APPENDIX I-D
REPORT OF SCHNEIDER CONSULTING ENGINEERS

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COMPUTER SIMULATION OF PREHEATER AND REACTOR IN DIRECT COAL LIQUEFACTION

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ABSTRACT

This report describes a comprehensive computer simulation program that predicts the performance of coal liquefaction preheater and reactor. The simulator is interactive and allows the user to input any linear kinetic network by specifying the reaction paths. The user must also specify the operating conditions and the physical dimensions of the units. The simulator will then provide detailed information on the performance of each unit, the characteristics of each flow stream, and an overall summary of the products leaving each unit. The simulator also provides graphical (pictorial) outputs of the results. The input/output results are stored in a database for any future processing.

Included in this report are model development, descriptions of the mathematical procedures used to predict the performance of the units, source code of the program, instructions for its use, and a sample problem showing both the input data and the resulting output, both in tabular and graphical form.

INTRODUCTION

Various processes are used for direct coal liquefaction (Whitehurst, et al., 1980; Shah, 1981). A typical coal liquefaction unit consists of a preheater and a reactor. Coal is mixed with recycle solvent and fed with hydrogen into a preheater, where the temperature of the mixture is raised to around 673 K. It is then fed into a reactor (dissolver), wherein the reaction is allowed to proceed. Recently, Albal et al., 1983, have qualitatively examined the performance of such preheaters and reactors.

This report describes a comprehensive computer program that allows the user to simulate the performance of coal liquefaction preheater and reactor units. The program is flexible in the sense that it can accommodate any reaction network as long as the reactions follow first order kinetics. The program is interactive and allows the user to execute it either in batch or time sharing mode.

The simulation program is written in modular form using the FORTRAN language. It can be implemented on virtually any large, scientific computer, though some customization may be required to ensure machine/language compatibility. The code has been developed on a DEC System-10 computer at the University of Pittsburgh. The programs necessary to convert the output from this simulator into a graphical form and to store it in a database, have been developed on a PDP-11/70 computer at Schneider Consulting Engineers, Bridgeville. These programs require the use of IGDS (Interactive Graphics Design System) and DMRS (Data Management and Retrieval System) software packages, developed by Intergraph Corporation, Huntsville, Alabama. The programs to display graphical outputs can only be used on computers supported by the Intergraph software.

Included in this report are a listing of the computer programs, instructions for its use and representative sample output, in addition to the general description of the methods used to carry out the simulation.

MODEL DEVELOPMENT

The direct coal liquefaction involves a three phase reaction mixture, wherein the hydrogen from the gas phase is absorbed into the liquid phase and reacts to form various products. The liquid phase consists of a mixture of coal and the solvent. The necessary equations to predict the thermal behavior of the preheater and reactor, include the material balance for hydrogen in the gas and liquid phases and the heat balances for both preheater and reactor. The heat generation in the dissolver is assumed to be proportional to the hydrogen consumption.

The mass and heat balance equations for the preheater can be derived with the assumption of plug flow condition. This assumption is justified considering that preheaters employed for coal liquefaction are usually in the form of coils with a length to diameter ratio of more than 100. In the reactor, the gas phase is assumed to flow in a plug flow, while standard axial dispersion model, with closed-closed boundary conditions is used to model liquid phase hydrogen balance and the energy balance equations. Other simplifying assumptions made in development are as follows:

1. Reactions occur in the bulk slurry phase only.

2. Mass transfer of hydrogen from gas phase to liquid phase is controlled by the liquid side mass transfer resistance.

3. The reactor operates under isobaric conditions. This assumption is justified since the pressure drop is not significant as compared to the actual pressure anywhere in the reactor.

4. The three phases are at the same temperature at any axial position.

5. The gas holdup is constant all along the preheater, and all along the reactor.

MODEL DEVELOPMENT (Continued)

6. The physical and thermal properties of the gas and the slurry (except the viscosity of the slurry), the mass transfer coefficient, gas liquid interfacial area, and the heats of reaction and dissolution are independent of the temperature and conversion.

7. Henry's law is applicable. The rate constant for hydrogen consumption and the Henry's constant are temperature dependent according to

$$k = \bar{k} \exp(-E/RT) \tag{1}$$

and

$$H = \bar{H} \exp(-\Delta H_r/RT) \tag{2}$$

8. As a consequence of assumption (6), the heat transfer coefficient can be obtained as a function of viscosity as

$$h = \beta\, \mu(\theta)^{-0.4667} \tag{3}$$

where h = heat transfer coefficient; β = constant depending on the coal, type of solvent and the coal to solvent ratio; $\mu(\theta)$ = viscosity, a function of temperature.

The exponent of the viscosity is in accordance with the Sieder-Tate equation (Shah, 1981) for heat transfer.

Based on the above assumptions, the following equations can be derived.

A. PREHEATER

1. Hydrogen Balance

(a) Gas Phase

$$\frac{da_g^i}{dx^i} + R_l^i\left(\frac{H}{H_l^i}\, a_g^i - a_l^i\right) = 0 \tag{4}$$

MODEL DEVELOPMENT (Continued)

where

$$R_i' = \frac{k_i' a L' H_i'}{v_g'} \tag{5}$$

$$H = \overline{H} \exp\left(-\Delta H_S^{\circ}/(1+\theta)\right) \tag{6}$$

and

$$\Delta H_S^{\circ} = \Delta H_S / RT_i' \tag{7}$$

$$a_g' = 1 \qquad \text{at } x' = 0 \tag{8}$$

(b) Slurry Phase

$$\frac{da_l'}{dx'} - \frac{R_l'}{H_i' \gamma'}\left(\frac{H}{H_i'} a_g' - a_l'\right) + \frac{R_p}{\gamma'} \exp\left(-E^{\circ}/(1+\theta')\right) a_l' = 0 \tag{9}$$

where

$$\gamma' = \frac{v_l'}{v_g'} \tag{10}$$

$$R_p = \frac{\overline{k}(1-\epsilon_g')L'}{v_g'} \tag{11}$$

and

$$E^{\circ} = E/RT_i' \tag{12}$$

Equation (9) is subject to the boundary condition

$$a_l' = 0 \text{ at } x' = 0 \tag{13}$$

MODEL DEVELOPMENT (Continued)

2. Energy Balance

In the preheater, the heat input is largely by the external heating and some by heat of reaction and heat of dissolution. The governing heat balance equation can be expressed as

$$\frac{d\theta^1}{dx^1} =$$

$$\alpha\mu(\theta^1)^{-0.4667}(\theta_w - \theta^1) + R_e\Gamma_R^1 H_i^1 \exp(-E^*/(1+\theta^1))a_i^1 + R_1^1\Gamma_S^1\left(\frac{H}{H_i^1}a_s^1 - a_i^1\right) \quad (14)$$

where

$$\alpha = \frac{\pi \cdot \beta \cdot L^1}{\dot{m}(v_s^1\rho_s C_{ps} + v_l^1\bar{\rho}_l\bar{C}_{pl})} \quad (15)$$

$$\Gamma_R^1 = \frac{C_R^1 \cdot v_s^1 \cdot \Delta H_R}{T_i^1(v_s^1\rho_s C_{ps} + v_l^1\bar{\rho}_l\bar{C}_{pl})} \quad (16)$$

and

$$\Gamma_S^1 = \frac{C_R^1 \cdot v_s^1 \cdot \Delta H_S}{T_i^1(v_s^1\rho_s C_{ps} + v_l^1\bar{\rho}_l\bar{C}_{pl})} \quad (17)$$

Here $\mu(\theta)$, viscosity is obtained from a fitted equation that accounts for the change in viscosity as a function of the temperature. Equation (14) is subject to the boundary condition

$$\theta^1 = 0 \qquad \text{at } x^1 = 0 \quad (18)$$

3. Chemical Species Balance

$$\frac{dc_j}{dx^1} - Ra_j^1 = 0 \quad ; \quad j = 1, N_s \quad (19)$$

where

$$Ra_j^1 = \bar{R}_j \frac{I}{I_L^2}(\quad) \quad j = 1, N_s \quad (20)$$

MODEL DEVELOPMENT (Continued)

The boundary condition for Equation (19) is

$$C_j = C_{j,i} \qquad \text{at} \quad x^{II} = 0 \; ; \quad j = 1, N_s \tag{21}$$

B. REACTOR

1. Hydrogen Balance

(a) Gas Phase

$$\frac{da_g^{II}}{dx^{II}} + R_l^{II}\left(\frac{H}{H_l'}a_g^{II} - a_l^{II}\right) = 0 \tag{22}$$

where

$$R_l^{II} = \frac{k_l a L^{II} H_l'}{v_g^{II}} \tag{23}$$

The boundary condition for Equation (22) is

$$a_g^{II}|_{x^{II}=0^-} = a_g^{II}|_{x^{II}=0^+} \tag{24}$$

(b) Slurry Phase

$$\frac{1}{Pe_l}\frac{d^2a_l^{II}}{(dx^{II})^2} - \frac{da_l^{II}}{dx^{II}} + \frac{R_l^{II}}{\gamma^{II}\cdot H_l'}\left(\frac{H}{H_l'}a_g^{II} - a_l^{II}\right) - \frac{Da}{\gamma^{II}}\exp\left(-E^*/(1+\theta^{II})\right)a_l = 0 \tag{25}$$

where

$$\gamma^{II} = \frac{v_l^{II}}{v_g^{II}} \tag{26}$$

$$Pe_l = \frac{v_l^{II}\cdot L^{II}}{D_l} \tag{27}$$

$$Da = \frac{\bar{k}(1-\epsilon_g^{II})L^{II}}{v_g^{II}} \tag{28}$$

MODEL DEVELOPMENT (Continued)

The boundary conditions for Equation (25) are

$$a_l^{II}|_{x^{II}=0^+} = a_l^{II}|_{x^{II}=0^-} - \frac{1}{Pe_l}\frac{da_l^{II}}{dx^{II}}\bigg|_{x^{II}=0^+} \tag{29}$$

and

$$\frac{da_l^{II}}{dx^{II}}\bigg|_{x^{II}=1} = 0 \tag{30}$$

2. Energy Balance

$$\frac{1}{Pe_h}\frac{d^2\theta^{II}}{(dx^{II})^2} - \frac{d\theta^{II}}{dx^{II}} + R_l^{II}\Gamma_S^{II}\left(\frac{H}{H_l'}a_g^{II} - a_l^{II}\right) + Da\Gamma_R^{II}H_l'\exp\left(E^*/(1+\theta^{II})\right)a_l^{II} = 0 \tag{31}$$

where

$$Pe_h = \frac{(v_g^{II}\rho_g C_{pg} + v_l^{II}\bar{\rho}_l\bar{C}_{pl})\cdot L^{II}}{D_H} \tag{32}$$

$$\Gamma_S^{II} = \frac{C_{gi}^{I}\cdot v_g^{II}\cdot \Delta H_S}{T_i^{I}(v_g^{II}\rho_g C_{pg} + v_l^{II}\bar{\rho}_l\bar{C}_{pl})} \tag{33}$$

$$\Gamma_R^{II} = \frac{C_{gi}^{I}\cdot v_g^{II}\cdot \Delta H_R}{T_i^{I}(v_g^{II}\rho_g C_{pg} + v_l^{II}\bar{\rho}_l\bar{C}_{pl})} \tag{34}$$

Boundary conditions for Equation (31) are

$$\theta^{II}|_{x^{II}=0} = \theta^{II}|_{x^{II}=0^-} - \frac{1}{Pe_h}\left(\frac{d\theta^{II}}{dx^{II}}\right)\bigg|_{x^{II}=0^+} \tag{35}$$

and

$$\frac{d\theta^{II}}{dx^{II}}\bigg|_{x^{II}=0} = 0 \tag{36}$$

3. Chemical Species Balance

$$\frac{1}{Pe_L}\frac{d^2C_j^{II}}{dx^{II^2}} - \frac{dC_j^{II}}{dx^{II}} + Ra_j^{II} = 0 \quad ; \quad j = 1, N_S \tag{37}$$

where

$$Ra_j^{II} = \bar{R}_j\frac{L^{II}}{V_l^{II}}\cdot\nu_j \quad ; \quad j = 1, N_S \tag{38}$$

MODEL DEVELOPMENT (Continued)

The boundary conditions for Equation (37) are

$$C_j^{II}\Big|_{x^{II}=0} = C_j^{II}\Big|_{x^{II}=s^{+}} - \frac{1}{E_{x_j}}\frac{dC_j^{II}}{dx^{II}}\Big|_{x^{II}=s^{+}} \qquad (39)$$

and

$$\frac{dC_j^{II}}{dx^{II}} \qquad (40)$$

SIMULATION TECHNIQUES

The hydroprocessing of coal involves a series of reactions, both homogeneous and heterogeneous. The consumption of hydrogen gas and coal conversion to soluble products occur simultaneously. Hence the equations described in the earlier section (plug flow equations for the preheater and axial dispersion equations for the reactor) are coupled and have to be solved simultaneously. The consumption of hydrogen is, however, generally used as a measure of the heat generation. This allows the uncoupling of the hydrogen balance equations (both gas and liquid phases) and energy balance equation from the chemical species balance equation. In this simulator, therefore, the hydrogen and energy balance equations are first solved simultaneously and the resulting temperature profile is superimposed on the chemical species balance equation.

The program code is written in a modular form for easy modification. For example, separate modules have been set up to calculate the gas holdups and viscosity (as function of temperature) in the preheater and reactor. Procedure for modification of these modules is explained in Section 6.

