLING

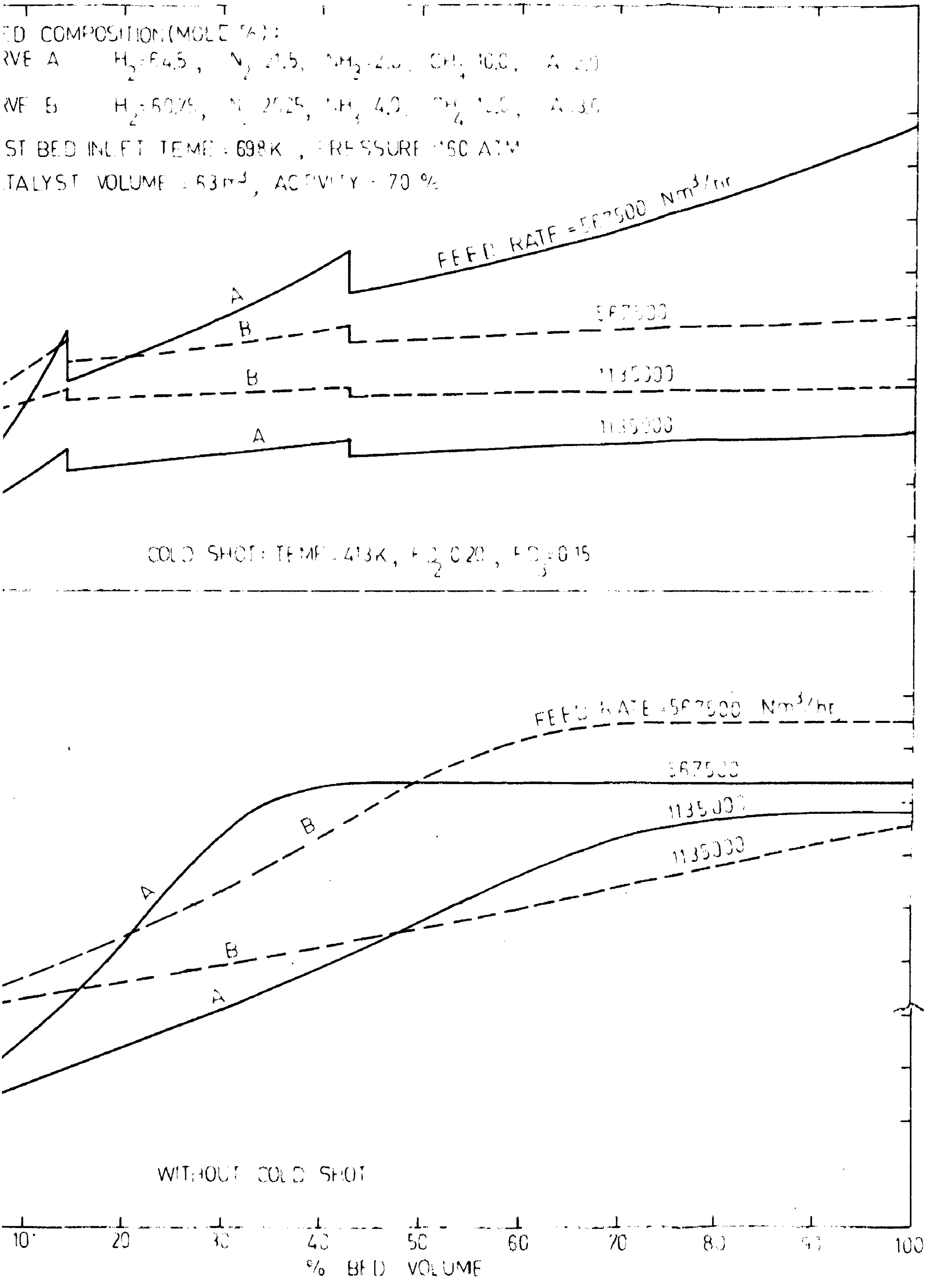


5.54 EFFECT OF FEED RATE ON CONVERSION AND BED TEMPERATURE WITH COLD SHOT COOLING



5.5 EFFECT OF COLD SHOT TEMPERATURE ON CONVERSION AND BED TEMPERA[illegible] DIFFERENT FIRST BED INLET TEMPERATURES T_{10}


MOLE % NH3
8
7
6
5
4
3
2
B
A
B
A
A
B
B
840
820
780
760
740
700
680
FEED COMPOSITION (MOLE %):
H_2 64.5, N_2 21.5, NH_3 2.0
CH_4 10.0, A 2.0
FIRST BED INLET TEMP. 698K, PRESSURE 150 ATM
CATALYST VOLUME 65 m³, F_{b2} 0.20, F_{b3} 0.15
CATALYST ACTIVITY 70 %
COLD SHOT TEMP.: CURVE A: 598K
CURVE B: 413K


ED COMPOSITION (MOLE %):
RVE A H_2=64.5, N_2=21.5, NH_3=2.0, CH_4=10.0, A=2.0
RVE B H_2=60.75, N_2=20.25, NH_3=4.0, CH_4=12.0, A=3.0
ST BED INLET TEMP.=698K, PRESSURE=150 ATM
TALYST VOLUME =63 m^3, ACTIVITY = 70 %
FEED RATE =567500 Nm^3/hr
A
B
567500
B
1135000
A
1135000
COLD SHOT: TEMP.=413K, F_2=0.20, F_3=0.15
FEED RATE =567500 Nm^3/hr
567500
1135000
1135000
B
A
B
A
WITHOUT COLD SHOT
10
20
30
40
50
60
70
80
90
100
% BED VOLUME

with synthesis gas composition (mole percent): $H_2=64\cdot5$, $N_2=21\cdot5$, $NH_3=2\cdot0$, $CH_4=10\cdot$ and $A=2\cdot0$ and for catalyst activity factor of 0·7, the use of first bed inlet temperature, T_{10}, as 598 °K gives extremely low conversion because of the very low catalyst bed temperature throughout the reactor. Increase in T_{10} to 648 °K increases the conversion and temperature rapidly but further increase in T_{10} to 698 °K may or may not be advantageous depending upon whether or not the reaction becomes equilibrium inhibited. It may be recalled that higher equilibrium ammonia conversion can be achieved at lower temperatures. At T_{10} value of 648 °K, ammonia percent in gases at the exit of catalyst section is 9·00 as compared to 8·33 when T_{10} is 698 °K because of the equilibrium inhibition after about 40 percent of the catalyst bed volume (Fig. 5·1 and Tables B·4 and B·7) without coldshot cooling. Shah[2] has also reported the existence of equilibrium conditions after about 30 percent of the catalyst bed volume for first bed inlet temperature of about 720 °K without coldshot cooling. The use of coldshot cooling at the inlet of second and third catalyst beds with coldshot temperature of 413 °K virtually quenches the reaction when first bed inlet temperature T_{10} is 648 °K but for T_{10} value of 698 °K increases ammonia concentration in exit gases in the range of 9·46 to 10·05 percent depending upon the distribution of coldshot and no equilibrium inhibition is observed (Fig. 5·2. and Tables B·4 and B·7). However, if the coldshot temperature is kept equal to first bed inlet temperature T_{10}, higher ammonia concentration in exit gases without any equilibrium inhibition is obtained for T_{10} value of 648 ^{O}K as compared to T_{10} value of 698 ^{O}K (Fig. 5·5 and Tables B·19 and B·19 and B·16).

It is, therefore, clear from the above discussion and summary of results given in Table 5·2 that the use of first bed inlet temperature T_{10} of 598 ^{O}K or less results in low catalyst bed temperature and ammonia production rate is always less than 100 metric tons per day. When T_{10} is raised to 648 ^{O}K, the catalyst bed temperatures and ammonia production rate increases rapidly. Further increase in T_{10} to 698 ^{O}K results in equilibrium limitations in some cases specially when coldshot cooling is not used or coldshot temperature is high or space velocity is low.

5.2 Effect of Space Velocity

The effect of feed rate can be explained in terms of space velocity. For the convenience of discussion, the space velocity is defined as cubic meter of total synthesis gas fed to reactor per hour per cubic meter of catalyst in the reactor obviously, actual velocity of synthesis gas at different points in catalyst bed will depend upon the distribution of coldshots, temperature, pressure and conversion and can be estimated from the results presented in Appendix B.

Increase in space velocity from $9{\cdot}0\times10^3$ to $18{\cdot}0\times10^3$ $Nm^3/(hr)(m^3)$ always decreases the ammonia concentration in the exit gas but the ammonia production rate may increase or decrease depending upon the first bed inlet temperature, coldshot distribution and the feed composition. For first bed inlet temperature of 598 and 648 ^{o}K increase in space velocity decrease the ammonia production rate because of lower temperature rise in catalyst bed temperature as a result of lower percent conversion at higher space velocity. (Tables 5·2, 5·3, 5·5 and 5·6). However, for T_{10} value of 698 ^{o}K the ammonia production rate increases with increase in space velocity if coldshot temperature is also 698 ^{o}K because of the equilibrium limitations at low space velocities. For T_{10} value of 698 ^{o}K and coldshot temperature of 413 ^{o}K, ammonia production rate may either increase with space velocity provided equilibrium limitations exists at low space velocity or decrease if catalyst bed 'temperature decreases rapidly due to excessive quenching effect (Tables 5·4 and 5·7 and Figs. 5·3, 5·6 and 5·7).

5·3 Effect of Cold Shot Distribution and Temperature

The advantage of the addition of cold shot cooling is to lower the temperature of reaction mixture as it passes through the catalyst bed so as to have more favourable equilibrium conditions. This enables the designer to keep high reaction temperature when the degree of conversion is still low and to drop the temperature as the conversion proceeds to achieve high production capacity and a high degree of conversion.

At low first bed inlet temperatures T_{10} of 598 and 648 ^{o}K the introduction of cold shot at 413 ^{o}K is always harmful due to excessive quenching effect but at cold shot temperatures equal to T_{10} some improvement in ammonia production capacity is possible in some cases. It may be observed that for T_{10} values of 598 and 648 ^{o}K the ammonia concentration in exit gas from the reactor is much below the equilibrium value. For T_{10} value of 698 ^{o}K, the beneficial effect of cold shot cooling is quite clear from the results presented in Table 5·4 and Figs. 5·1 to 5·4. The introduction of the cold shot at 698 ^{o}K is not of much advantage because temperature of the reaction mixtures after the addition of cold shot is still quite high for the reaction mixture to attain equilibrium composition quickly. The introduction of cold shot of 413 ^{o}K with proper distribution can improve the ammonia concentration in exit gas and the ammonia production rate quite significantly because the addition of cold shot lowers the temperature sufficiently for the reaction not to be inhibited by equilibrium limitations as the reaction mixture passes through catalyst bed (Fig. 5·5). Results in Table 5·4 indicate that at a space velocity of $9{\cdot}0 \times 10^{3}$ $Nm^{3}/(hr)(m^{3})$ ammonia production rate can be increased from 603·7 to 756·0 tons/day by adding 20% of the total feed as cold shot at a temperature of 413 ^{o}K at the inlet of second catalyst bed. Similarily, at space velocity of $13{\cdot}5 \times 10^{3}$ $Nm^{3}/(hr)(m^{3})$ ammonia production rate is increased from 878·5 to 1037·0 tons/day by adding 15% of the total feed as cold shot at a temperature of 413 ^{o}K at the inlet of the third bed. However, the use of cold shot cooling at a higher space velocity of $18{\cdot}0 \times 10^{3}$ $Nm^{3}/(hr)(m^{3})$ has resulted in either inappreciable improvement in production rate or a significant decline from 1113·5 to 391·0 tons/day due to quenching effect by the addition of cold shot at 413 °K.

When feed contains higher ammonia and **inerts** concentration even for T_{10} value of 698 °K the addition of cold shot also at 698 °K does not improve the production rate appreciably and when colder cold shot at 413 °K is added, the ammonia production rate decreases significantly in most of the cases (Table 5·7).

5.4 Effect of Ammonia And Inerts in the Feed

Ammonia synthesis reaction is reversible and increased ammonia concentration in feed is bound to slow down the rate of ammonia formation and the ammonia production will be adversely effected. The presence of inert gases will also reduce the ammonia synthesis reaction and production rates due to the diluent action. Further, the presence of inerts can also moderate the temperature rise in catalyst bed by acting as heat carriers and this may or may not be beneficial depending upon whether reaction does or does not become equilibrium inhibited at low ammonia and inerts concentration in feed.

For the first bed inlet temperature T_{10} values of 598 and 648 ^{o}K the increase in ammonia concentration from 2·0 to 4·0 mole percent and that of methane and argon from 10·0 and 2·0 to 12·0 and 3·0 mole percent respectively decreases the ammonia production rate to about 35 to 45 percent of the value at low ammonia and inerts concentration in feed depending upon the cold shot temperature and distribution. However, at T_{10} value of 698 ^{o}K and cold shot temperature equal to T_{10} the increase in ammonia and inerts concentration as mentioned above is not as deterimental for ammonia production rate due to more favourable equilibrium conditions due to slower rise in reaction temperature since the production rate decreases only to about 65 to 85 percent of the value at low ammonia and inerts concentration in feed. But when the cold shot temperature is 413 ^{o}K, the reduction in ammonia production rate is as significant as that for T_{10} values of 598 and 648 ^{o}K. (Fig 5·7 and Tables 5·4 and 5·7).

5.5 Effect of Pressure

Effect of pressure is not investigated in the present study and synthesis feed gas presence is taken at 160 ATM. But the sensitivity of the reaction system on operating presence can be understood from the results presented in Tables B·7 and B·8 and Fig. 5·3. For first bed inlet temperature T_{10} of 698 °K and for feed rate of $5\cdot675\times10^5$ and $8\cdot513\times10^5$ Nm^3/hr when equilibrium composition reaches at some position in the bed, as this equilibrium mixture passes further down the bed pressure decreases due to frictional losses and results in the reverse reaction depending upon the extent of pressure drop. In such a situation, conversionand temperature at the exit of the bed is somewhat lower than the maximum conversion and temperature position in the bed where equilibrium is first achieved. The position in the bed where the maxima is achieved is indicated in the lost two columns of the table giving summary of the computed results (Table 5·4).

CHAPTER-VI

CONCLUSIONS AND RECOMMENDATIONS

6.1 CONCLUSIONS:

Results of simulation for ammonia synthesis reactor leads to following conclusions:

1. The net ammonia production rate is quite sensitive to the operating parameters, such as, first bed inlet temperature, space velocity, cold shot temperature and distribution, concentration of ammonia and inerts in synthesis gas feed and pressure, and design parameters, such as, cold shot location and internal and external heat exchange capacities.

2. For operation at 160 ATM and catalyst activity factor of 0·70 and with normal synthesis gas compositions and space velocity, the use of first bed inlet temperature less than 648 °K results in poor conversion. The use of first bed inlet temperature of 698 °K at space velocity much less than $18 \cdot 0 \times 10^3$ $Nm^2/(hr)(m^3)$ without cold shot cooling is also undesirable because of the attainment of equilibrium before the end of the catalyst bed. The use of cold shot cooling improves the reactor performance provided that an excessive cooling of the reaction mixture and catalyst is avoided. The highest

ammonia production rate of over 19 Tons/(day)(m^3 of catalyst) is obtained at a space velocity of $18\cdot0\times10^3$ $Nm^3/(hr)(m^3)$ first bed inlet temperature of 698 ^{o}K and with 15 percent of total feed added at 413 ^{o}K as cold shot at the inlet of the third bed for a feed composition of $H_2=64\cdot5$, $N_2=21\cdot5$, $NH_3=2\cdot0$, $CH_4=10\cdot0$ and $A=2\cdot0$ (mole percent).

3. Use of higher space velocity improves the ammonia production rate provided equilibrium limitations are observed before exit end of the bed.

4. Use of proper amount of cold shot at proper position and temperature with higher first bed inlet temperature is desirable to improve the conversion and ammonia production rate. However, indiscriminate use of cold shot at low temperature is disasterous for ammonia conversion and production rate.

5. For higher conversion and ammonia production rate, it is desirable to ensure that the synthesis gas feed contains minimum of ammonia and inerts.

6.2 RECOMMENDATIONS

1. The present study is restricted to adiabatic operation of multibed reactor with or without cold shot cooling. The simulation model, even though quite general to take care of internal and external

heat exchange, could not be used for autothermal operation due to convergence difficulties. It is recommended that suitable convergence techniques be developed so as to study the reactor performance under stable operating conditions.

2. The optimal distribution of catalyst and cold shot in different beds will definitely improve the conversion and ammonia production rate and needs the development of suitable strategies.

3. The use of one-dimensional ideal plug flow model without inter-and intra-particle transport limitations is a gross simplification of modern reactors. It is desirable to analyze the significance of the above non-ideal reactor behaviour.

