

KINETICS OF METHANE-AIR COMBUSTION
AT
THE LOWER FLAMMABILITY LIMIT

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ABSTRACT

KINETICS OF METHANE-AIR COMBUSTION
AT LOWER LIMIT OF FLAMMABILITY

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A 30 reaction step kinetic model of methane-air combustion at lower limit of flammability. (5.3 % methane in air), 1000 K temperature and one atmosphere pressure is developed and used to predict flame structure while diffusion and heat conduction are neglected. The species and energy conservation equations and solved by a computer code, give Species concentrations, thermodynamic properties at 40 interval of time and distance. Ignition is defined and occurs at 1109 K. Flame length is estimated to be 1.5 cm. The model permits a detailed discussion of the role of each equation in the reaction scheme. Nitrogen is treated as inert.

DEDICATION

This work is dedicated to my mother.

Acknowledgements

The author is grateful to all the members of the combustion research group at Concordia University: They have contributed immeasurably to the research involved and to the production of this thesis. In particular, the author thanks Dr. A.J. Saber, his research advisor and the leader of the group. Dr. Saber gave freely of his time and shared his insight at times when problems seemed insurmountable and understanding seemed elusive.

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1.0.0 FLAMMABILITY LIMITS

The flammability limits of a fuel/oxidizer gas mixture at given thermodynamic boundary conditions are the proportions between which the gas can support flame propagation.(19) At the limits, therefore, a change in the mixture composition in one direction permits flame propagation, while a change in the other does not.

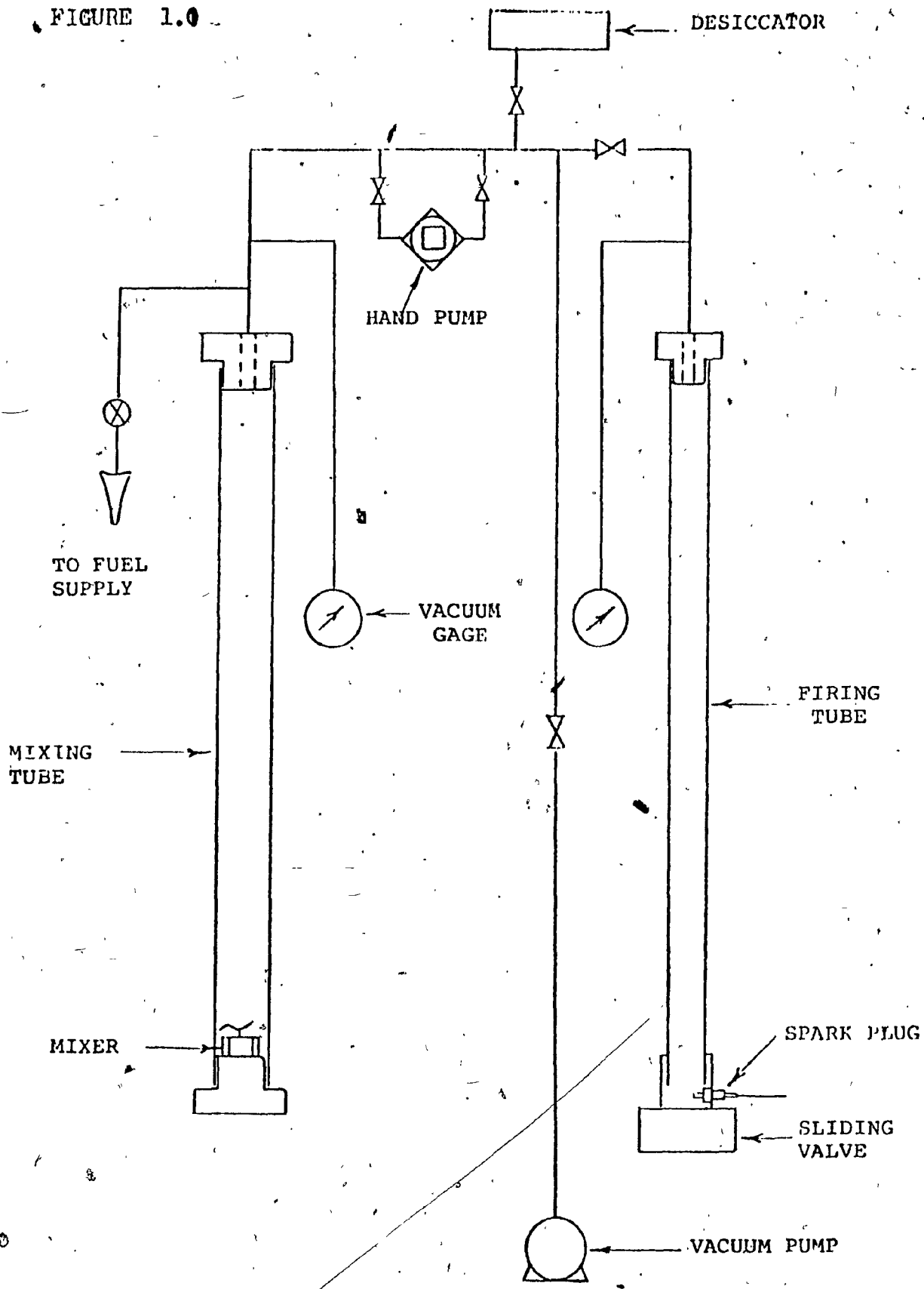
There are two distinctly separate flammability limits corresponding to the minimum (lower) and maximum (upper) ratios of fuel to oxidizer reactants which will support flame propagation. Although these flammability limits are believed to be physiochemical constants for flammable gases or vapours of flammable liquids,(19) no such consistent physiochemical constants are yet evident.(45) Consequently, flammability limits are determined experimentally, usually by the observation of flame propagation in wide vertical tubes, open at one end. Indeed, such flame propagation measurements have been standardized by the U.S. Bureau of Mines.(3)

Experimentation is conducted at atmospheric pressure using 5.0 diameter, 120 to 180 cm long tubes.(3) The basic operating principles of the flammability tester are in accordance with specifications set by U.S. Bureau of mines.(3) Such flammability limit measurements are conducted at Concordia University, in a vertical pyrex glass tube, 5 cm in diameter and 160 cm long, shown in Fig. 1.1. A fuel-oxidizer mixture of given composition is obtained by mixing appropriate volumes of each in a previously evacuated, 10 cm diameter, 160 cm long mixing tube. The gases are then transferred to the firing tube, which has also been evacuated. Then, the slide valve at the base of the tube is opened to atmosphere and ignition is induced by a small electric spark at the lower end. The flammability tester is used to obtain comparison data for parameters used in this kinetic study.

Flammable mixtures are then defined operationally as those mixtures which support flame propagation throughout the tube length, and the flammability limits are the limiting fuel/oxidizer ratios for propagation.

In the U.S Bureau of Mines method, the mixture may be ignited at either end of the vertical tube. If the

FIGURE 1.0



mixture is ignited at the top, the flame propagates downward. However, if the ignition occurs at the base of the tube, the flame propagates upwards.

It has also been demonstrated that the flammability limits depend on pressure and temperature, although normal variations in atmospheric pressure do not cause any noticeable effect.(19) However, as pressure is decreased below atmospheric, the flammability limits meet a critical condition representing the lower pressure for that test vessel.(30) Furthermore, at pressures exceeding atmospheric, some observers state that flammability limits spread apart,(20) while others claim the opposite effect.(35,41) Indeed, for certain combustible mixtures, the range may first narrow and then broaden.(20)

1.1.0 EFFECT OF TUBE DIAMETER

The limits of flammability widen as the diameter of the apparatus is increased, rapidly at first and then slowly as the diameter approaches 5 cm.(1) However, in test work at the U.S. Bureau of Mines, Coward and Jones show that an increase in diameter above 5 cm rarely shows

more than a few tenths of one percent change in the limit air/fuel ratios.(3) However, at the small diameter end, the apparatus limits narrow markedly. Indeed, a methane/air mixture propagating from an open-end 5 cm diameter tube is quenched by a tube of 0.30 cm or less.(20) This latter effect of tube diameter is expressed as a quenching diameter and the boundary condition at the large diameter limit has been called the true flammability limit.(3)

1.2.0 EFFECT OF CONVECTION

If the mixture is ignited at of top of the vertical tube, the flame propagates downward. This can occur only when the flame speed exceeds the convective draught of the hot combustion products.(3) However, if the ignition occurs at the base of tube, the flame propagates upward: Convection enhances the apparent flame speed.(8) Consequently, the flammability limits for upward and downward propagation are different. Furthermore, experimentation shows that the flammability range for upward flame propagation in a vertical tube is wider than that for downward propagation.(11) Correspondingly, for

horizontal tubes, the limiting values for the same fuel and oxidizer lie somewhere between those determined from vertical tests.(13)

It is believed that the effect of convection is greater the larger the tubes. However, the difference between upward and downward propagation limits does not change with larger diameter tubes. To explain this, the following mechanisms have been suggested, but they are contradictory.

Linnet and Simpson,(9) for example, believe that the surface of a flame propagating upward under the action of convection is larger, and the flame speed is correspondingly higher, than for the downward propagation. Consequently, for downward propagation the slower flame speed allows more heat to be lost to the walls.

Lewis and Von Elbe,(20) however, explain the difference between upward and downward propagation limits by a "flame stretch" concept. In the case of upward propagation, the gas speed gradients at the surface of the flame are presumed lower than those for downward propagating. As a result, the flame propagation upward

suffers "stretch" and hence propagates through a more dilute mixture.

Next, Lovachev attempts to explain convection in his theory of limits.(11) Lovachev assumes:

- a) The flame acts like a solid sphere.
- b) The limit flame speed equals the convection velocity.
- c) A drag force acts on the core of the limit flame.(13)
- d) The radius of the limit core equals the flame thickness, calculated from flame theory.

The first assumption is a limiting condition for downward propagation, although upward propagation is still possible. The convective motion of the hot gases develop unsteady phenomena in the formation of the flame front. Hot and less dense gases rise and consequently the fresh mixture flows round the flame core. The state at which the flame core stops rising and the visible flame speed becomes zero is defined as limiting.

Lovachev bases flammability limits on the solution of a set of non-stationary equations for energy conversion and diffusion of all reaction component, the Navier-stokes equations and the continuity equation. He suggests the following relation, which determines the convective rise velocity at the limit.

$$U = 2 \left[\frac{2}{3} \frac{L'}{CDP} \left(1 - \frac{D'}{D}\right) \left(\frac{D'}{D}\right)^2 \frac{G}{C'} \right]^{1/3}$$

U = convective rise velocity

L' = thermal conductivity.

C = heat capacity.

D = unburnt gas density.

P = co-efficient dependent on the form of heat release.

D' = burnt gas density.

G = gravitational constant.

C' = resistance coefficient.

The result may be interpreted as a minimum to which propagation is possible.

Lovachev assumes that the flame can be modelled like a solid sphere, submerged in a gas. This model may be used for the motion of vapours and gas bubbles in liquids.

However, since the flaming gas density and surrounding gas density are about the same, the basic drag force assumption of unequal densities does not apply. Also, the continuing consumption of the surrounding unburnt gas by the flame front results in an unburnt gas velocity normal to and away from the flame surface, which is a thrust to the flame rather than a drag force.

Next, Andrew and Bradley have a theory which neglects this drag force.(10) They assume that any buoyancy force acting on the hot core of the flame is equal to the flame's rate of change of momentum. Balancing the buoyancy and rate of change of momentum, they suggest the convective rise velocity at the limit is

$$Y = S'T(D/D') + [(D/D') - 1]GT^2/8$$

S' = Near limit burning velocity.

D = Unburnt gas density.

T = Time.

Y = Distance travelled.

G = Gravitational constant.

D' = Burnt gas density.

1.3.0 EFFECT OF TEMPERATURE

The lower limit decreases and upper limit increases with temperature, since the degree of preheat required decreases with temperature. Also, it has been shown that radiation losses represent so small an effect that they can be neglected. Furthermore, at excessively elevated pre-ignition temperatures, the occurrence of preflame reactions can result in changes in mixture composition and state:(3)

1.4.0 EFFECT OF HUMIDITY

The normal quantity of water vapour present in air does effect lower flammability limits, but the effect is usually very small.(1) It appears in the upper limit, which may be significantly reduced because some of the oxygen in the mixture is displaced. Indeed, the oxygen concentration is the important factor in an upper limit mixture, since lowering the oxygen fraction reduces the degree of completion of the combustion train.

1.5.0 EFFECT OF COMPOSITION

For mixtures of various fuel species the knowledge of the limits of each component in air and the percentage of each combustible present in the mixture can be used to calculate flammability limits for a mixture. (18) For a large number of compositions, these limits can be calculated by the following relation:

$$L = 100 / \left[\left(\frac{P_1}{N_1} \right) + \left(\frac{P_2}{N_2} \right) + \dots + \left(\frac{P_n}{N_n} \right) \right]$$

Where P_1, P_2, \dots, P_n are percentages of each combustible component, and N_1, N_2, \dots, N_n are the lower limits of flammability of each combustible in air.

2.0.0 OBJECTIVE

It is believed that a knowledge of the fundamental mechanisms are key to understanding flammability limits. To that end, the focus here is the chemical kinetics at atmospheric pressure of a methane/air mixture at the lower limit of flammability. In the following, the structure of the flame is calculated and shown at the lower limit (5.3 % methane in air) for a one atmosphere pressure mixture at 1000 K initial temperature:

Usually approximate kinetic schemes are used to describe the oxidation of the gaseous hydrocarbon fuels in air.(31) These schemes generally assume relative fast partial oxidation of the hydrocarbon to carbon monoxide in the $H_2/O_2/CO/N_2$ system.(30) However, these approximate kinetic models have been shown to be unreliable when incorporated to predict formation of different species, such as the oxides of nitrogen.(30) Consequently, more detailed kinetics are demanded.

This present study uses a detailed kinetic scheme in a "stiff system" approach involving the energy, overall-mass and elemental conservation equations which

are coupled and solved in a chemical kinetic code.(33) The calculation neglects diffusion and thermal conduction, which are important in laminar flames. As such the approach is restrictive since this simplification effects the calculated species concentration profiles near the flame interior, where gradients are large. However, results below provide qualitative information about the trend of various species concentration. The work leads the way to further study of the parametric effect of key species formation on the limits. Specific species restrictions include neglecting nitrogen reactions, except for third body effects.