1. Numerical Solution of Hydrogen and Energy balance equations:

   The preheater is assumed to be plug flow and therefore the equations are coupled first order differential equations [Equations (4), (9) and (14)] with initial conditions [Equations (8), (13) and (18)]. These equations are solved simultaneously by using fourth-order Runge-Kutta method of integration (Carnahan et al., 1969).

   The gas in the reactor is assumed to be plug flow. This results in one first order differential equation [Equation (22)] with an initial condition [Equation (24)]. The axial dispersion model is used to model the slurry phase in the reactor. This results in two second order differential equations [Equations (25) and (31)], with four boundary conditions [Equations (29), (30), (35) and (36)]. Again all the reactor model equations are coupled. The second order equations are also non-linear. A shooting technique is required to solve this boundary value problem. The problem is first converted to an initial

SIMULATION TECHNIQUES (Continued)

value problem by guessing the concentration of hydrogen and the temperature in the phase at the reactor entrance. Again the Runge-Kutta fourth-order technique is used to intergrate the equations. The method of interval-halving is used to refine the guesses at the reactor inlet so as to satisfy the exit boundary conditions.

2. Numerical solution of chemical species balance equations:

Equation (19) describes a set of equations for the chemical species balances in the preheater. These equations along with the set of boundary conditions [Equation (21)] are solved by the same technique as used above.

Equation (37) with boundary conditions (39) and (40) are a set of equations for chemical species balance in the reactor. Initially a computer code similar to the one used to solve the hydrogen and temperature balance equations, was developed to solve these equations. The computation time required to arrive at the final solution increased exponentially with the number of species. Computation time of the order of one hour was required to solve the equations for three (3) species, on the DEC-10 computer at the University of Pittsburgh. As the computation time was prohibitively high, it was decided to develop a code for solving coal liquefaction reaction networks involving only first order reactions. This code is used for simultaneous solution of coupled linear equations.

The code takes advantage of the fact that a linear combination of several solutions of a differential equation, obtained for different initial conditions, is also a solution of the differential equation, if the differential equation is linear in the dependant variable. For example, if C_1 and C_2 are two independent solutions of a second order linear differential equation, then $C = \delta_1 C_1 + \delta_2 C_2$ is also a solution of the differential equation. The coefficients δ_1 and δ_2 can be calculated so as to satisfy the boundary conditions.

SIMULATION TECHNIQUES (Continued)

The computer code developed makes $2N_S$ (N_S = number of species) independent guesses, at the reactor inlet, and performs the integration using Runge-Kutta fourth-order technique. The independent guesses are made by using a random number generation routine. The coefficients C_i are calculated by matrix inversion (Gerald, 1978), so as to satisfy the required initial and boundary conditions.

Computer programs to generate graphical outputs were developed on the PDP-11/70 computer at Schneider Consulting Engineers, Bridgeville, Pennsylvania. IDGS and DMRS software developed by Intergraph Corporation, Huntsville, Alabama was used in these programs.

USE OF SIMULATOR

To use the simulator, the following information must be provided:

- Flow rate of gas to preheater, (cm^3/s)
- Flow rate of slurry to preheater, (cm^3/s)
- Length of preheater, (cm)
- Length of reactor, (cm)
- Diameter of preheater, (cm)
- Diameter of reactor, (cm)
- Inlet temperature of slurry to preheater, (°C)
- Operating Pressure, (atm)
- Mole fraction of hydrogen in gas to preheater, (dimensionless)
- Temperature of furnace, (°C)
- Heat capacity of gas, (cal/gm°C)
- Heat capacity of slurry, (cal/gm°C)
- Arrhenius frequency factor for hydrogen consumption kinetics, (s^{-1})
- Activation energy for hydrogen consumption kinetics, (cal/gmol)
- Heat of reaction of hydrogen, (cal/gm)
- Heat of dissolution of hydrogen, (cal/gm)
- Solubility constant, [(gm/cm^3 l)/(gm/cm^3 g)]
- Diffusivity of the gas, (cm^2/s)
- Surface tension of the slurry, (gm/cm^3)
- Total number of chemical species
- Name and code number of each species
- Total number of non-zero rate constants
- For each rate constant:
  - Code of reacting species
  - Code of product species
  - Arrhenius frequency factor, (s^{-1})
  - Activation energy, (cal/gmol)
- For each species:
  - Initial concentration, (gm/gm_{total})

USE OF SIMULATOR (Continued)

The input data is entered interactively by executing a program "SIMDAT.FOR". This program prompts the user for the input information. The data are stored in a file 'SIM.DAT'. The main simulator program 'SIM.FOR' can next be executed either in batch or time sharing mode.

Output is contained in the following files:

Output Summary	SUMRY.DAT
Preheater:	
Temperature Profile	PTEMP.DAT
Hydrogen Profile (Gas Phase)	PHYGAS.DAT
Hydrogen Profile (Liquid Phase)	PHYLIQ.DAT
Viscosity Profile	PVISCO.DAT
Species Concentration Profile	PCONC.DAT
Reactor:	
Temperature Profile	RTEMP.DAT
Hydrogen Profile (Gas Phase)	RHYGAS.DAT
Hydrogen Profile (Liquid Phase)	RHYLIQ.DAT
Species Concentration Profile	RCONC.DAT

Graphical output can be obtained on the PDP-11/70 computer at Schneider Consulting Engineers.

The simulation program has been written in standard FORTRAN (except for programs needed to obtain the output in a graphical form).

The program typically requires about one to one and a half minutes of computation (CPU) time on a large computer.

A representative set of output data is shown in Appendix B.

SIMULATOR MODIFICATION

The simulator has been written in a modular form so as to allow easy modification.

The viscosity in the gel region is a strong function of the type of coal, type of solvent and the coal to solvent ratio. In the present simulator, the viscosity of the coal-oil slurry is calculated from a equation fitted to data reported for 35 wt % Kentucky No. 9 coal with Wilsonville recycle solvent (McNeese, 1980). A separate function subroutine VISCOS has been written to calculate the viscosity as a function of temperature. The user need only modify this function routine to incorporate different viscosity dependence on temperature.

Similarly, a separate function routine FEG has been written to calculate the gas hold up in preheater and reactor. Presently correlations suggested by Akita (Akita and Yoshida, 1973) have been incorporated in the simulator to calculate the gas hold up. If the user desires to use some other correlations, he need only modify the routine FEG.

CONCLUSIONS AND RECOMMENDATIONS

The simulation program described in this report is a convenient tool for analyzing the performance of coal liquefaction plants. It could assist a decision maker in arriving at optimum equipment sizes and operating conditions.

Additional features can be added to this simulator to enhance its value. The following additions are recommended.

1. The simulator in its present state is not limited to the type of process,(SRC-I, SRC-II, EDS or H-Coal), as long as the processes have only one preheater and one reactor. The simulator should be modified to include two and more stage processes.

2. The simulator requires the user to input data, such as hydrogen conversion and coal liquefaction kinetics, physical properties, etc. In many cases, the user will be unaware of these data. A numerical database of the required data should be developed to assist the user in selecting the input data. At least some default values for these data should be set up in case the user has no idea about the range of the input data.

3. Coal conversion reactions are exothermic and they are carried out in adiabatic partially backmixed bubble columns. Such reactors can exhibit multiple steady states. (Nunez et al., 1982). In the present state, the simulator converges to one steady state and has no way of determining whether other steady states exit. Nunez et al. have presented graphs showing regions of multiple steady states for various operating conditions. This information should be incorporated in the simulator and if the user input data results in the reactor operation in the multiple steady states region, appropriate messages should be relayed to the user.

4. Subroutines should be developed to permit non-linear kinetics and also rate expression of other than the Arrhenius form.

CONCLUSIONS AND RECOMMENDATIONS (Continued)

5. Similar programs should be developed for other unit operations, such as coal preparation, separation units, etc. In some cases such as coal preparation, simulation programs already exist (Gottfried, et al., 1982). Software should be developed to depict the output from such simulators in pictorial/graphical form to enhance their value to the user.

NOMENCLATURE

a_g	dimensionless concentration of hydrogen in gas phase (C_g/C'_{gi})
a_l	dimensionless concentration of hydrogen in liquid phase $(C_l/H_iC'_{gi})$
C	concentration of hydrogen, g/cm^3
C_p	specific heat, cal/g K
$\bar{C}_p$	weighted average specific heat, cal/g K
c	dimensionless concentration of chemical species, (gm/gm)
D	diameter, cm
Da	Damkohler number, defined in Equation (28)
D_H	thermal dispersion coefficient, cal/cm s K
D_l	mass diffusivity, cm^2/s
E	activation energy, cal/gmol K
E*	dimensionless activation energy, defined in Equation (12)
H	Henry's law constant
$\bar{H}$	pre-exponential factor in Equation 2
h	heat transfer coefficient, cal/cm^2s K
$\triangle H_R$	heat of reaction, cal/gmol
$\triangle H_S$	heat of dissolution, cal/gmol
$\triangle H_S^*$	dimensionless heat of dissolution, defined in Equation (7)
k	rate constant, s^{-1}
$\bar{k}$	Arrhenius frequency factor, s^{-1}
k_la	volumetric liquid phase mass transfer coefficient, s^{-1}
L	length, cm
N_s	number of chemical species
Pe_h	Peclet number for heat, defined in Equation (32)
Pe_l	Peclet number for mass, defined in Equation (27)

NOMENCLATURE (Continued)

R	gas law constant, cal/gmol K
R_a	dimensionless parameter, defined in Equations (20) and (38)
R_1	dimensionless parameter, defined in Equations (5) and (23)
R_p	dimensionless parameter, defined in Equation (11)
$\bar{R}$	rate of generation of chemical species, s^{-1}
T	temperature, K
v	superficial velocity, cm/s
x	dimensionless axial distance, (Z/L)
	axial distance, cm

Greek Symbols

α	dimensionless parameter, defined in Equation (15)
β	constant in Equation (3)
δ	coefficients of solutions of differential equations
Γ_R	dimensionless parameter, defined in Equations (16) and (34)
Γ_T	dimensionless parameter, defined in Equations (17) and (33)
μ	viscosity, g/cm s
ρ	density, g/cm^3
$\bar{\rho}$	weighted average density, g/cm^3
θ	dimensionless temperature
ϵ_g	gas holdup
γ	dimensionless parameter, defined in Equations (10) and (26)

Superscripts

I	in preheater
II	in reactor

NOMENCLATURE (Continued)

Subscripts

g	gas phase
i	inlet condition
j	chemical species number
o	outlet condition
l	liquid phase
w	wall condition

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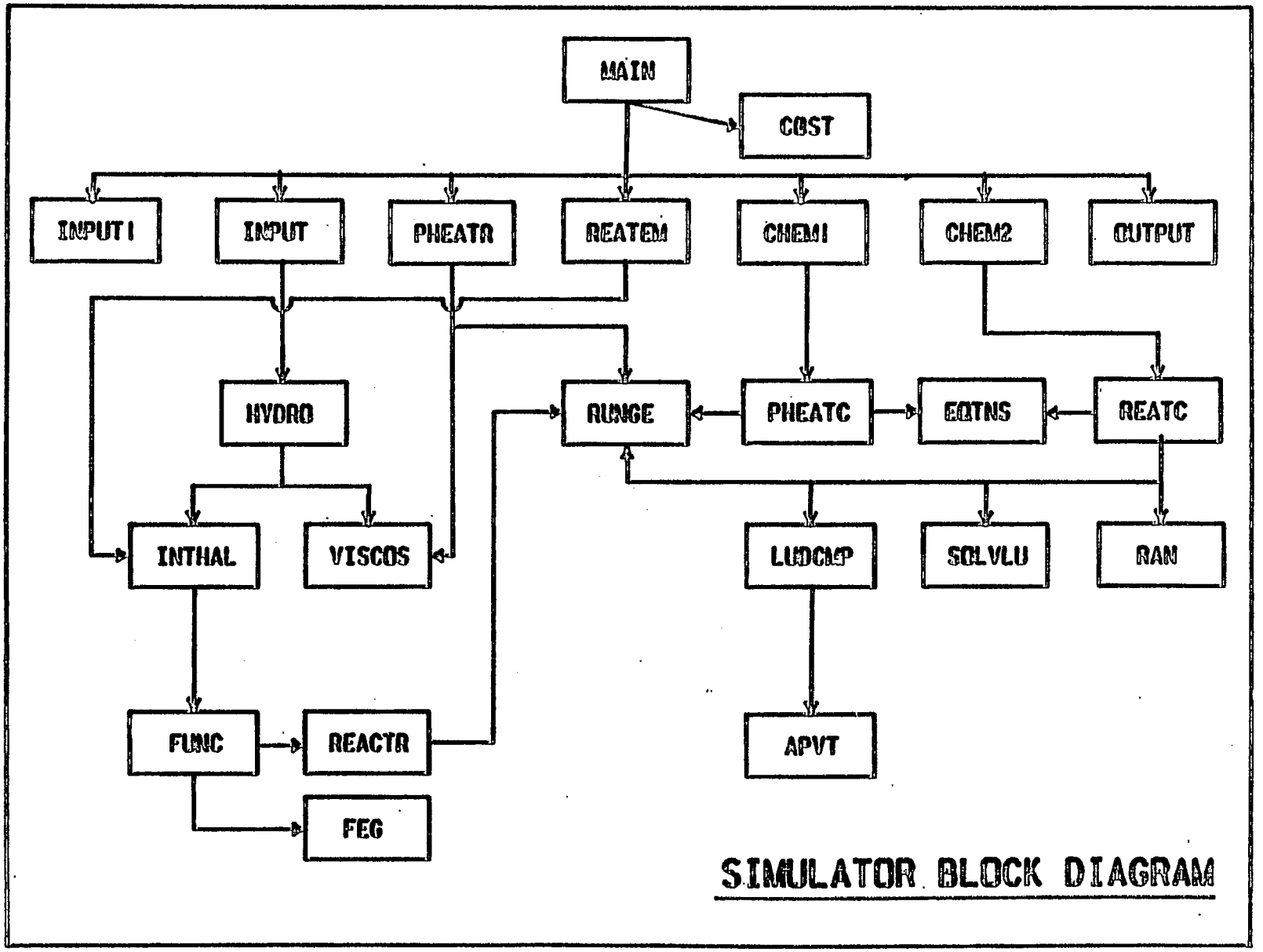
APPENDIX A

This section includes the program source code and a simulator block diagram.