4. The work should be extended to analyze the dynamic behaviour of ammonia reactor so as to have better understanding of the parameteric sensitivity and the region of safe stable operation at high conversion conditions.

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NOMENCLATURE

C_{pi}	Heat capacity of component i,	cal/(gm mole)(K)
F_{DH}	Fraction of total feed entering through preheating section	
F_{Dj}	Fraction of total feed entering as cold shot in bed j	
F_i	Total moles of component i fed to the reactor,	gm moles/sec
F_1	Total moles of hydrogen fed to the reactor,	gm moles/sec
$-\Delta H_{R1}$	Heat of exothermic reaction,	Cal/(gm mole of Hydrogen reacted)
N_i	Flow rate of component i,	gm moles/sec
N_{Tj}	Total flow rate of gas in bed j,	gm moles/sec.
P_j	Pressure at any point in bed j,	ATM
$-r_1$	Rate of reaction of hydrogen,	gm moles of hydrogen reacted/(sec)(cm^3 of catalyst volume)
T_{10}	First bed inlet temperature,	K
T_{jo}	Bed number j inlet temperature,	K
T_F	Feed temperature,	K
T_H	Gas temperature in heat exchanger in reaction product side,	K
T	Gas temperature,	K
T_S	Gas temperature on internal preheating section of catalyst bed,	K

T_{SH}	Gas temperature in external heat exchanger on cold feed side,	K
T_{SHE}	Temperature of preheated feed gas after passing through external and internal preheating sections,	K
T'_{SHI}	Temperature of feed gas at the inlet of external preheating section,	K
UA_H	Heat exchange capacity per unit of external heat exchanger vol.,	Cal/(sec)(K)(cm^3)
UA_j	Heat exchange capacity per unit of catalyst bed volume,	Cal/(sec)(K) (cm^3)
V_H	Volume of heat exchanger,	cm^3
V_j	Volume of catalyst in bed number j,	cm^3
X_{1j}	Fraction conversion of hydrogen in bed number j	
α_i	Coefficient proportional to stoichiometric coefficient for component i ($\alpha_1=1, \alpha_2= -1/3, \alpha_3=2/3, \alpha_4=\alpha_5=0$)	
$\underline{\omega}$	Coefficient of pressure drop,	ATM/cm^3
i	Designates component (1-hydrogen, 2-nitrogen, 3-ammonia, 4-methane and 5-argon)	
j	Designates number of catalyst bed (1,2,3)	
O	Designates entry of a bed	
L	Designates exit of a bed	
N	Designates normal or reference value	

APPENDIX

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PART 1 OF THE MAIN PROGRAM FOR SIMULATION OF AMMONIA SYNTHESIS REACTOR
ICI QUENCH TYPE HIGH CAPACITY REACTOR
INPUT STATEMENT PROGRAM
DIMENSION PF(50),TF(50),F11(50),F22(50),F33(50 ),F44(50),
. F55(50),FD22(50),FD33(50),FD44(50),Z11(50 ),Z22(50),Z33(50),
2HLL(50),UAR(50),UAH(50), AZ(110,4),AP(110,4),AX(110,4),AT(110,4),
3ATH(110,4),ACX(110,4),ACT(110,4),ACTH(110,4),ATH12(10)
4,ATEM(100),ADEL(100),ATEP(100),ATEMP(100),ADET(100)
5,ANX(110,4),AZP(110,4)
 COMMON/CB1/F1,F2,F3,F4,F5/CB2/AZ,AP,AX,AT,ATH,ACX,ACT,ACTH/CB3/
1AFD1,AFD2,AFD3,AFD4,Z1,Z2,Z3,HL,XW,UV,C4,RUA,HUA,C5,C61,C62,M15,K7
2,FI11,FI12,FI13,FI21,FI22,FI23,FI31,FI32,FI33,FI41,FI42,FI43,
3FI51,FI52,FI53,PH1,PH2,PB11,S2,S11,S12,FTF1,S112,S122,AR1,AR2,
4AR3,AR4,AR5,Q11,Q21,Q31,Q41,Q51, Q12,Q22,Q32,Q42,Q52, M12,K5,
5Q13,Q23,Q33,Q43,Q53,HA11,HA21,HA31,HA41,HA51,HA61,HA71,HA12 ,M16,
6HA22,HA32,HA42,HA52,HA62,HA72,HA13,HA23,HA33,HA43,HA53,HA63, K8,
7HA73, HA14,HA24,HA34,HA44,HA54,HA64,HA74,NZ1,NZ2,NZ3,NZ4, MZ1,MZ2,
8MZ3,MZ4, HAA21,HAA22,HAA23,HAA24,AHA21,AHA22,AHA23,AHA24, BHA21,
9BHA22,BHA23,BHA24,HAB21,HAB22,HAB23,HAB24,AHA31,AHA32,AHA33,AHA34
A/CB4/ANX,ZTI,PAM,AZP
 READ 51,W11,C3,C2,C4,C51,C611,C621,VW,H1,H2,H3,H4,C71,C72,C73,C74,
1F,M5,M8,IJ1,IJ2,IJ3,IJ4,J5,M12,K5,M15,M16,K7,K8,FF
 FORMAT(8E10.2/8E10.2/E10.2,7I10/6I10,F10.2)
 READ 52,(PF(I),TF(I),F11(I),F22(I),F33(I),F44(I),F55(I),FD22(I),
1FD33(I),FD44(I),Z11(I),Z22(I),Z33(I),HLL(I), UAR(I),UAH(I),I=1,M5)
 FORMAT(8E10.2)

 SEE READ STATEMENT FOR DATA BEFORE OUTPUT STATEMENTS PROGRAM AFTER
 STATEMENT NO.203 IN THE MAIN PROGRAM

 GO TO 404


 PART 2 OF THE MAIN PROGRAM FOR SIMULATION OF AMMONIA SYNTHESIS REACTOR
 FROM INTERNAL PREHEATER  OUTLET STREAM TEMPERATURES PREDICTION BY TRIAL
 AND ERROR TECHNIQUE BY MATCHING CALCULATED FEED TEMPERATURE WITH KNOWN
 FEED TEMPERATURES
 M=1
 HA11=0.5*H1
 HA21=0.083333*H1
 HA31=0.5*HA21
 HA41=4.0*H1
 HA51=2.666667*H1
 HA61=2.0*H1
 HA71=0.333333*H1
 HA12=0.5*H2
 HA13=0.5*H3
 HA14=0.5*H4
 HA22=0.0833333*H2
```

```
HA23=0.0833333*H3
HA24=0.0833333*H4
HA32=0.5*HA22
HA33=0.5*HA23
HA34=0.5*HA24
HA42=4.0*H2
HA43=4.0*H3
HA44=4.0*H4
HA52=2.666667*H2
HA53=2.666667*H3
HA54=2.666667*H4
HA62=2.0*H2
HA63=2.0*H3
HA64=2.0*H4
HA72=0.333333 *H2
HA73=0.333333*H3
HA74=0.333333*H4
HAA21=5.0*HA21
HAA22=5.0*HA22
HAA23=5.0*HA23
HAA24=5.0*HA24
AHA21=23.0*HA21
AHA22=23.0*HA22
AHA23=23.0*HA23
AHA24=23.0*HA24
BHA21=16.0*HA21
BHA22=16.0*HA22
BHA23=16.0*HA23
BHA24=16.0*HA24
HAB21=8.0*HA21
HAB22=8.0*HA22
HAB23=8.0*HA23
HAB24=8.0*HA24
AHA31=9.0*HA31
AHA32=9.0*HA32
AHA33=9.0*HA33
AHA34=9.0*HA34
BHA31=19.0*HA31
BHA32=19.0*HA32
BHA33=19.0*HA33
BHA34=19.0*HA34
CHA31=5.0*HA31
CHA32=5.0*HA32
CHA33=5.0*HA33
CHA34=5.0*HA34
XW=PF(M)
UV=TF(M)
J=1
T=TF(M)
Z1=Z11(M)
Z2=Z22(M)
```

```
Z3=Z33(M)
HL=HLL(M)
F1=F11(M)
F2=F22(M)
F3=F33(M)
F4=F44(M)
F5=F55(M)
FTT=F1+F2+F3+F4+F5
FTV=FTT*80.64
FTT1=100./FTT
PHY=F1*FTT1
PNI=F2*FTT1
PAM=F3*FTT1
PME=F4*FTT1
PAR=F5*FTT1
RHN=F1/F2
ZTI=100./(Z1+Z2+Z3+HL)
C5=C51*FF**1.8
C61=C611*FF**1.8
C62=C621*FF**1.8
UAH )M*=40.0(E-04
RUA=UAR(M)
HUA=UAH(M)
ZC1=Z1*0.000001
ZC3=Z3*0.000001
ZC2=Z2*0.000001
HCL=HL*0.000001
RUAI=RUA*1.0E+06
HUAI=HUA*1.0E+06
CTVO=ZC1+ZC2+ZC3+HCL
AFD2=FD22(M)
AFD3=FD33(M)
AFD4=FD44(M)
AFD1=1.0-AFD2-AFD3-AFD4
W1=W11
C2=20.0
C21=C2
XWC5=C5*XW *AFD1 **1.8
PH1=XW-0.75*XWC5
PB11=XW-XWC5
S2=AFD1+AFD4
S11=S2+AFD2
S12=S11+AFD3
PH2=XW-0.25*XWC5
FT=F1+F2+F3+F4+F5
FTF1=2.0*F1/(3.0*FT*S2)
S112=S11/S2
S122=S12/S2
FI11=F1*S2
FI21= F2*S2
```

```
FI31=F3*S2
FI41=F4*S2
FI51=F5*S2
FI12=F1*S11
FI22=F2*S11
FI32=F3*S11
FI42=F4*S11
FI52=F5*S11
FI13=F1*S12
FI23=F2*S12
FI33=F3*S12
FI43=F4*S12
FI53=F5*S12
ZH1=Z1/H1
ZH2=Z2/H2
ZH3=Z3/H3
ZH4=ZL/H4
NZ1=ZH1-3.0
MZ1=ZH1/C71
NZ2=ZH2-3.0
NZ3=ZH3-3.0
NZ4=ZH4-3.0
MZ2=ZH2/C72
MZ3=ZH3/C73
MZ4=ZH4/C74
AR1=F1*AFD1
AR2=F2*AFD1
AR3=F3*AFD1
AR4=F4*AFD1
AR5=F5*AFD1
Q11=FI11-AR1
Q21=FI21-AR
Q31=FI31-AR3
Q41=FI41-AR4
Q51=FI51-AR5
Q12=F1*AFD2
Q22=F2*AFD2
Q32=F3*AFD2
Q42=F4*AFD2
Q52=F5*AFD2
Q13=F1*AFD3
Q23=F2*AFD3
Q33=F3*AFD3
Q43=F4*AFD3
Q53=F5*AFD3
KAA=0
KAA1=M8*10
NJ1=1
NJM=1
KNN=1
```

```
      KNA1=2
      KNA=1
      NJN=1
      KAB=1
      ATEMP(KAB)=W1
      KAD=1
      GO TO 407
  100 TH12=W1
      K2A=1
      K2A=K2A.1
      M7=1
      IF(KAD.LE.1)GO TO 119
      KAC=0
  114 KAC=KAC+1
      IF(ATEMP(KAC).EQ.W1)GO TO 112
      IF(KAC.LT.KAB)GO TO 114
      KAB=KAB+1
      ATEMP(KAB)=W1
  119 KAD=2
      CALL FEEDT( TF1,W1,F,H1,H2,H3,H4,VW,C71,C72,C73,C74   ,BHA31,BHA32,
     1BHA33,BHA34,CHA31,CHA32,CHA33,CHA34,J1,K11)
      KAA=KAA+1
      ATEM(KAA)=W1
      IF(AT(J1,K11))61,61,62
   62 DELT1=TF1-T
      ADEL(KAB)=DELT1
      ADET(KAA)=ADEL(KAB)
      GO TO 421
   61 GO TO 71
   67 DELT1=0.3*W1
      ADEL(KAB)=DELT1
      ADET(KAA)=ADEL(KAB)
      GO TO 422
  112 DELT1=ADEL(KAC)
      IF(NJ1.LE.1)GO TO 422
      IF(ADET(KAA).LT.0.0.AND.ADEL(KAC).LT.0.0.OR.ADET(KAA).GE.0.0
     1.AND.ADEL(KAC).GE.0.0)GO TO 312
      KAA=KAA+1
      ADET(KAA)=ADEL(KAC)
      ATEM(KAA)=W1
  422 IF(ABS(DELT1)-C4)101,101,102
  102 W2=W1-C21
  152 TH12=W2
      K2A=K2A.1
      KAC=0
  115 KAC=KAC+1
      IF(ATEMP(KAC).EQ.W2)GO TO 116
      IF(KAC.LT.KAB)GO TO 115
      KAB=KAB+1
      ATEMP(KAB)=W2
```

```
      M7=M7+1
      CALL FEEDT( TF2,W2,F,H1,H2,H3,H4,VW,C71,C72,C73,C74   ,BHA31,BHA32,
     1BHA33,BHA34,CHA31,CHA32,CHA33,CHA34,J1,K11)
      KAA=KAA+1
      ATEM(KAA)=W2
      IF(AT(J1,K11))63,63,64
   64 DELT2=TF2-T
      ADEL(KAB)=DELT2
      ADET(KAA)=ADEL(KAB)
      GO TO 424
   63 GO TO 72
   68 DELT2=0.2*W2
      ADEL(KAB)=DELT2
      ADET(KAA)=ADEL(KAB)
      GO TO 426
  116 DELT2=ADEL(KAC)
      IF(NJ1.LE.1)GO TO 426
      IF(ADET(KAA).LT.0.0.AND.ADEL(KAC).LT.0.0.OR.ADET(KAA).GE.0.0
     1.AND.ADEL(KAC).GE.0.0)GO TO 312
      KAA=KAA+1
      ADET(KAA)=ADEL(KAC)
      ATEM(KAA)=W2
  426 IF(ABS(DELT2)-C4)103,103,104
  103 W1=W2
      GO TO 101
  104 IF(M7-M8)504,504,312
  504 W12=(W1+W2)*0.5
      IF)K2A.GE.KA/1* GO TO 312
      DW12=W1-W2
      IF(ABS(ATEM(KAA)-ATEM(KAA-1)).GT.2.0)GO TO 42
      IF(ADET(KAA).GT.0.0.AND.ADET(KAA-1).LT.0.0.OR.ADET(KAA).LT.0.0
     1.AND.ADET(KAA-1).GT.0.0.OR.ABS(ADET(KAA)).LT.5.0.AND.
     2ABS((ADET(KAA)-ADET(KAA-1))).GE.0.1)GO TO 42
   41 DW12=(W1-W2)*8.0
      GO TO 48
   42 IF(KAA.LT.3)GO TO 48
      IF(ADET(KAA-2).GT.0.0.AND.ADET(KAA-1).GT.0.0.AND.ADET(KAA).GT.0.0
     1.OR.ADET(KAA-2).LT.0.0.AND.ADET(KAA-1).LT.0.0.AND.ADET(KAA)
     2.LT.0.0)GO TO 27
      GO TO 48
   27 IF)ABS)ADET)KAA-2**.GT. ABS)ADET)KAA**.AND.ABS)ADET)KAA-1**.GT.
     1ABS(ADET(KAA)).OR.ABS(ADET(KAA-2)).GT.ABS(ADET(KAA-1)).AND.
     2ABS(ADET(KAA-1)).LT.ABS(ADET( KAA)))GO TO 38
      GO TO 48
   38 DW12=DW12*0.5
      IF(KNN.GT.1)GO TO 39
      ATEP(KNA)=ATEM(KAA-2)
      ATEP(KNA+1)=ATEM(KAA-1)
      ATEP(KNA+2)=ATEM(KAA)
   39 KNA3=KNA+2
```