The 1000 K initial temperature is selected, since it has been found that the pure methane and air reactants must be at 1000 K or higher for the reactions to proceed within a reasonable time (1000 sec). Although reactions initiated at a lower temperature are calculated to proceed to completion, in a much longer time, such a calculation is not warranted, since heat transfer effects are no longer negligible and the system cannot be treated as adiabatic.

In the course of studying the methane/air system, the following additional questions were also addressed.

- a) What reaction controls the pyrolysis of methane?
- b) What reaction controls the oxidation of methane?
- c) What is the thickness of flame?

3.0.0 CALCULATIONS OUTLINE

Many integration techniques have been derived which are stable and efficient methods for integrating the stiff systems. Among these are Treanor's modified Runge-Kutta method(25) and Moretti's method which involves exact solution of locally linearized equations.(26)

A method which falls logically between these two is the implicit integration method of Tyson.(27,28) Tyson's method has the advantage of being inherently stable and computationally efficient. The approach used here involve a computer code developed by NASA,(33) which uses the Tyson approach. The calculation follows a particle of fluid and traces its time and distance history.

3.1.0 COMPUTER CODE CHARACTERISTICS

For the calculations, the flame is divided into intervals called station points. At each station point, existing species are used in the reaction scheme to calculate products. The products then become the existing species for the next station point.

To get a clear picture of concentration, temperature, enthalpy and entropy changes, 40 stations points are chosen. The intervals, which have variable sizes, are large where changes are small (e.g., over 1 cm or 0.033 sec), but significantly smaller (e.g., 0.02 cm or 0.35 msec.) where rapid changes occur.

A minimum integration step size of 0.0001 cm is chosen, while a maximum integration step size is kept at 1.0 cm. The initial step size is 1.0 mm. The precision for each integration step is 0.001. About 600-650 steps of varying sizes are required to reach the last station point.

The execution times on the CONCORDIA UNIVERSITY COMPUTER CENTER CDC-CYBER 172/2 operating under NOS 1.3-485, are in the range of 300 CPU Seconds.

4.0.0 SELECTION OF THE KINETIC SCHEME

The kinetics of the methane/air system have been studied extensively. Noticeable are studies by Cooke and Williams,(34) Peeters and Mahnen,(35) Dryer,(36) Bowman,(37) Heffington, et al,(38) Smoot, Hecker and Williams,(49) Boni and Penner,(39) Tsatsaronis,(32) Tabayushi and Bauer,(40) Ay and Sichel,(46) Olson and Gardner, (47) Bendik, et al, (48) and Waldman, Wilson and Maloney.(31)

4.1.0 SELECTED SCHEMES

Four specific schemes have been selected as a basis for this study of methane/air combustion at the lower limit of flammability.

These schemes are associated with.

- 1- BOWMAN (37)
- 2- AY and SICHEL (46)
- 3- WALDMAN, WILSON and MALONEY (31)
- 4- TSATSARONIS (32)

4:1.1 BOWMAN'S SCHEME

Bowman conducted an analytical study of nitrous oxide formation in the shock-induced combustion of a methane/air mixture.(37) In his calculations, the time-dependent species concentrations and thermodynamic properties during combustion were obtained by numerically integrating the coupled equations for reaction kinetics, state and energy. Bowman modelled the methane flame in an isothermal, constant pressure flow reactor, neglecting mass and energy transfer processes.

The Bowman kinetics model cannot properly describe the combustion processes of hydrocarbon flames, unless combustion is shock-induced. Such is not the case here and it is confirmed in this work that the Bowman scheme should not be used for a self-heating mixture approach to flammability limits modelling.

4.1.2 AY and SICHEL

Bowman kinetics have been extended by Ay and Sichel (46) using the findings of Homer and Sutton.(52) The latter suggest that HO_2 has an important influence on radical recombination, hence on the radical over-shoot immediately downstream of the flame. Consequently, Ay and Sichel supplemented Bowman's scheme by involving HO_2 reactions, a result derived from their use of the equivalence ratio (i.e., mixture fuel-air ratio/stoichiometric fuel-air ratio). The Ay and Sichel calculations resulted in a 5 %, 20 % and 35 % decrease in OH, O and H concentration respectively, at 1000 K for the equivalence ratio of 0.6. Whereas at equivalence ratio of unity and a temperature 1000 K, the effect of HO_2 reactions was negligible.

4.1.3 WALDMAN, WILSON and MALONEY

The Waldman, et al, kinetic scheme has been suggested for an equivalence ratio less than one.(31) The scheme consists of 27 reactions for low temperature flows. ($T < 1500$), but gives enormously long preheat times and

works only for supersonic combustion.

4.1.4 TSATSARONIS' KINETIC SCHEME

A methane/oxygen reaction mechanism consisting of 29 elementary reactions is used by Tsatsaronis.(32) In his study, flame speed and thickness at the different temperature and equivalence ratios are predicted. However, it is found in the present study that this kinetic scheme works only when a methane pyrolysis reaction is added to the chain. With such an addition, the kinetic scheme operates and has been selected for use here.

4.2.0 FINAL CHEMICAL SCHEME

With the addition of an initiating pyrolysis step, the basic Tsatsaronis chemical kinetics scheme has been selected for use here. However, each equation was examined in the literature, to find its agreement with other published results. The examination resulted in the overall scheme shown in the Table 4.1. The quantities represents values which give reasonable induction times.

It is important to note that changes in the activation energy and frequency factor strongly affect the reactions rates and must carefully assessed.

In the present study 13 chemical species are recognized. They are shown in Table 4.2.

TABLE 4.1

METHANE COMBUSTION SCHEME

REACTIONS					F	N	A			
1	M	+	CH ₄	-->	CH ₃	+	H	1.00E+18	0.	88420.
2	CH ₄	+	OH	-->	CH ₃	+	H ₂ O	2.20E+13	0.	4967.
3	CO	+	O	-->	CO ₂	+	M	3.60E+15	-1.	2583.
4	H	+	O ₂	-->	OH	+	O	2.20E+14	0.	16690.
5	CO	+	OH	-->	CO	+	H	2.50E+12	0.	5762.
6	CH ₃	+	O ₂	-->	CH ₂ O	+	OH	1.00E+11	0.	9935.
7	H ₃	+	CH ₄	-->	CH ₃	+	H ₂	2.24E+04	3.	8742.
8	O	+	CH ₄	-->	CH ₃	+	OH	1.26E+14	0.	11922.
9	H	+	O ₂	-->	HO ₂	+	M	1.40E+13	0.	-994.
10	HO ₂	+	H ₂	-->	H ₂	+	O ₂	6.00E+13	0.	1987.
11	O	+	H ₂	-->	OH	+	H ₂	1.80E+10	1.	8942.
12	H ₂	+	OH	-->	H ₂ O	+	H	2.20E+13	0.	5166.
13	H ₂	+	H	-->	H ₂	+	M	2.00E+16	-1.	0.
14	CH ₃	+	O	-->	CH ₂ O	+	H	2.00E+13	0.	1987.
15	CH ₂ O	+	H	-->	HCO	+	H ₂	1.25E+10	1.	3179.
16	CH ₂ O	+	OH	-->	HCO	+	H ₂ O	4.80E+13	0.	0.
17	CH ₂ O	+	O	-->	HCO	+	OH	5.00E+13	0.	4570.
18	HCO	+	O	-->	CO	+	OH	3.00E+11	1.0	497.
19	HCO	+	OH	-->	CO	+	H ₂ O	1.00E+14	0.	0.
20	HCO	+	H	-->	CO	+	H ₂	2.00E+14	0.	0.
21	M	+	HCO	-->	H	+	CO	5.00E+12	0.	19075.
22	HCO	+	O ₂	-->	CO	+	HO ₂	3.00E+13	0.	0.
23	H	+	HO ₂	-->	OH	+	OH ₂	2.00E+14	0.	1987.
24	H	+	HO ₂	-->	H ₂ O	+	O	5.00E+13	0.	994.
25	O	+	HO ₂	-->	OH	+	O ₂	6.00E+13	0.	0.
26	OH	+	HO ₂	-->	H ₂ O	+	O ₂	4.00E+13	0.	0.
27	H	+	OH	-->	H ₂ O	+	M	2.30E+19	-2.	0.
28	H	+	O	-->	OH	+	M	6.20E+23	-0.6	0.
29	OH	+	OH	-->	O	+	H ₂ O	6.30E+12	0.	1093.
30	M	+	CH ₂ O	-->	CO	+	H ₂	2.00E+16	0.	37753.

WHERE:

F = Frequency factor

N = Nondimensional temperature factor.

A = Activation energy.

Units: mole, cm, K

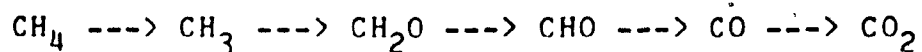
TABLE 4.2

SPECIES INCLUDED IN THE STUDY

CHO	FORMYL	OH	HYDROXYL
CH ₃	METHYL	HO ₂	HYDROPEROXYL
CH ₄	METHANE	H ₂ O	WATER
CO	CARBON MONOXIDE	O	MONOATOMIC OXYGEN
CO ₂	CARBON DIOXIDE	O ₂	DIATOMIC OXYGEN
H	ATOMIC HYDROGEN	H ₂	MOLECULAR HYDROGEN
CH ₂ O	FORMALDEHYDE		

It is noted that CH_4 , CH_3 , CH_2O , HCO , and CO are key species, since their reaction with the oxidizer results in the release of heat.

An examination of the scheme shows the sequence for combustion of methane with oxygen is



Each path of the chain is discussed below and shown in figure 4.1.

4.2.1 $\text{CH}_4 \text{ ---> } \text{CH}_3$ PATH

There are four paths for formation of methyl radicals from methane molecules.

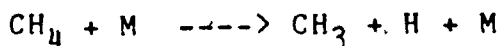
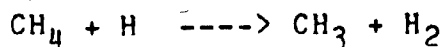
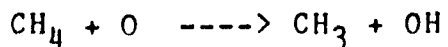
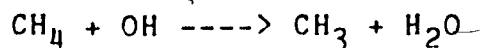
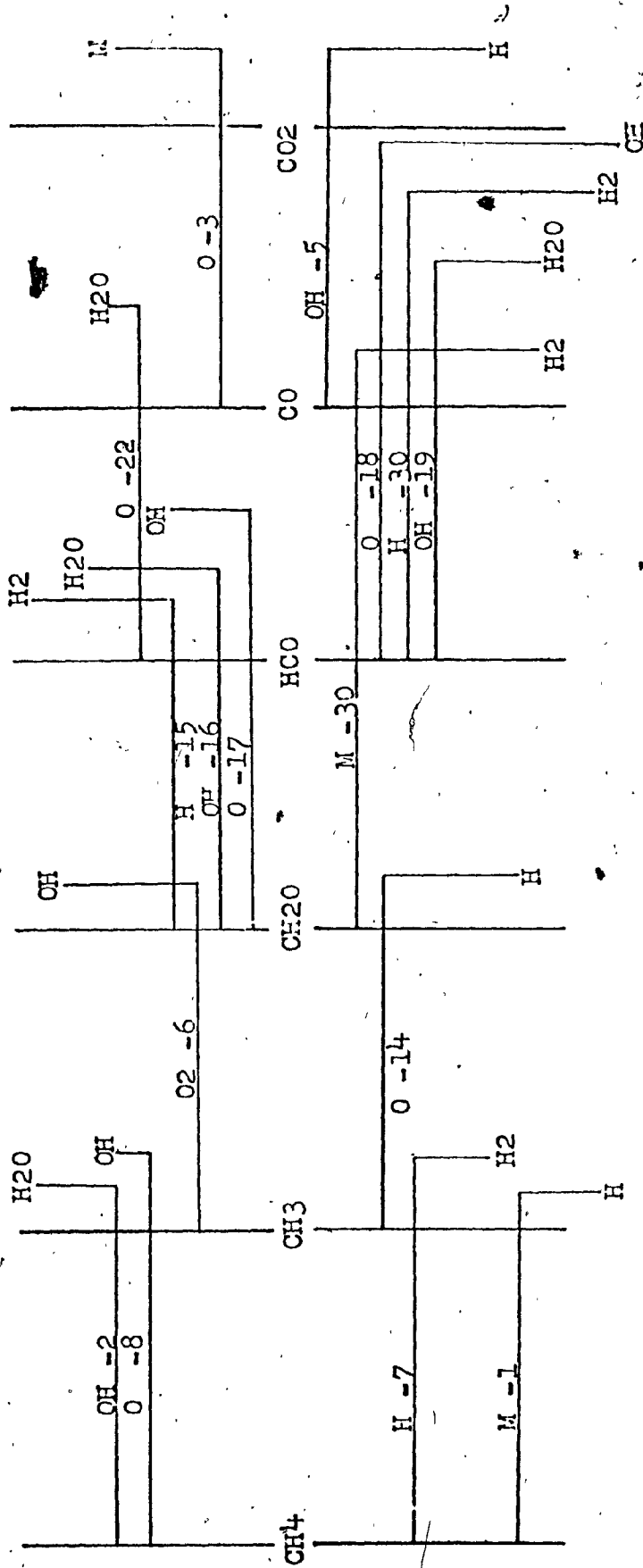


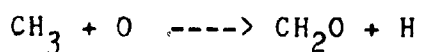
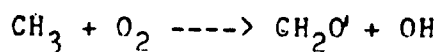
FIGURE 4.1



where -xx is reaction number

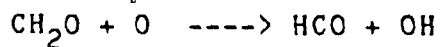
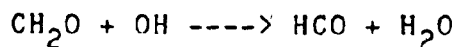
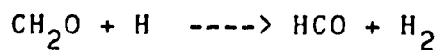
4.2.2 CH₃ ----> CH₂O PATH

Oxidation of methyl radicals results in the formation of formaldehyde. This formation occurs because of two paths:



4.2.3 CH₂O ----> HCO PATH

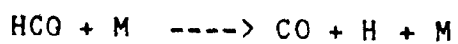
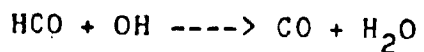
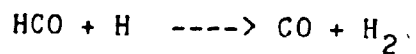
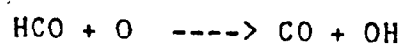
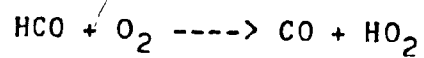
Formaldehyde breaks and forms formyl radicals by the following three reactions:



4.2.4 HCO ----> CO PATH

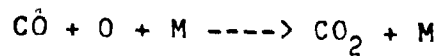
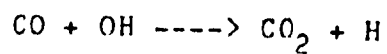
Formation of carbon monoxide occurs by the oxidation of formyl species and by the pyrolysis of formyl groups. The following are reactions showing the transformation of

formyl to carbon monoxide:



4.2.5 CO ----> CO₂ PATH

Oxidation of carbon monoxide to carbon dioxide takes place via the following two reactions:



5.0.0 INITIAL CONDITIONS

In this study, conditions at which the flammability tester discussed above operates are selected.