MAIN
COST
INPUT1
INPUT
PHEATR
REATEM
CHEM1
CHEM2
OUTPUT
HYDRO
RUNGE
PHEATC
EQTNS
REATC
INTHAL
VISCOS
LUDCMP
SOLVLU
RAN
FUNC
REACTR
APVT
FEG
SIMULATOR BLOCK DIAGRAM

SUBROUTINE/FUNCTION NAME	PURPOSE
INPUT 1	Reads input data: viz. coal conversion kinetics
INPUT	Reads input data: viz. Physical dimensions of the units, physical and thermal properties and hydrogen consumption kinetics
PHEATR:	Simulates preheater performance: Thermal and hydrogen consumption only
REATEM:	Simulates reactor performance: Thermal balance only
CHEM1:	Initializes simulation of preheater: Chemical species conversion
CHEM2:	Initializes simulation of reactor: Chemical species conversion
OUTPUT:	Prints output
HYDRO:	Calculates hydrodynamic parameters
RUNGE:	Runge-Kutta fourth-order integrator
PHEATC:	Simulates preheater performance: Chemical species conversion
EQTNS:	Calculates chemical species conversion rates
REATC:	Simulates reactor performance: Chemical species conversion
INTHAL:	Interval halving program to solve implicit equations
VISCOS:	Calculates viscosity of coal slurry in preheaters
LUDCMP:	Calculates lower and upper triangular matrices
SOLVLU:	Finds solution of matrix AX=B, after finding its LU equivalent matrices
RAN:	Random numbers generator
FUNC:	Function routine that calls REACTR and FEG
REACTR:	Simulates reactor performance: Hydrogen consumption only.
APVT:	Finds largest element for pivot and performs interchanges
FEG:	Provides equations for calculation of gas holdup

PROGRAMS TO GENERATE GRAPHICAL OUTPUT

PLOT.FTN

(SOURCE PROGRAM)

```
0195            ORIGIN(1)=I0-JIFIX(0.267*8000.0)
0196            ORIGIN(2)=I1+JIFIX(3.6*8000.0)
0197            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNP,TSP,TS,ORIGIN,RTNCD,
              1 YLABEL(4),NOATT)
0198            WRITE(10,236) RTNCD
0199            ORIGIN(1)=I0-JIFIX(0.267*8000.0)
0200            ORIGIN(2)=I1+JIFIX(4.8*8000.0)
0201            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNP,TSP,TS,ORIGIN,RTNCD,
              1 YLABEL(5),NOATT)
0202            WRITE(10,236) RTNCD
0203            ORIGIN(1)=I0-JIFIX(0.267*8000.0)
0204            ORIGIN(2)=I1+JIFIX(6.0*8000.0)
0205            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNP,TSP,TS,ORIGIN,RTNCD,
              1 YLABEL(6),NOATT)
0206            WRITE(10,236) RTNCD
0207            TNP(4)=3
0208            TSP(6)=3
0209            ORIGIN(1)=I0-JIFIX(1.03*8000.0)
0210            ORIGIN(2)=I1+JIFIX(5.752*8000.0)
0211            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNP,TSP,TS,ORIGIN,RTNCD,
              * ONY,NOATT)
0212            WRITE(10,237) RTNCD
0213     237    FORMAT('        RET FORM TNDFPI 2',I)
0214            TNP(4)=2
0215            TSP(6)=2
0216            ORIGIN(1)=I0-JIFIX(1.2375*8000.0)
0217            ORIGIN(2)=I1+JIFIX(5.13*8000.0)
0218            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNP,TSP,TS,ORIGIN,
              1 RTNCL,RR1,NOATT)
0219            WRITE(10,238) RTNCD
0220     238    FORMAT('        RET CODE FROM TNDFPI 3'=I)
0221            NN=2*M
0222            WRITE(10,245) M,NN
0223     245    FORMAT('  M=NN',2I)
0224            J=0
0225            DO 25 I=1,NN,2
0226            J=J+1
0227            WRITE(10,234) J,X(J),Y(J)
0228     234    FORMAT('   J,X(J),Y(J)',I,2E)
0229            OR(I)=I0+JIFIX(5.0*X(J)*8000.0)
0230            OR(I+1)=I1+JIFIX((Y(J)/10.0*HY-YTICK(1))/(YTICK(6)-YTICK(1))
              1 *6.0*8000.0)
0231            WRITE(10,*) I,OR(I),OR(I+1),J,X(J),Y(J)
0232     25     CONTINUE
               C
0233            CALL LSDFPI(GGROUP,LEVEL,SPEC3,OR,N,RTNCD,NOATT)
0234            WRITE(10,235) RTNCD
0235     235    FORMAT('        RET FROM LSDFPI',I)
0236            CLOSE (UNIT=10)
0237            CALL DEDFPI(1)
0238            TSKCI(1)=IBUFF(1)
0239            TSKCI(2)=IBUFF(2)
0240            CALL VSENDM(TSKCI,OBUFF,,1,IDS)
0241            CALL RESUME(TSKCI,IDS)
0242            END
```

```
0144            DO 55 I=1,6
0145            WRITE(9,501) YTICK(I)
0146      501   FORMAT(F4.1)
0147      55    CONTINUE
0148            IF(R1.NE.0) WRITE(9,503) R1
0149      503   FORMAT(I2)
0150            CLOSE (UNIT=9)
0151            OPEN (UNIT=9,FILE='DS1:[50,15]FLOT.DAT',STATUS='OLD')
0152            READ(9,300) CNY
0153            WRITE(10,300) CNY
0154      300   FORMAT(A3)
0155            DO 56 I=1,6
0156            READ(9,301) YLABEL(I)
0157            WRITE(10,301) YLABEL(I)
0158      301   FORMAT(A4)
0159      56    CONTINUE
0160            IF(R1.NE.0) READ(9,303) RR1
0161      303   FORMAT(A2)
0162            IF(R1.NE.0) WRITE(10,303) RR1
0163            CLOSE (UNIT=9)
0164            ANGL=90
0165            TNF(1)=0
0166            TNF(2)=800.0
0167            TNF(4)=4
0168            TNF(5)=6
0169            TSF(1)=800.0
0170            TSF(3)=800.0
0171            TSF(3)=10
0172            TSF(6)=4
0173            TS(1)=0
0174            TS(2)=0
0175            TS(3)=0
0176            TS(4)=1
0177            TS(5)=0
0178            TS(6)=0
0179            TS(7)=2
0180            ORIGIN(1)=I0-JIFIX(0.267*8000.0)
0181            ORIGIN(2)=I1+JIFIX(0.03*8000.0)
        C
0182            WRITE(10,568) I0,I1,ORIGIN(1),ORIGIN(2)
0183      568   FORMAT('       I0,I1,ORIGIN(1),ORIGIN(2)',4I)
0184            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNF,TSF,TS,ORIGIN,RTNCD,
           *    YLABEL(1),NOATT)
0185            WRITE(10,236) RTNCD
0186      236   FORMAT('       RET FROM TNDFPI 1',I)
        C
0187            ORIGIN(1)=I0-JIFIX(0.267*8000.0)
0188            ORIGIN(2)=I1+JIFIX(1.23*8000.0)
0189            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNF,TSF,TS,ORIGIN,RTNCD,
           1    YLABEL(2),NOATT)
0190            WRITE(10,236) RTNCD
0191            ORIGIN(1)=I0-JIFIX(0.267*8000.0)
0192            ORIGIN(2)=I1+JIFIX(2.4*8000.0)
0193            CALL TNDFPI(GGROUP,ANGL,LEVEL,TNF,TSF,TS,ORIGIN,RTNCD,
           1    YLABEL(3),NOATT)
0194            WRITE(10,236) RTNCD
```

```
0096            IXLAST=XMAX/10.0**NX
0097            JXMIN=XMIN
0098            ZJXMIN=JXMIN
0099            IF(XMIN.EQ.ZJXMIN) GO TO 9
0100            IF(XMIN.LT.0.0) IXFRST=IXFRST-1
0101     9      JXMAX=XMAX
0102            ZJXMAX=JXMAX
0103            IF(XMAX.EQ.ZJXMAX) GO TO 10
0104            IF(XMAX.GT.0.0) IXLAST=IXLAST+1
0105     10     CONTINUE
               C
               C
0106            XLAST=IXLAST
0107            XFRST=IXFRST
0108            XDIFF=(XLAST-XFRST)/5.0
0109            DO 7 I=1,6
0110            XTICK(I)=XFRST+(I-1)*XDIFF
0111     7      CONTINUE
               C
               C
0112     500    FORMAT(6(2X,F8.1))
0113            YY=ABS(YMIN)
0114            IF(ABS(YMAX).GT.ABS(YMIN)) YY=ABS(YMAX)
0115            IF(YY.LT.1.0) GO TO 14
0116     15     YY=YY/10.0
0117            IF(YY.LE.1.0) GO TO 16
0118            NY=NY+1
0119            GO TO 15
0120     14     YY=YY*10.0
0121            IF(YY.GE.10.0) GO TO 16
0122            NY=NY-1
0123            GO TO 14
0124     16     IYFRST=YMIN/10.0**NY
0125            IYLAST=YMAX/10.0**NY
0126            JYMIN=YMIN
0127            ZJYMIN=JYMIN
0128            IF(YMIN.EQ.ZJYMIN) GO TO 19
0129            IF(YMIN.LT.0.0) IYFRST=IYFRST-1
0130     19     JYMAX=YMAX
0131            ZJYMAX=JYMAX
0132            IF(YMAX.EQ.ZJYMAX) GO TO 20
0133            IF(YMAX.GT.0.0) IYLAST=IYLAST+1
0134     20     CONTINUE
               C
               C
0135            YLAST=IYLAST
0136            YFRST=IYFRST
0137            YDIFF=(YLAST-YFRST)/5.0
0138            DO 17 I=1,6
0139            YTICK(I)=YFRST+(I-1)*YDIFF
0140     17     CONTINUE
               C
               C
0141            WRITE(10,*) YMIN,YMAX
0142            WRITE(9,502) NY
0143     502    FORMAT(I3)
```

```
0046            LEVEL=63
0047            ANGL=0.0
0048            ORIGIN(1)=I0
0049            ORIGIN(2)=I1
0050            CALL CLDFFI(LEVEL,GGROUP,ANGL,SC,CELL,ORIGIN,VIEW,
     *  RTNCD,NDATT,SPECS)
0051            OPEN (UNIT=9,FILE='DS1:[50,15]PLOT.DAT',STATUS='OLD')
      C
0052            IF(RO.EQ.1) OPEN(UNIT=8,FILE='DS1:[50,15]PTEMP.DAT',STATUS='OLD')
0053            IF(RO.EQ.2) OPEN(UNIT=8,FILE='DS1:[50,15]PHYGAS.DAT',STATUS='OLD')
0054            IF(RO.EQ.3) OPEN(UNIT=8,FILE='DS1:[50,15]PHYLIQ.DAT',STATUS='OLD')
0055            IF(RO.EQ.4) OPEN(UNIT=8,FILE='DS1:[50,15]PCONC.DAT',STATUS='OLD')
0056            IF(RO.EQ.5) OPEN(UNIT=8,FILE='DS1:[50,15]PVISCO.DAT',STATUS='OLD')
0057            IF(RO.EQ.6) OPEN(UNIT=8,FILE='DS1:[50,15]RTEMP.DAT',STATUS='OLD')
0058            IF(RO.EQ.7) OPEN(UNIT=8,FILE='DS1:[50,15]RHYGAS.DAT',STATUS='OLD')
0059            IF(RO.EQ.8) OPEN(UNIT=8,FILE='DS1:[50,15]RHYLIQ.DAT',STATUS='OLD')
0060            IF(RO.EQ.9) OPEN(UNIT=8,FILE='DS1:[50,15]RCONC.DAT',STATUS='OLD')
      C
      C
0061            JMAX=R1+2
0062            IF(R1.EQ.0) JMAX=4
0063            IF(RO.EQ.5) JMAX=3
0064            DO 1 I=1,101
0065     26     READ(8,*,ERR=26,END=2) (A(J),J=1,JMAX)
0066            X(I)=A(1)
0067            Y(I)=A(JMAX)
0068            WRITE(10,*) I,X(I),Y(I)
0069     1      CONTINUE
0070     2      CLOSE (UNIT=8)
0071            N=I-1
0072            XMIN=X(1)
0073            YMIN=Y(1)
0074            XMAX=X(1)
0075            YMAX=Y(1)
0076            DO 3 I=1,N
0077            IF(X(I).LT.XMIN) XMIN=X(I)
0078            IF(Y(I).LT.YMIN) YMIN=Y(I)
0079            IF(X(I).GT.XMAX) XMAX=X(I)
0080            IF(Y(I).GT.YMAX) YMAX=Y(I)
0081     3      CONTINUE
      C
      C
0082            NX=0
0083            NY=0
0084            XX=ABS(XMIN)
0085            IF(ABS(XMAX).GT.ABS(XMIN)) XX=ABS(XMAX)
0086            IF(XX.LT.1.0) GO TO 4
0087     5      XX=XX/10.0
0088            IF(XX.LE.1.0) GO TO 6
0089            NX=NX+1
0090            GO TO 5
0091     4      XX=XX*10.0
0092            IF(XX.GE.1.0) GO TO 6
0093            NX=NX-1
0094            GO TO 4
0095     6      IXFRST=XMIN/10.0**NX
```

```
PDP-11 FORTRAN-77 V4.0-1       10:26:40    14-May-84          Page 1
PLOT.FTN;202            /F77/TR:BLOCKS/WR

 001            REAL*4 X,Y,XFRST,YFRST,XLAST,YLAST,XMIN,XMAX,YMIN,YMAX
0002            REAL*4 A
0003            INTEGER*2 I,N,NX,NY,IXFRST,IYFRST,IXLAST,IYLAST,IX,IY
 004            INTEGER*2 JMAX,J,NN
 005            DIMENSION X(101),Y(101),IX(101),IY(101)
 006            DIMENSION A(12)
0007            DIMENSION XTICK(6),YTICK(6)
0008            REAL*8 ANGL,SC(2)
 009            CHARACTER*2 RR1
 010            CHARACTER*25 DGNFIL,DGNF
0011            CHARACTER*3 CHX,CHY
0012            CHARACTER*6 CELL
0013            CHARACTER*4 YLABEL(6)
 014            INTEGER*2 TMP(5),TSP(6),TS(7)
 015            INTEGER*2 OBUFF(1),IDS
0016            INTEGER*2 IBUFF(9),ITERM,LEVEL,GGROUP(2),VIEW(2),RTNCD,R0,R1
0017            INTEGER*2 NOATT(2),SPECS(5)
 018            INTEGER*2 TSKCI(2),DGNBLK(7),WHATEV
 019            INTEGER*4 I0,I1,ORIGIN(2),OR(10)
 020            EQUIVALENCE (ITERM,IBUFF(3))
0021            EQUIVALENCE (R0,IBUFF(4))
0022            EQUIVALENCE (R1,IBUFF(5))
 023            EQUIVALENCE (I0,IBUFF(6))
 024            EQUIVALENCE (I1,IBUFF(8))
0025            DATA GGROUP/0,0/
0026            DATA SC/1.0,1.0/
 027            DATA NOATT/0,0/
 028            DATA VIEW/1,1/
 029            DATA SPECS/0,0,0,1,0/
0030            DATA DGNFIL/'DB1:[050,015]BINCHART.DGN'/
C
C
C
C
0031            OPEN (UNIT=10,FILE='DB1:[50,153]OUT.DAT',STATUS='NEW')
C
 032            CALL VREDVM(,IBUFF,9,IDS)
C
0033            CALL SWFWRD(I0,1)
C
 034            CALL SWFWRD(I1,1)
C
 035            CALL LKTCSI(DGNFIL,DGNBLK,25,0,RTNCD)
C
0036            CALL INQFFI(WHATEV,DGNBLK,0,0,0,1,RTNCD,ITERM)
 037            IF(R0.EQ.1) CELL='RTEMP'
 038            IF(R0.EQ.2) CELL='PHYGAS'
 039            IF(R0.EQ.3) CELL='PHYLIQ'
 040            IF(R0.EQ.4) CELL='PCONC'
 041            IF(R0.EQ.5) CELL='PVISCO'
 042            IF(R0.EQ.6) CELL='RTEMP'
 043            IF(R0.EQ.7) CELL='RPHYGAS'
0044            IF(R0.EQ.8) CELL='RPHYLIQ'
0045            IF(R0.EQ.9) CELL='RCONC'
C
C
```