```
      KAA3=KAA-KNN-1
      DO 37 LM=KNA,KNA3
      DO 37 LM1=KAA3,KAA
      IF(ABS(ATEM(LM1)).EQ.ATEP(LM))GO TO 32
   37 CONTINUE
      KNN=1
      ATEP(KNA)=ATEM(KAA-2)
      ATEP(KNA+1)=ATEM(KAA-1)
      ATEP(KNA+2)=ATEM(KAA)
      GO TO 34
   32 IF(KNN.LT.KNA1)GO TO 34
      DW12=DW12*8.0
      KNN=0
   34 KNN=KNN+1
   48 DELT12=DELT1+DELT2
      IF(KAA.GE.KAA1)GO TO 312
  107 IF(DELT1)1,101,5
    1 IF(DELT2)2,103,3
    5 IF(DELT2)7,103,2
    2 IF(ABS(DELT1)-ABS(DELT2))161,161,162
  161 W2=W1.DW12
      GO TO 152
  162 W1=W2-DW12
  163 TH12=W1
      K2A=K2A.1
      KAC=0
  117 KAC=KAC+1
      IF(ATEMP(KAC).EQ.W1)GO TO 118
      IF(KAC.LT.KAB)GO TO 117
      KAB=KAB+1
      ATEMP(KAB)=W1
      M7=M7+1
      CALL FEEDT( TF1,W1,F,H1,H2,H3,H4,VW,C71,C72,C73,C74   ,BHA31,BHA32,
     1BHA33,BHA34,CHA31,CHA32,CHA33,CHA34,J1,K11)
      KAA=KAA+1
      ATEM(KAA)=W1
      IF(AT(J1,K11))65,65,66
   66 DELT1=TF1-T
      ADEL(KA3)=DELT1
      ADET(KAA)=ADEL(KAB)
      GO TO 427
   65 GO TO 73
   69 DELT1=0.2*W1
      ADEL(KA3)=DELT1
      ADET(KAA)=ADEL(KAB)
      GO TO 429
  118 DELT1=ADEL(KAC)
      IF(NJ1.LE.1)GO TO 429
      IF(ADET(KAA).LT.0.0.AND.ADEL(KAC).LT.0.0.OR.ADET(KAA).GE.0.0
     1.AND.ADEL(KAC).GE.0.0)GO TO 312
      KAA=KAA+1
      ADET(KAA)=ADEL(KAC)
      ATEM(KAA)=W1
  429 IF(ABS(DELT1)-C4)101,101,104
    3 IF(DELT12)181,181,184
    7 IF(DELT12)184,184,181
```

```
184 W2=W12
    GO TO 152
181 W1=W12
    GO TO 163
101 ATH12(J)=W1
    NJM=1
    PATD=F1*0.9792*AX(M12,K5)
    NJN=NJN+1
    GO TO 401
321 CONTINUE
    IF(J.EQ.J5)GO TO 202
    GO TO 316
312 NJ1=NJ1+1
    PATD=F1*0.9792*AX(M12,K5)
    GO TO 138
139 CONTINUE
    IF(J-J5)319,319,202
319 IF(NJN.GT.1)GO TO 316
    IF)NJM.EQ.1*GO TO 315
    IF)NJM.EQ.2* GO TO 314
    GO TO 316
315 W1=W11+C3*3.
    NJN=NJN.1
    NJM=NJM+1
    GO TO 100
314 W1=W11-C3*3.
    NJN=NJN+1
    GO TO 100
316 IF(NJN.GT.2)GO TO 311
318 IF(NJM.LE.1)GO TO 207
    IF(NJM.EQ.2)GO TO 315
    GO TO 314
311 J=J+1
201 IF(J.LE.2)GO TO 207
    IF)J.GT.J5*GO TO 202
    GO TO 208
207 W1=W11-C3
    J=J+1
    NJM=NJM+1
    GO TO 100
208 W1=TF(M)
    GO TO 100
202 IF(M-M5)203,204,204
203 M=M+1
```

APPENDIX-A9

```
    READ 911,H1,H2,H3,H4,F,W11  ,J5,M8,M15,M16,K7,K8,C71,C72,C73,C74
911 FORMAT(6E10.2,2I10/4I10,4E10.2)
    READ 821,FF,UV,C2
821 FORMAT(3F10.2)
    GO TO 205
C
C     OUTPUT STATEMENTS PROGRAM
C
404 PRINT 403,IJ1,IJ2,IJ3,IJ4
403 FORMAT( 1X,57X,6HSTART  //   42X,6HDATE..,I3,2H..,I3,2H..,I5,9H,RU
   1N NO. ,I6    //   12X, 94HNAME OF THE STUDENT...SUDHINDRA NATH SIN
   2HA,CLASS...MASTER OF ENGINEERING(CHEM.ENGG.)FINAL YE R     //  20X
   3,81HDEPARTMENT OF CHEMICAL ENGINEERING,UNIVERSITY OF ROORKEE,ROORK
   4EE(U.P.),PIN 247672    //5X,  109HM.E.THESIS PROBLEM ON SIMULATION
   5 AND OPTIMISATION OF AMMONIA SYNTHESIS REACTOR(ICI   ENCH TYPE HIG
   6H CAPACITY)   //   1X,119HM.E.THESIS SUPERVISOR...D  SHANT KUMAR S
   7ARAF,SC.D.(M.I.T.,U.S.A.),PROFESSOR,DEPTT.OF CHEM.E  G.,UNIVERSITY
   8 OF ROORKEE       //    )
    GO TO 405
407 PRINT408,UV,XW,F1,F2,F3,F4,F5,AFD4,AFD2,AFD3,AFD1,ZC1,ZC2,ZC3,
   1HCL, RUAI
408 FORMAT(  1X,14X,14HFEED TEMP.(K)=,F7.2,21H,FEED PRES URE(ATM.)=,
   1F7.2,31H,HYDROGEN IN FEED( GMOLES/SEC)=, F10.3  //   X, 30HNITROGE
   2N IN FEED( GMOLES/SEC)=, F9.2,30H,AMMONIA IN FEED( G OLES/SEC)=,
   3F9.2,30H,METHANE IN FEED( GMOLES/SEC)=,F9.2 //1X,27H RGON IN FEED(
   4 GMOLES/SEC)=,F9.3,21H,FIRST BED COLD SHOT=,F6.3,22H,SECOND BED CO
   5LD SHOT= ,F6.3,21H,THIRD BED COLD SHOT=,F6.3 //        4X,20HHEAT E
   6XCHANGER FEED=,F7.3,42H,CATALYST SPLIT IN CUBIC METER..FIRST BED=,
   7F7.3,12H,SECOND BED=,F7.3,11H,THIRD BED=,F7.3   //  6X,40HHEAT EXC
   8HANGER TUBE SIDE VOLUME(CU.MR.)=,F7.3,52H,RATE OF HE T TRANSFER/(T
   9EMP.DIFFERENCE)FOR REACTOR=,F9.3     /)
806 PRINT807,HUAI ,F

   1T EXCHANGER=,F9.4,41HCAL./(SEC)(K)(CU.MR.OF TUBE SIDE VOLUME) //
   22X, 25HCATALYST ACTIVITY FACTOR=  ,F10.7//)
    GO TO 100
401 PRINT406,((AZ(M1,K1),AP(M1,K1),AX(M1,K1),AT(M1,K1),ATH(M1,K1),
   1ACX(M1,K1),ACT(M1,K1),ACTH(M1,K1),M1=M15,M12,M16),K1=K7,K5,K8)
406 FORMAT(  1X,38X,44HREACTOR CONVERSION AND TEMPERATURE PROFILES  //
   1     3X,16HREACTOR CATALYST,5X,8HPRESSURE,2X,14HFR. C NVERSION,3X,
   29HBED TEMP.,2X,9HPREHEATER,3X,42HDIFF.IN VALUE OBTAI ED AND LAST I
   3TERATION     /    3X,18HBED VOLUME(CU.MR.),3X,6H(ATM ),5X,11HOF HY
   4DROGEN,5X,10H(DEGREE K),2X,8HTEMP.(K),3X,10HCONVERS  N,5X,9HBED TE
   5MP. ,5X,15HPFEHEATER TEMP.      //(4X,F10.3,10X,F8.3,3X,F10.6,5X,
   6F8.3,3X,F8.3,4X,F10.6,4X,F10.6,8X,F10.6   /  ))
    GO TO 321
138 PRINT 406,((AZ(M1,K1),AZP(M1,K1),AP(M1,K1),ANX(M1,K1),AX(M1,K1),
   1AT(M1,K1),ATH(M1,K1),ACX(M1,K1),ACT(M1,K1),ACTH(M1,K ), M1=M15,
   2M12,M16),K1=K7,K5,K8)
    GO TO 139
```

```
421 PRINT 423,M7,W1,DELT1,AX(M12,K5),AT(M12,K5)
423 FORMAT(1X,14HITERATION NO.=,I3,51H,ASSUMED INTERNAL PREHEATER OUT
   1LET STREAM TEMP.(K)=,F7.2,35H,CAL.AND GIVEN FEED TEMP.DIFF.(K)=
   2,F8.3//2X,49HFRACTIONAL CONVERSION AT THE EXIT OF TH  REACTOR=  ,
   3F15.10,40H,TEMP. OF BED AT HEAT EXCHANGER EXIT(K)=    ,F10.2/)
    GO TO 422
424 PRINT425,M7,W2,DELT2 ,AX(M12,K5),AT(M12,K5)
425 FORMAT(1X,14HITERATION NO.=,I3,51H,ASSUMED INTERNAL PREHEATER OUT
   1LET STREAM TEMP.(K)=,F7.2,35H,CAL.AND GIVEN FEED TEMP.DIFF.(K)=
   2,F8.3//2X,49HFRACTIONAL CONVERSION AT THE EXIT OF THE REACTOR=  ,
   3F15.10,40H,TEMP. OF BED AT HEAT EXCHANGER EXIT(K)=    ,F10.2/)
    GO TO 426
427 PRINT 428,M7,W1,DELT1,AX(M12,K5),AT(M12,K5)
428 FORMAT(1X,14HITERATION NO.=,I3,51H,ASSUMED INTERNAL  REHEATER OUT
   1LET STREAM TEMP.(K)=,F7.2,35H,CAL.AND GIVEN FEED TEM .DIFF.(K)=
   2,F8.3//2X,49HFRACTIONAL CONVERSION AT THE EXIT OF THE REACTOR=  ,
   3F15.10,40H,TEMP. OF BED AT HEAT EXCHANGER EXIT(K)=    ,F10.2/)
    GO TO 429
 71 PRINT74,M7,K11,J1,AT(J1,K11),AX(J1,K11),ATH(J1,K11)
 74 FORMAT(1X,14HITERATION NO.= ,I3,21H,CATALYST BED NU   ER= ,I3,
   115H,BED POINT NO.= ,I5,36H,BED TEMP.AT THIS POINT IS  EGATIVE= ,
   2F8.2//2X,38HAT THIS PT.FR. CONVERSION OF HYDROGEN=    5.10,
   332H,AT THIS PT.SHELL SIDE TEMP.(K)= ,F10.4//1X,115HT  REFORE SWITC
   4HING TO NEXT TEMPERATURE BY ASSUMING A FICTITIOUS VA  E OF TEMPERA
   5TURE DIFFERENCE FOR NEXT ITERATION      /)
    GO TO 67
 72 PRINT75,M7,K11,J1,AT(J1,K11),AX(J1,K11),ATH(J1,K11)
 75 FORMAT(1X,14HITERATION NO.= ,I3,21H,CATALYST BED NUM ER= ,I3,
   115H,BED POINT NO.= ,I5,36H,BED TEMP.AT THIS POINT IS NEGATIVE= ,
   2F8.2//2X,38HAT THIS PT.FR. CONVERSION OF HYDROGEN= , 15.10,
   332H,AT THIS PT.SHELL SIDE TEMP.(K)= ,F10.4//1X,115HT EREFORE SWITC
   4HING TO NEXT TEMPERATURE BY ASSUMING A FICTITIOUS VA UE OF TEMPERA
   5TURE DIFFERENCE FOR NEXT ITERATION      /)
    GO TO 68
 73 PRINT76,M7,K11,J1,AT(J1,K11),AX(J1,K11),ATH(J1,K11)
 76 FORMAT(1X,14HITERATION NO.= ,I3,21H,CATALYST BED NU    R= ,I3,
   115H,BED POINT NO.= ,I5,36H,BED TEMP.AT THIS POINT IS  EGATIVE= ,
   2F8.2//2X,38HAT THIS PT.FR. CONVERSION OF HYDROGEN=    5.10,
   332H,AT THIS PT.SHELL SIDE TEMP.(K)= ,F10.4//1X,115HT  REFORE SWITC
   4HING TO NEXT TEMPERATURE BY ASSUMING A FICTITIOUS VA  E OF TEMPERA
   5TURE DIFFERENCE FOR NEXT ITERATION      /)
    GO TO 69
204 PRINT 231
231 FORMAT(  1X,56X,7HTHE END     )
    STOP
    END
```

```
      SUBROUTINE FEEDT(T2,W1,F,H1,H2 H3,H4,VW,C71,C72,C73,C74,BHA31,
     1BHA32,BHA33,BHA34,CHA31,CHA32,CHA33,CHA34,J,K1    )
C     SUBROUTINE NO.1 FOR CALCULATION OF  FEED TEMPERATURE TO AMMONIA SYNTHES
C     REACTOR
      DIMENSION AZ(110,4),AP(110,4),AX(110,4),AT(110,4),ATH(110,4),
     1ACX(110,4),ACT(110,4),ACTH(110,4)
     2,ANX(110,4),AZP(110,4)
      COMMON/CB1/F1,F2,F3,F4,F5/CB2/AZ,AP,AX,AT,ATH,ACX,AC ,ACTH/CB3/
     1AFD1,AFD2,AFD3,AFD4,Z1,Z2,Z3,HL,XW,UV,C4,RUA,HUA,C5, 61,C62 ,M15,K7
     2,FI11,FI12,FI13,FI21,FI22,FI23,FI31,FI32,FI33,FI41,FI42,FI43,
     3FI51,FI52,FI53,PH1,PH2,PB11,S2,S11,S12,FTF1,S112,S122,AR1,AR2,
     4AR3,AR4,AR5,Q11,Q21,Q31,Q41,Q51, Q12,Q22,Q32,Q42,Q52, M12,K5,
     5Q13,Q23,Q33,Q43,Q53,HA11,HA21,HA31,HA41,HA51,HA61,HA71,HA12,M16,
     6HA22,HA32,HA42,HA52,HA62,HA72,HA13,HA23,HA33,HA43,HA53,HA63, K8,
     7HA73, HA14,HA24,HA34,HA44,HA54,HA64,HA74,NZ1,NZ2,NZ3,NZ4, MZ1,MZ2,
     8MZ3,MZ4, HAA21,HAA22,HAA23,HAA24,AHA21,AHA22,AHA23,AHA24, BHA21,
     9BHA22,BHA23,BHA24,HAB21,HAB22,HAB23,HAB24,AHA31,AHA32,AHA33,AHA34
     A/CB4/ANX,ZTI,PAM,AZP/CB5/LK,AN3T1 ,ZCTV
C     CALCULATION OF FIRST REACTOR BED CONVERSION AND TEMPERATURE PROFILES
      M1=1
      K1=1
      K3=1
      LK=1
      ZCTV=0.
      UA1=RUA
      AX(M1,K1)=0.0
      ATH(M1,K1)=W1
C     CALCULATION FOR MIXTURE TEMPERATURE ENTERING FIRST BED
      XB12=0.0
      IF(AFD4)21,22,21
   22 TB=ATH(M1,K1)
      GO TO 23
   21 CALL MTEMP(TB,W1,F1,AR1,AR2,AR3,AR4,AR5, Q11,Q21,Q31,Q41,Q51,
     1XB12,PB11,UV,C4       )
   23 AP(M1,K1)=PB11
      C6=C61*(AFD1+AFD4)**1.8
C     CALCULATION FOR REACTOR PROFILES BY MILNE PREDICTOR  CORRECTOR METHOD OF
C     NUMERICAL INTEGRATION
      CALL RNUMI(M1,K1,K3,TB,AFD1,NZ1,MZ1,HA11,HA21,HAA21,AHA21,BHA21,
     1HA31,HA41,HA51,HA61,HA71,FI11,FI21,FI31,FI41,FI51,Z1,HL,H1,C6,
     2VW,C71,UA1,F,PH1,HAB21,AHA31,BHA31,CHA31,J    )
      IF(AT(J,K1))11,11,12
C     CALCULATION FOR SECOND BED PROFILES
   12 TH12=AT(M1,K1)
      PB1=AP(M1,K1)
```