5.1.0 PRESSURE

Flammability of the gases are determined at a constant pressure of one atmosphere.

5.2.0 AREA

The nominal initial gas flow area has been rounded down from 19.63 sq.cm to 19.50 sq.cm.

5.3.0 TEMPERATURE

We presume that there is a non-chemical kinetic preheat mechanism that the code does not consider. Using that unspecified mechanism, the gas mixture temperature is

increased from a standard, at say 293 K, to 1000 K at which temperature the kinetic calculations considered here begin.

This temperature is consistent with reference (31) which cites that the ignition occurs at approximately 1200 K in combustors, and reference(52) which cites 810 K for ignition of methane/air mixtures at atmospheric conditions.

5.4.0 BURNING VELOCITY

The burning velocity of a methane/air mixture increases from the lower limit to a maximum on the fuel rich side of stoichiometric. It then declines to a low value at the upper flammability limit.

Andrew and Bradley(42) have reported a steady increase in the burning velocity as the mixture is preheated. They have suggest the following relation to estimate the burning velocity V of a stoichiometric mixture at the unburnt gas mixture T :

$$V = 10 + 0.000371 * T^2, \text{ cm/sec}$$

Table 5.1 lists the burning velocities reported at standard conditions. (2,32,42)

5.5.0 COMPOSITION OF AIR.

Air used in the study is assumed to have following composition:

NITROGEN = 78.85 %

OXYGEN = 21.15 %

TABLE 5.1

BURNING VELOCITIES AT STANDARD CONDITIONS

BURNING VELOCITY cm/sec	LOWER FL. LIMITS % BY VOLUME	REF.
30-37.0	5.30	51
-	5.26	3
5-10	5.35	2
33.50	4.6	50
28.00	5.3	44

6.0.0 DISCUSSION:

Combustion is modelled using the kinetic scheme, without back flow of any product species. The scheme is presumed initiated thermally, when the rate of slow reactions becomes high enough that the ensemble is self-heating.(31)

6.1.0 REACTION ZONES

The process is analyzed below by first considering that the entire flame is broken into four distinct regions (Table 6.1) Then, the species history is presented followed by a discussion of the salient events for each reaction. The zone limits are defined by the breaks in the calculated temperature vs distance and temperature vs time curves and by studying the behaviour of different reactions.

TABLE 6.1
REACTION ZONES

ZONES	EXTENT (cm)
INDUCTION	00.0-32.0
FLAME REACTION	32.0-33.4
RADICAL RECOMBINATION	33.4-33.5
POST FLAME REACTION	33.50-...

6.1.1 INDUCTION ZONE

In this study, ignition is modelled as a plug flow i.e, there is no back-mixing.

It is observed that rapid changes occur in the reaction rates where the slope of the temperature vs distance/time curve breaks. This behavior is exhibited at 32.0 cm. in to the flame where, the temperature is 1109 K as shown in Fig. B-58. (Figures labelled B- refer to illustrations in Appendix B) In this situation, the time 1.067 sec, (Fig. B-57) is the ignition delay and the temperature is the ignition temperature. This agrees with observations of Waldman, et al, in a study of methane/air combustion, (31) where ignition occurs at 1200 K. Although the Waldman reactants enter the combustor and are mixed with equilibrium combustion products, Norrish and Foord (43) report CO, CO₂ and H₂O vapours have no appreciable influence on the velocity of the reactions. This implies these vapours do not effect the ignition temperature.

In the induction region, reactions proceed isothermally, i.e., without raising the temperature. This zone ends with ignition and at ignition, 30 % of the methane is consumed.

6.1.2 FLAME REACTION ZONE

The flame reaction zone starts with ignition. This zone is defined as the region for which about 90 % of the temperature rise in combustion occurs. In it the remaining seventy percent of the methane is essentially consumed. The width of the flame reaction zone is about 1.4 cm.

6.1.3 RADICAL RECOMBINATION ZONE

This is the region where left-over radicals combine and raise the temperature to its final value. The calculations show the boundaries at 33.4-33.5 cm. It is noted that some of the reactions e.g. 1,12,21,25, etc. reverse direction in this zone.

6.1.4 POST FLAME REACTION ZONE

This is the zone where post flame reactions proceed at low speed, as the mixture drives to equilibrium. The end of the zone occurs when the Gibbs' free energy vs distance diagram, Fig. B-62, shows a minimum signalling completion of the process.

6.2.0 FLAME THICKNESS

The flame thickness is defined here as the distance necessary for the methane to decrease its concentration by 99 % of its initial value, and the thickness of the radical recombinaton zone. The flame thickness thus estimated at the lower limit of flammability is 1.5 cm.

6.3.0 SPECIES HISTORY

In this study, calculations follow a particle of fluid and trace its reactions. The results are presented as time and distance histories, in Appendix C.

6.3.1 METHANE

In the induction zone reactions proceed with a very low thermal gradient. The concentration of methane starts at about 6.44×10^{-7} moles/cm³ (Fig. B-1, B-2). It decreases first at about 10^{-11} mole/cm³/sec then speeding to 10^{-5} cm³/gm²/sec, in the main reaction zone. The integrated result illustrated in Figs. B-1 and B-2, is that about 30% of the methane is consumed in 168 seconds and rest is consumed in 0.042 seconds.

6.3.2 METHYL

Methyl radicals are generated in significant quantities only after, about 0.917 seconds. At 0.917 sec., the concentration of methyl radicals increase as this is

shown in Figs. B-3 and B-4, at 10^{-19} moles/cm³/sec. Later the rate increases further to 10^{-5} cm³/gm²/sec at the maximum, where the concentration is $1.11 \cdot 10^{-8}$ cm³/gm²/sec at 1.114 seconds. The concentration then falls to about $5 \cdot 10^{-19}$ moles/cm³. This change occurs in the short interval of 0.055 sec. in a 1.257 cm wide band, at a rate as high as 10^{-5} moles/cm³/sec. The slope of the curve suggests that reactions involving methyl radicals are very fast, implying reactions 6 and 14 are particularly rapid, see reaction histories below.

6.3.3 ATOMIC HYDROGEN

The concentration of atomic hydrogen becomes significant much later than the maximum methyl radical concentration. After 1.70 sec, atomic hydrogen as shown in Figs. B-5 and B-6, has an apparent two branch curve. The first branch occurs at 0.90 sec., when the methyl radical concentration is at maximum. However, following that time the concentration continues to grow at a rate of $9 \cdot 10^{-9}$ cm³/gm²/sec.

Figures B-33 and B-34 confirms these observations, by showing an isolated high production rate, fourteen orders

of magnitude above the baseline.

6.3.3 WATER

Water starts forming after 0.915 sec. at 27.44 cm into the flame, when the concentration starts increasing as shown in Figs. B-9 and B-10. Nevertheless, it is not until 0.154 sec. that the concentration of the water molecules makes its most significant gains. The water concentration reaches a maximum at 1.1033 seconds. Figures B-37 and B-38 show that, in the post-flame reaction zone water molecules starts decomposition at very low rate.

6.3.5 CARBON MONOXIDE

The concentration of carbon monoxide becomes significant after 0.87 sec. at 26.12 cm. The concentration starts rising at $1.48 \cdot 10^{-6}$ $\text{cm}^3/\text{gm}^2/\text{sec}$ after 1.04 sec, at 31.425 cm distance as shown in Figs. B-11 and B-12. After reaching a maximum rate of $2.5 \cdot 10^{-7}$ $\text{cm}^3/\text{gm}^2/\text{sec}$ it starts declining, to reach near zero concentration at 1.1033 seconds.

The return curve between the maximum and minimum concentrations is almost vertical, showing a very thin radical recombination zone. Oxidation of CO in this region is achieved through combination with hydroxyl radicals. These findings are further displayed by Figs. B-15 and B-14 showing CO₂ concentration profiles.

6.3.6 ATOMIC OXYGEN

Atomic oxygen starts production only towards the end of the reaction zone. Figures B-83 and B-84 suggests atomic oxygen concentration remains small, until 0.9 sec, but then increases to its maximum at the end of the reaction zone. Such results are demonstrated by the four order of magnitude increase in production rate, as shown in Figs. B-41 and B-42.

6.3.7 CARBON DIOXIDE

At ignition, 1.067 sec and 32.0 cm, the temperature is 1109 K and the concentration of CO₂ is 1.43×10^{-9} cm³/gm²/sec. However with the rise of temperature to 1147 K the concentration increases by 40 % as shown in figs. B-15 and B-16. However, CO₂ forms mainly at the

end of the reaction zone. The production of 3×10^{-7} moles/ cm^3 occurs at the 1.1 sec. in less than 0.3 msec (Figs. B-43 and B-44) time.

6.3.8 FORMALDEHYDE

Seen in the Fig. B-23 and B-24, the concentration of CH_2O species rises sharply after 0.817 sec. At 24.5115 cm, i.e. before ignition, it reaches a maximum at 0.991 sec. and then starts decaying, to a minimum at the end of the reaction zone.

The concentration of is 2.115×10^{-11} moles/ cm^3 at 33.42 cm and 1750 K. It then starts decreasing at 33.44 cm when the temperature is 1989 K and the concentration is down by one order of magnitude to 4.09×10^{-12} moles/ cm^3 .

6.3.9 MOLECULAR HYDROGEN

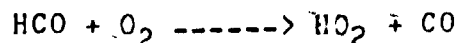
Concentration profiles of molecular hydrogen are shown in Figs. B-21 and B-22. The high rate of formation toward the reaction zone and high rate of depletion at the end of the reaction zone are indicated. Again, the double

humped concentration profile appears. Furthermore, the concentration profile suggests that there may be a 0.05 sec. wide molecular hydrogen plateau.

6.3.10 HYDROGEN PEROXIDE

Figures B-23 to B-24 suggest the HO_2 concentration rises comparatively slowly for the first 0.824 sec., at $1 \cdot 10^{-10} \text{ cm}^3/\text{gm}^2/\text{sec}$ (Figs. B-51 and B-52), and then rises at a two order of magnitude higher rate. It reaches a maximum at 0.824 sec. and 28.911 cm. and next the concentration starts decreasing.

It is noted here, that the reaction 22



becomes abnormally fast. At 33.40 K and 1626 K, there is a significant decrease in HO_2 concentration, indicating the beginning of the radical recombination zone.

6.3.11 FORMYL

The concentration profiles for formyl radicals are shown in Figs. B-25 and B-26. The concentration rises toward the reaction zone and then continues to a maximum at 1.087. After an additional 0.0139 seconds, it reaches a minimum at the end of the reaction. This shows that reactions consuming HCO radicals accelerate after 1.1033 seconds. Figures also suggest the high rate of depletion of HCO radicals at 1.1033 seconds.

6.3.12 NITROGEN

The nitrogen concentration does not change; since nitrogen is not involved in any of the reactions. However, changes in mole fraction appear as an artifact because the total number of particles in the system change as a result of the reactions. This appears in Figs. B-27 and B-28.

6.3.13 MOLECULAR OXYGEN

Concentration profiles Figs. B-17 and B-18 are

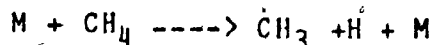
similar to concentration profiles of methane. Concentration of oxygen drops to $5.399 \cdot 10^{-7}$ from $2.438 \cdot 10^{-6}$ moles/cm³ at the end of the radical recombination zone.

Figures B-45 and B-46 show high depletion rates of oxygen at ignition.

6.4.0 REACTION HISTORIES

The reaction calculation results are compiled in Appendix C.

6.4.1 REACTION # 1

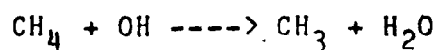


This is the initiating step. It represents the pyrolysis of methane, generating CH_3 and H radicals. This equation is fundamental, since no reaction can occur unless atomic hydrogen is produced. This is because atomic hydrogen frees the atomic oxygen required for subsequent reactions. A similar role is also played by the methyl radical produced, although the effective rate constant in methyl reactions is three orders of magnitude lower.

The reaction's conversion rate, initially at 3.16×10^{-6} $cm^3/gm^2/sec.$, increases very slowly over a

temperature rise of magnitude 0.01 K. However, as soon as the temperature increases by 0.50 K, the reaction reverses with a conversion rate of $11.9 \text{ cm}^3/\text{gm}^2/\text{sec}$.

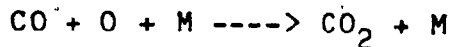
6.4.2 REACTION # 2



This reaction is responsible for 90% of the methyl radical and water molecule production, in the induction and reaction zones, and so is the major route for such production. When some CH_3 radicals and atomic hydrogen are produced oxygen molecules later react with methyl radicals and atomic hydrogen, producing hydroxyl groups, which later react with methane molecules as the step suggests.

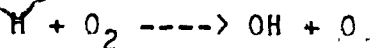
The reaction becomes faster in the radical recombination zone with a rate of $519 \text{ mole-cm}^3/\text{gm}^2/\text{sec}$ It then decreases in the post flame reaction to $9.5 \cdot 10^{-18} \text{ mole-cm}^3/\text{gm}^2/\text{sec}$.