PLOT.UCM

(USER COMMAND PROGRAM)

```
        SET     CONTRL=CONTRL! 768
        KEY     'RC=GS1:C50,153DOE.CEL'
        KEY     'LV=63'
        KEY     'AS=1'
        KEY     'AA=0'
        KEY     'WT=1'
        KEY     'FT=10'
        KEY     'TH=1.1'
        KEY     'TW=1.1'
        SET     R0=0
        SET     R1=0
        CMD     TXJ96
        KEY     'DR=DOEMENU.DAT'
        MSG     'ER '
A:      MSG     'PREnter Key from Menu'
        MSG     'STORE TO EXIT'
        GET     P,S,R,B,K,C,C,B
B:      TST     NUM EQ 8,EX
        MSG     'ERINVALID INPUT!   ENTER AGAIN'
        GO      A
C:      MSG     'ER '
        SET     R0=KEY
        TST     KEY EQ 4,H
        GO      I
D:      TST     KEY EQ 9,H
        GO      J
H:      MSG     'PREnter Species Code'
        MSG     'STORE TO EXIT'
        GET     P,K,R,K,K,L,C,K
E:      TST     NUM EQ 3,EX
        MSG     'ERINVALID INPUT!   ENTER AGAIN'
        GO      H
L:      SET     R1=KEY
        CMD     UPDAT2
I:      MSG     'PREnter Start Point'
        MSG     'STORE TO EXIT'
        GET     P,F,F,3,K,E,C,E
J:      TST     NUM EQ 6,EX
        MSG     'ERINVALID INPUT!   ENTER AGAIN'
        GO      D
F:      MSG     'ERPROCESSING'
        SET     I0=XUR
        SET     I1=YUR
        TSK     'PLOT',R0,R1,I0,I1
        WT      'PLOT'
        MSG     'PRPLOT COMPLETE'
        MSG     'ERNORMAL EXIT'
        GO      G
K:      MSG     'STOP EXITED'
G:      UCM     'GS1:C17,173EXIT.UCM'
        END
```

DATABASE SCHEMA

```
PR='GS1:I50;15ISIM1.PRT'
DB='GS1:I50;15ISIM1.DBS'
;
1.   PROCESS_CONDITIONS   DF='GS1:I50;15ICONDITIG1.ENT'  OCC=100
    .1 LINE_DESIGNATION   F=AN(20)
    .2 FLOW_RATE_SLURRY   F=F
    .3 FLOW_RATE_GAS      F=F
    .4 TEMPERATURE        F=F
    .5 HYD_CONC_GAS       F=F
    .6 HYD_CONC_LIQ       F=F
    .7 CONC_SPECIES_1     F=F
    .8 CONC_SPECIES_2     F=F
    .9 CONC_SPECIES_3     F=F
    .10 CONC_SPECIES_4     F=F
    .11 CONC_SPECIES_5     F=F
    .12 CONC_SPECIES_6     F=F
    .13 CONC_SPECIES_7     F=F
    .14 CONC_SPECIES_8     F=F
    .15 CONC_SPECIES_9     F=F
    .16 CONC_SPECIES_10    F=F
    .17 SPARE_A            F=F
    .18 SPARE_B            F=F
    .19 SPARE_C            F=I(10I197)
    .20 SPARE_D            F=I(10I990)
    .21 SPARE_E            F=AN(5)
    .22 SPARE_F            F=AN(30)
    .23 LEVEL              F=AN(2)
2.   EQUIPMENT_COST  P=0   DF='GS1:I50;15IEQUIPCOG1.ENT'  OCC=100
    .1 EQUIPMENT_TYPE      F=AN(20)
    .2 CAPITAL_COST        F=F
    .3 OPERATING_COST      F=F
    .4 MAINTENANCE_COST    F=F
    .5 FIXED_COST          F=F
    .6 VARIABLE_COST       F=F
    .7 SPARE_A             F=F
    .8 SPARE_B             F=F
    .9 SPARE_C             F=I(10I197)
    .10 SPARE_D            F=I(10I990)
    .11 SPARE_E            F=AN(5)
    .12 SPARE_F            F=AN(30)
    .13 LEVEL              F=AN(2)
END
```

SOURCE PROGRAM TO ATTACH DATA TO GRAPHICS

```
SET     CONTRL=CONTRL! 768
KEY     'RA=1.*.1!'
SET     I0=960000000
SET     I1=960000000
SET     MSG='AE=1.*.1=0047Preheater Inlet0047!'
KEY     MSG
CMD     ATCPTO
SET     I2=I0+28524
SET     I3=I1+43712
PNT     I2,I3
PNT     1000,1000
SET     MSG='AE=1.*.1=0047Preheater Outlet0047!'
KEY     MSG
CMD     ATCPTO
SET     I2=I0+36188
SET     I3=I1+38961
PNT     I2,I3
PNT     1000,1000
SET     MSG='AE=1.*.1=0047Reactor Outlet0047!'
KEY     MSG
CMD     ATCPTO
SET     I2=I0+40840
SET     I3=I1+39731
PNT     I2,I3
PNT     1000,1000
KEY     'RA=2.*.1!'
SET     MSG='AE=2.*.1=0047Preheater0047!'
KEY     MSG
CMD     ATCPTO
SET     I2=I0+31044
SET     I3=I1+38403
PNT     I2,I3
PNT     1000,1000
SET     MSG='AE=2.*.1=0047Reactor0047!'
KEY     MSG
CMD     ATCPTO
SET     I2=I0+36804
SET     I3=I1+42824
PNT     I2,I3
PNT     1000,1000
MSG     'PRUCM COMPLETE'
UCM     'DS1:[17,17]EXIT.UCM'
END
```

SOURCE PROGRAM FOR DATA ENTRY INTO DATABASE

```
0001            IMPLICIT INTEGER*2 (A-Z)
0002            CHARACTER*30 A
0003            CHARACTER*20 LINE
0004            CHARACTER*42 L
0005            REAL X,X1,X2
0006            LOGICAL SETCB
        C
0007            INCLUDE 'DB0:[14,35]HOL.PAR/NOLIST'
0074            INCLUDE 'DB0:[14,35]HOLCB.COM/NOLIST'
        C
0150            CBMIG1=0
0151            IF(SETCB(ATTACH,0)) STOP 'ATTACH'
0152            IF(SETCB(USECP,'DB='//'DB1:[50,15]SIM1.DB0'//')) STOP 'USE'
0153            OPEN (UNIT=1,FILE='DB1:[50,15]SIM1.DAT',STATUS='OLD')
        C
0154            DO 1 I=1,4
0155     1      READ(1,2) A
0156            WRITE(5,2) A
0157     2      FORMAT(A30)
0158            READ(1,3) NOSPEC
0159            WRITE(5,3) NOSPEC
0160     3      FORMAT(59X,I2)
0161            READ(1,7) X1
0162            WRITE(5,7) X1
0163            READ(1,7) X2
0164            WRITE(5,7) X2
0165            DO 4 I=1,2
0166     4      READ(1,2) A
0167            WRITE(5,2) A
        C
0168            DO 100 J=1,3
0169            READ(1,5) LINE
0170            WRITE(5,5) LINE
0171     5      FORMAT(30X,A20)
0172            ENCODE(42,6,L) LINE
0173     6      FORMAT(9H1,1.1,1='',A20,2H'')
0174            IF(SETCB(FINDCP,L)) STOP 'FIND1'
0175            ENCODE(42,16,L) X1
0176    16      FORMAT(9H1,1.1,2='',E20.8,2H'')
0177            IF(SETCB(CHNGCP,L)) STOP 'CHNG0.1'
0178            ENCODE(42,17,L) X2
0179    17      FORMAT(9H1,1.1,3='',E20.8,2H'')
0180            IF(SETCB(CHNGCP,L)) STOP 'CHNG0.2'
0181            READ(1,7) X
0182            WRITE(5,7) X
0183     7      FORMAT(59X,E)
0184            ENCODE(42,8,L) X
0185     8      FORMAT(9H1,1.1,4='',E20.8,2H'')
0186            IF(SETCB(CHNGCP,L)) STOP 'CHNG1'
0187            READ(1,7) X
0188            WRITE(5,7) X
0189            ENCODE(42,9,L) X
0190     9      FORMAT(9H1,1.1,5='',E20.8,2H'')
0191            IF(SETCB(CHNGCP,L)) STOP 'CHANG2'
0192            READ(1,7) X
0193            WRITE(5,7) X
```

```
0194            ENCODE(42,10,L) X
0195      10    FORMAT(9H1,1.1.6=',E20.9,2H'1)
0196            IF(SETCB(CHNGCP,L)) STOP 'CHNG3'
0197            READ(1,2) A
0198            WRITE(5,2) A
0199            DO 200  K=1,NOSPEC
0200            K1=K+6
0201            READ(1,7) X
0202            WRITE(5,7) X
0203            ENCODE(42,11,L) K1,X
0204      11    FORMAT(6H1,1.1.,I2,2H=',E19.9,2H'1)
0205            IF(SETCB(CHNGCP,L)) STOP 'CHNG4'
0206      200   CONTINUE
0207            READ(1,2) A
0208            WRITE(5,2) A
0209      100   CONTINUE
        C
0210            DO 12 I=1,3
0211      12    READ(1,2) A
0212            WRITE(5,2) A
0213            DO 300 J=1,2
0214            READ(1,13) LINE
0215            WRITE(5,13) LINE
0216      13    FORMAT(14X,A20)
0217            ENCODE(42,14,L) LINE
0218      14    FORMAT(9H1,2.1.1='A20,2H'1)
0219            IF(SETCB(FINDCP,L)) STOP 'FIND3'
0220            DO 400 K=1,5
0221            K1=K+1
0222            READ(1,7) X
0223            WRITE(5,7) X
0224            ENCODE(42,15,L) K1,X
0225      15    FORMAT(6H1,2.1.,I2,2H=',E19.9,2H'1)
0226            IF(SETCB(CHNGCP,L)) STOP 'CHNG5'
0227      400   CONTINUE
0228            READ(1,2) A
0229            WRITE(5,2) A
0230      300   CONTINUE
0231            IF(SETCB(DETACH,0)) STOP 'DETACH'
0232            CLOSE (UNIT=1)
0233            STOP 'JOB DONE'
0234            END
```