```
      XB12=AX(M1,K1)
      IF(AFD2)24,25,24
   25 TB=AT(M1,K1)
      GC TO 26
   24 CALL MTEMP(TB,TH12, F1,FI11,FI21,FI31,FI41,FI51,Q12,Q22,Q32,
     1Q42,Q52,XB12,PB1,UV,C4                       )
   26 C6=((S112-FTF1*XB12)*(AFD1+AFD4))**1.8*C61
      ZCTV=Z1
      CALL RNUMI(M1,K1,K3,TB,AFD1,NZ2,MZ2,HA12,HA22,HAA22,AHA22,
     1BHA22,HA32,HA42,HA52,HA62,HA72,FI12,FI22,FI32,FI42,FI52,      Z2,
     2HL,H2,C6,VW,C72,UA1,F,PH1,HAB22,AHA32,BHA32,CHA32,J    )
      IF(AT(J,K1))11,11,14
C     CALCULATION OF THIRD BED REACTOR PROFILES
   14 XB12=AX(M1,K1)
      PB1=AP(M1,K1)
      TH12=AT(M1,K1)
      IF(AFD3)27,28,27
   28 TB=AT(M1,K1)
      GO TO 29
   27 CALL MTEMP(TB,TH12,F1,FI12,FI22,FI32,FI42,FI52,Q13,Q23,Q33,Q43,
     1Q53,XB12,PB1,UV,C4                    )
   29 C6=((S122-FTF1*XB12)*(AFD1+AFD4))**1.8*C61
      ZCTV=Z2  +Z1
      CALL RNUMI(M1,K1,K3,TB,AFD1,NZ3,MZ3,HA13,HA23,HAA23, HA23,BHA23,
     1HA33,HA43,HA53,HA63,HA73,FI13,FI23,FI33,FI43,FI53,Z3,HL,H3,C6,
     2VW,C73,UA1,F,PH1,HAB23,AHA33,BHA33,CHA33,J  )
      IF(AT(J,K1))11,11,15
C     CALCULATION OF HEAT EXCHANGER PROFILES
   15 UA1=HUA
      TB=AT(M1,K1)
      C6=C62
      LK=2
      ZCTV=Z1+Z2+Z3
      CALL RNUMI(M1,K1,K3,TB,AFD1,NZ4,MZ4,HA14,HA24,HAA24,AHA24,BHA24,
     1HA34,HA44,HA54,HA64,HA74,FI13,FI23,FI33,FI43,FI53,HL,HL,H4,C6,
     2VW,C74,UA1,F,PH2,HAB24,AHA34,BHA34,CHA34,J     )
   11 TF=ATH(M1,K1)
      RETURN
      END
```

```
      SUBROUTINE RNUMI (M1,K1,K3,TB, D1,N,M2,HA1,HA2,HAA2,AHA2,BHA2,
     1HA3,HA4,HA5,HA6,HA7,FI1,FI2,FI3,FI4,FI5,Z1,HL,H,C6,VW,C7,UA1,F,
     2PH,   HAB2,AHA3,BHA3,CHA3,J   )
C     SUBROUTINE NO.2 FOR NUMERICAL INTEGRATION OF AMMONIA SYNTHESIS REACTOR
C     DIFFERENTIAL EQUATIONS BY MILNE PREDICTOR AND CORRECTOR METHOD
      DIMENSION WX(110),WT(110),WTH(110),P(110),T(110),TH(110),
     1AZ(110,4),AP(110,4),AX(110,4),AT(110,4),ATH(110,4),ACX(110,4),
     2ACT(110,4),ACTH(110,4),XN(110),TN(110),THN(110),Z(110),X(110),
     3CX(110),CT(110),CTH(110)
     4,ANX(110,4),AZP(110,4)
      COMMON/CB1/F1,F2,F3,F4,F5/CB2/AZ,AP,AX,AT,ATH,ACX,ACT,ACTH
     1/CB4/ANX,ZTI,PAM,AZP/CB5/LK,AN3T ,ZCTV
      AZ1=Z1
      I=1
      Z(I)=0.0
      P(I)=AP(M1,K1)
      X(I)=AX(M1,K1)
      T(I)=TB
      TH(I)=ATH(M1,K1)
      IF(K3-1)302,301,302
  302 K1=K1+1
  301 M1=1
      J=I
      AZ(M1,K1)=Z(I)
      AZP(M1,K1)=(Z(I)+ZCTV)*ZTI
      AP(M1,K1)=P(I)
      AX(M1,K1)=X(I)
      AT(M1,K1)=T(I)
      ACX(M1,K1)=0.0
      ACT(M1,K1)=0.0
      ACTH(M1,K1)=0.0
      ANX(M1,K1)=PAM
      IF(T(J))304,304,303
  303 ATH(M1,K1)=TH(I)
      CALL DEV(I,WX,WT,WTH,P,T,TH,X,FD1,
     1FI1,FI2,FI3,FI4,FI5,F,AZ1,HL,UA1,PH           )
      HC6=C6*H
      ANX(M1,K1)=AN3T
      Z(I+1)=H
      P(I+1)=P(I)-HC6
      X(I+1)=X(I)+H*WX(I)
      T(I+1)=T(I)+H*WT(I)
      TH(I+1)=TH(I)+H*WTH(I)
    4 J=I+1
      IF(T(J))304,304,305
  305 CALL DEV(J,WX,WT,WTH,P,T,TH,X,FD1,
     1FI1,FI2,FI3,FI4,FI5,F,AZ1,HL,UA1,PH           )
      XN(I+1)=X(I)+HA1*(WX(J)+WX(I))
```

```
      TN(I+1)=T(I)+HA1*(WT(J)+WT(I))
      THN(I+1)=TH(I)+HA1*(WTH(J)+WTH(I))
      CX(I+1)=(XN(I+1)-X(I+1))
      CT(I+1)=(TN(I+1)-T(I+1))
      CTH(I+1)=(THN(I+1)-TH(I+1))
      X(I+1)=XN(I+1)
      T(I+1)=TN(I+1)
      TH(I+1)=THN(I+1)
      IF(ABS (CX(I+1))-VW*0.01)1,1,4
    1 IF(ABS(CT(I+1))-VW)5,5,4
    5 IF(ABS(CTH(I+1))-VW)3,3,4


    3 M1=M1+1
      AX(M1,K1)=X(I+1)
      AT(M1,K1)=T(I+1)
      ATH(M1,K1)=TH(I+1)
      ACT(M1,K1)= CT(I+1)
      ACX(M1,K1)=CX(I+1)
      ACTH(M1,K1)=CTH(I+1)
      AZ(M1,K1)=Z(I+1) *0.000001
      AZP(M1,K1)=(Z(I+1)+ZCTV) *ZTI
      ANX(M1,K1)=AN3T
      AP(M1,K1)=P(I+1)
      X(I+2)=X(I+1)+HA1*(3.0*WX(J)-WX(I))
      T(I+2)=T(I+1)+HA1*(3.0*WT(J)-WT(I))
      TH(I+2)=TH(I+1)+HA1*(3.0*WTH(J)-WTH(I))
      Z(I+2)=Z(I+1)+H
      P(I+2)=P(I+1)-HC6
      WXI1=HAB2*WX(I+1)
      WXI2=HA2*WX(I)
      WTI1=HAB2*WT(I+1)
      WTI2=HA2*WT(I)
      WTHI1=HAB2*WTH(I+1)
      WTHI2=HA2*WTH(I)
   12 J=I+2
      IF(T(J))304,304,306
  306 CALL DEV(J,WX,WT,WTH,P,T,TH,X,FD1,
     1FI1,FI2,FI3,FI4,FI5,F,AZ1,HL,UA1,PH                    )
      XN(I+2)=X(I+1)+HAA2*WX(J)+WXI1-WXI2
      TN(I+2)=T(I+1)+HAA2*WT(J)+WTI1-WTI2
      THN(I+2)=TH(I+1)+HAA2*WTH(J)+WTHI1-WTHI2
      CX(I+2)=(XN(I+2)-X(I+2))
      CT(I+2)=(TN(I+2)-T(I+2))
      CTH(I+2)=(THN(I+2)-TH(I+2))
      X(I+2)=XN(I+2)
      T(I+2)=TN(I+2)
      TH(I+2)=THN(I+2)
      IF(ABS(CX(I+2))-VW*0.01)11,11,12
   11 IF(ABS(CT(I+2))-VW)14,14,12
   14 IF(ABS(CTH(I+2))-VW)15,15,12
   15 M1=M1+1
      AX(M1,K1)=X(J)
      AT(M1,K1)=T(J)
```

```
      ATH(M1,K1)=TH(J)
      ACT(M1,K1)=CT(J)
      ACTH(M1,K1)=CTH(J)
      ACX(M1,K1)=CX(J)
      AZ(M1,K1)=Z(J)*0.000001
      AZP(M1,K1)=(Z(J)+ZCTV)*ZTI
      ANX(M1,K1)=AN3T
        AP(M1,K1)=P(J)
      X(I+3)=X(I+2)+AHA2*WX(I+2)-BHA2*WX(I+1)+HAA2*WX(I)
      T(I+3)=T(I+2)+AHA2*WT(I+2)-BHA2*WT(I+1)+HAA2*WT(I)
      TH(I+3)=TH(I+2)+AHA2*WTH(I+2)-BHA2*WTH(I+1)+HAA2*WTH(I)
      Z(I+3)=Z(I+2)+H
      P(I+3)=P(I+2)-HC6
      WXN1=BHA3*WX(I+2)
      WXN2=CHA3*WX(I+1)
      WXN3= HA3*WX(I)
      WTN1=BHA3*WT(I+2)
      WTN2=CHA3*WT(I+1)
      WTN3=HA3*WT(I)
      WTHN1=BHA3*WTH(I+2)
      WTHN2=CHA3*WTH(I+1)
      WTHN3=HA3*WTH(I)
   22 J=I+3
      IF(T(J))304,304,307
  307 CALL DEV(J,WX,WT,WTH,P,T,TH,X,FD1,
     1FI1,FI2,FI3,FI4,FI5,F,AZ1,HL,UA1,PH          )
      XN(I+3)=X(I+2)+AHA3*WX(I+3)+WXN1-WXN2+WXN3
      TN(I+3)=T(I+2)+AHA3*WT(I+3)+WTN1-WTN2+WTN3
      THN(I+3)=TH(I+2)+AHA3*WTH(I+3)+WTHN1-WTHN2+WTHN3
      CX(I+3)=(XN(I+3)-X(I+3))
      CT(I+3)=(TN(I+3)-T(I+3))
      CTH(I+3)=(THN(I+3)-TH(I+3))
      X(I+3)=XN(I+3)
      T(I+3)=TN(I+3)
      TH(I+3)=THN(I+3)
      IF(ABS(CX(I+3))-VW*0.01)21,21,22
   21 IF(ABS (CT(I+3))-VW)23,23,22
   23 IF(ABS (CTH(I+3))-VW)24,24,22
   24 M1=M1+1
      AX(M1,K1)=X(J)
      AT(M1,K1)=T(J)
      ATH(M1,K1)=TH(J)
      ACT(M1,K1)=CT(J)
      ACTH(M1,K1)=CTH(J)
      ACX(M1,K1)=CX(J)
      AZ(M1,K1)=Z(J)*0.000001
      AZP(M1,K1)=(Z(J)+ZCTV)*ZTI
      ANX(M1,K1)=AN3T
        AP(M1,K1)=P(J)
```

```
      L11=1
      K=1
  101 X(K+4)=X(K)+ HA4*WX(K+2)+HA5*(WX(K+3)-2.0*WX(K+2)+WX(K+1))
      T(K+4)=T(K)+HA4*WT(K+2)+HA5*(WT(K+3)-2.0*WT(K+2)+WT(K+1))
      TH(K+4)=TH(K)+HA4*WTH(K+2)+HA5*(WTH(K+3)-2.0*WTH(K+2)+WTH(K+1))
      Z(K+4)=Z(K+3)+H
      P(K+4)=P(K+3)-HC6
      IF(L11-1) 25,89,25
   25 X(K+4)=X(K+4)+CX(K+3)
      T(K+4)=T(K+4)+CT(K+3)
      TH(K+4)=TH(K+4)+CTH(K+3)
   89 L11=2
      WXK1=HA6*WX(K+3)
      WTK1=HA6*WT(K+3)
      WTHK1=HA6*WTH(K+3)
      WXK2=WXK1/3.0
      WXK3=HA7*WX(K+2)
      WTK2=WTK1/3.0
      WTK3=HA7*WT(K+2)
      WTHK2=WTHK1/3.0
      WTHK3=HA7*WTH(K+2)
   29 J=K+4
      IF(T(J))304,304,308
  308 CALL DEV(J,WX,WT,WTH,P,T,TH,X,FD1,
     1FI1,FI2,FI3,FI4,FI5,F,AZ1,HL,UA1,PH          )
      XN(K+4)=X(K+2)+WXK1+HA7*WX(K+4)-WXK2+WXK3
      TN(K+4)=T(K+2)+WTK1+HA7*WT(K+4)-WTK2+WTK3
      THN(K+4)=TH(K+2)+WTHK1+HA7*WTH(K+4)-WTHK2+WTHK3
      CX(K+4)=(XN(K+4)-X(K+4))
      CT(K+4)=(TN(K+4)-T(K+4))
      CTH(K+4)=(THN(K+4)-TH(K+4))
      X(K+4)=XN(  K+4)
      T(K+4)=TN(K+4)
      TH(K+4)=THN(K+4)
```

```
      IF(ABS(CX(K+4))-VW*0.01)31,31,29
  31  IF(ABS (CT(K+4))-VW)32,32,29
  32  IF(ABS (CTH(K+4))-VW)33,33,29
  33  M3=K+4
      M4=M2*(M1-3)
      IF(M3-M4)34,34,35
  35  M1=M1+1
      AZ(M1,K1)=Z(M3) *0.000001
      AP(M1,K1)=P(M3)
      AX(M1,K1)=X(M3)
      AT(M1,K1)=T(M3)
      ATH(M1,K1)=TH(M3)
      ACX(M1,K1)=CX(M3)
      ACT(M1,K1)=CT(M3)
      ACTH(M1,K1)=CTH(M3)
      AZP(M1,K1)=(Z(J)+ZCTV)*ZTI
      ANX(M1,K1)=AN3T
  34  IF(K-N)191,192,192
 191  K=K+1
      GO TO 101
 192  K3=K3+1
      GO TO 309
 304  AT(J,K1)=T(J)
      AX(J,K1)=X(J)
      ATH(J,K1)=TH(J)
 309  RETURN
      END
```

APPENDIX-A18

```
      SUBROUTINE DEV(I,WX,WT,WTH,P,T,TH,X,FD1,
     1FI1,FI2,FI3,FI4,FI5,F,AZ1,HL,UA1,PH                )
C     SUBROUTINE NO.3 FOR CALCULATION OF DERIVATIVE VALUES FROM AMMONIA
C     SYNTHESIS REACTOR
C     EQUATIONS FOR NUMERICAL INTEGRATION
      DIMENSION WX(110),WT(110),WTH(110),P(110),T(110 ),TH(110),X(110)
      COMMON/CB1/F1,F2,F3,F4,F5
     1/CB5/LK,AN3T,ZCTV
      PP=P(I)
      TT=T(I)
      THH=TH(I)
      AB=F1*X(I)
      AN1=FI1-AB
      AN2=FI2-0.333333  *AB
      AN3=FI3+0.66667*AB
      AN4=FI4
      AN5=FI5
      ANT=AN1+AN2+AN3+AN4+AN5
      AN3T=100.*AN3/ANT
      IF(LK.EQ.2)GO TO 202
  201 HR3=-15564.51+(7.0646-(14.8399E-03-(3.3563E-07-1.1625E-10*TT)*
     1TT)*TT)*TT-PP*(3.01975-(4.4552E-03-1.928E-06*TT)*TT)
      AK=EXP (0.50327*(9184.0/TT-7.2949*ALOG (TT)+(3.4966E-03+
     1(1.6781E-07-3.875E-11*TT)*TT)*TT+23.05))
      AKF=1.7343-8.143E-04*PP+(5.714E-07*PP-2.6714E-03+2.0E-06*TT)*TT
      PANT=PP*AN1/ANT
      IF(PP)11,11,15
   15 IF(PANT)11,11,12
   11 PRINT 14,PANT,PP
   14 FORMAT(1X,5HPANT= ,E15.6,10H,PRESSURE= ,F10.4   /)
   12 SPANT=SQRT(PANT)
      PANTS=AN3/SPANT
      AKR=(300.0/PP)**0.63*EXP (-24092.2/TT+33.5566)
      R1=29.4204*((AK/AKF)**2*PANT*AN2/PANTS-PANTS/AN1)*F*AKR*1.0E-06
      B7=-0.666667*HR3*R1
      GO TO 203
  202 R1=0.0
      B7=0.0
  203 WX(I)=R1/F1
      B4=-UA1*(TT-THH)
      B1=B7+B4
      CALL HEATC (CP1,CP2,CP3,CP4,CP5,PP,TT         )
      B2=AN1*CP1+AN2*CP2+AN3*CP3+AN4*CP4+AN5*CP5
      WT(I)=B1/B2
      CALL HEATC (CP1,CP2,CP3,CP4,CP5,PH,THH      )
      B3=FD1*(F1*CP1+F2*CP2+F3*CP3+F4*CP4+F5*CP5        )
      WTH(I)=B4/B3
      RETURN
      END
```

APPENDIX-A19