6.4.3 REACTION # 3



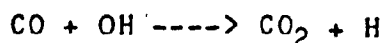
Reactions 3 and 5 produce carbon-dioxide. Reaction 3, in particular, is a very slow reaction, with the very low conversion rate of about 1.079×10^{-7} mole-cm³/gm²/sec, in the induction zone. In the main reaction zone, reaction 3 reverses and starts decomposing the carbon dioxide at a rate of 1.0×10^{-6} mole-cm³/gm²/sec. The computations show, however, that this reaction does not play an important role in methane/air combustion.

6.4.4 REACTION # 4



Ten reactions produce hydroxyl radicals. This reaction moves fast, reaching a maximum rate of about 76,200 mole-cm³/gm²/sec, as the temperature increases, and then starts slowing down in the post flame reaction zone. Finally, it reverses direction and starts decomposing hydroxyl radicals at 0.7 mole-cm³/gm²/sec.

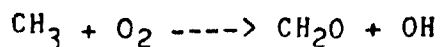
6.4.5 REACTION # 5



More than 99 % of the CO_2 production occurs by this reaction. Indeed, in the reaction zone, its carbon dioxide production rates are much higher than those of reaction 3.

Its rate increases with temperature and reaches about 12000 mole-cm³-gm²/sec maximum, at the end of radical recombination zone. In the post flame reaction, the reaction reverses.

6.4.6 REACTION # 6

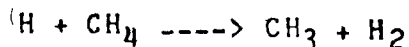


Formaldehyde is produced by reactions 6 and 14. However, reaction 6 dominates, and is the major formaldehyde producing step, accounting for more than 95 % production.

This reaction is fastest in the temperature range of

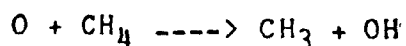
1626-2103 K. After 2103 K the reaction becomes slow.

6.4.7 REACTION # 7



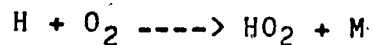
In the early stages of the induction zone, this reaction generates methyl radicals at the low rate of $1.87 \cdot 10^{-6}$ mole-cm³/gm²/sec, lower than that of reaction 1. However, part way through the flame the reactions starts regenerating CH₄ and in the post flame reaction zone it again moves forward.

6.4.8 REACTION # 8



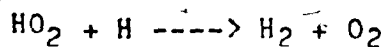
This reaction has a conversion rates in the induction zone of 2.845 mole-cm³/gm²/sec. However, the rate increases in the flame reaction zone, in the temperature range of 1043-1626 K, to 91 mole-cm³/gm²/sec, about a factor of 30. In the post flame reaction zone, reaction 8 slows down considerably to $1.56 \cdot 10^{-18}$ mole-cm³/gm²/sec.

6.4.9 REACTION # 9



Both reaction 9 and 22 produce HO₂ at the slow rate of 7.32*10⁻⁹ mole-cm³/gm²/sec in the temperature range 1000-1001 K. Then, its conversion rate rises to 5.32*10⁻² mole-cm³/gm²/sec, in the temperature range of 1001-1630 K subsequently slowing down. In the post flame reaction zone, the reaction decomposes HO₂ groups at the rate of 3.55*10⁻⁷ mole-cm³/gm²/sec.

6.4.10 REACTION # 10



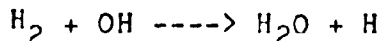
This reaction decomposes HO₂ groups, in the temperature range of 1000-1001 K. In the flame reaction zone, it reverses to start generating HO₂. Finally, in the post flame reaction zone, it again decomposes the HO₂ groups.

6.4.11 REACTION # 11



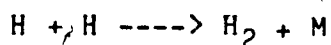
This reaction does not play an important role in induction zone, but it speeds up to a rate of 69.49 mole-cm³/gm²/sec, as the temperature increases. The rate then increases in the flame reaction zone over the temperature range of 1220-1626 K. Finally, at the end of the reaction zone it slows down to 0.29 mole-cm³/gm²/sec. In the post flame reaction zone reaction 11 reverses.

6.4.13 REACTION # 12



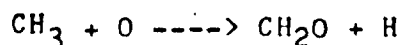
This reaction is slow in the induction zone, but speeds up after ignition, in the temperature range of 1109-1626 K. It reaches a maximum rate of 1349.98 mole-cm³/gm²/sec at 1989 K and 33.44 cm, and then reverses, operating at the rate of 0.8215 mole-cm³/gm²/sec at 2103 K. Finally in the post flame zone, it again starts to proceed forward at 3.95*10⁻³ mole-cm³/gm²/sec, to the end of the flame.

6.4.13 REACTION # 13



This reaction has a low conversion rate of $4.97 \cdot 10^{-19}$ mole-cm³/gm²/sec. These rates suggests that the reaction is not playing an important role in methane-air kinetics. In the high temperature range of 1042-2103 K, however, its rate improves to $2.70 \cdot 10^{-5}$ mole-cm³/gm²/sec.

6.4.14 REACTION # 14



This reaction produces 90 % of the CH₂O species, although it is a slow reaction initially. However, the reaction becomes important in the temperature range of 1626-1989 K, with the rate of 711 mole-cm³/gm²/sec. After the increase of temperature to 1989 K, reaction 14 reaches the maximum rate of 711 mole-cm³/gm²/sec then slows to $10.3 \cdot 10^{-16}$ mole-cm³/gm²/sec.

In the post flame reaction zone, reaction 14/reverses and starts decomposing the HCO groups.

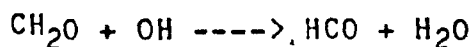
6.4.15 REACTION # 15



This reaction begin slowly with a rate of 0.29 mole-cm³/gm²/sec, but reverses in the post flame reaction zone.

Conversion rates show its insignificant role at the lower limits, producing only about 1% of the HCO molecules in the reaction zone.

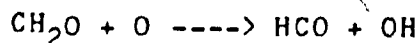
6.4.16 REACTION # 16



Reaction 16 is fast both in the induction and the flame reaction zones. In the induction zone its rate is 0.08 mole-cm³/gm²/sec, but in the flame reaction zone its rate increases very steadily and reaches at maximum of 44.4 mole-cm³/gm²/sec at 1989.38 K. There is a tremendous

reduction in its speed, as the reaction continues in the post flame reaction zone.

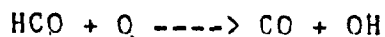
6.4.17 REACTION # 17



This reaction is slower than reaction 16. with increases of temperature. In particular, its speed increases to a maximum of about 1.1909 mole-cm³/gm²/sec, in flame reaction zone. Then, in the radical recombination zone its speed decreases by 10 orders of magnitude to 2.34*10⁻⁹ mole-cm³/gm²/sec, where it reverses direction and starts decomposition of HCO radicals.

Its low reaction rate suggests that reaction 17 is not important to the overall problem at hand.

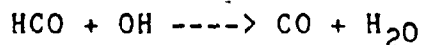
6.4.18 REACTION # 18



This reaction is slow in induction, flame reaction and post flame reaction zones. Its maximum conversion

rate is 0.654 mole-cm³/gm²/sec, which is among the lowest of all reaction considered. It produces very small amounts of OH and CO species (less than 1.5 %).

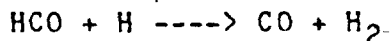
6.4.20 REACTION # 19



This reaction is also slow: the effect of temperature on the speed of this reaction is negligible. At the end of flame reaction zone, its rate becomes 1.552 mole-cm³/gm²/sec. It reverses its direction in radical and post flame reaction zones.

It produces less than 0.5 % of CO and H₂O in the system.

6.4.20 REACTION # 20



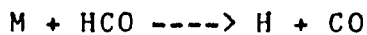
This is a slow reaction, when compared to the very slow rates of reaction 1. In the induction zone, however, its conversion speed exceeds that of reaction 1 as

temperature increases to 1229 K, thus causing the atomic hydrogen produced by reaction 1 to be consumed rapidly. In the temperature range 1626-1989 K the reaction again becomes slow.

In the radical recombination and flame reaction zones, reaction 20 has a rate of $4.3 \cdot 10^{-12}$ mole-cm³/gm²/sec and does not reverse in the post flame reaction zone.

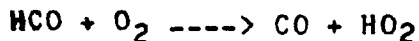
It is so slow, that reaction 12 produces less than 0.1 % of the H₂ and CO in the different zones.

6.4.21 REACTION # 21



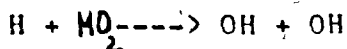
This reaction is also slow. However, its rate increases through the flame and reaches a maximum with conversion rate of 0.566 mole-cm³/gm²/sec, at the end of the reaction zone. It also reverses direction in radical recombination zone, and in the post flame reaction zone, it starts forward again.

6.4.22 REACTION # 22



This is the fastest HCO group destroying reaction. It is also very temperature sensitive. In the flame reaction zone, it increases speed by five order of magnitude to a maximum of 43.19 mole-cm³/gm²/sec at 1989 K. In the radical recombination zone, it reverses direction and decomposes the CO and HO₂ species.

6.4.23 REACTION # 23

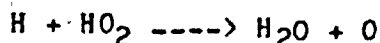


Reaction 23 is slow in the induction zone, but the conversion rate increases as ignition is approached. At ignition there is a sharp rise in its conversion rate. The conversion rates reaches a maximum of 5.44 mole-cm³/gm²/sec in the flame reaction zone. However, in the radical recombination zone, the rate drops down to 0.0405 mole-cm³/gm²/sec.

In post flame reaction zone the reaction reverses

direction and ~~states~~ producing HO₂ species at a rate of
1.578*10⁻⁴ mole-cm³/gm²/sec.

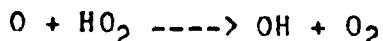
6.4.24 REACTION # 24



This reaction speeds up in the ignition temperature range of 1009.48-1147 K. Then in the temperature range of 1229-1989.38 K it also show a significant rise, reaches to 1.74 mole-cm³/gm²/sec. Then, in the radical recombination zone, reaction 24 slows down and indeed in the post flame reaction zone the direction is reversed.

It is important to note that the contribution of this reaction is significant in the kinetics at the lower limit.

6.4.25 REACTION # 25



This reaction proceeds in reverse, in the early portion of the induction zone. Through the flame, with the rise of temperature, its rate of conversion increases toward the flame reaction zone; and through that zone, the reaction reaches to a maximum rate of 4.043

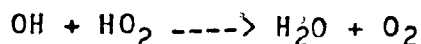
mole-cm³/gm²/sec.

In the radical recombination zone, reaction 25 starts producing HO₂ species at 0.027 mole-cm³/gm²/sec.

In post flame reaction zone it again proceeds forward.

This is an important reaction in the kinetic scheme, because of its high rates of conversion and energy exchange.

6.4.26 REACTION # 26

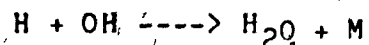


The behaviour of this reaction is similar to that of reaction 25, but faster.

In the early period of induction, this process decomposes water molecules. Then, as the temperature increases, it moves forward and its speed increases through-out the flame reaction zone. The maximum conversion rate of 30.266 mole-cm³/gm²/sec is attained in the flame reaction zone.

Reaction 26 reverses in the radical recombination zone, to shift direction again in the post flame reaction zone. (The complicated nature expected from this reaction should be verified in the laboratory.)

6.4.27 REACTION # 27



This reaction is slow: Its conversion rates are very low, attaining a maximum rate of 6.356×10^{-5} mole-cm³/gm²/sec in the flame reaction zone. After the flame reaction zone the reaction reverses direction. The conversion rates show that this reaction does not contribute much to methane-air kinetics at the lower limit.

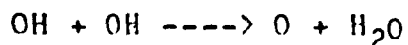
6.4.28 REACTION # 28



In the early portion of the induction period this reaction is slow. However, this is a significant reaction in the flame reaction zone, since it reaches a maximum

conversion rate of 6000 mole-cm³/gm²/sec at the end of the flame reaction zone. In the radical recombination zone however, its speed, reduced to 85.1 mole-cm³/gm²/sec is still high compared to other reactions. In the later post-flame reaction zone, it too reverses.

6.4.29 REACTION # 29



This reaction competes with reaction 23, since it consumes hydroxyl groups in the forward direction. It is slow in the early induction zone, however, as ignition is approached it changes direction and starts decomposing the water molecules present. This is one of the major hydroxyl group producing reactions.

The rate of reaction 29 reaches a maximum of 85.46 mole-cm³/gm²/sec in the flame reaction zone, but slows down in the radical recombination zone. Then, in the post flame reaction zone, it again starts producing water.

6.4.30 REACTION # 30



This reaction is very efficient. It has the high conversion rate of 6.28 mole-cm³/gm²/sec in the induction zone and increases to over 1200 mole-cm³/gm²/sec, in the flame reaction zone. In the radical recombination zone it has a value of 7.55*10⁻⁷ mole-cm³/gm²/sec and in the post-flame reaction zone it reverses direction and starts forming OH₂ groups. This reaction appears to be important in the kinetics at the lower limit.

7.0.0 CONCLUDING REMARKS

This study presents the flame structure for methane/air combustion at the lower flammability limit, using chemical kinetics calculations.

The Kinetic model is based on following assumptions:

1-Plug flow, i.e. no back mixing

2-There is no convective and radiative heat transfer.

3-There is no mass transfer by diffusion.

4-Flammability limits are independent of unburnt gas temperature.

5-Flame velocity is independent of unburnt gas temperature.

6-All third body ratios are unity.

The mixture initially at one atmosphere, 1000 K temperature with 5.3 % methane in air, is thermally preheated from 293 K to 1000 K and burns at a velocity of 30.0 cm/sec. This velocity falls in the laminar regime for the standard flammability tube, and permits an uncomplicated visualization of the non-back flow flame.

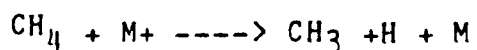
The 30.0 cm/sec velocity assumption is supported even though it is noted that flame velocity is dependent on the unburnt gas temperature, as mentioned earlier and at 1000 K the velocity using the Andrew and Bradley approach(42) has been calculated as 380 cm/sec.