PROGRAMS TO GENERATE GRAPHICAL REPORT

SIMREPORT.UCM

(USER COMMAND PROGRAM)

```
SET     CONTRL=CONTRL ! 748
MSG     'CF GRAPHICAL REPORT'
MSG     'ST CBS TO EXIT'
SET     MSG='Q81:[50,15]SIMREPORT.RPT'
CMD     REPORT
KEY     ' '
KEY     ' '
KEY     MSG
MSG     'ST NORMAL EXIT'
UCM     'Q81:[17,17]EXIT.UCM'
END
```

SIMREPORT.RPT

(OUTPUT FORMATING PROGRAM)

```
ORDER 11,2,2,1,4!
REPORT
=U(2)
J=50,131,,'DS1:[50,15]SIMREPORT.OUT'
C T
  L=2,1
   V='COMPREHENSIVE GRAPHICAL-REPORT',0(45)
  L=0,1
    V='DATE: ',0(10)
    V=%D%,0(18),'ZZ/ZZ/ZZ'
    V='PAGE',0(115)
    V=%P%,*,'Z9'
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        V='OPERATING',0(45)
        V='MAINTENENCE',0(60)
        V='FIXED',0(75)
        V='VARIABLE',0(90)
L=0,0
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        V='COST',0(47)
        V='COST',0(63)
        V='COST',0(75)
        V='COST',0(92)
 =0,0
        V='( $ )',0(31)
        V='($/YR)',0(46)
        V='($/YR)',0(62)
        V='($/YR)',0(75)
        V='($/YR)',0(91)
 =0,2
        V='-------',0(30)
        V='---------',0(45)
        V='-----------',0(60)
        V='-----',0(75)
        V='--------',0(90)
C=0
 L=2,0
        V=E(2)A(1),0(10)
        V=E(2)A(2),0(30),'E10.4'
        V=E(2)A(3),0(45),'E10.4'
        V=E(2)A(4),0(60),'E10.4'
        V=E(2)A(5),0(75),'E10.4'
        V=E(2)A(6),0(90),'E10.4'
 =F
 L=1,0
   V='----------',0(30)
   V='----------',0(45)
   V='----------',0(60)
   V='----------',0(75)
   V='----------',0(90)
 L=0,0
   V='Total',0(10)
   V=+E(2)A(2),0(30),'E10.4'
   V=+E(2)A(3),0(45),'E10.4'
   V=+E(2)A(4),0(60),'E10.4'