```
      SUBROUTINE MTEMP(TB21,TB12,F1,R11,R22,R33,R44,R55,Q1,Q2,Q3,Q4,Q5,
     1XB12,PB1,UV,C4                         )
C     SUBROUTINE NO.4 FOR CALCULATION OF MIXTURE STREAM TEMPERATURE BY TRIAL
C     AND ERROR TECHNIGUE
      I=1
      TBUV=0.33333*(TB12-UV)
      W1=TB12-TBUV
      W2=UV+TBUV
  192 TB21=W1
      CALL TEMP(AT1,F1,R11,R22,R33,R44,R55,Q1,Q2,Q3,Q4,Q5,XB12,PB1,
     1TB12,TB21,UV                           )
      DELT1=AT1-W1
      IF(ABS(DELT1)-C4) 151,151,191
  191 IF(I-1)153,152,153
  152 TB21=W2
      CALL TEMP(AT2,F1,R11,R22,R33,R44,R55,Q1,Q2,Q3,Q4,Q5,XB12,PB1,
     1TB12,TB21,UV                             )
      DELT2=AT2-W2
      IF(ABS(DELT2)-C4)154,154,153
  153 DW12=(W1-W2)*0.5
      DELT12=DELT1+DELT2
      W12=(W1+W2)*0.5
      I=I+1
      IF(DELT1)1,151,5
    1 IF(DELT2)2,154,3
    5 IF(DELT2)7,154,2
    2 IF(ABS(DELT1)-ABS(DELT2))161,161,162
  161 W2=W1+DW12
      GO TO 152
  162 W1=W2-DW12
      GO TO 192
    3 IF(DELT12)181,181,184
    7 IF(DELT12)184,184,181
  184 W2=W12
      GO TO 152
  181 W1=W12
      GO TO 192
  154 TB21=AT2
      GO TO 155
  151 TB21=AT1
  155 RETURN
      END
```

```
      SUBROUTINE TEMP(T,F1,R11,R22,R33,R44,R55,Q1,Q2,Q3,Q4,Q5,XB12,
     1PB1,TB12,TB21,UV                     )
C     SUBROUTINE NO. 5 FOR CALCULATION OF MIXTURE TEMPERATURE FROM ENTHALAPY
C     BALANCE
      XBF1=F1*XB12
      R1=R11-XBF1
      R2=R22-0.33333*XBF1
      R3=R33+0.66667*XBF1
      R4=R44
      R5=R55
      CALL HEATC(CP1,CP2,CP3,CP4,CP5,PB1,TB12    )
      C1=TB12*(R1*CP1+R2*CP2+R3*CP3+R4*CP4+R5*CP5        )
      CALL HEATC(CP1,CP2,CP3,CP4,CP5,PB1,UV        )
      C2=UV*(Q1*CP1+Q2*CP2+Q3*CP3+Q4*CP4+Q5*CP5        )
      CALL HEATC(CP1,CP2,CP3,CP4,CP5,PB1,TB21      )
      C3=(R1+Q1)*CP1+(R2+Q2)*CP2+(R3+Q3)*CP3+(R4+Q4)*CP4+(R5+Q5)*CP5
      T=(C1+C2)/C3
      RETURN
      END
```

APPENDIX-A21

```
      SUBROUTINE HEATC( CP1,CP2,CP3,CP4,CP5,P,T                  )
C     SUBROUTINE NO. 6 FOR CALCULATION OF HEAT CAPACITY AT GIVEN TEMPERATURE
C     AND PRESSURE
      CP1=6.952-(4.576E-04-(9.563E-07-2.079E-10*T)* T)*T
      CP2=6.903-(3.753E-04-(1.93E-06-6.861E-10*T)*T)*T
      CP3=102.7524-(21.63767E-02-(13.12707E-05-1.5981E-09*T)*T)*T-
     1P*(6.7571E-02-(1.6847E-04-1.009514E-07*T)*T)
      CP4=4,750+(1.2E-02+(3.03E-06-2.63E-09*T)*T)*T
      CP5=4.9675