For completeness, it is pointed out here that the lower limit of flammability decreases as the temperature of unburnt gas increases. Indeed, at 1000 K, the lower limit drops to 1.5 % methane.(52) Nevertheless, the 1000 K was selected at 5.3 % since significant reactions do not occur without preheat. However, on the application of these conditions to the system, it is observed that length of the induction period is in the range of minutes, and flame width becomes enormously large.

The study shows methane is oxidized by a straight

chain with production of comparable stable intermediates. The oxidation step, although key to initiation, may also become significant, since it is capable from time to time of starting the fresh methane chains. Indeed, the initial step serves as a seed to the overall process.

In detail, the pyrolysis reaction



is the major initiating step.

Reaction 2 is responsible for 90 % of methyl radicals and water molecules production.

Reaction 3 has low conversion rates, which indicates its unimportant role in kinetics.

Reaction 4 has the highest conversion rate in the flame reaction zone.

Reaction 5 is responsible for 99 % of the CO_2 production.

Reaction 6 becomes significantly fast in the temperature range of 1626-2103 K and at 2103 K it becomes slow.

Reaction 7 consumes methyl radicals, in the flame reaction zone.

It is noted that the reaction 24 is significant in the kinetics at the lower limit.

Reaction 26 should be studied in the laboratory as it changes its direction quickly in the different zones of the the flame.

Reaction 27 does not contribute much to the kinetics at the lower limit.

Reaction 28 is a significant reaction in the flame reaction zone.

Reaction 29 is the one of major hydroxyl group producing reaction.

Reaction 30 is very efficient: it has high conversion rates.

Based on this study of the thirty reaction steps, it can be concluded that reactions 3 and 27 can be neglected for 1000 K kinetics, if desired, while equations 1,2,4,5,7,24,26,28,29 and 30 should always be present. Using only the 10 important reactions could produce a simple kinetic scheme which could be used in a model where some of the simplifying assumptions used here have been

relaxed.

Finally, this study should be extended by a detailed experimental effort examining the flame structure.

APPENDIX A

REACTIONS AND KINETIC DATA

	FRE.	FAC.	N	ACT.	ENG.
$M + CH_4 = CH_3 + H$	1.00E+18	0.		88400.	

BOWMAN, C.T.

REFERENCE 32

$CH_4 + OH = CH_3 + H_2O$	2.20E+13	0.		2500.	
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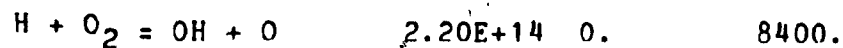
UNIVERSITY OF LEADS, NOV.. 1975.

$CO + O = CO_2 + M$	3.60E+12	-1.		1300.	
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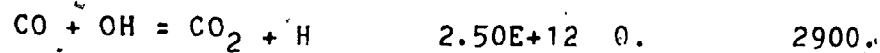
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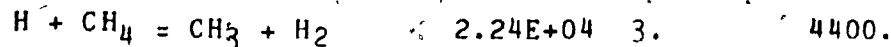


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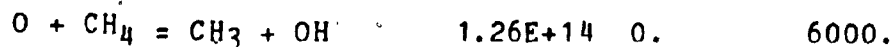
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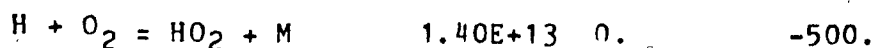
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869 882, 1972

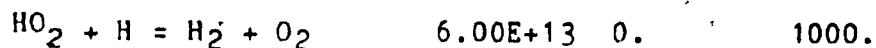


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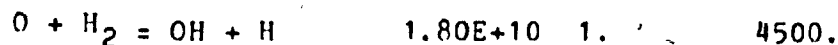
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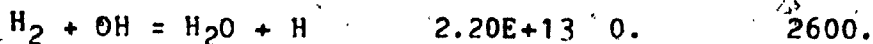


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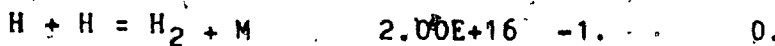


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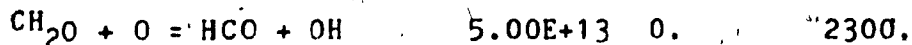
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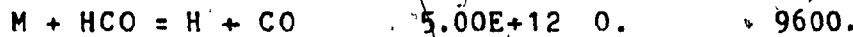


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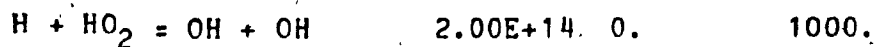


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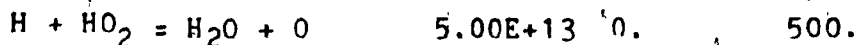
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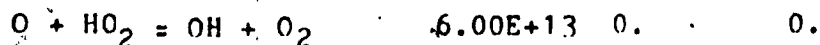


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SAME AS ABOVE

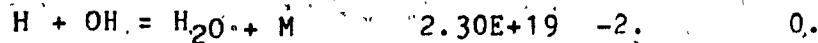


PEETERS, J.M AND MAHNEN, G.

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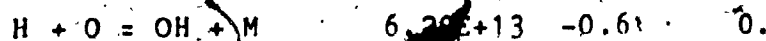


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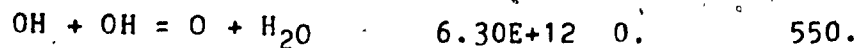
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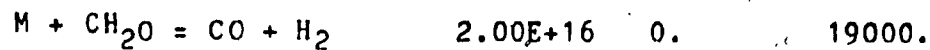
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BUTTERWORTH, LONDON, 1972.



PEETERS AND MAHNEN.

FOURTEENTH SYMP. INT. ON COMBUSTION 133-146, 1973

UNITS=MOLE, CM, SEC.