   V=+E(2)A(5),0(75),'E10.4'
   V=+E(2)A(6),0(90),'E10.4'
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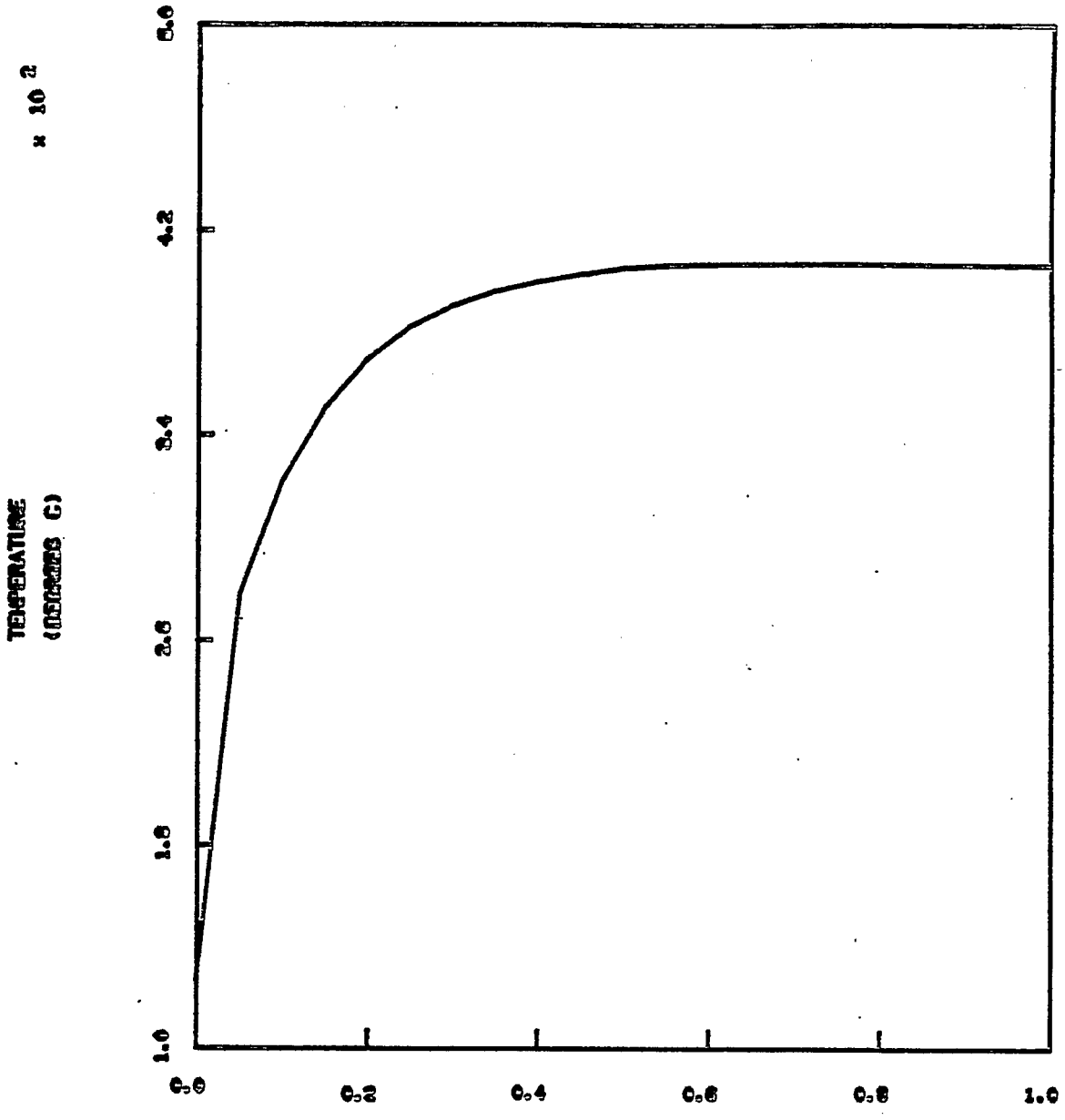
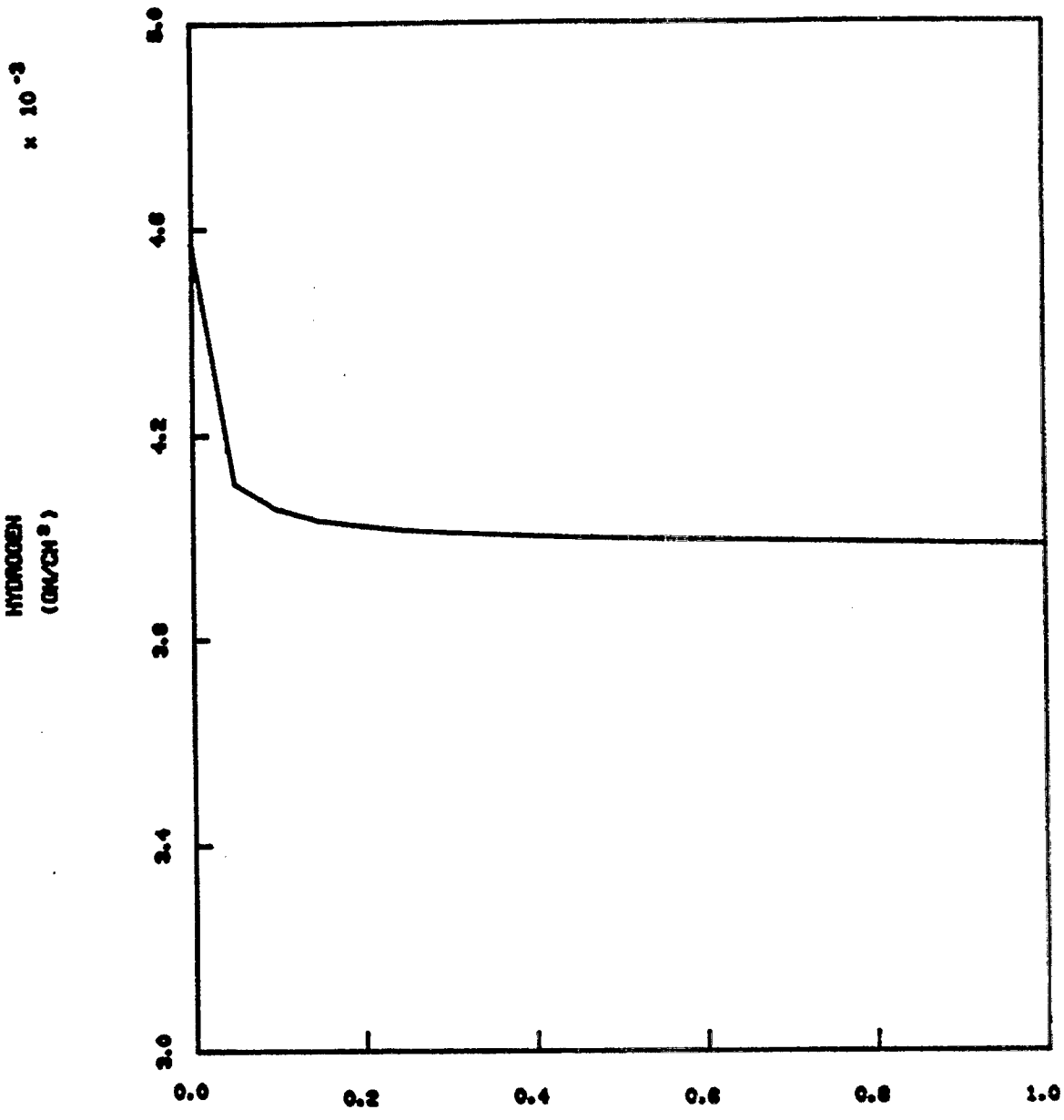
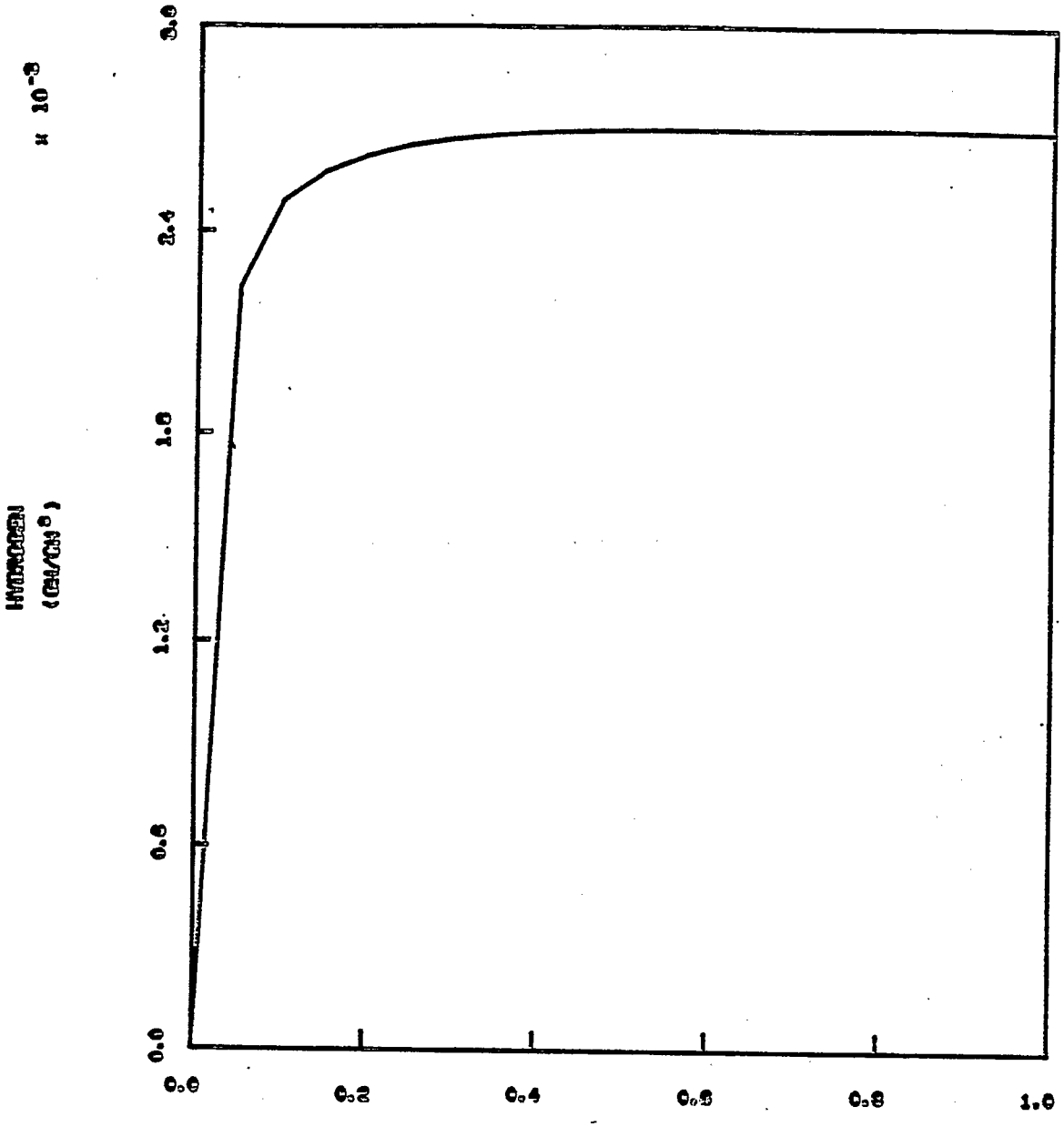
GRAPHICAL OUTPUT



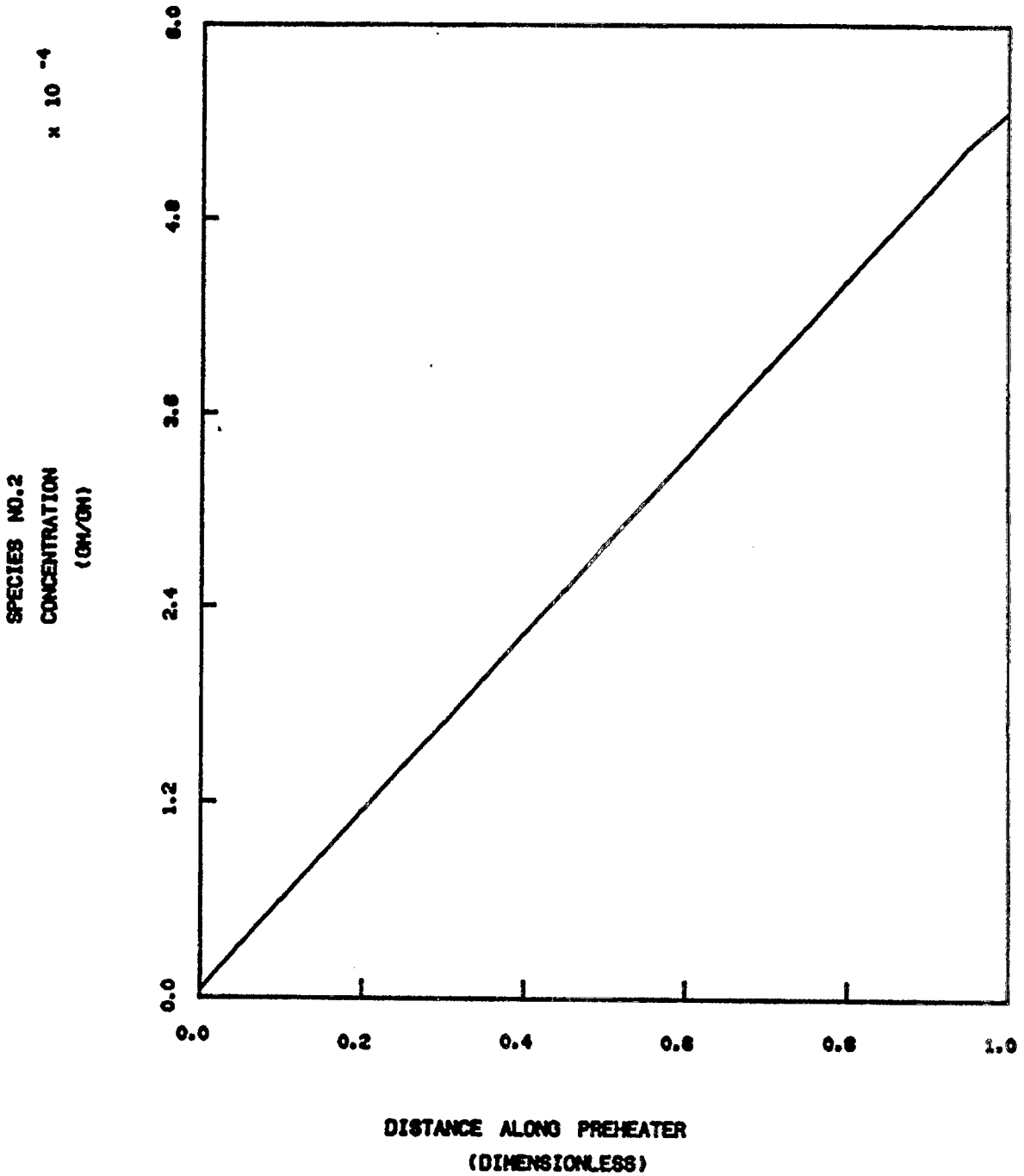
PREHEATER TEMPERATURE PROFILE



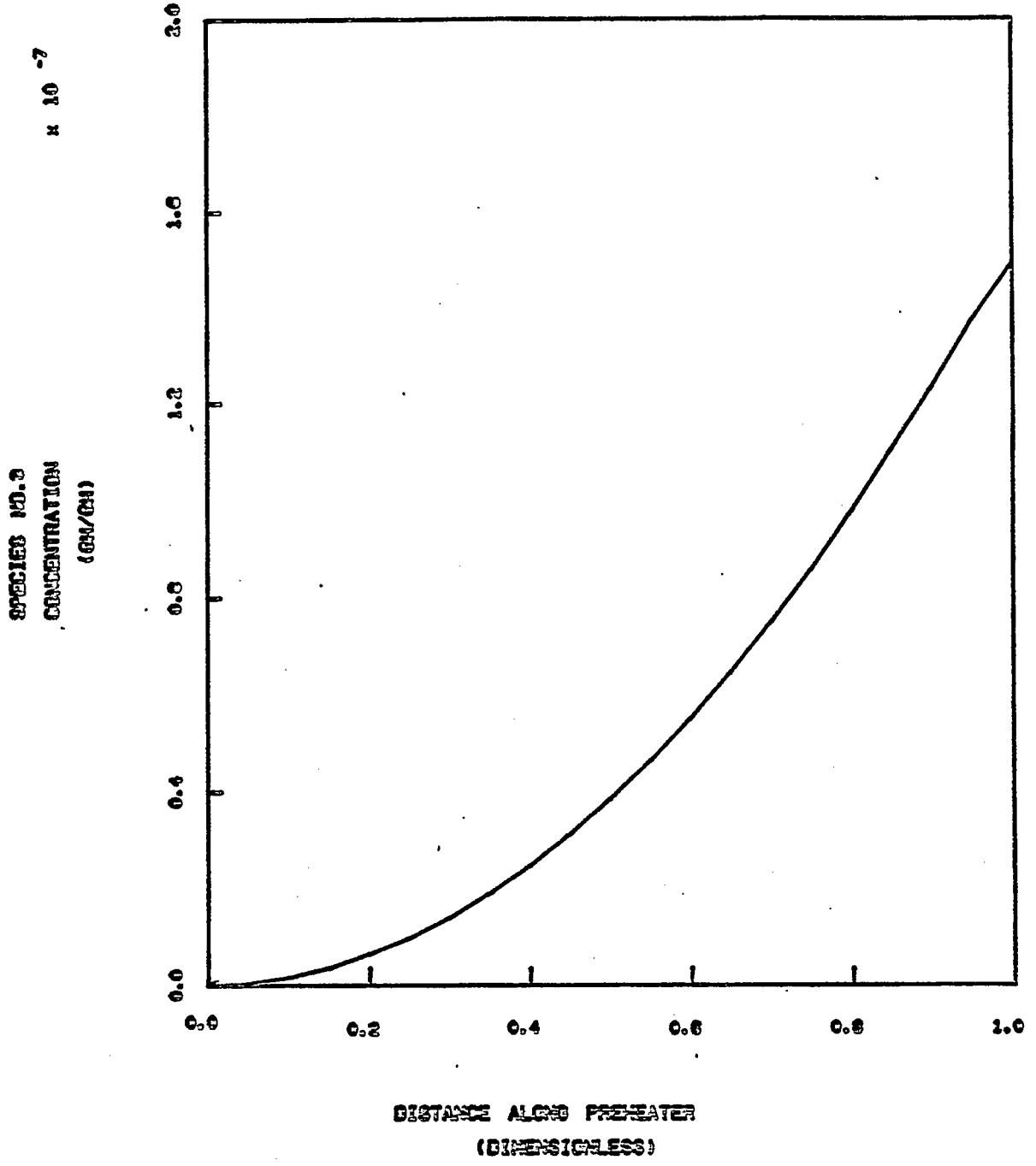
PREHEATER HYDROGEN PROFILE
(GAS PHASE)



PREHEATER HYDROGEN PROFILE
(LIQUID PHASE)



PREHEATER CONCENTRATION PROFILE



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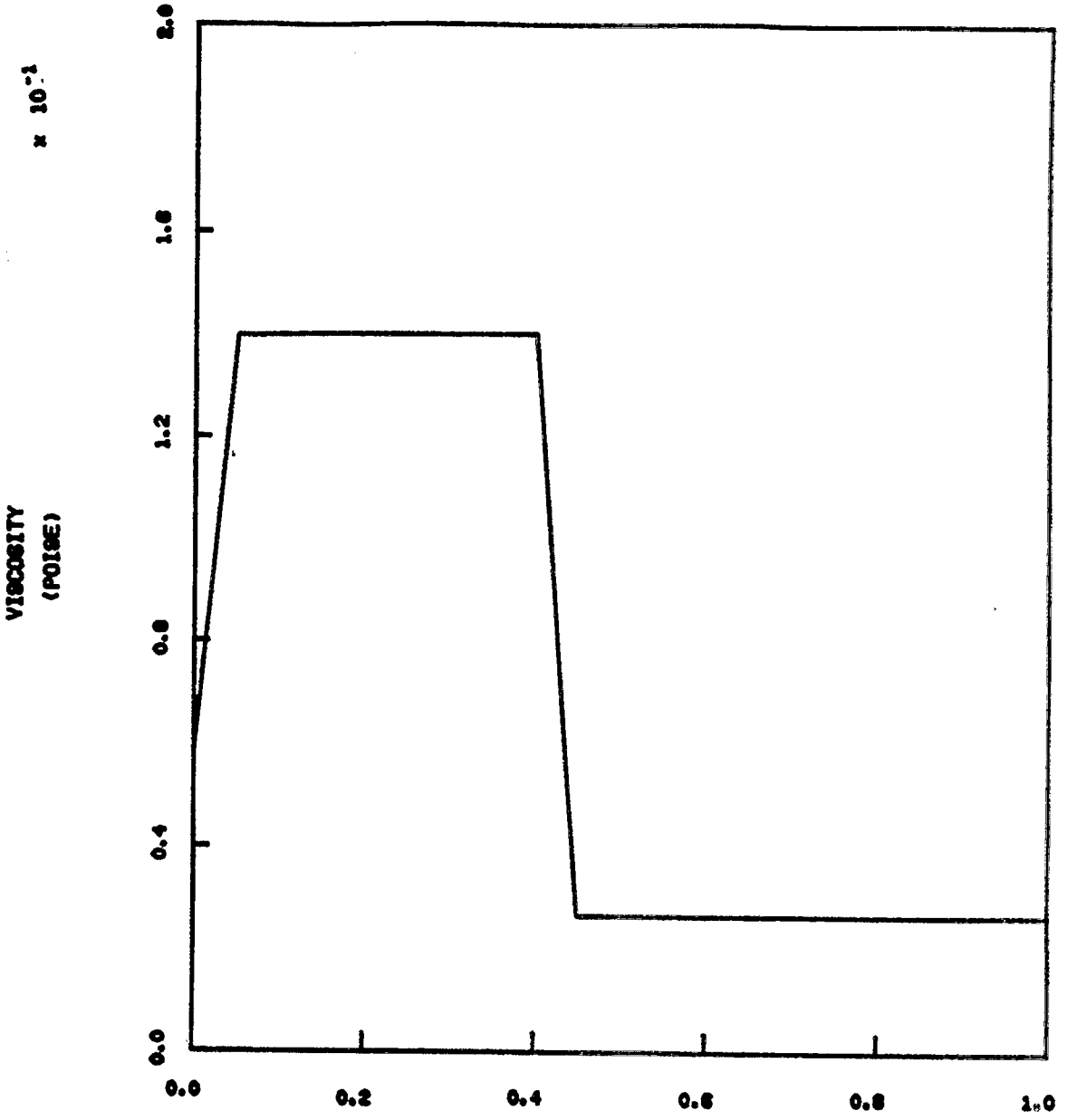
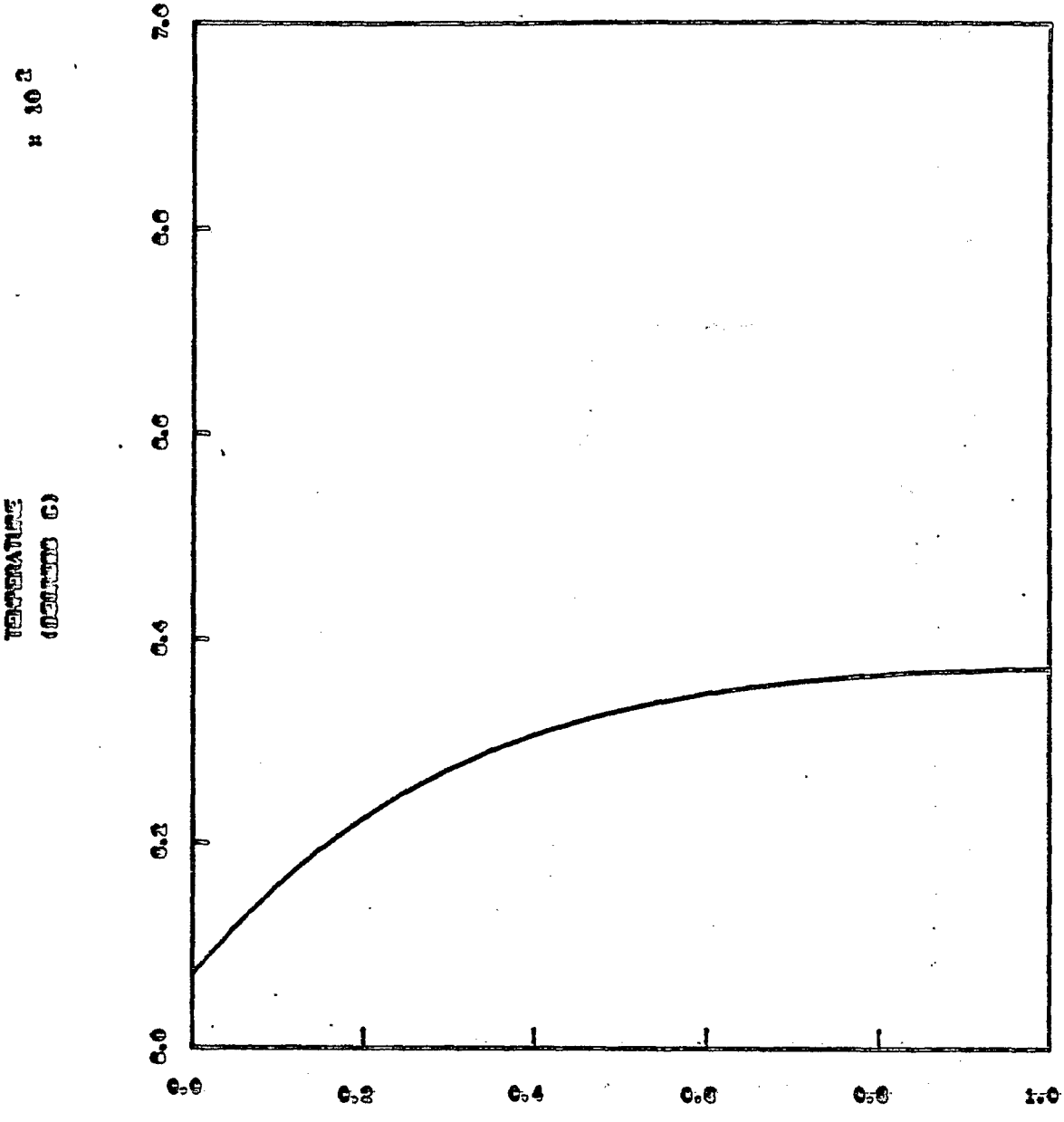
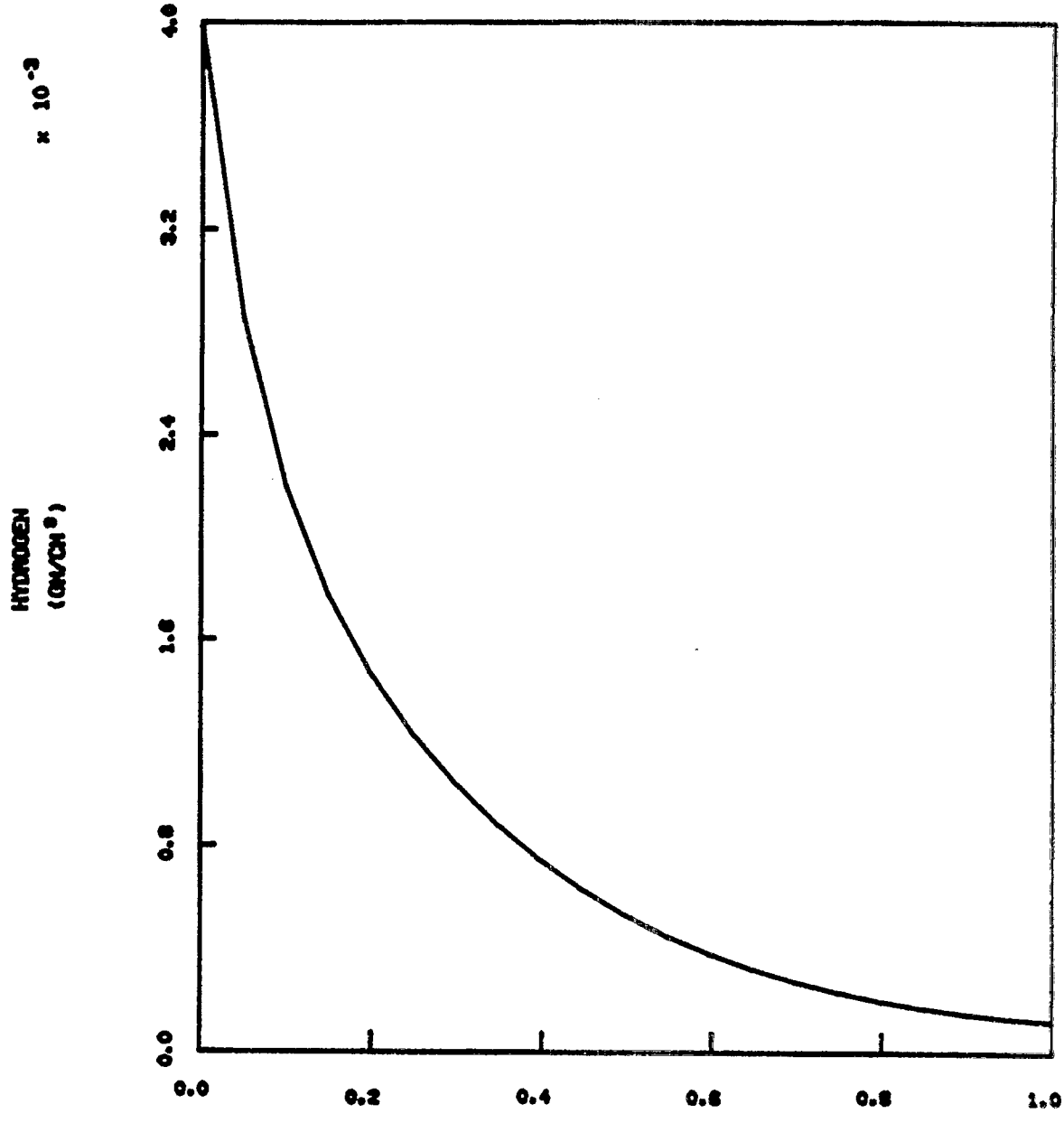


PREHEATER VISCOSITY PROFILE

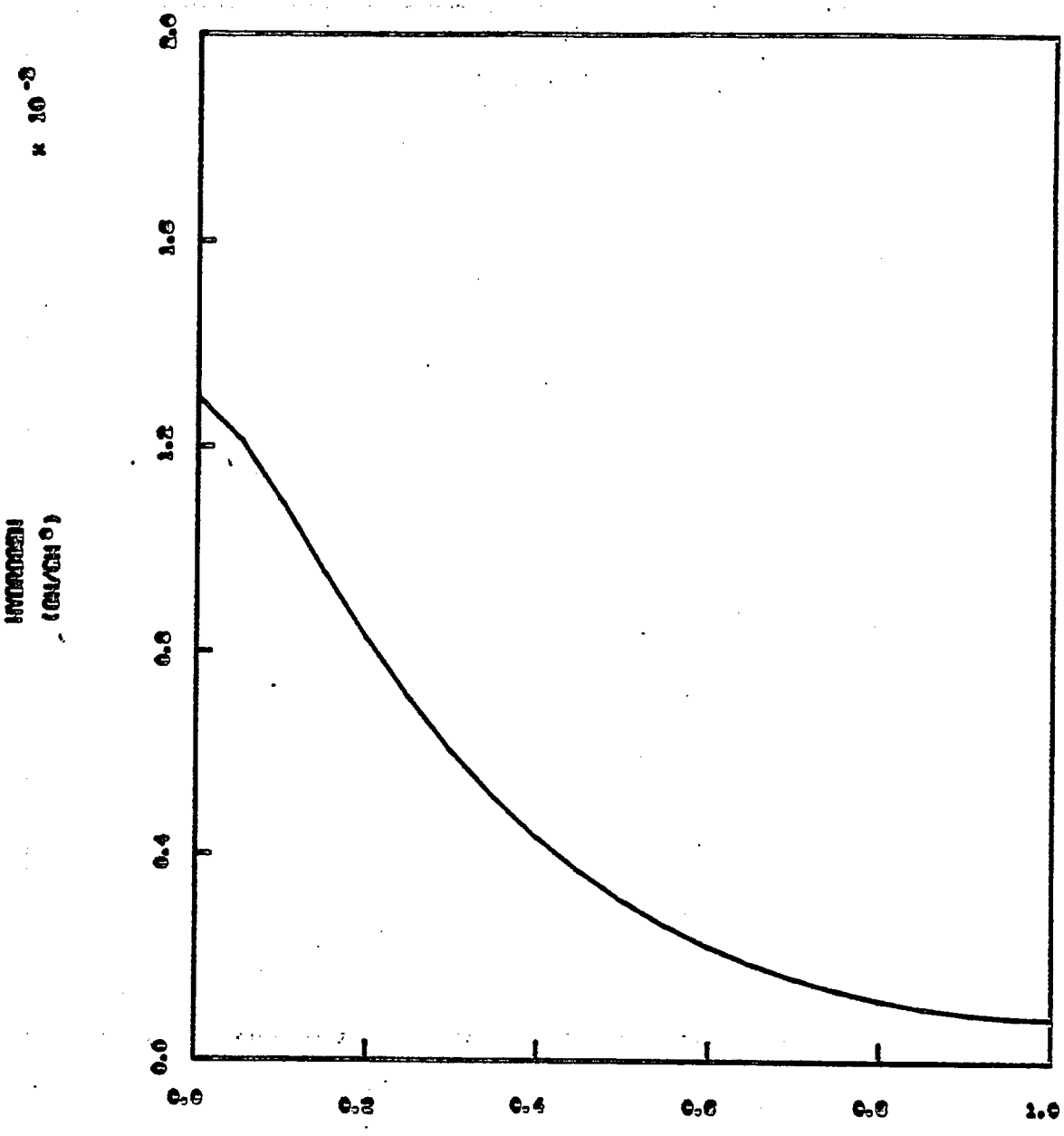


DISTANCE ALONG REACTOR
(DIMENSIONLESS)

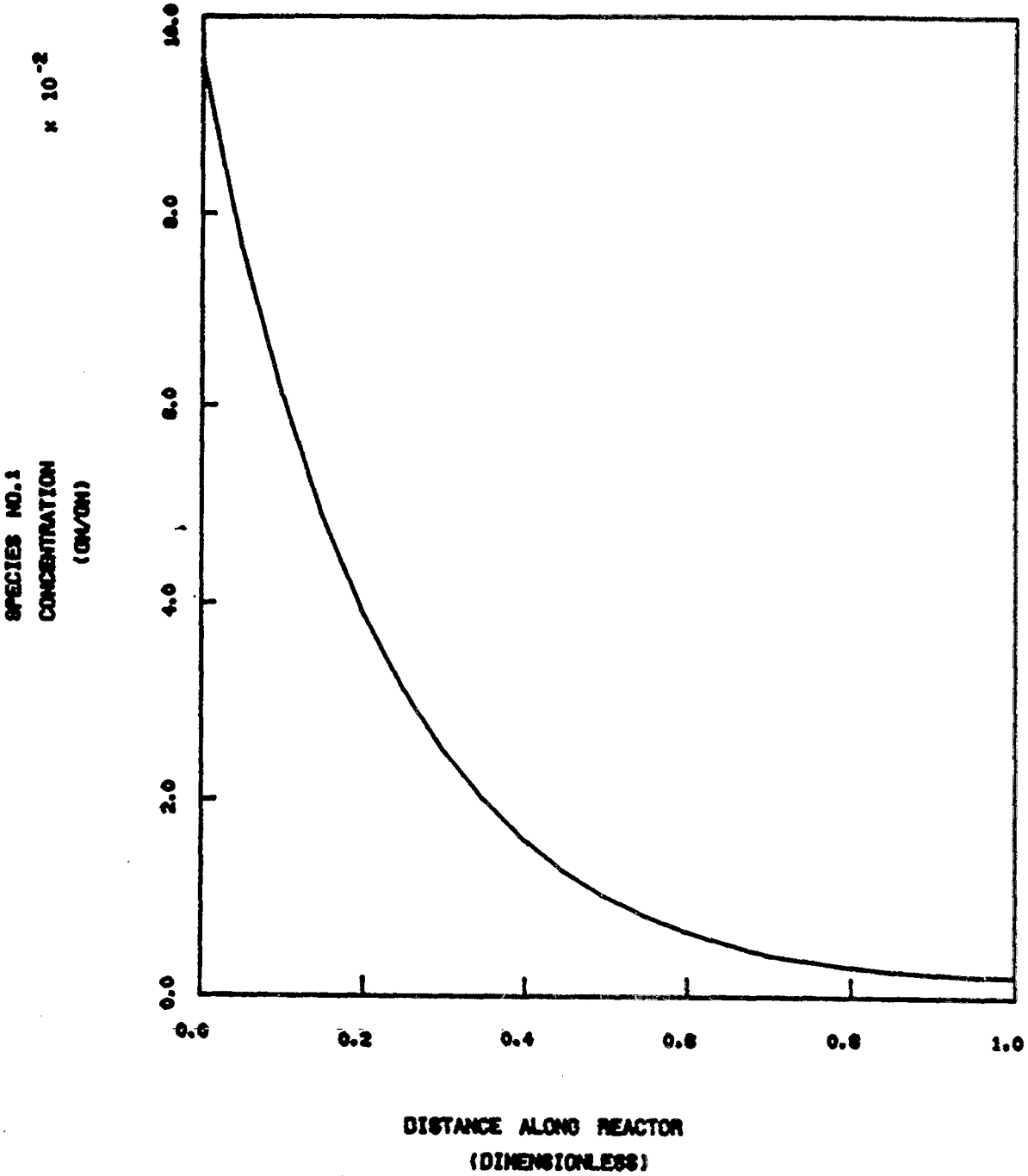