      RETURN
      END
```

APPENDIX

TABLE NO.B1: COMPUTED CONVERSION AND BED TEMPERATURE PROFILE:FEED COMPOSITION (IN MOLE %) H_2=64·5, N_2=21·5,NH_3=2,CH_4=10,A=2. FEED RATE=567500 Nm^3/hr,PRESSURE=160 ATM, COLDSHOT TEMPERATURE= 413K CATALYST VOLUME=63 m^3, ACTIVITY=70%

S. No.	% BED VOLUME	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)
		1st bed feed fr= 1,cold shot fr= 0,1st bed % H_2 conv= ·29		1st bed feed fr.=·85, coldshot fr.=0,1st bed % H_2 conv. = ·29		1st bed feed fr= ·8, coldshot fr.=0,1st bed % H_2 conv= ·29		1st bed feed fr.=·65,. coldshot fr.=0,1st bed % H_2 conv. =·29	
1	0·00	2·00	598·0	2·00	598·0	2·00	598·0	2·00	598·0
2	2·86	2·03	598·5	2·03	598·6	2·04	598·7	2·04	598·8
3	5·72	2·05	599·0	2·06	599·2	2·07	599·3	2·08	599·6
4	8·58	2·08	599·6	2·09	600·0	2·10	600·0	2·12	600·5
5	11·42	2·10	600·1	2·12	600·5	2·13	600·7	2·16	601·3
6	14·28	2·13	600·6	2·15	601·1	2·16	601·3	2·20	602·2
		2nd bed feed fr.=1,cold shot fr.=0,2nd bed % H_2 conv.=·88		2nd bed feed fr.=·85, coldshot fr.=0,2nd bed % H_2 conv.=·89		2nd bed feed fr.=1, coldshot fr.=·2, 2nd bed % H_2 conv.=·46		2nd bed feed fr.=·85, coldshot fr.=·2,2nd bed % H_2 conv.=·42	
7	14·28	2·13	600·6	2·15	601·1	2·13	564·8	2·16	558·9
8	20·00	2·18	601·7	2·22	602·4	2·15	565·1	2·17	559·1
9	25·72	2·23	602·8	2·28	603·7	2·16	565·4	2·18	559·4
.0	31·43	2·28	603·9	2·34	605·0	2·18	565·7	2·20	559·7
.1	37·14	2·34	605·0	2·40	606·3	2·19	566·0	2·21	560·0
.2	42·86	2·39	606·1	2·47	607·7	2·20	566·3	2·22	560·2
		3rd bed feed fr.=1,cold shot fr= 0,3rd bed % H_2 conv.=2·15		3rd bed feed fr.=1, coldshot fr.=·15,3rd bed % H_2 conv.=1·39		3rd bed feed fr.=1, coldshot fr.=0,3rd bed % H_2 conv.=·79		3rd bed feed fr.=1, coldshot fr.=·15,3rd bed % H_2 conv.=·54	
.3	42·86	2·39	606·1	2·40	579·2	2·20	566·3	2·19	538·6
.4	54·28	2·50	608·3	2·44	580·1	2·23	566·9	2·20	538·8
.5	65·72	2·61	610·6	2·48	581·0	2·26	567·5	2·21	539·0
.6	77·14	2·72	613·0	2·53	581·9	2·29	568·1	2·22	539·2
7	88·57	2·84	615·4	2·57	582·8	2·32	568·7	2·23	539·4
8	100·0	2·96	617·9	2·62	583·7	2·35	569·3	2·24	539·6
		Pressure drop =10·5 ATM		Pressure drop =8·6 ATM		Pressure drop=8·6 ATM		Pressure drop=7ATM	

NOTE: H_2 conversion is based on total H_2 in feed

TABLE NO D·2: COMPUTED CONVERSION AND BED TEMPERATURE PROFILE: FEED COMPOSITION (IN MOLE %): H_2=64·5, N_2=21·5, NH_3=2, CH_4=10, A=2, FEED RATE=851300 Nm³/hr, PRESSURE=160 ATM, COLDSHOT TEMPERATURE= 413K CATALYST VOLUME=63 m³, ACTIVITY=70%

S. No.	% BED VOLUME	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)
		1st bed feed fr.=1, cold shot fr.=0, 1st bed % H_2 conv.= ·18		1st bed feed fr.= ·85, coldshot fr.=0, 1st bed % H_2 conv.= ·19		1st bed feed fr.= ·8, coldshot fr.=0, 1st bed % H_2 conv.= ·19		1st bed feed fr.= ·65, coldshot fr.= 0, 1st bed % H_2 conv.= ·19	
1	0·0	2·00	598·0	2·0	598·0	2·0	598·0	2·0	598·0
2	2.86	2·02	598·3	2·02	598·4	2·02	598·4	2·03	598·5
3	5·72	2·04	598·7	2·04	598·8	2·05	598·9	2·06	599·1
4	8·58	2·05	599·0	2·06	599·2	2·07	599·3	2·08	599·6
5	11·42	2·07	599·3	2·08	599·6	2·09	599·7	2·11	600·2
6	14·28	2·08	599·7	2·10	600·0	2·11	600·1	2·13	600·7
		2nd bed feed fr= 1, cold shot fr.=0, 2nd bed % H_2 conv. = 55		2nd bed feed fr.= ·85, coldshot fr.= 0, 2nd bed % H_2 conv.= ·57		2nd bed feed fr.=1, coldshot fr.= ·2, 2nd bed % H_2 conv.= ·29		2nd bed feed fr.= ·85, coldshot fr.= ·2, 2nd bed % H_2 conv.= ·28	
7	14·28	2·08	599·7	2·10	600·0	2·09	563·9	2·10	557·8
8	20·00	2·12	600·3	2·14	600·8	2·10	564·1	2·11	558·0
9	25·72	2·15	601·0	2·18	601·6	2·11	564·3	2·12	558·2
10	31·43	2·18	601·7	2·22	602·5	2·11	564·5	2·13	558·3
11	37·14	2·21	602·4	2·26	603·3	2·12	564·6	2·14	558·5
12	42·86	2·25	603·1	2·30	604·1	2·13	564·8	2·15	558·7
		3rd bed feed fr.=1, cold shot fr.=0, 3rd bed % H_2 conv.= 1·30		3rd bed feed fr.= 1, coldshot fr·= ·15, 3rd bed % H_2 conv.= ·86		3rd bed feed fr.= 1, coldshot fr= 0, 3rd bed % H_2 conv.= ·50		3rd bed feed fr.=1, coldshot fr.= ·15, 3rd bed % H_2 conv.= 0·34	
13	42·86	2·25	603·1	2·25	576·3	2·13	564·8	2·13	537·3
14	54·28	2·31	604·4	2·28	576·8	2·15	565·2	2·13	537·4
15	65·72	2·38	605·8	2·31	577·3	2·17	565·6	2·14	537·5
16	77·14	2·44	607·2	2·33	577·9	2·19	565·9	2·14	537·7
17	88·57	2·51	608·6	2·36	578·4	2·21	566·3	2·15	537·8
18	100·0	2·58	609·9	2·38	579·0	2·22	566·7	2·16	537·9
		Pressure drop=21·7 ATM		Pressure drop=17·9 ATM		Pressure drop=17·8 ATM		Pressure drop=14·6ATM	

TABLE NoB3: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %) : H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0; Feed rate=1135000 Nm^3/hr
Feed pressure=160·0 ATM, coldshot temperature=413·0K; catalyst vol = 63m^3, Activity = 70%

S. No.	% Bed Volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction		: 1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1	0·00	2·00	598·0	2·00	598·0	2·00	598·0	2·00	598·0
2	2·86	2·02	598·2	2·02	598·3	2·02	598·3	2·02	598·4
3	5·72	2·03	598·5	2·03	598·6	2·03	598·6	2·04	598·8
4	8·58	2·04	598·7	2·05	598·9	2·05	598·9	2·06	599·2
5	11·42	2·05	598·9	2·06	599·1	2·06	599·2	2·08	599·6
6	14·28	2·06	599·2	2·07	599·4	2·08	599·6	2·10	600·0
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7	14·28	2·06	599·2	2·07	599·4	2·06	563·4	2·08	557·3
8	20·00	2·08	599·7	2·10	600·0	2·07	563·6	2·08	557·4
9	25·72	2·11	600·1	2·13	600·6	2·08	563·7	2·09	557·5
10	31·43	2·13	600·6	2·16	601·2	2·08	563·8	2·10	557·6
11	37·14	2·15	601·1	2·18	601·7	2·09	564·0	2·10	557·8
12	42·86	2·17	601·5	2·21	602·3	2·10	564·1	2·11	557·9
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13	42·86	2·17	601·5	2·18	574·8	2·10	564·1	2·09	536·6
14	54·28	2·22	602·5	2·20	575·2	2·11	564·4	2·10	536·7
15	65·72	2·26	603·4	2·22	575·5	2·12	564·6	2·10	536·8
16	77·14	2·31	604·3	2·24	575·9	2·13	564·9	2·10	536·9
17	88·57	2·35	605·2	2·25	576·3	2·15	565·1	2·11	537·0
18	100·00	2·39	606·1	2·27	576·6	2·16	565·4	2·11	537·0

Total H_2 feed conversion, %				
First bed	0·13	0·13	0·14	0·14
Second bed	0·39	0·40	0·21	0·20
Third bed	0·88	0·61	0·35	0·25
Total pressure drop, ATM	36·40	30·00	30·00	24·50

TABLE No.34: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed Comp.(Mole %) : H_2=64·5,N_2=21·5,NH_3=2·0,CH_4=10·0,A=2·0;Feed rate=567500 Nm^3/hr
Feed pressure=160·0 ATM,coldshot temperature=413·0K;catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction		:1·00		0·85		0·80		0·65	
Coldshot fraction		:0·00		0·00		0·00		0·00	
1.	0·0	2·00	648·0	2·00	648·0	2·00	648·0	2·00	648·0
2.	2·86	2·12	650·5	2·14	650·9	2·15	651·1	2·18	651·9
3.	5·72	2·24	653·0	2·28	653·9	2·30	654·3	2·37	655·9
4.	8·58	2·35	655·5	2·42	657·0	2·45	657·6	2·56	659·9
5.	11·42	2·47	658·1	2·56	660·0	2·60	660·9	2·75	664·1
6.	14·28	2·59	660·7	2·71	663·2	2·76	664·2	2·95	668·4
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	2·59	660·7	2·71	663·2	2·61	615·6	2·73	610·0
8.	20·00	2·84	666·1	3·02	669·8	2·68	617·0	2·79	611·3
9.	25·72	3·11	671·7	3·34	676·7	2·74	618·5	2·86	612·7
10.	31·43	3·38	677·6	3·69	684·1	2·81	620·0	2·93	614·1
11.	37·14	3·68	683·9	4·07	692·2	2·89	621·5	3·00	615·5
12.	42·86	3·99	690·5	4·48	701·0	2·96	623·0	3·06	616·9
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	3·99	690·5	4·10	653·2	2·96	623·0	2·90	586·7
14.	54·28	4·70	705·5	4·40	664·4	3·11	626·1	2·95	587·6
15.	65·72	5·54	723·2	4·72	671·0	3·27	629·3	3·00	588·6
16.	77·14	6·56	744·7	5·08	678·4	3·43	632·7	3·05	589·6
17.	88·57	7·78	770·3	5·47	686·5	3·60	636·2	3·09	590·6
18.	100·00	9·00	795·6	5·92	695·6	3·78	639·9	3·14	591·6
Total H_2 feed conversion, %									
First bed		1·30		1·36		1·37		1·40	
Second bed		4·44		4·69		2·16		2·03	
Third bed		14·91		8·59		3·98		2·57	
Total pressure drop ATM		10·30		8·50		8·50		7·0	

TABLE NoB5: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %) : H_2=64·5,N_2=21·5,NH_3=2·0,CH_4=10·0,A=2·0;Feed rate=351300 Nm^3/hr.

Feed pressure=160·0 ATM,coldshot temperature=413·0K;catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	2·00	648·0	2·00	648·0	2·00	648·0	2·00	643·0
2.	2·36	2·03	649·6	2·09	649·9	2·10	650·0	2·12	650·5
3.	5·72	2·15	651·2	2·18	651·8	2·19	652·1	2·24	653·1
4.	8·58	2·23	652·8	2·27	653·8	2·29	654·2	2·36	655·7
5.	11·42	2·30	654·4	2·36	655·7	2·39	656·2	2·49	658·4
6.	14·23	2·38	656·0	2·45	657·7	2·49	658·4	2·61	661·1
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	2·38	656·0	2·45	657·0	2·39	611·1	2·47	604·6
8.	20·00	2·53	659·3	2·64	661·7	2·43	612·0	2·51	605·5
9.	25·72	2·69	662·7	2·83	665·8	2·47	612·9	2·55	606·3
10.	31·43	2·85	666·1	3·03	670·1	2·51	613·7	2·59	607·1
11.	37·14	3·01	669·6	3·24	674·5	2·56	614·6	2·63	607·9
12.	42·86	3·18	673·2	3·45	679·0	2·60	615·5	2·67	608·8
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	3·18	673·2	3·23	640·1	2·60	615·5	2·57	580·0
14.	54.28	3·53	680·8	3·33	643·1	2·69	617·3	2·59	580·5
15.	65·72	3·91	688·9	3·53	646·2	2·77	619·1	2·62	581·1
16.	77·14	4·33	697·6	3·68	649·4	2·86	621·0	2·65	581·6
17.	83·57	4·78	707·2	3·84	652·7	2·95	622·9	2·67	582·2
18.	100·00	5·28	717·7	4·01	656·2	3·04	624·8	2·70	582·7
Total H_2 feed conversion, %									
First bed		0·85		0·87		0·87		0·89	
Second bed		2·65		2·77		1·35		1·23	
Third bed		7·23		4·47		2·35		1·58	
Total pressure drop ATM		21·60		17·80		17·80		14·50	

TABLE NO.B6: COMPUTED CONVERSION AND BED TEMPERATURE PROFILE: FEED COMPOSITION (IN MOLE %) $H_2=64\cdot5$, $N_2=21\cdot5$, $NH_3=2$, $CH_4=10$, A=2. FEED RATE=1135000 Nm^3/hr, PRESSURE=160 ATM, COLDSHOT TEMPERATURE=413K CATALYST VOLUME=63 m^3, ACTIVITY=70%

S. No.	% BED VOLUME	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)	MOLE % NH_3	BED TEMP (K)
		1st bed feed fr=1, cold shot fr.=0, 1st bed % H_2 conv.=·60		1st bed feed fr.=·85, coldshot fr.=0, 1st bed % H_2 conv.=·62		1st bed feed fr.=·8, coldshot fr.=0, 1st bed % H_2 conv.=·63		1st bed feed fr.=·65, coldshot fr.=0, 1st bed % H_2 conv.=·65	
1	0·0	2·00	648·0	2·0	648·0	2·00	648·0	2·00	648·0
2	2·86	2·06	649·1	2·07	649·4	2·07	649·5	2·09	649·9
3	5·72	2·11	650·3	2·13	650·8	2·14	651·0	2·18	651·7
4	8·58	2·16	651·4	2·20	652·1	2·21	652·4	2·27	653·6
5	11·42	2·21	652·5	2·26	653·5	2·28	653·9	2·35	655·5
6	14·28	2·27	653·7	2·33	654·9	2·35	655·4	2·44	657·5
		2nd bed feed fr.=1, cold shot fr.=0, 2nd bed % H_2 conv.=1·82		2nd bed feed fr.=·85, coldshot fr.=0, 2nd bed % H_2 conv=1·92		2nd bed feed fr.=1, coldshot fr.=·2, 2nd bed % H_2 conv.=·96		2nd bed feed fr.=·85, coldshot fr.=·2, 2nd bed % H_2 conv.=0·92	
7	14·28	2·27	653·7	2·33	654·9	2·28	608·9	2·34	602·0
8	20·00	2·37	655·9	2·46	657·7	2·31	609·5	2·37	602·6
9	25·72	2·48	658·2	2·59	660·6	2·34	610·1	2·40	603·2
10	31·43	2·59	660·6	2·72	663·5	2·37	610·7	2·42	603·8
11	37·14	2·70	662·9	2·86	666·4	2·40	611·3	2·45	604·3
12	42·86	2·81	665·2	3·00	669·4	2·43	611·9	2·48	604·9
		3rd bed feed fr.=1, cold shot fr.=0, 3rd bed % H_2 conv.=4·47		3rd bed feed fr.=1, coldshot fr.=·15, 3rd bed % H_2 conv.=2·96		3rd bed feed fr.=1, coldshot fr.=0, 3rd bed % H_2 conv.=1·61		3rd bed feed fr.=1, coldshot fr.=·15, 3rd bed % H_2 conv.=1·12	
13	42·86	2·81	665·2	2·85	632·2	2·43	611·9	2·41	576·8
14	54·28	3·03	670·0	2·94	634·1	2·49	613·2	2·43	577·2
15	65·72	3·26	675·0	3·04	636·0	2·54	614·4	2·44	577·6
16	77·14	3·50	680·0	3·13	638·0	2·60	615·6	2·46	577·9
17	88·57	3·75	685·3	3·22	639·9	2·66	616·8	2·48	578·3
18	100·00	4·00	690·7	3·32	641·9	2·72	618·0	2·50	578·7
		Pressure drop=36·3 ATM		Pressure drop=29·9 ATM		Pressure drop=29·9 ATM		Pressure drop=24·4 ATM	

TABLE NO. B7: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp. (Mole %) : H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0; Feed rate=567500 Nm^3/hr
Feed pressure=160·0 ATM, coldshot temperature=413·0K; catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1	0·0	2·00	698·0	2·00	698·0	2·00	698·0	2·00	698·0
2	2·86	2·41	707·0	2·49	708·7	2·52	709·4	2·64	712·2
3	5·72	2·83	716·2	2·99	719·8	3·05	721·3	3·32	727·2
4	8·58	3·26	725·8	3·52	731·5	3·63	733·8	4·07	743·5
5	11·42	3·72	736·0	4·09	744·0	4·25	747·5	4·90	761·8
6	14·28	4·21	746·8	4·71	757·7	4·93	762·4	5·83	782·2
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7	14·28	4·21	746·8	4·71	757·7	4·33	694·8	4·90	697·8
8	20·00	5·31	770·9	6·12	738·4	4·68	702·3	5·30	706·0
9	25·72	6·54	797·6	7·51	818·7	5·06	710·4	5·73	715·1
10	31·43	7·63	821·3	8·24	834·4	5·49	719·2	6·22	725·2
11	37·14	8·19	833·5	8·40	838·0	5·95	729·0	6·76	736·5
12	42·86	8·35	836·9	8·42	833·5	6·46	739·8	7·37	749·1
Coldshot fraction		0·00		0·15		0·00		0·15	
13	42·86	8·35	836·9	7·41	779·2	6·46	739·8	6·53	698·0
14	54·28	8·38	837·6	8·85	809·6	7·65	764·6	7·02	707·9
15	65·72	8·37	837·3	9·39	821·1	8·92	790·9	7·53	719·2
16	77·14	8·36	837·1	9·47	822·7	9·75	808·3	8·22	732·2
17	83·57	8·35	836·8	9·47	822·6	10·01	813·6	8·95	746·8
18	100·00	8·33	836·4	9·46	822·4	10·05	814·5	9·74	762·7
Total H_2 feed conversion, %									
First bed		4·93		5·11		5·18		5·47	
Second bed		13·62		11·70		9·74		9·87	
Third bed		13·58		15·83		17·00		16·38	
Total pressure drop, ATM		10·08		8·30		8·30		6·70	

TABLE NO.B8: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %) : H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0; Feed rate=351300·00 Nm^3/hr
Feed pressure=160·0 ATM, coldshot temperature=413·0K; catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	2·00	698·0	2·00	698·0	2·00	698·0	2·00	698·0
2.	2·86	2·26	703·8	2·32	704·9	2·34	705·4	2·42	707·3
3.	5·72	2·53	709·6	2·63	712·0	2·68	712·9	2·85	716·8
4.	8·58	2·80	715·5	2·96	719·2	3·03	720·7	3·30	726·7
5.	11·42	3·07	721·6	3·30	726·6	3·39	728·7	3·77	737·1
6.	14·28	3·35	727·9	3·65	734·3	3·77	737·1	4·28	748·3
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	3·35	727·9	3·65	734·3	3·41	674·9	3·73	672·0
8.	20·00	3·95	741·0	4·41	751·0	3·59	678·6	3·92	675·8
9.	25.72	4·61	755·3	5·26	769·6	3·78	682·5	4·11	679·8
10.	31·43	5·32	770·9	6·18	789·7	3·97	686·6	4·30	683·9
11.	37·14	6·07	787·4	7·08	809·4	4·17	690·8	4·51	688·3
12.	42·86	6·82	803·7	7·77	824·2	4·38	695·2	4·73	692·8
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	6·82	803·7	6·87	766·1	4·38	695·2	4·30	650·9
14.	54·28	7·86	826·3	7·85	787·1	4·82	704·7	4·46	653·9
15.	65·72	8·15	832·4	8·69	804·7	5·32	715·1	4·61	657·0
16.	77·14	8·17	833·0	9·14	814·2	5·88	726·8	4·77	660·3
17.	88·57	8·15	832·6	9·29	817·3	6·50	739·8	4·94	663·7
18.	100·00	8·13	832·1	9·31	817·8	7·19	754·3	5·11	667·3
Total H_2 feed conversion, %									
First bed		3·04		3·14		3·17		3·31	
Second bed		10·49		10·57		5·28		5·14	
Third bed		13·17		15·54		11·26		6·88	