FIGURE D-1 NAME CH4
CONCENTRATION (MOLES/CM**3) VS TIME

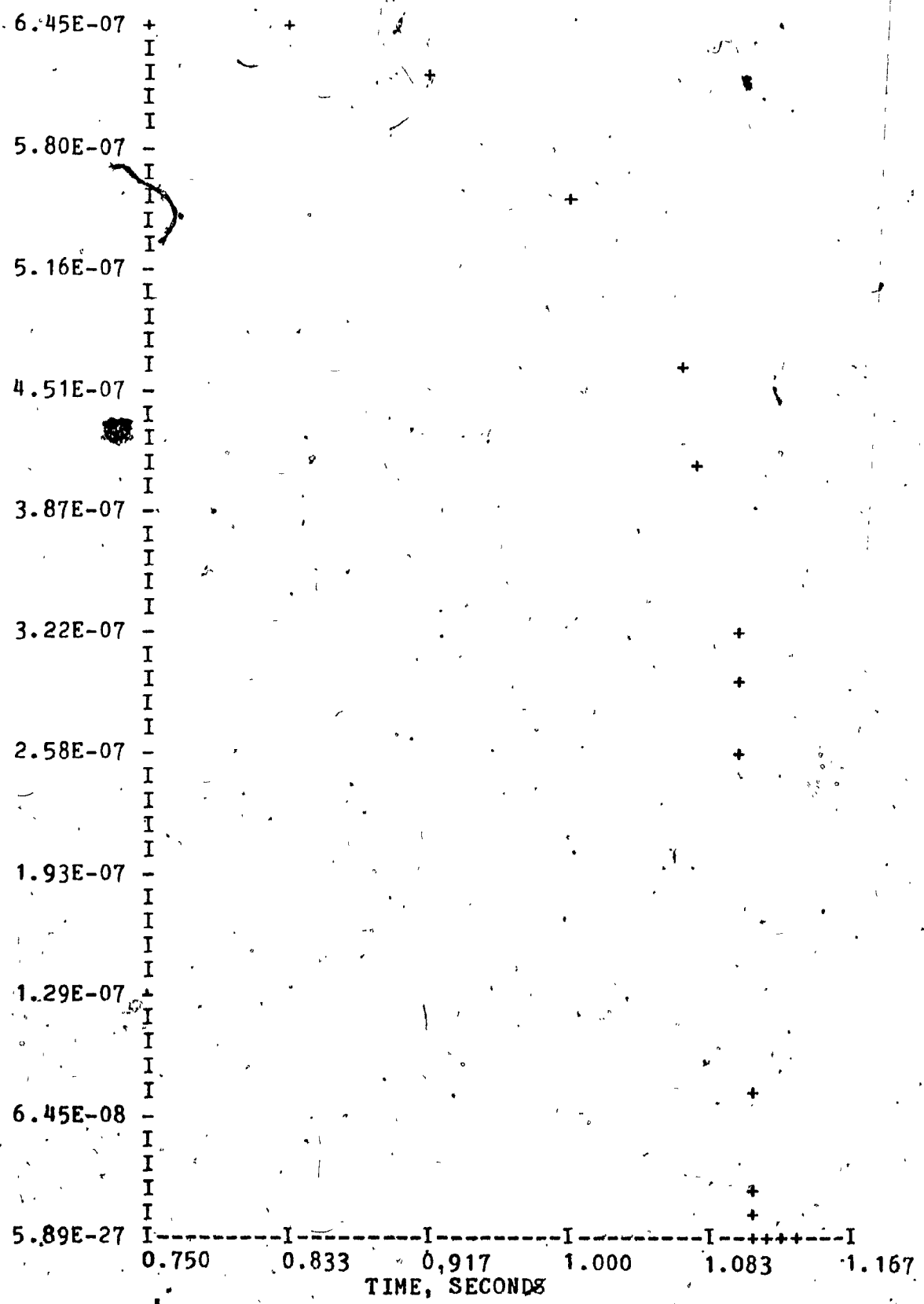


FIGURE B-2 NAME CH4
CONCENTRATION (MOLES/CM**3) VS DISTANCE

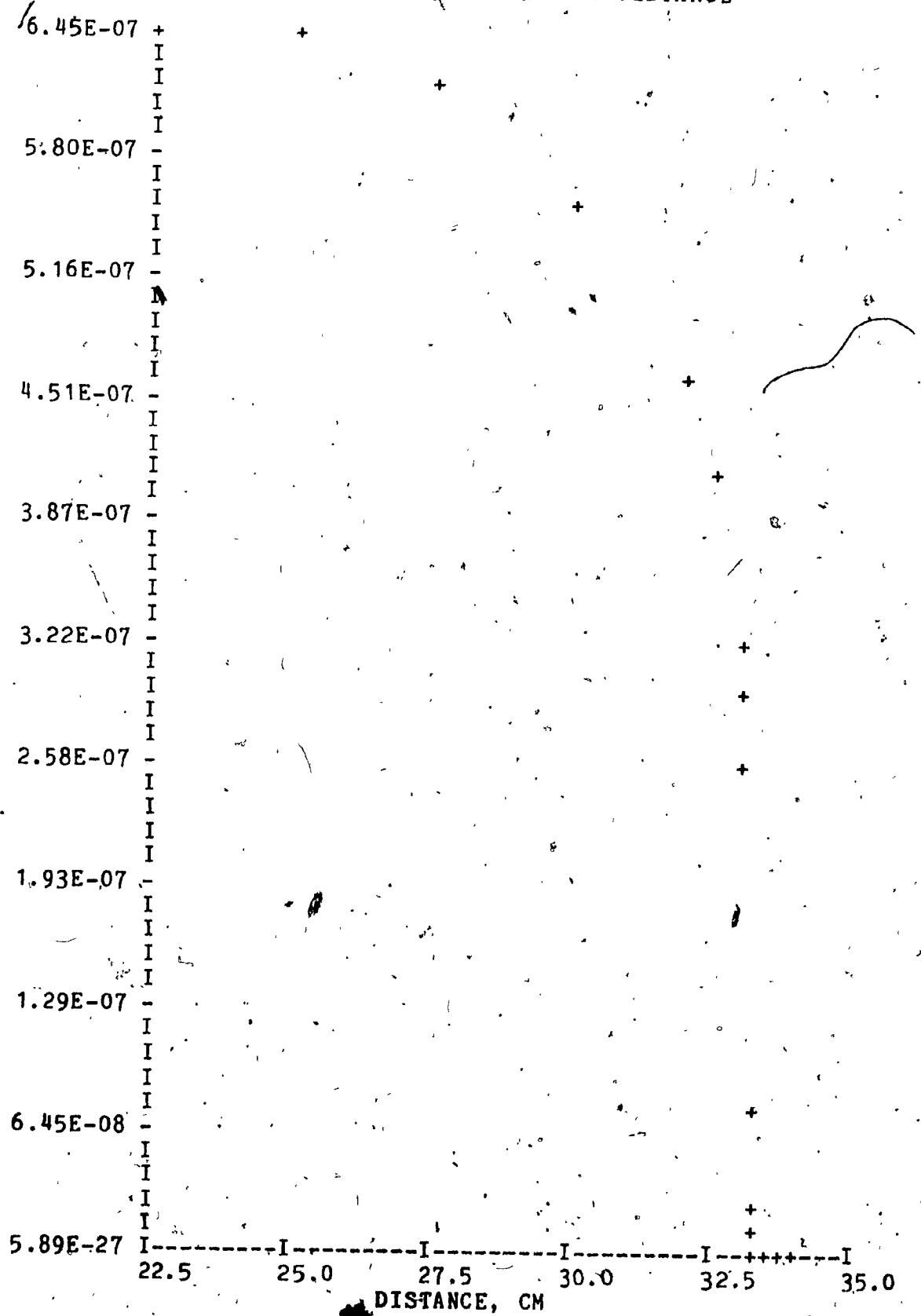


FIGURE B-3 NAME CH3
 CONCENTRATION (MOLES/CM**3) VS TIME

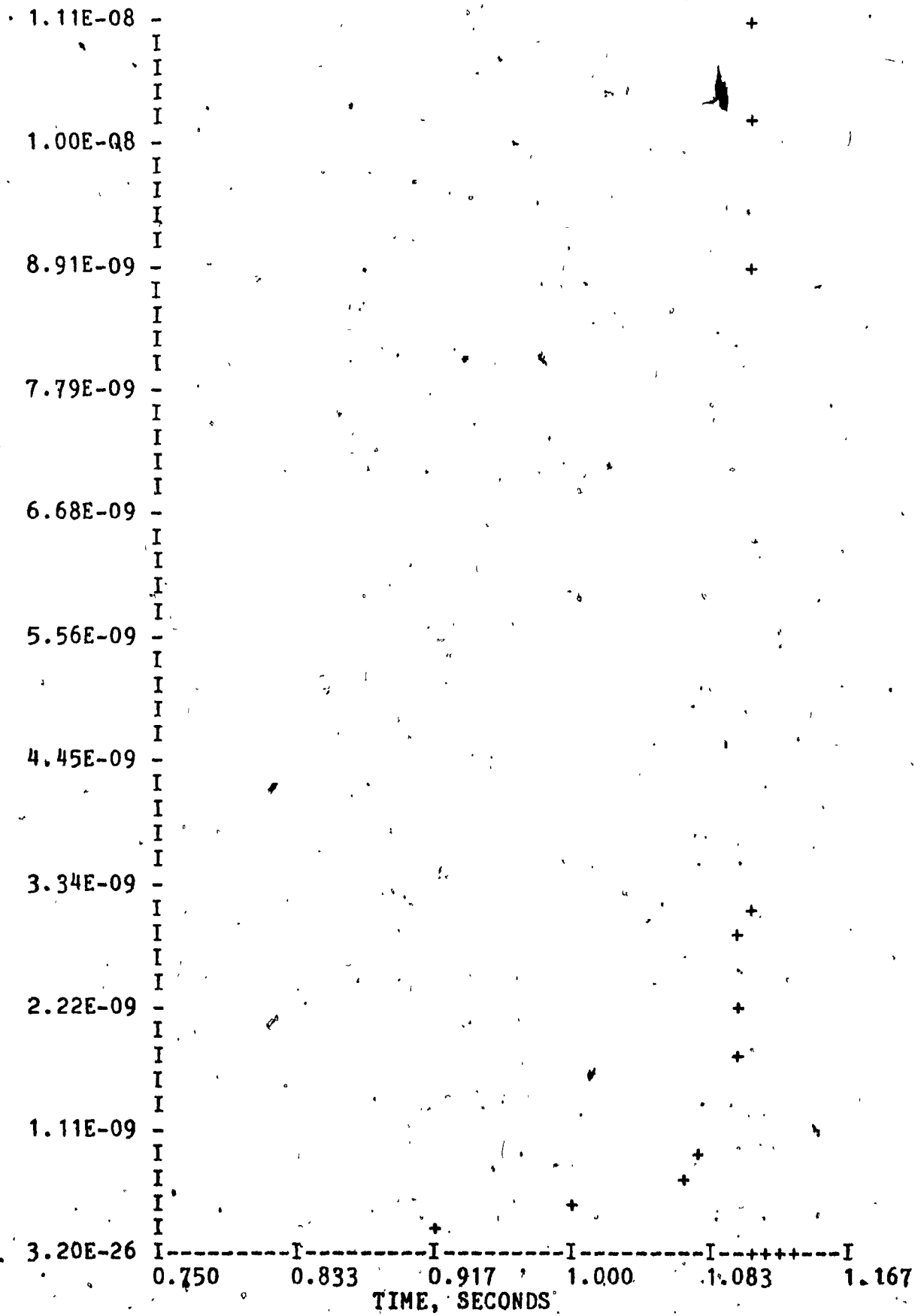


FIGURE B-11

NAME CH3

CONCENTRATION (MOLES/CM**3) VS DISTANCE

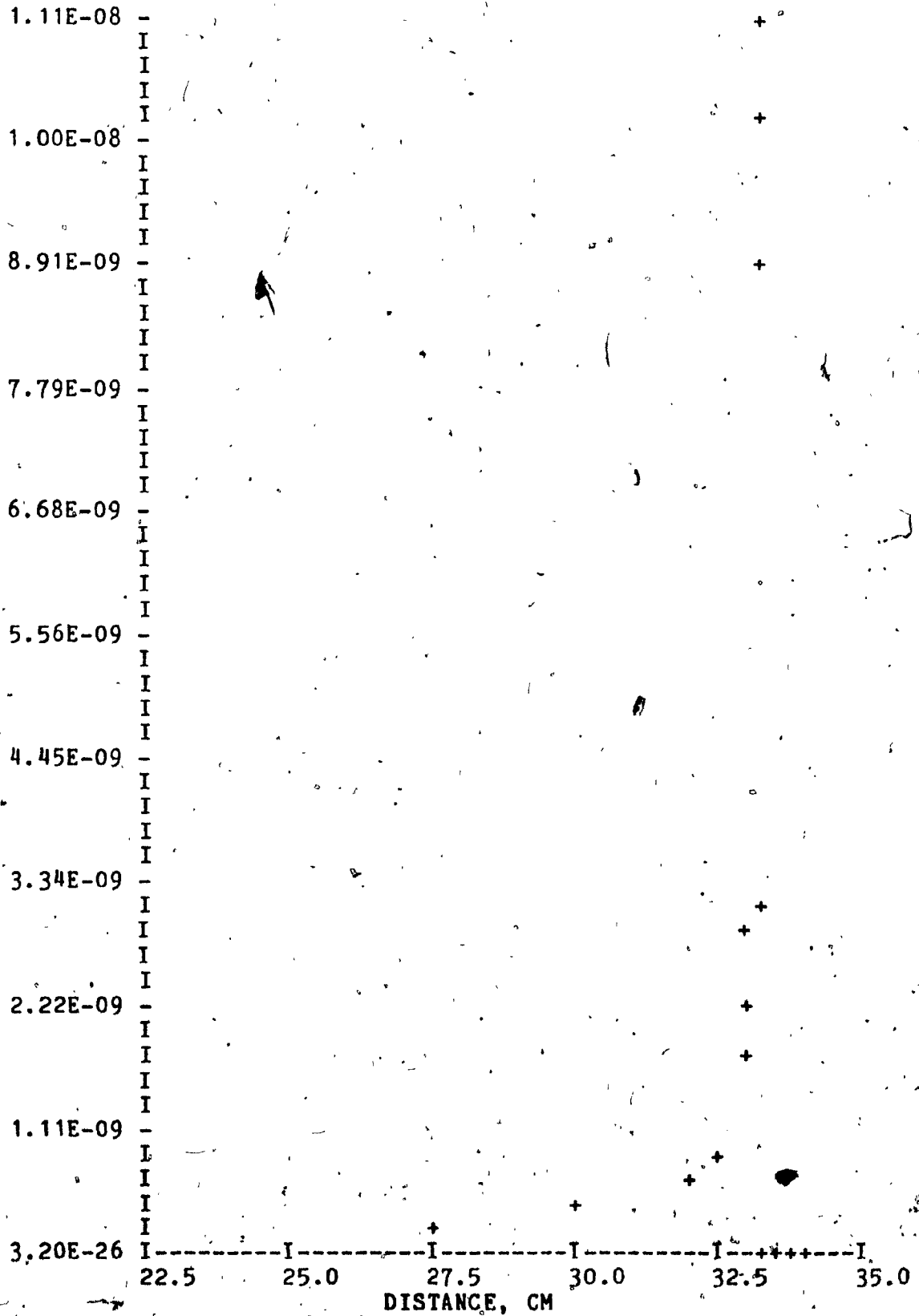


FIGURE B-5 NAME H
 CONCENTRATION (MOLES/CM**3) VS TIME