REACTOR TEMPERATURE PROFILE



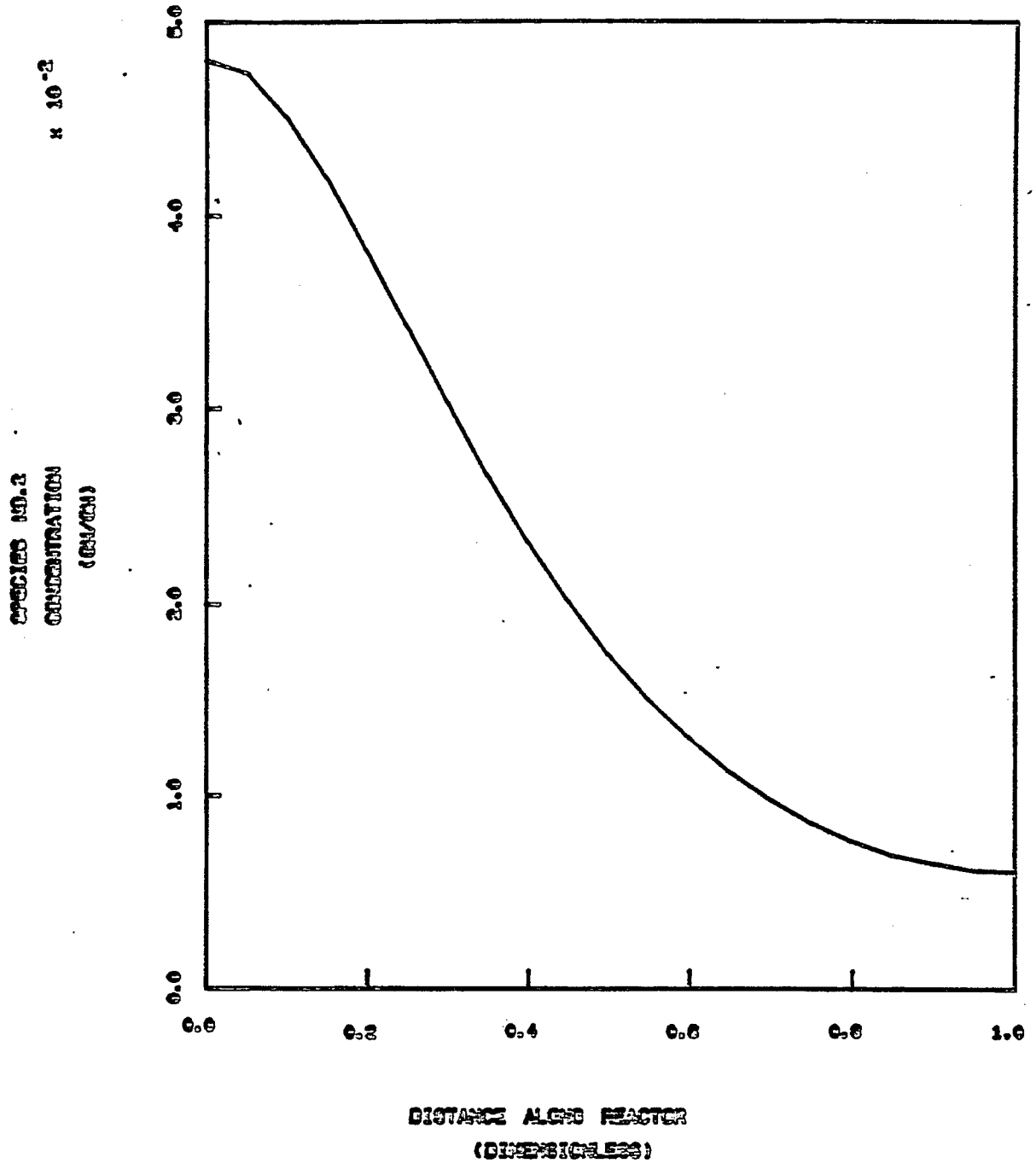
REACTOR HYDROGEN PROFILE
(GAS PHASE)



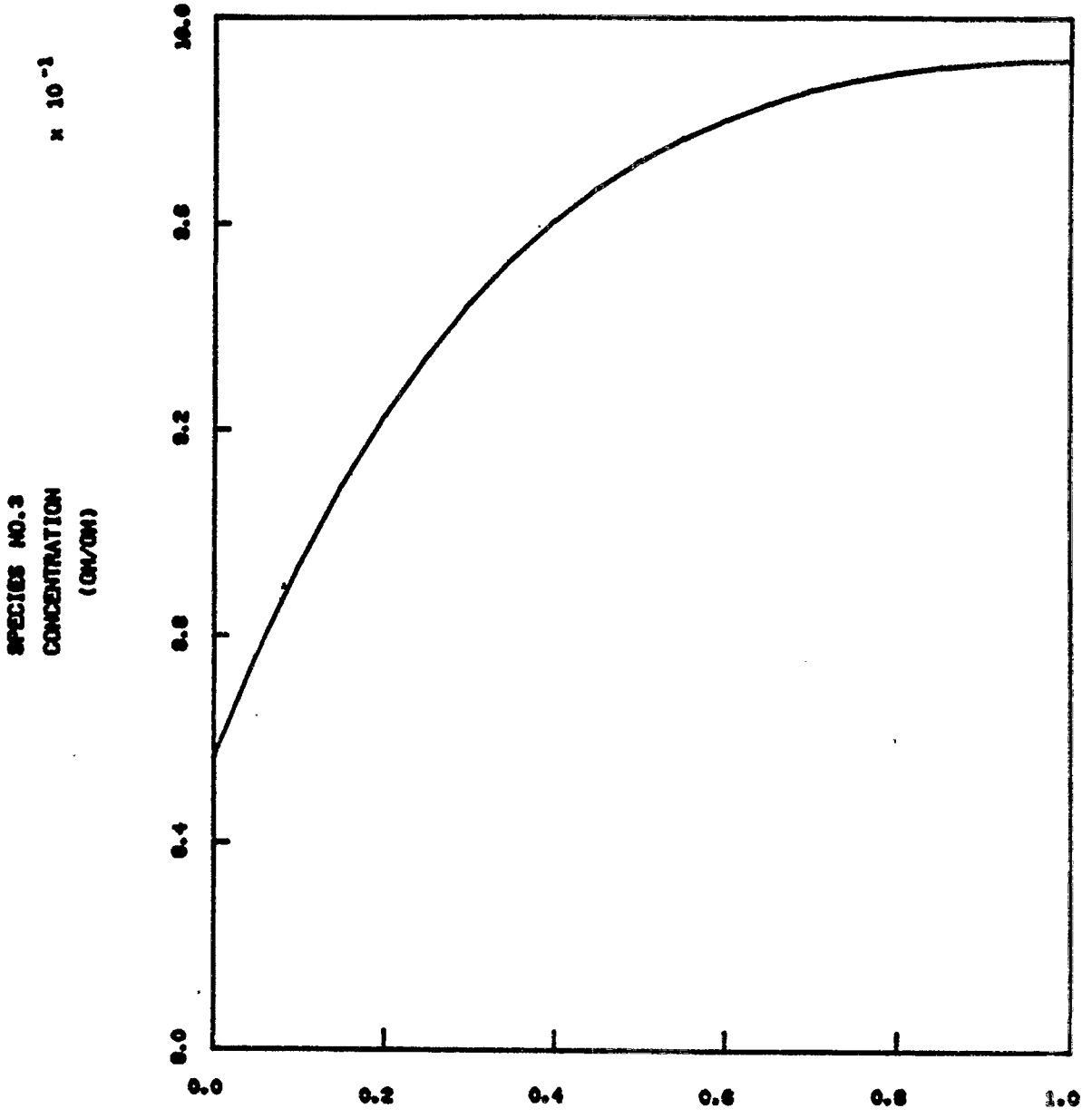
REACTOR HYDROGEN PROFILE
(LIQUID PHASE)



REACTOR CONCENTRATION PROFILE



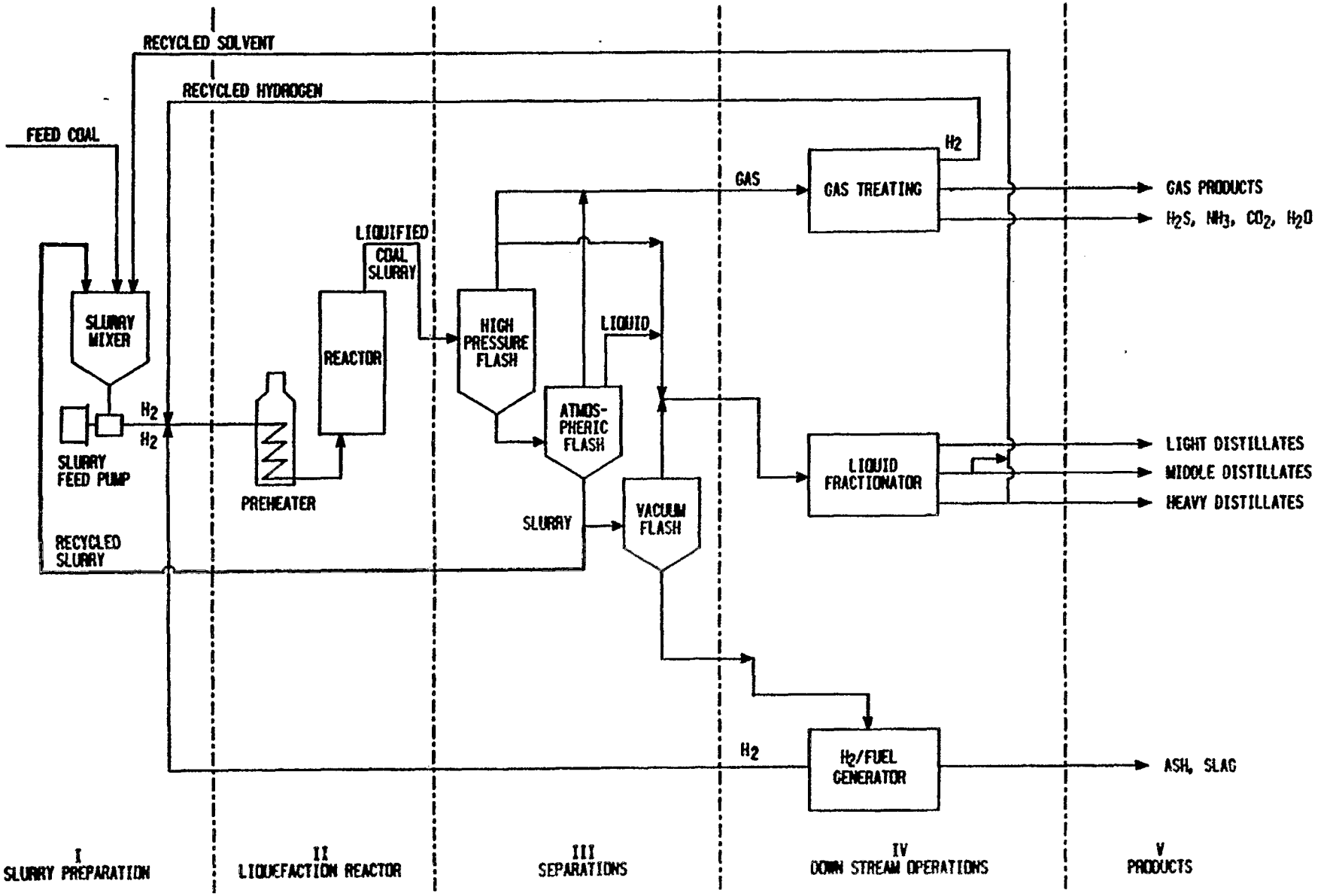
REACTOR CONCENTRATION PROFILE



REACTOR CONCENTRATION PROFILE

PROCESS FLOWSHEET AND GRAPHICAL REPORT

SRC-II PROCESS



COMPREHENSIVE GRAPHICAL-REPORT

DATE: 5/07/84

	CAPITAL COST ($)	OPERATING COST ($/YR)	MAINTENENCE COST ($/YR)	FIXED COST ($/YR)	VARIABLE COST ($/YR)
Reactor	0.6361D+08	0.1738D+07	0.1738D+07	0.9541D+06	0.7812D+06
Preheater	0.6699D+08	0.4368D+09	0.1831D+07	0.1005D+07	0.4359D+09
Total	0.1306D+09	0.4385D+09	0.3569D+07	0.1959D+07	0.4366D+09

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