Total pressure drop, ATM		21·10		17·30		17·50		14·20	

TABLE NO B10: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %) : H_2 60·75,% N_2=20·25,% NH_3=4·0,% CH_4=12·0,% A=3·0,Feed rate=567500 $\frac{Nm^3}{hr}$
Feed pressure=100·0 ATM,coldshot temperature=413·0K,catalyst vol=63 m^3 Activity=70%

No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		0·00		0·00		0·00		0·00	
1.	0·00	4·00	643·0	4·00	648·0	4·00	648·0	4·00	648·0
2.	2·86	4·05	649·0	4·06	649·2	4·06	649·3	4·08	649·6
3.	5·72	4·10	650·1	4·12	650·5	4·13	650·6	4·16	651·3
4.	8·58	4·15	651·1	4·18	651·7	4·20	652·0	4·25	653·0
5.	11·42	4·21	652·2	4·25	653·0	4·26	653·4	4·33	654·7
6.	14·28	4·26	653·3	4·31	654·3	4·33	654·8	4·42	656·5
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·26	653·3	4·31	654·3	4·27	608·6	4·32	601·6
8.	20·00	4·37	655·5	4·44	657·0	4·30	609·2	4·35	602·1
9.	25·72	4·48	657·8	4·58	659·8	4·33	609·8	4·37	602·6
10.	31·43	4·60	660·2	4·73	662·7	4·36	610·4	4·40	603·2
11.	37·14	4·72	662·6	4·88	665·8	4·39	611·0	4·43	603·7
12.	42·86	4·85	665·2	5·03	669·0	4·42	611·6	4·46	604·3
Coldshot fraction		0·00		0·15		0·00		0·15	
13.	42·86	4·85	665·2	4·83	632·0	4·42	611·6	4·39	576·3
14.	54·28	5·11	670·5	4·98	634·1	4·48	612·8	4·41	576·7
15.	65·72	5·39	676·3	5·09	636·2	4·54	614·0	4·43	577·1
16.	77·14	5·70	682·5	5·20	638·4	4·61	615·3	4·45	577·4
17.	88·57	6·04	689·3	5·32	640·7	4·67	616·6	4·47	577·8
18.	100·00	6·41	696·8	5·44	643·1	4·74	617·9	4·48	578·1
Total H_2 feed conversion, %									
First bed		0·62		0·63		0·63		0·64	
Second bed		2·00		2·05		0·98		0·92	
Third bed		5·60		3·36		1·74		1·14	
Total pressure drop, ATM		10·42		8·58		8·59		7·01	

TABLE NoB9: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %) : H_2=64·5,N_2=21·5,NH_3= 2·0,CH_4=10·0,A=2·0;Feed rate=1135000 Nm^3/hr.

Feed pressure=160·0 ATM,coldshot temperature=413·OK;catalyst vol=63 m^3,Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·35		0·80		0·65	
Coldshot fraction		0·00		0·00		0·00		0·00	
1.	0·00	2·00	698·0	2·00	698·0	2·00	698·0	2·00	698·0
2.	2·86	2·19	702·1	2·23	703·0	2·25	703·4	2·31	704·8
3.	5·72	2·33	706·3	2·46	708·0	2·49	708·8	2·62	711·7
4.	8·58	2·56	710·4	2·69	713·1	2·74	714·3	2·94	718·7
5.	11·42	2·75	714·6	2·92	718·3	2·99	719·9	3·27	725·9
6.	14·28	2·95	718·9	3·16	723·6	3·25	725·6	3·61	733·5
Coldshot fraction		0·00		0·00		0·20		0·20	
7.	14·28	2·95	718·9	3·16	723·6	3·00	665·9	3·23	661·0
8.	20·00	3·34	727·6	3·66	734·6	3·12	668·3	3·34	663·4
9.	25.72	3·76	736·7	4·20	746·4	3·23	670·8	3·46	665·9
10.	31·43	4·19	746·3	4·77	759·0	3·35	673·4	3·58	668·4
11.	37·14	4·65	756·3	5·39	772·4	3·47	676·0	3·70	671·0
12.	42·86	5·13	766·9	6·03	786·4	3·60	678·6	3·83	673·6
Coldshot fraction		0·00		0·15		0·00		0·15	
13.	42·86	5·13	766·9	5·41	732·7	3·60	678·6	3·55	635·0
14.	54·28	6·14	788·8	5·96	744·4	3·86	684·1	3·63	636·7
15.	65·72	7·04	808·3	6·56	757·1	4·12	689·8	3·72	638·4
16.	77·14	7·59	820·3	7·18	770·3	4·41	695·7	3·80	640·2
17.	88·57	7·78	824·5	7·79	783·2	4·70	702·0	3·89	641·9
18.	100·00	7·81	825·1	8·31	794·1	5·02	708·6	3·97	643·7
Total H_2 feed conversion, %									
First bed		2·13		2·22		2·25		2·34	
Second bed		6·92		7·50		3·58		3·47	
Third bbed		12·52		13·54		6·67		4·40	
Total pressure drop, ATM		35·73		29·37		29·59		24·10	

TABLE NO B11: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp. (Mole %) : H_2=60·75, N_2=20·25, NH_3=4·0, CH_4=12·0, A=3·0; Feed rate=851300 $\frac{Nm^3}{hr.}$

Feed pressure=160·0 ATM, coldshot temperature=413·OK; catalyst vol=63 m^3 Activity=70%.

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·30		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	4·00	648·00	4·00	648·00	4·00	648·0	4·00	648·00
2	2·86	4·03	648·7	4·04	648·8	4·04	648·8	4·05	649·1
3.	5·72	4·07	649·3	4·08	649·6	4·08	649·7	4·11	650·1
4.	8·58	4·10	650·0	4·12	650·4	4·13	650·6	4·16	651·2
5.	11·42	4·13	650·7	4·16	651·2	4·17	651·4	4·21	652·3
6.	14·23	4·17	65 ·0	4·20	652·0	4·21	652·3	4·27	653·4
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·23	4·17	651·3	4·20	652·0	4·17	606·7	4·21	599·3
8.	20·00	4·23	652·7	4·23	653·7	4·19	607·1	4·22	599·7
9.	25·72	4·30	654·1	4·37	655·4	4·21	607·4	4·24	600·0
10.	31·43	4·37	655·5	4·45	657·1	4·23	607·8	4·26	600·3
11.	37·14	4·44	657·0	4·54	658·9	4·24	608·2	4·27	600·7
12.	42·86	4·51	658·4	4·63	660·8	4·26	608·5	4·29	601·0
Coldshot fraction		: 0 00		0·15		0·00		0·15	
13.	42·86	4·51	658·4	4·53	625·2	4·26	608·5	4·25	573·6
14.	54·28	4·66	661·4	4·59	626·4	4·30	609·2	4·26	573·8
15.	65·72	4·81	664·5	4·65	627·6	4·34	610·0	4·27	574·1
16.	77·14	4·97	667·7	4·71	628·8	4·37	610·7	4·28	574·3
17.	88·57	5·14	671·1	4·77	630·0	4·41	611·4	4·29	574·5
18.	100·00	5·31	674·5	4·83	631·2	4·45	612·2	4·30	574·7
Total H_2 feed conversion, %									
First bed		0·39		0·40		0·40		0·41	
Second bed		1·21		1·26		0·62		0·58	
Third bed		3·07		1·96		1·06		0·72	
Total pressure drop, ATM		21·66		17·85		17·83		14·56	

TABLE NO.312: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %): H_2=60·75, N_2=20·25, NH_3=4·0, CH_4=12·0, A=3·0; Feed rate=1135000 $\frac{Nm^3}{hr}$
Feed pressure=160·0 ATM, coldshot temperature=413·OK; catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	4·00	648·0	4·00	648·0	4·00	648·0	4·00	648·0
2.	2·86	4·02	648·5	4·03	648·6	4·03	648·6	4·04	648·8
3.	5·72	4·05	648·9	4·06	649·1	4·06	649·2	4·08	649·6
4.	8·58	4·07	649·4	4·09	649·7	4·09	649·8	4·12	650·3
5.	11·42	4·09	649·9	4·11	650·3	4·12	650·5	4·16	651·1
6.	14·28	4·12	650·4	4·14	650·9	4·15	651·1	4·19	651·9
Coldshot fraction		0·00		0·00		0·20		0·20	
7.	14·28	4·12	650·4	4·14	650·9	4·12	605·8	4·15	598·2
8.	20·00	4·16	651·3	4·20	652·1	4·14	606·0	4·16	598·5
9.	25·72	4·21	652·3	4·26	653·2	4·15	606·3	4·17	598·7
10.	31·43	4·26	653·2	4·32	654·4	4·16	606·5	4·19	599·0
11.	37·14	4·31	654·2	4·38	655·7	4·17	606·8	4·20	599·2
12.	42·86	4·35	655·2	4·44	656·9	4·19	607·0	4·21	599·4
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	4·35	655·2	4·37	622·0	4·19	607·0	4·18	572·3
14.	54·28	4·45	657·1	4·41	622·8	4·21	607·5	4·19	572·5
15.	65·72	4·55	659·1	4·45	623·6	4·24	608·0	4·19	572·6
16.	77·14	4·65	661·1	4·49	624·3	4·26	608·5	4·20	572·8
17.	88·57	4·75	663·2	4·53	625·1	4·29	609·0	4·21	572·9
18.	100·00	4·85	665·2	4·57	625·9	4·31	609·5	4·22	573·0
Total H_2 feed conversion, %									
First bed		0·28		0·29		0·29		0·30	
Second bed		0·84		0·88		0·44		0·42	
Third bed		2·00		1·34		0·74		0·51	
Total pressure drop ATM		36·38		30·00		29·95		24·45	

TABLE NO B13:COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %): H_2=60·75,N_2=20·25,NH_3=4·0,CH_4=12·0,A=3·0;Feed rate 567500 $\frac{Nm^3}{hr.}$

Feed pressure=160·0 ATM,coldshot temperature=413·OK;catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	4·00	698·0	4·00	698·0	4·00	698·00	4·00	698·0
2.	2·86	4·18	701·8	4·22	702·5	4·23	702·8	4·29	704·0
3.	5·72	4·37	705·7	4·44	707·3	4·47	707·9	4·59	710·4
4.	8·58	4·56	709·8	4·68	712·2	4·72	713·2	4·92	717·2
5.	11·42	4·77	714·1	4·93	717·4	4·99	718·8	5·27	724·5
6.	14·28	4·98	718·6	5·19	722·9	5·28	724·8	5·64	732·4
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·98	718·6	5·19	722·9	5·02	666·1	5·25	661·2
8.	20·00	5·43	728·1	5·76	734·8	5·15	668·7	5·38	663·8
9.	25·72	5·93	738·4	6·39	748·1	5·28	671·4	5·52	666·5
10.	31·43	6·48	749·8	7·09	762·6	5·43	674·3	5·66	669·3
11.	37·14	7·06	762·0	7·83	777·9	5·57	677·2	5·80	672·2
12.	42·86	7·68	774·7	8·52	792·2	5·73	680·3	5·96	675·3
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	7·68	774·7	7·82	739·3	5·73	680·3	5·66	636·7
14.	54·28	8·78	797·5	8·59	754·8	6·05	686·9	5·76	638·7
15.	65·72	9·36	809·4	9·39	770·7	6·41	694·1	5·87	640·8
16.	77·14	9·51	812·5	10·06	784·2	6·81	702·0	5·98	642·9
17.	88·57	9·53	813·0	10·48	792·7	7·25	710·8	6·09	645·2
18.	100·00	9·53	812·9	10·67	796·5	7·74	720·6	6·21	647·5
Total H_2 feed conversion, %									
First bed		2·30		2·37		2·39		2·49	
Second bed		8·43		8·75		4·03		3·88	
Third bed		12·46		14·88		8·57		5·14	
Total pressure drop, ATM		10·25		8·41		8·49		6·92	

TABLE NO.D14: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %): H_2=60·75, N_2=20·25, NH_3=4·0, CH_4=12·0, A=3·0; Feed rate 851300 $\frac{Nm^3}{hr}$

Feed pressure=160·0 ATM, coldshot temperature=413·0K; catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		0·00		0·00		0·00		0·00	
1.	0·00	4·00	698·0	4·00	698·0	4·00	698·0	4·00	698·0
2.	2·86	4·12	700·4	4·14	700·9	4·15	701·1	4·19	701·9
3.	5·72	4·23	702·9	4·28	703·9	4·30	704·3	4·38	706·0
4.	8·58	4·35	705·4	4·43	707·0	4·46	707·6	4·58	710·2
5.	11·42	4·48	708·0	4·58	710·1	4·62	711·0	4·79	714·6
6.	14·28	4·60	710·7	4·73	713·4	4·79	714·6	5·01	719·2
Coldshot fraction		0·0		0·00		0·20		0·20	
7.	14·28	4·60	710·7	4·73	713·4	4·63	658·0	4·77	651·2
8.	20·00	4·87	716·2	5·06	720·3	4·70	659·5	4·84	652·6
9.	25·72	5·14	722·0	5·41	727·6	4·78	661·0	4·91	654·1
10.	31·43	5·43	728·1	5·78	735·4	4·86	662·6	4·99	655·6
11.	37·14	5·74	734·5	6·18	743·7	4·94	664·2	5·07	657·1
12.	42·86	6·07	741·2	6·61	752·5	5·02	665·8	5·14	658·7
Coldshot fraction		0·00		0·15		0·00		0·15	
13.	42·86	6·07	741·2	6·21	704·6	5·02	665·8	4·97	623·0
14.	54·28	6·76	755·7	6·54	711·3	5·18	669·1	5·02	623·9
15.	65·72	7·49	770·9	6·90	718·5	5·35	672·6	5·07	624·9
16.	77·14	8·19	785·3	7·28	726·2	5·53	676·2	5·12	626·0
17.	88·57	8·73	796·4	7·69	734·5	5·72	679·9	5·17	627·0
18.	100·00	9·04	802·9	8·12	743·2	5·91	683·9	5·23	628·0
Total H_2 feed conversion, %									
First bed		1·42		1·47		1·49		1·54	
Second bed		4·81		5·13		2·39		2·28	
Third bed		11·42		9·41		4·46		2·83	
Total pressure drop ATM		21·46		17·64		17·72		14·45	

TABLE NO.B15: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %): H_2=60·75, N_2=20·25, NH_3=4·0, CH_4=12·0, A=3·0; Feed rate=1135000 $\frac{Nm^3}{hr}$

Feed pressure =160·0 ATM, coldshot temperature=413·0K; catalyst vol=63 m^3 Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	4·00	698·0	4·00	698·0	4·00	698·0	4·00	698·00
2.	2·86	4·08	699·7	4·10	700·1	4·11	700·3	4·14	700·8
3.	5·72	4·17	701·5	4·20	702·2	4·22	702·5	4·28	703·8
4.	8·58	4·25	703·2	4·31	704·4	4·33	704·9	4·42	706·8
5.	11·42	4·34	705·0	4·41	706·6	4·44	707·3	4·57	709·9
6.	14·28	4·42	706·8	4·52	708·9	4·56	709·7	4·72	713·1
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·42	706·8	4·52	708·9	4·45	654·2	4·55	646·6
8.	20·00	4·60	710·6	4·74	713·5	4·50	655·2	4·60	647·6
9.	25·72	4·78	714·4	4·97	718·4	4·55	656·3	4·65	648·6
10.	31·43	4·97	718·3	5·21	723·4	4·60	657·3	4·69	649·6
11.	37·14	5·16	722·3	5·46	728·6	4·65	658·3	4·74	650·6
12.	42·86	5·36	726·5	5·73	734·1	4·70	659·4	4·79	651·6
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	5·36	726·5	5·46	688·9	4·70	659·4	4·67	617·1
14.	54·28	5·78	735·2	5·65	692·7	4·81	661·5	4·71	617·7
15.	65·72	6·22	744·3	5·84	696·7	4·91	663·6	4·74	618·3
16.	77·14	6·67	753·8	6·04	700·7	5·02	665·8	4·77	619·0
17.	88·57	7·13	763·3	6·25	704·9	5·13	668·0	4·80	619·6
18.	100·00	7·57	772·3	6·47	709·2	5·24	670·3	4·84	620·2
Total H_2 feed conversion, %									
First bed		1·00		1·04		1·05		1·10	
Second bed		3·19		3·42		1·65		1·59	
Third bbed		8·18		5·72		2·91		1·97	
Total pressure drop, ATM		36·16		29·76		29·82		24·32	

TABLE No. B. 16: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp. (mole %): H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0, Feed rate =567500 $\frac{Nm^3}{hr.}$
Feed pressure=160·0 ATM, coldshot temperature=698·0K; catalyst vol=63 m^3, Activity =70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:									
Coldshot fraction		:							
1.	0·00	2·00	698·0	2·00	698·0	2·00	698·0	2·00	698·0
2.	2·86	2·41	707·0	2·49	708·7	2·52	709·4	2·64	712·2
3.	5·72	2·83	716·3	2·99	719·8	3·05	721·3	3·32	727·2
4.	8·58	3·26	725·8	3·52	731·5	3·63	733·8	4·07	743·5
5.	11·42	3·72	736·0	4·09	744·0	4·25	747·5	4·90	761·8
6.	14·28	4·21	746·8	4·71	757·7	4·93	762·4	5·83	782·2
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·21	746·8	4·71	757·7	4·33	749·3	4·90	762·1
8.	20·00	5·31	770·9	6·12	788·4	5·46	774·1	6·36	794·0
9.	25·72	6·54	797·6	7·51	818·7	6·71	801·4	7·71	823·3
10.	31·43	7·63	821·3	8·24	834·4	7·77	824·4	8·32	836·4
11.	37·14	8·19	833·5	8·40	838·0	8·27	835·1	8·44	838·9
12.	42·86	8·35	836·9	8·42	838·5	8·40	837·9	8·45	839·2
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	8·35	836·9	7·41	817·8	8·40	837·9	7·43	818·5
14.	54·28	8·38	837·6	8·32	837·6	8·42	838·3	8·35	838·4
15.	65·72	8·37	837·3	8·37	838·6	8·41	838·1	8·39	839·3
16.	77·14	8·36	837·1	8·36	838·4	8·40	837·9	8·38	839·2
17.	88·57	8·35	836·8	8·35	838·2	8·38	837·6	8·38	839·0
18.	100·00	8·33	836·4	8·35	838·1	8·37	837·2	8·37	838·9
Total H_2 feed conversion, %									
First bed		4:93		5·11		5·18		5·47	
Second bed		13·62		11·70		13·71		11·75	
Third bed		13·58		13·61		13·65		13·67	
Total pressure drop ATM		10·08		8·29		8·22		6·69	

TABLE NO.B17: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %): H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0; Feed rate=351300 $\frac{Nm^3}{hr}$

Feed pressure-160·0 ATM, coldshot temperature=693·0K, catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	2·00	698·0	2·00	698·0	2·00	698·0	2·00	698·0
2.	2·86	2·26	703·8	2·32	704·9	2·34	705·4	2·42	707·3
3.	5·72	2·53	709·6	2·63	712·0	2·68	712·9	2·85	716·8
4.	8·58	2·80	715·6	2·96	719·2	3·03	720·7	3·30	726·7
5.	11·42	3·07	721·6	3·30	726·6	3·39	728·7	3·77	731·1
6.	14·28	3·35	727·9	3·65	734·3	3·77	737·1	4·28	748·3
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	3·35	727·9	3·65	734·3	3·41	729·2	3·73	736·3
8.	20·00	3·95	741·0	4·41	751·0	4·04	742·8	4·53	753·7
9.	25·72	4·61	755·3	5·26	769·6	4·72	757·7	5·41	773·0
10.	31·43	5·32	770·9	6·18	789·7	5·46	774·0	6·37	793·9
11.	37·14	6·07	787·4	7·08	809·4	6·25	791·2	7·28	813·7
12.	42·86	6·82	803·7	7·77	824·2	7·02	807·9	7·93	827·7
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	6·82	803·7	6·87	805·3	7·02	807·9	7·00	808·4
14.	54·28	7·86	826·3	7·94	828·7	8·01	829·4	8·04	831·2
15.	65·72	8·15	832·4	8·21	834·6	8·24	834·4	8·28	836·2
16.	77·14	8·17	833·0	8·23	835·0	8·25	834·7	8·29	836·5
17.	88·57	8·15	832·6	8·21	834·6	8·23	834·2	8·27	836·1
18.	100·00	8·13	832·1	8·18	834·1	8·21	833·7	8·25	835·6
Total H_2 feed conversion, %									
First bed		3·04		3·14		3·17		3·31	
Second bed		10·49		10·57		10·89		10·85	
Third bed		13·17		13·28		13·33		13·41	
Total pressure drop ATM		21·10		17·31		17·23		13·96	

TABLE NO.B.13: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES