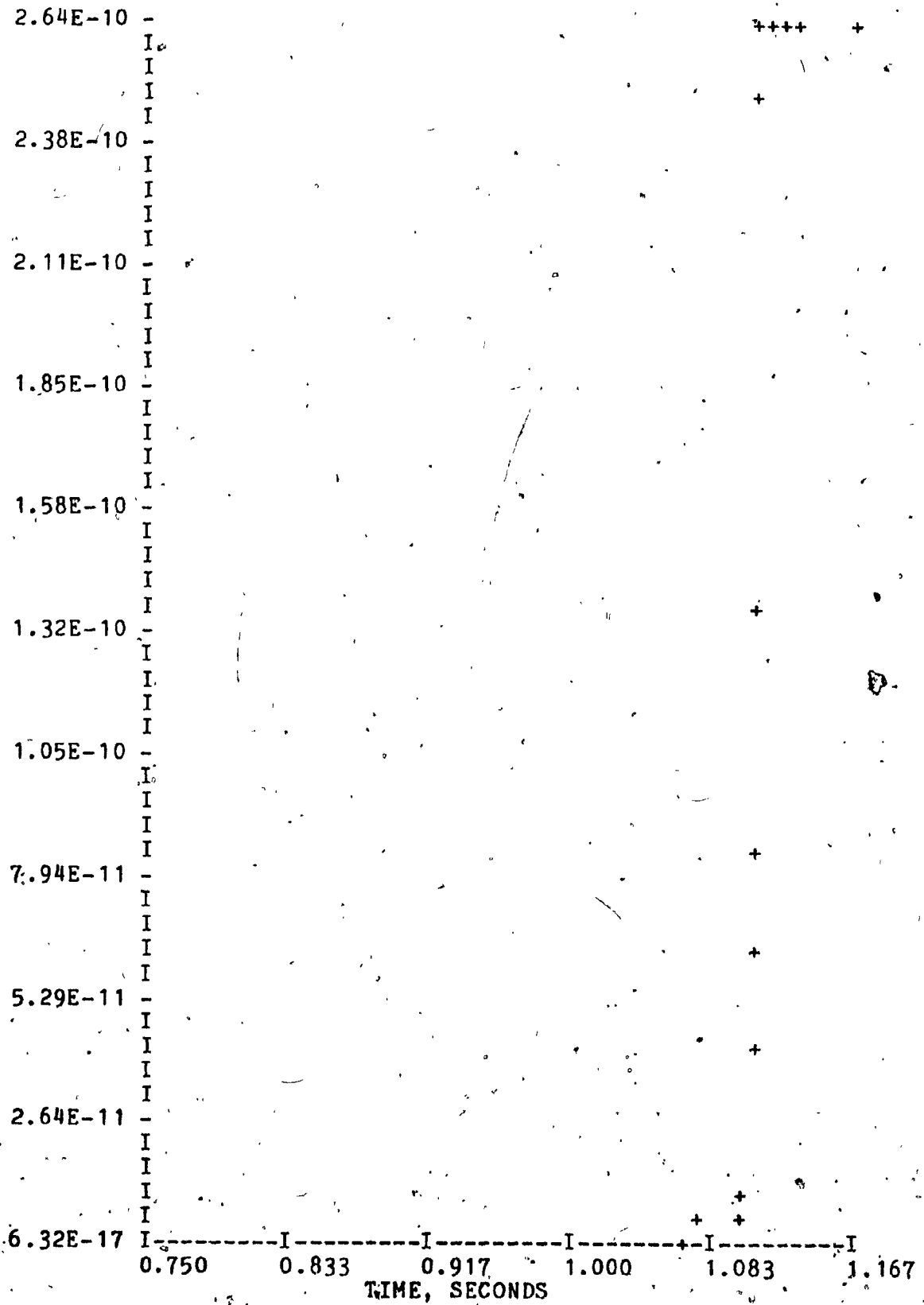


FIGURE B-6 NAME H
CONCENTRATION (MOLES/CM**3) VS DISTANCE

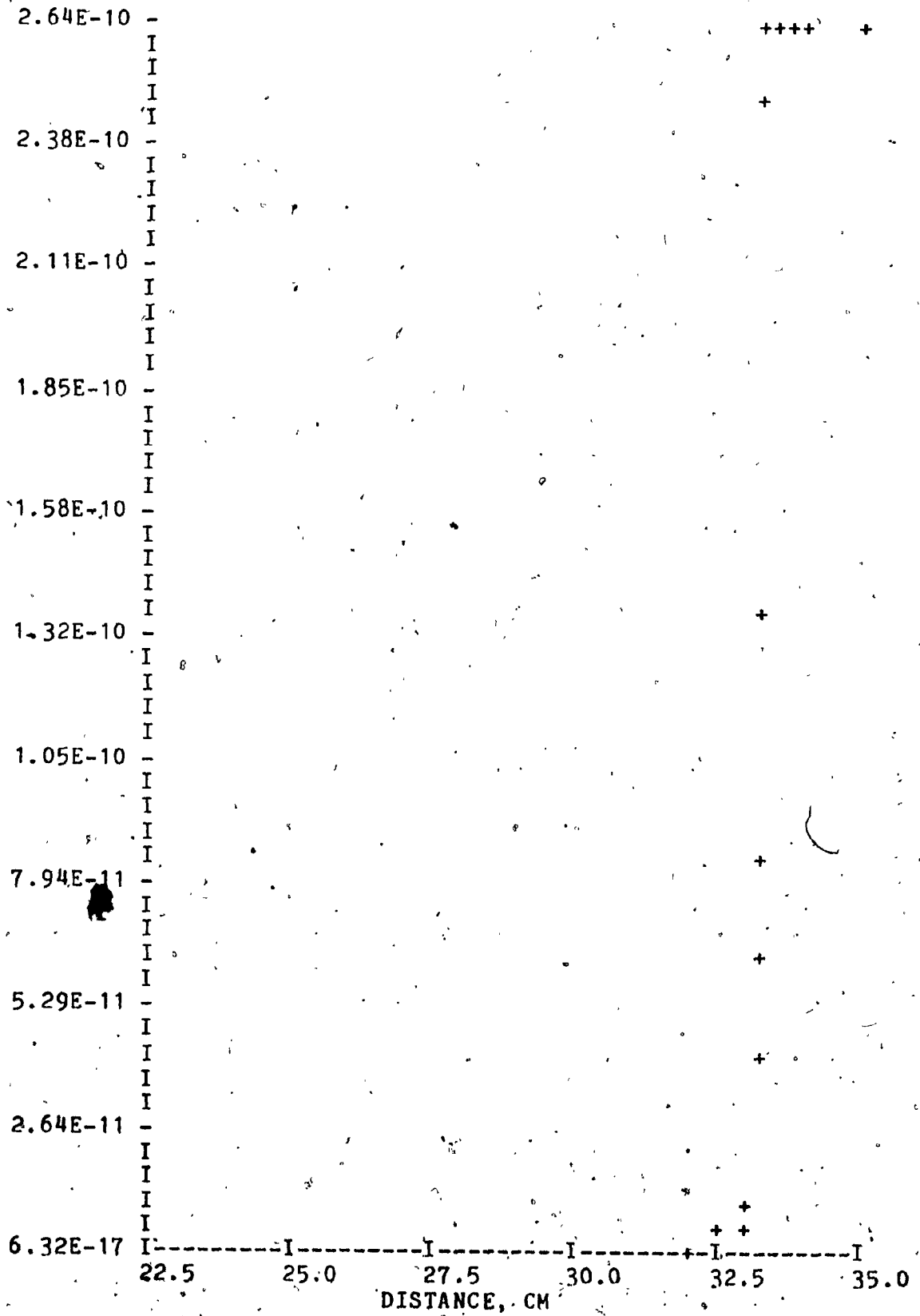


FIGURE B-7 NAME OH
 CONCENTRATION (MOLES/CM**3) VS TIME

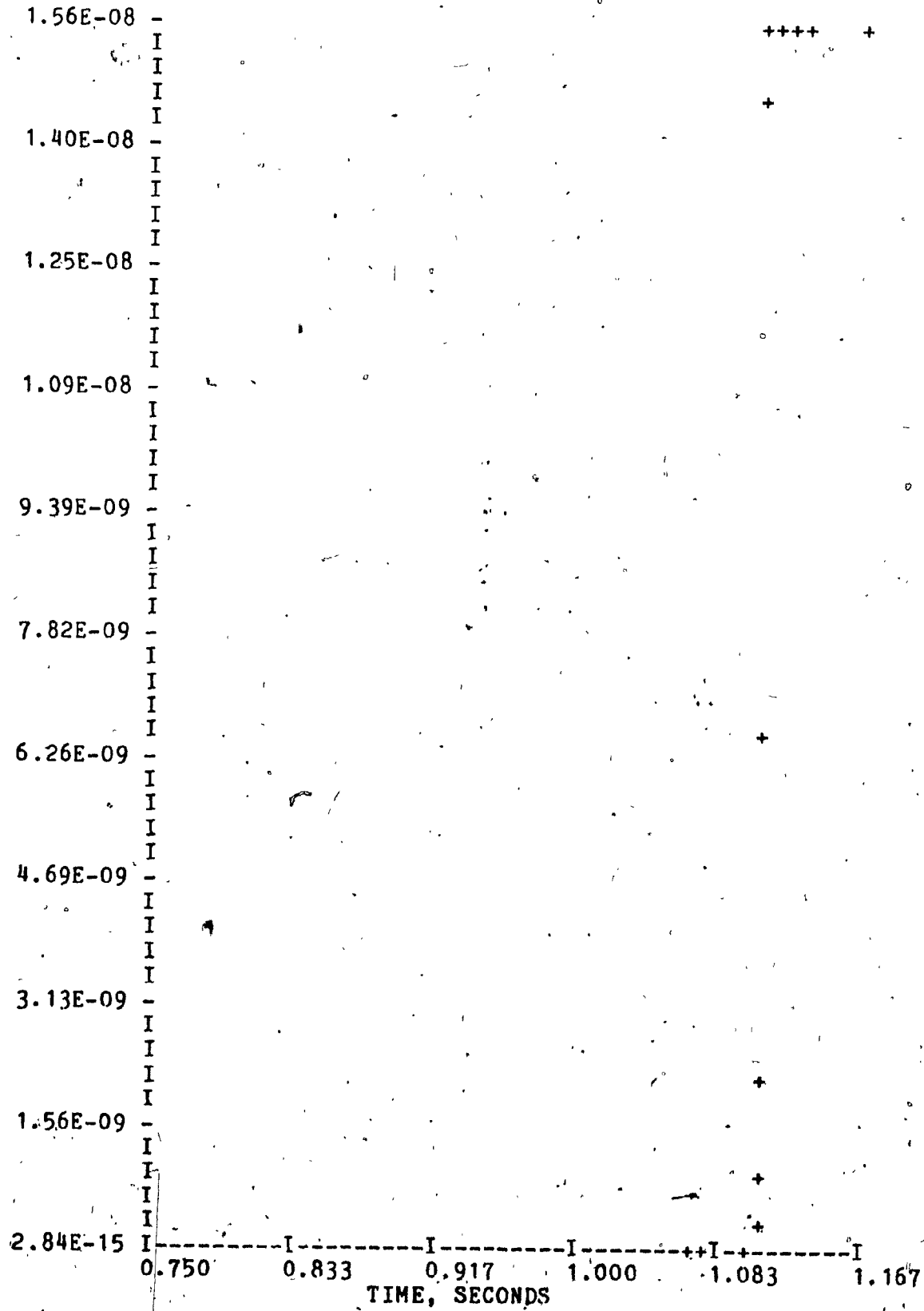


FIGURE B-8 NAME OH
 CONCENTRATION (MOLES/CM**3) VS DISTANCE

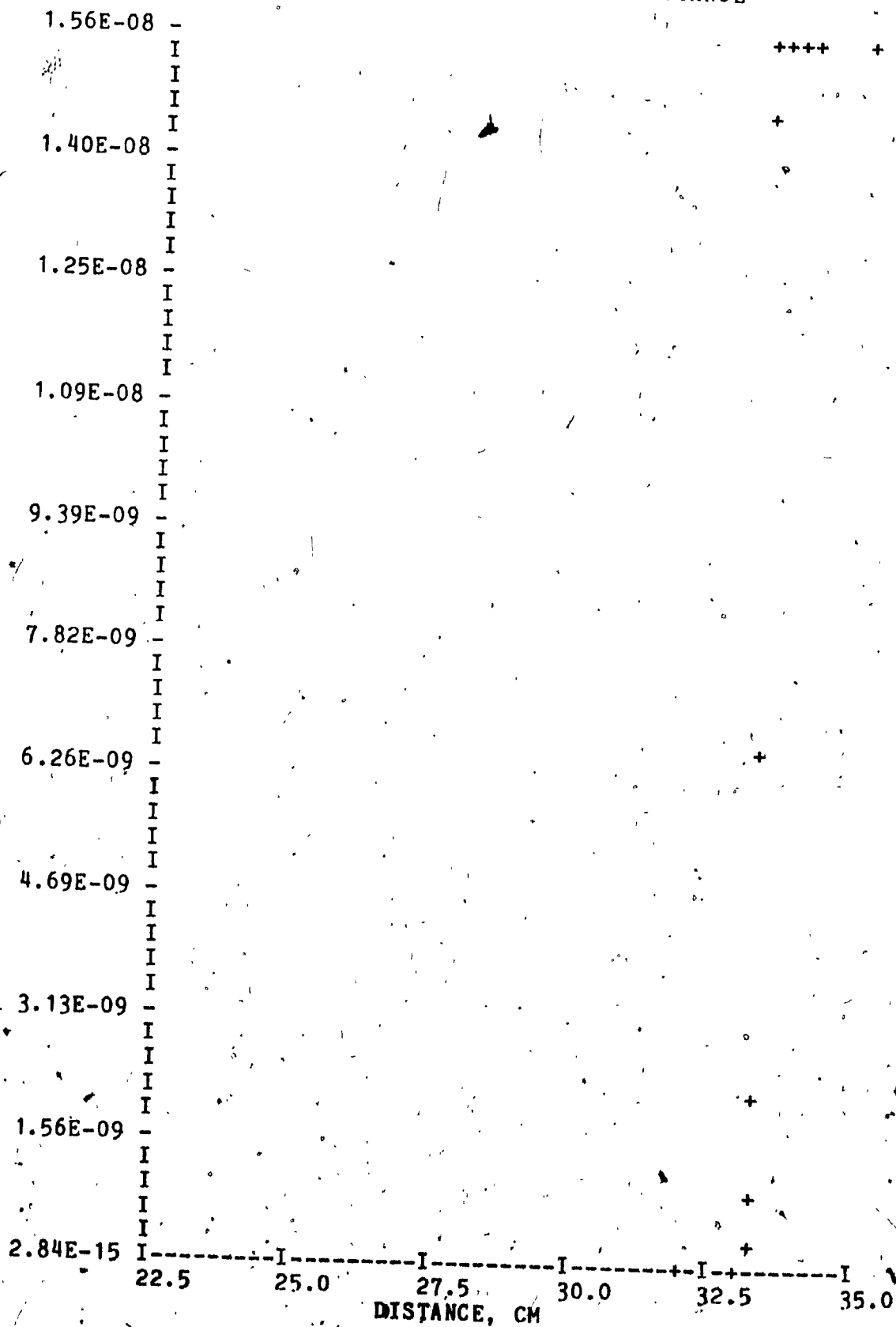


FIGURE D-9 NAME H₂O
 CONCENTRATION (MOLES/CM³) VS TIME

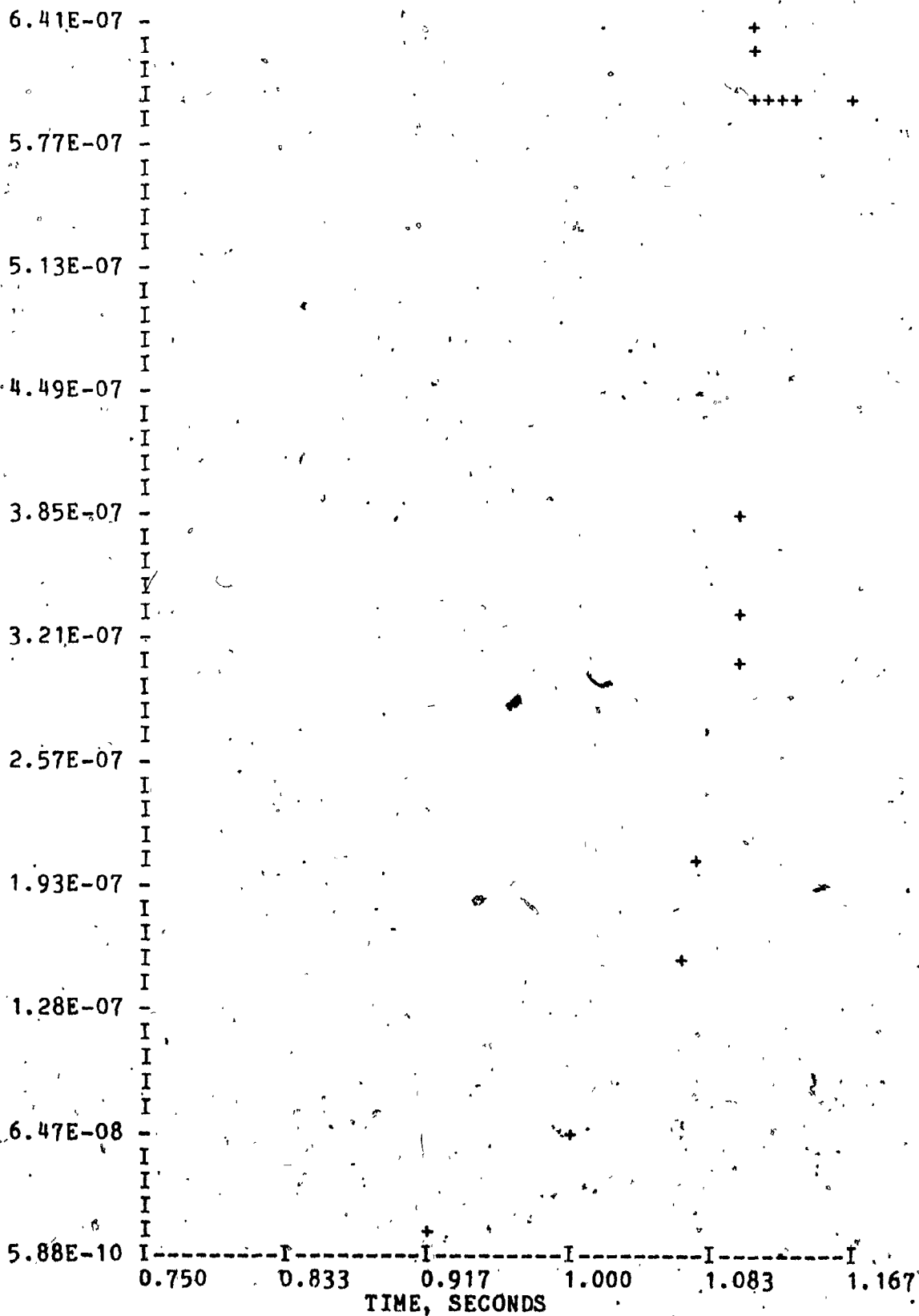