Feed comp.(Mole %): H_2=64·5, N_2=21·5, NH_3=2·0, CH_4=10·0, A=2·0, Feed rate=1135000 $\frac{Nm^3}{hr}$

Feed pressure=160·0 ATM, coldshot temperature=693·0K; catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fracrton		: 0·00		0·00		0·00		0·00	
1.	0·00	2·00	698·0	2·00	698·0	2·00	698·0	2·00	698·0
2.	2·86	2·19	702·1	2·23	703·0	2·25	703·4	2·31	704·8
3.	5·72	2·38	706·3	2·46	708·0	2·49	708·8	2·62	711·7
4.	8·58	2·56	710·4	2·69	713·1	2·74	714·3	2·94	718·7
5.	11·42	2·75	714·6	2·92	718·3	2·99	719·9	3·27	725·2
6.	14·28	2·95	718·9	3·16	723·6	3·25	725·6	3·61	733·5
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	2·95	718·9	3·16	723·6	3·00	720·0	3·23	725·1
8.	20·00	3·34	727·6	3·66	734·6	3·42	729·2	3·75	736·6
9.	25·72	3·76	736·7	4·20	746·4	3·86	738·9	4·32	749·1
10.	31·43	4·19	746·3	4·77	759·0	4·32	749·1	4·93	762·4
11.	37·14	4·65	756·3	5·39	772·4	4·81	759·9	5·59	776·8
12.	42·86	5·13	766·9	6·03	786·4	5·33	771·2	6·27	791·6
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	5·13	766·9	5·41	772·9	5·33	771·2	5·61	777·3
14.	54·28	6·14	788·8	6·48	796·3	6·41	794·7	6·74	802·1
15.	65·72	7·04	808·3	7·38	815·8	7·33	814·7	7·63	821·2
16.	77·14	7·59	820·3	7·83	825·7	7·82	825·2	8·01	829·6
17.	88·57	7·78	824·5	7·96	828·4	7·96	828·3	8·09	831·4
18.	100·00	7·81	825·1	7·96	828·4	7·96	828·4	8·08	831·1

Total H_2 feed conversion, %				
First bed	2·13	2·22	2·25	2·34
Second bed	6·92	7·50	7·35	7·93
Third bed	12·52	12·83	12·83	13·07
Total pressure drop ATM	35·73	29·34	29·27	23·72

TABLE NO.B.19: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %): H_2=64·5,N_2=21·5,NH_3=2·0,CH_4=10·0,A=2·0,Feed rate=567500 Nm^3/hr.
Feed pressure=160·0 ATM,coldshot temperature=648 K;catalyst vol=63 m^3,Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	2·00	648·0	2·00	648·0	2·00	648·0	2·00	648·0
2.	2·86	2·12	650·5	2·14	650·9	2·15	651·1	2·18	651·9
3.	5·72	2·24	653·0	2·28	653·9	2·30	654·3	2·37	655·9
4.	8·58	2·35	655·5	2·42	657·0	2·45	657·6	2·56	659·9
5.	11·42	2·47	658·1	2·56	660·0	2·60	660·9	2·75	664·1
6.	14·28	2·59	660·7	2·71	663·2	2·76	664·2	2·95	668·4
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	2·59	660·7	2·71	663·2	2·61	660·9	2·73	663·6
8.	20·00	2·84	666·1	3·02	669·8	2·86	666·4	3·04	670·2
9.	25·72	3·11	671·7	3·34	676·7	3·13	672·1	3·37	677·3
10.	31·43	3·38	677·6	3·69	684·1	3·41	678·1	3·72	684·8
11.	37·14	3·68	633·9	4·07	692·2	3·71	684·4	4·11	693·0
12.	42·86	3·99	690·5	4·48	701·0	4·03	691·2	4·54	702·0
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	3·99	690·5	4·10	692·8	4·03	691·2	4·15	693·6
14.	54·28	4·70	705·5	4·84	708·3	4·75	706·5	4·89	709·5
15.	65·72	5·54	723·2	5·72	726·8	5·61	724·7	5·80	728·5
16.	77·14	6·56	741·7	6·79	749·4	6·66	746·8	6·91	751·8
17.	88·57	7·78	770·3	8·07	776·1	7·92	773·2	8·56	779·1
18.	100·00	9·00	795·6	9·23	800·4	9·13	798·4	9·56	803·0
Total H_2 feed conversion, %									
First bed		1·36		1·36		1·37		1·40	
Second bed		4·44		4·69		4·52		4·78	
Third bed		14·91		15·39		15·19		15·64	
Total pressure drop ATM		10·30		8·51		8·49		6·90	

TABLE NO.B.20: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %): H_2=64·5,N_2=21·5,NH_3=2·0,CH_4=10·0,A=2·0,Feed rate=1135000 Nm^3/hr.
Feed pressure 160·0 ATM,coldshot temperature=648 K;catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	2·00	648·0	2·00	648·0	2·00	648·0	2·00	648·0
2.	2·86	2·06	649·1	2·07	649·4	2·07	649·5	2·09	649·9
3.	5·72	2·11	650·3	2·13	650·8	2·14	651·0	2·18	651·7
4.	8·58	2·16	651·4	2·20	652·1	2·21	652·4	2·27	653·6
5.	11·42	2·21	652·5	2·26	653·5	2·28	653·9	2·35	655·5
6.	14·28	2·27	653·7	2·33	654·9	2·35	655·4	2·44	657·5
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	2·27	653·7	2·33	654·9	2·28	653·9	2·34	655·3
8.	20·00	2·37	655·9	2·46	657·7	2·39	656·3	2·48	658·2
9.	25·72	2·48	658·2	2·59	660·6	2·50	658·7	2·62	661·2
10.	31·43	2·59	660·6	2·72	663·5	2·62	661·2	2·76	664·2
11.	37·14	2·70	662·9	2·86	666·4	2·73	663·6	2·90	667·3
12.	42·86	2·81	665·2	3·00	669·4	2·85	666·1	3·05	670·5
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	2·81	665·2	2·85	666·2	2·85	666·1	2·89	667·1
14.	54·28	3·03	670·0	3·09	671·3	3·09	671·2	3·14	672·4
15.	65·72	3·26	675·0	3·33	676·5	3·33	676·4	3·40	678·0
16.	77·14	3·50	680·0	3·59	681·9	3·59	681·9	3·67	683·7
17.	88·57	3·75	685·3	3·86	687·6	3·85	687·5	3·95	689·7
18.	100·00	4·00	690·7	4·13	693·5	4·13	693·4	4·25	696·0

Total H_2 feed conversion, %				
First bed	0·60	0·62	0·63	0·65
Second bed	1·82	1·92	1·91	2·00
Third bed	4·47	4·75	4·75	5·01
Total pressure drop, ATM	36·30	29·88	29·80	24·29

TABLE NO.B.21: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(Mole %): H_2=64·5,N_2=21·5,NH_3=2·0,CH_4=10·0,A=2·0,Feed rate=567500 Nm^3/hr.
Feed pressure=160·0 ATM,coldshot temperature=593 K;catalyst vol=63 M^3,Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction	:	0·00		0·00		0·00		0·00	
1.	0·00	2·00	598·0	2·00	598·0	2·00	598·0	2·00	598·0
2.	2·86	2·03	598·5	2·03	598·6	2·04	598·7	2·04	598·8
3.	5·72	2·05	599·0	2·06	599·2	2·07	599·3	2·08	599·6
4.	8·58	2·08	599·6	2·09	600·0	2·10	600·0	2·12	600·5
5.	11·42	2·10	600·1	2·12	600·5	2·13	600·7	2·16	601·3
6.	14·28	2·13	600·6	2·15	601·1	2·16	601·3	2·20	602·7
Coldshot fraction	:	0·00		0·00		0·20		0·20	
7.	14·28	2·13	600·6	2·15	601·1	2·13	600·7	2·16	601·2
8.	20·00	2·18	601·7	2·22	602·4	2·18	601·8	2·22	602·5
9.	25·72	2·23	602·8	2·28	603·7	2·24	602·9	2·28	603·8
10.	31·43	2·28	603·9	2·34	605·0	2·29	604·0	2·35	605·1
11.	37·14	2·34	605·0	2·40	606·3	2·34	605·1	2·41	606·5
12.	42·86	2·39	606·1	2·47	607·7	2·40	606·2	2·48	607·8
Coldshot fraction	:	0·00		0·15		0·00		0·15	
13.	42·86	2·39	606·1	2·40	606·2	2·40	606·2	2·41	606·4
14.	54·28	2·50	608·3	2·51	608·5	2·51	608·5	2·52	608·7
15.	65·72	2·61	610·6	2·62	610·9	2·62	610·9	2·63	611·0
16.	77·14	2·72	613·0	2·73	613·3	2·73	613·3	2·74	613·5
17.	88·57	2·84	615·4	2·85	615·7	2·85	615·7	2·86	616·0
18.	100·00	2·96	617·9	2·97	618·3	2·97	618·3	2·99	618·6
Total H_2 feed conversion, %									
First bed	:	0·29		0·29		0·29		0·29	
Second bed		0·88		0·89		0·89		0·91	
Third bed		2·15		2·19		2·19		2·22	
Total pressure drop ATM		10·50		8·60		8·60		7·00	

TABLE NO.B.22: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(mole %): H_2=60·75, N_2=20·25, NH_3=4·0, CH_4=12·0, A=3·0, Feed rate=567500 Nm^3/hr
Feed pressure=160·0 ATM, coldshot temp=6;3 K; catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	4·00	648·0	4·00	648·0	4·00	648·0	4·00	648·0
2.	2·86	4·05	649·0	4·06	649·2	4·06	649·3	4·06	649·6
3.	5·72	4·10	650·1	4·12	650·5	4·13	650·6	4·16	651·3
4.	8·58	4·15	651·1	4·18	651·7	4·20	652·0	4·25	653·0
5.	11·42	4·21	652·2	4·25	653·0	4·26	653·4	4·33	654·7
6.	14·28	4·26	653·3	4·31	654·3	4·33	654·8	4·42	656·5
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·26	653·3	4·31	654·3	4·27	653·4	4·32	654·5
8.	20·00	4·37	655·5	4·44	657·0	4·38	655·7	4·45	657·2
9.	25·72	4·48	657·8	4·58	659·8	4·49	658·0	4·61	660·1
10.	31·43	4·60	660·2	4·73	662·7	4·61	660·4	4·74	663·0
11.	37·14	4·72	662·6	4·88	665·8	4·73	662·9	4·89	666·1
12.	42·86	4·85	665·2	5·03	669·0	4·86	665·5	5·05	669·4
Coldshot fraction		0·00		0·15		0·00		0·15	
13.	42·86	4·85	665·2	4·88	665·8	4·86	665·5	4·89	666·1
14.	54·28	5·11	670·5	5·14	671·2	5·13	670·9	5·17	671·7
15.	65·72	5·39	676·3	5·44	677·1	5·42	676·8	5·46	677·7
16.	77·14	5·70	682·5	5·75	683·5	5·74	683·2	5·79	684·2
17.	88·57	6·04	689·3	6·10	690·5	6·08	690·2	6·14	691·3
18.	100·00	6·41	696·8	6·48	698·2	6·46	697·8	6·53	699·2
Total H_2 feed conversion, %									
First bed		0·62		0·63		0·63		0·64	
Second bed		2·00		2·06		2·03		2·10	
Third bed		5·60		5·76		5·71		5·87	
Total pressure drop ATM		10·42		8·58		8·56		6·98	

TABLE NO.B.24: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(mole %): H_2=60·75, N_2=20·25, NH_3=4·0, CH_4=12·0, A=3·0, Feed rate=567500 $\frac{Nm^3}{hr}$
Feed pressure=160·0 ATM, coldshot temp=698 K; catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00		0·00		0·00		0·00	
1.	0·00	4·00	698·0	4·00	698·0	4·00	698·0	4·00	698·0
2.	2·86	4·18	701·8	4·22	702·5	4·23	702·8	4·29	704·0
3.	5·72	4·37	705·7	4·44	707·3	4·47	707·9	4·59	710·4
4.	8·58	4·56	709·8	4·68	712·2	4·72	713·2	4·92	717·2
5.	11·42	4·77	714·1	4·93	712·4	4·99	718·8	5·27	724·5
6.	14·28	4·98	718·6	5·19	722·9	5·28	724·8	5·64	732·4
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·98	718·6	5·19	722·9	5·02	719·4	5·25	724·2
8.	20·00	5·43	728·1	5·76	734·8	5·48	729·1	5·83	736·4
9.	25·72	5·93	738·4	6·39	748·1	5·99	739·7	6·49	750·0
10.	31·43	6·48	749·8	7·09	762·6	6·55	751·4	7·21	765·0
11.	37·14	7·06	762·0	7·83	777·9	7·15	763·9	7·96	780·5
12.	42·86	7·68	774·7	8·52	792·2	7·78	776·9	8·65	794·8
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	7·68	774·7	7·82	778·0	7·78	776·9	7·92	780·2
14.	54·28	8·78	797·5	8·91	800·5	8·87	799·6	9·00	802·4
15.	65·72	9·36	809·4	9·42	811·1	9·42	810·7	9·47	812·2
16.	77·14	9·51	812·5	9·54	813·6	9·55	813·4	9·58	814·4
17.	88·57	9·53	813·0	9·56	813·9	9·57	813·8	9·59	814·6
18.	100·00	9·53	812·9	9·55	813·8	9·56	813·6	9·58	814·4
Total H_2 feed conversion, %									
First bed		2·30		2·37		2·39		2·49	
Second bed		8·43		8·75		8·66		8·97	
Third bed		12·46		12·51		12·54		12·58	
Total pressure drop ATM		10·25		8·41		8·39		6·80	

TABLE NO.B.25: COMPUTED CONVERSION AND BED TEMPERATURE PROFILES
Feed comp.(mole %): H_2=60·75,N_2=20·25,NH_3=4·0,CH_4=12·0,A=3·0,Feed rate=1135000 $\frac{Nm^3}{hr}$
Feed pressure=160·0 ATM,coldshot temp=698 K,catalyst vol=63 m^3, Activity=70%

S. No.	% Bed volume	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)	Mole % NH_3	Bed temp. (K)
1st bed feed fraction:		1·00		0·85		0·80		0·65	
Coldshot fraction		: 0·00						0·00	
1.	0·00	4·00	698·0	4·00	698·0	4·00	698·0	4·00	698·0
2.	2·86	4·08	699·7	4·10	700·1	4·11	700·3	4·14	700·8
3.	5·72	4·17	701·5	4·20	702·2	4·22	702·5	4·28	703·8
4.	8·58	4·25	703·2	4·31	704·4	4·33	704·9	4·42	706·8
5.	11·42	4·34	705·0	4·41	706·6	4·44	707·3	4·57	709·9
6.	14·28	4·42	706·8	4·52	708·9	4·56	709·7	4·72	713·1
Coldshot fraction		: 0·00		0·00		0·20		0·20	
7.	14·28	4·42	706·8	4·52	708·9	4·45	707·3	4·55	709·5
8.	20·00	4·60	710·6	4·74	713·5	4·63	711·3	4·78	714·4
9.	25·72	4·78	714·4	4·97	718·4	4·83	715·3	5·02	719·5
10.	31·43	4·97	718·3	5·21	723·4	5·02	719·5	5·28	724·8
11.	37·14	5·16	722·3	5·46	728·6	5·23	723·8	5·54	730·4
12.	42·86	5·36	726·5	5·73	734·1	5·44	728·2	5·82	736·2
Coldshot fraction		: 0·00		0·15		0·00		0·15	
13.	42·86	5·36	726·5	5·46	728·7	5·44	728·2	5·54	730·4
14.	54·28	5·78	735·2	5·91	738·0	5·89	737·5	6·02	740·3
15.	65·72	6·22	744·3	6·39	747·9	6·36	747·4	6·53	750·9
16.	77·14	6·67	753·8	6·88	758·2	6·85	757·6	7·06	761·9
17.	88·57	7·13	763·3	7·38	768·5	7·35	767·9	7·59	772·9
18.	100·00	7·57	772·3	7·84	778·1	7·82	777·6	8·08	783·0
Total H_2 feed conversion, %									
First bed		1·00		1·04		1·05		1·10	
Second bed		3·19		3·42		3·38		3·61	
Third bed		8·18		8·80		8·74		9·31	
Total pressure drop ATM		36·16		29·76		29·68		24·16	

APPENDIX-C

TABLE NO.C.1: RELATIONSHIPS FOR HEAT CAPACITIES, HEAT OF REACTION AND REACTION RATE

Heat Capacities: $[\mathrm{Cal}/(\mathrm{g\ mole})(^{\circ}\mathrm{K})]$

Hydrogen : $$C_{p1} = 6\cdot952-4\cdot576\times10^{-4}T+9\cdot563\times10^{-7}T^2-2\cdot079\times10^{-10}T^3 \qquad \dots C\cdot1$$

Nitrogen : $$C_{p2} = 6\cdot903-3\cdot753\times10^{-4}T+1\cdot93\times10^{-6}T^2-6\cdot861\times10^{-10}T^3 \qquad \dots C\cdot2$$

Ammonia : $$C_{p3} =102\cdot7524-21\cdot63767\times10^{-2}T+13\cdot12707\times10^{-5}T^2-1\cdot5981\times10^{-9}T^3 -P(6\cdot7571\times10^{-2}-1\cdot6847\times10^{-4}T+1\cdot009514\times10^{-7}T^2) \qquad \dots C\cdot3$$

Methane : $$C_{p4} = 4\cdot75+1\cdot2\times10^{-2}T+3\cdot03\times10^{-6}T^2-2\cdot63\times10^{-9}T^3 \qquad \dots C\cdot4$$

Argon : $$C_{p5} = 4\cdot9675 \qquad \dots C\cdot5$$

Heat of Reaction [Cal/g mole of H_2 reacted]

$$\Delta H_{R1} = \frac{2}{3}\left\{-15564\cdot51+,\cdot0646T-14\cdot8399\times10^{-3}T^2+3\cdot3563\times10^{-7}T^3-1\cdot1625\times10^{-10}T^4 -P(3\cdot01975-4\cdot4552\times10^{-3}T+1\cdot928\times10^{-6}T^2)\right\} \qquad \dots C\cdot6$$

Reaction Rate [g mole H_2 reacted/(sec)(M^3 of catalyst volume)]

$$-r_1 = 29\cdot4204\ f\ k_r \left\{\left(\frac{k}{k_\nu}\right)^2 \left[P^{1\cdot5}N_1^{1\cdot5}N_2/(N_3N_T^{1\cdot5}) \right] -N_3N_T^{0\cdot5}/(P^{0\cdot5}N_1^{1\cdot5})\right\} \qquad \dots C\cdot7$$

where f is the catalyst activity factor

$$k_r = \left(\frac{300}{P}\right)^{0\cdot63} \exp\left(\frac{-24092\cdot2}{T} + 33\cdot5566\right) \qquad \dots C\cdot8$$

[illegible] $$= \exp\left[0\cdot50327\left(\frac{9184\cdot0}{T} - 7\cdot2949\ \ln T+3\cdot4966\times10^{-3}T+1\cdot6781\times10^{-7}T^2 -3\cdot875\times10^{-11}T^3+23\cdot05\right)\right] \qquad \dots C\cdot9$$

$$K_\nu = 1\cdot7343-8\cdot143\times10^{-4}P+5\cdot714\times10^{-7}PT-2\cdot6714\times10^{-3}T+2\times10^{-6}T^2 \qquad C\cdot10$$

and subscript j deontes the catalyst bed number.

The energy balance equation for the gas in internal preheating section is

$$F_{DH}\left(\sum_{i=1}^{5} F_i \; Cp_i\right) d\, T_{sj} = -\,(UA)_j\,(T_j - T_{sj})\; d\, V_j \qquad \ldots\ (3\cdot4)$$

where F_{DH} is the fraction of total feed entering through preheating section and negative sign on right hand side takes into account that the flow direction of gases in internal preheating section is opposite to that in the reaction section. Equations 3·2, 3·3 and 3·4 are applicable to each of the catalyst bed when proper values to variables for bed j are assigned. It may be noted that X_1 fractional conversion based on total moles of hydrogen fed to reactor including all the coldshots, increases monotonically as reaction mixture passes through the catalyst beds.

Eventhough Eqn. 3·2, 3·3 and 3·4 are applicable to each of the catalyst bed but since the coldshots of feed gases are added at the entry of each of the catalyst bed, additional mass and energy balance equations are necessary to obtain the boundary conditions for the solution of above equations .

Mass Balance Equations for Catalyst Bed j

At the entry (subscript 0)

The simulation model thus consists of Eqns. 3·2 to 3·12 and C·1–C·10. Eqns. 3·2, 3·3 and 3·4 are repeated for consecutive catalyst beds; however, the initial temperature, pressure and composition for each bed (the initial boundary values for the solution of differential equations) will be different for each bed.