FIGURE B-10 NAME H2O

CONCENTRATION (MOLES/CM**3) VS DISTANCE

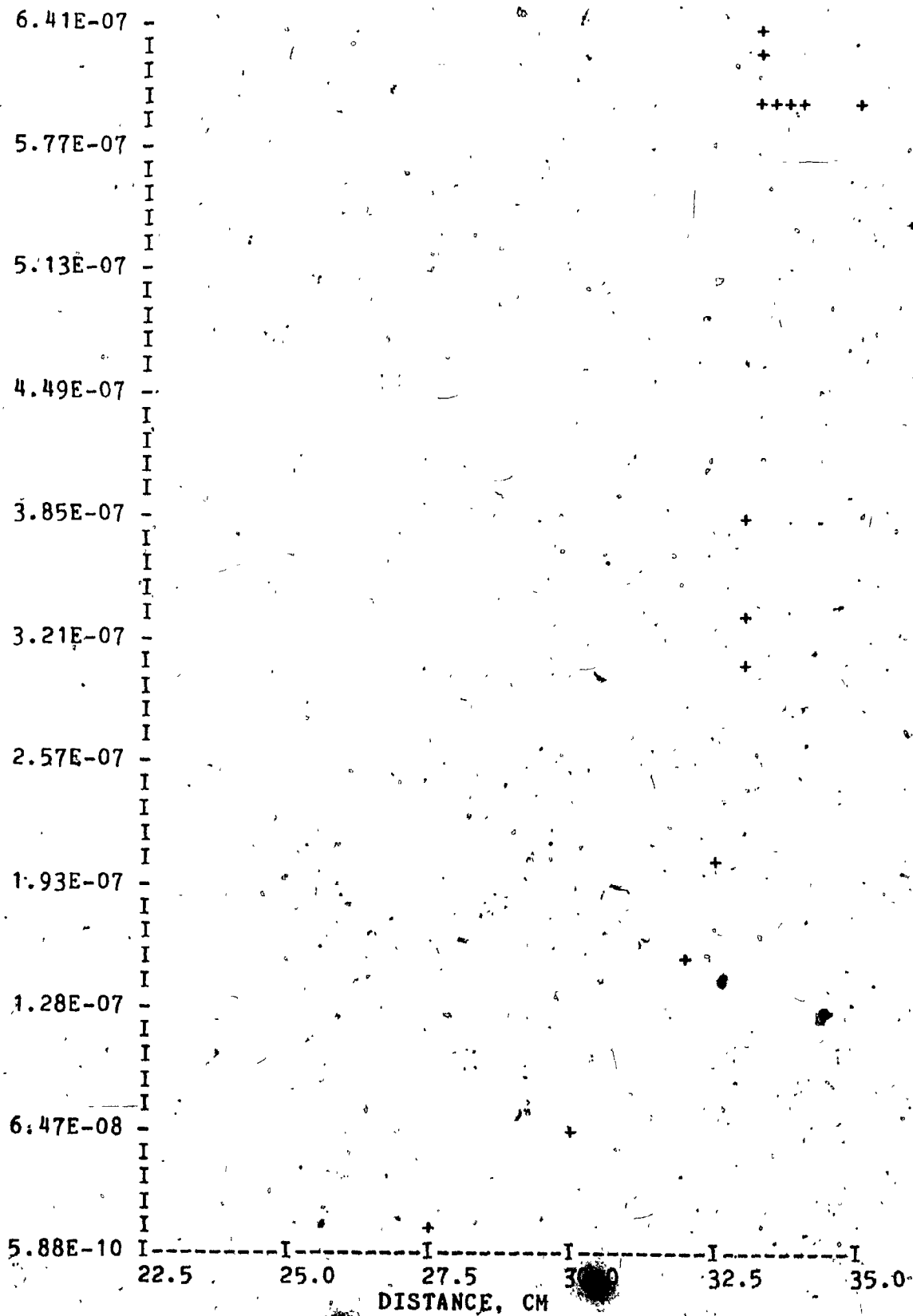


FIGURE D-11

NAME CO _____

CONCENTRATION (MOLES/CM³) VS TIME

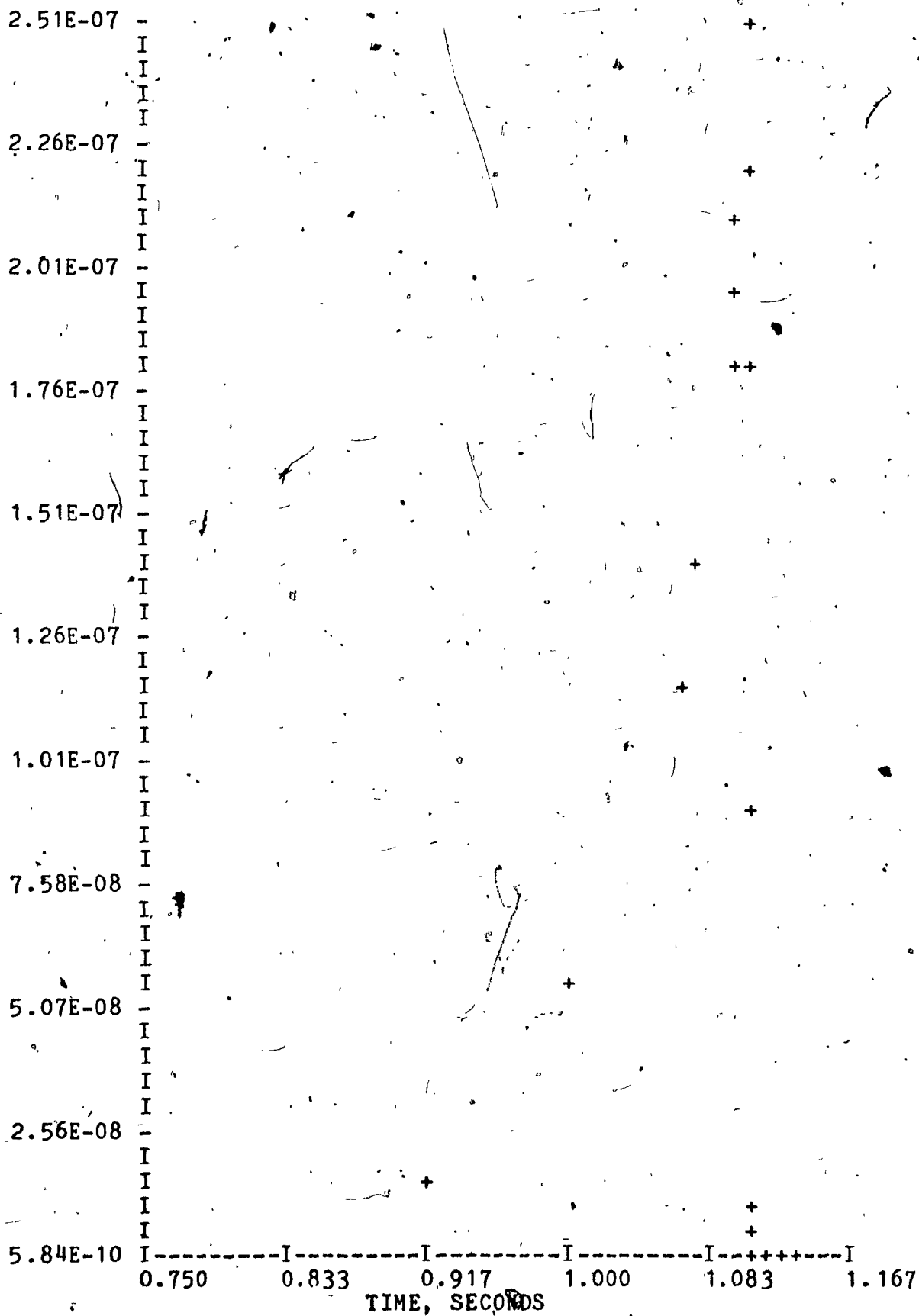
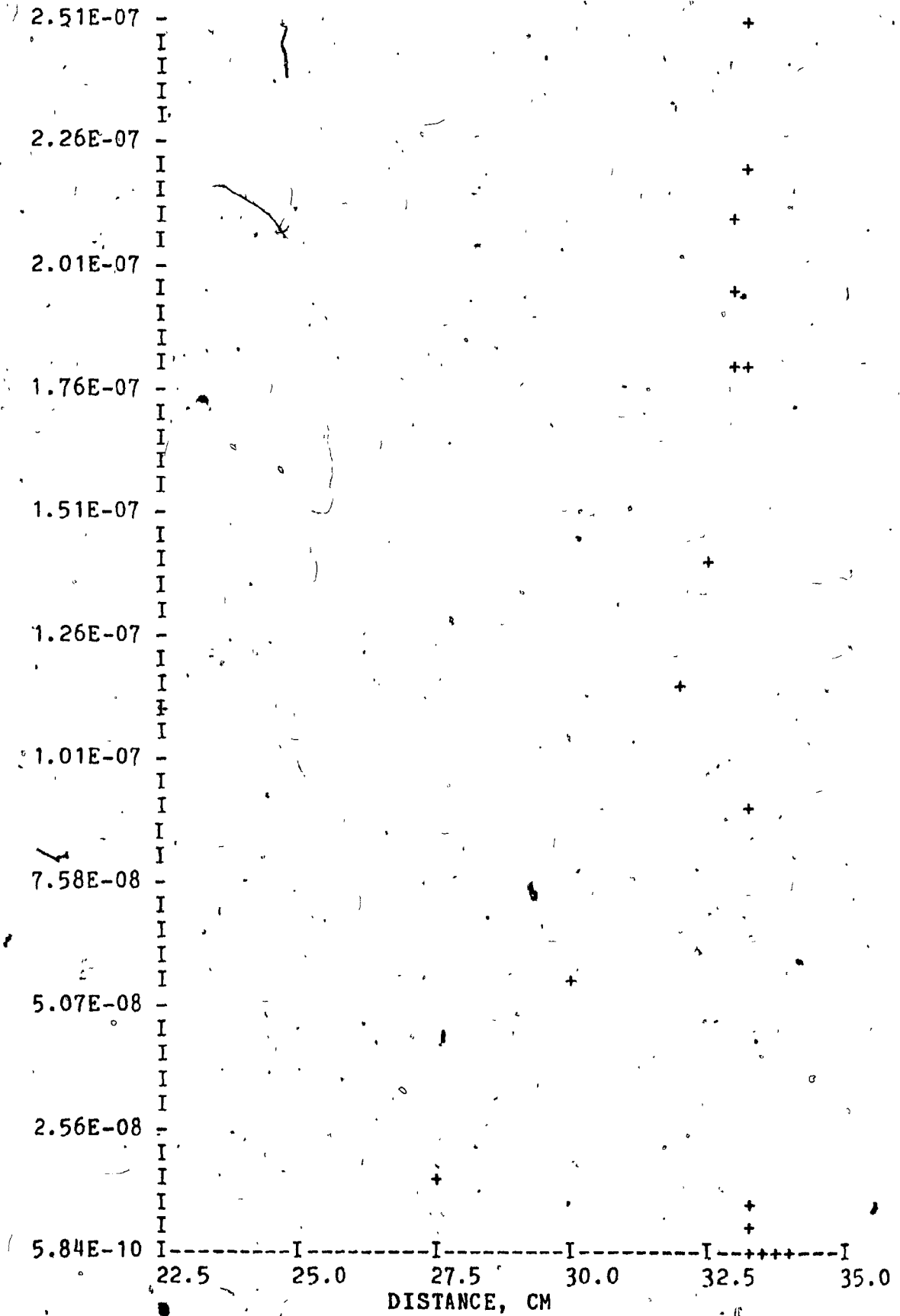


FIGURE B-12

NAME CO

CONCENTRATION (MOLES/CM**3) VS DISTANCE



CONCENTRATION. (MOLES/CM**3) VS TIME

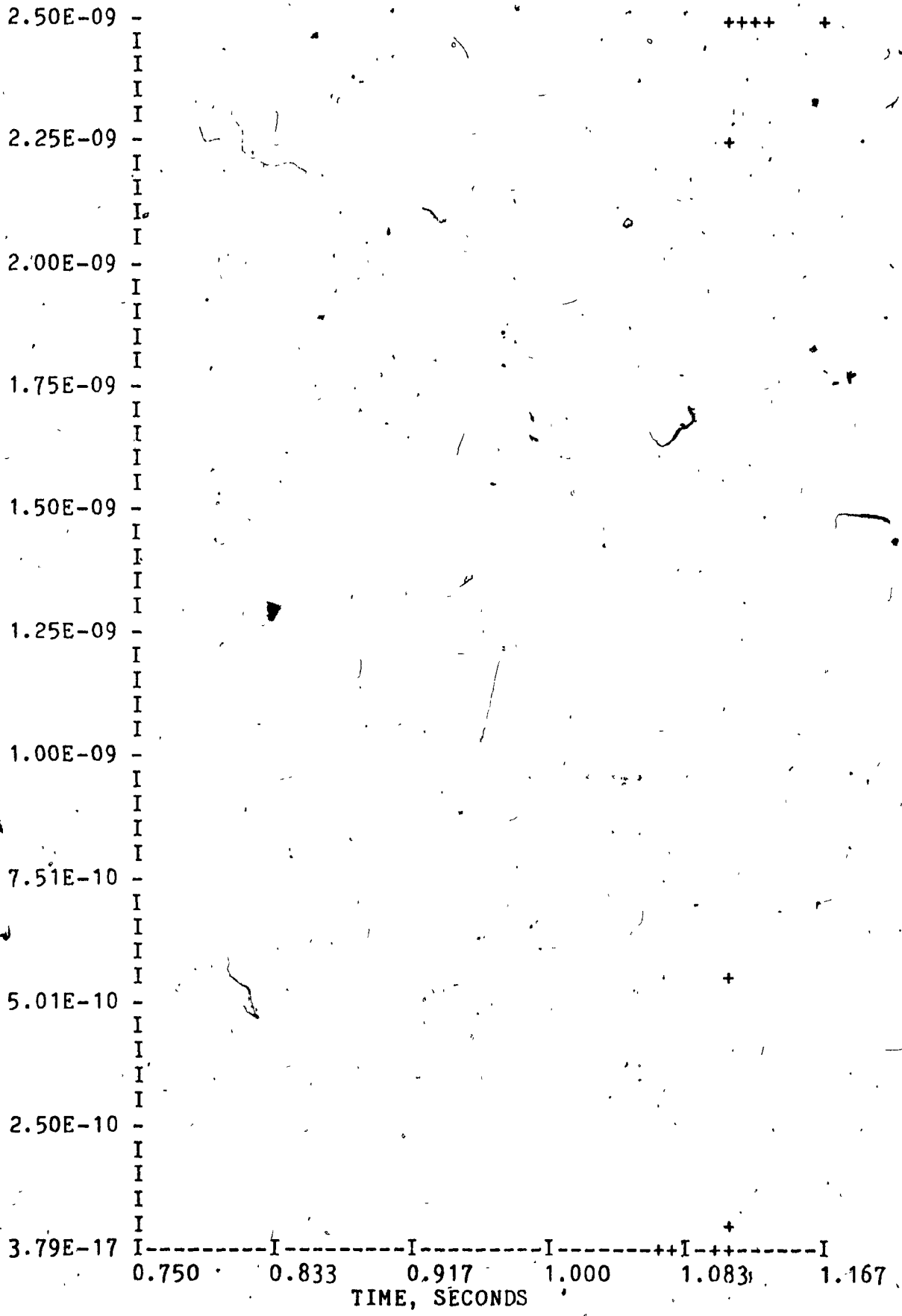


FIGURE R-14

NAME O

CONCENTRATION (MOLES/CM**3) VS DISTANCE

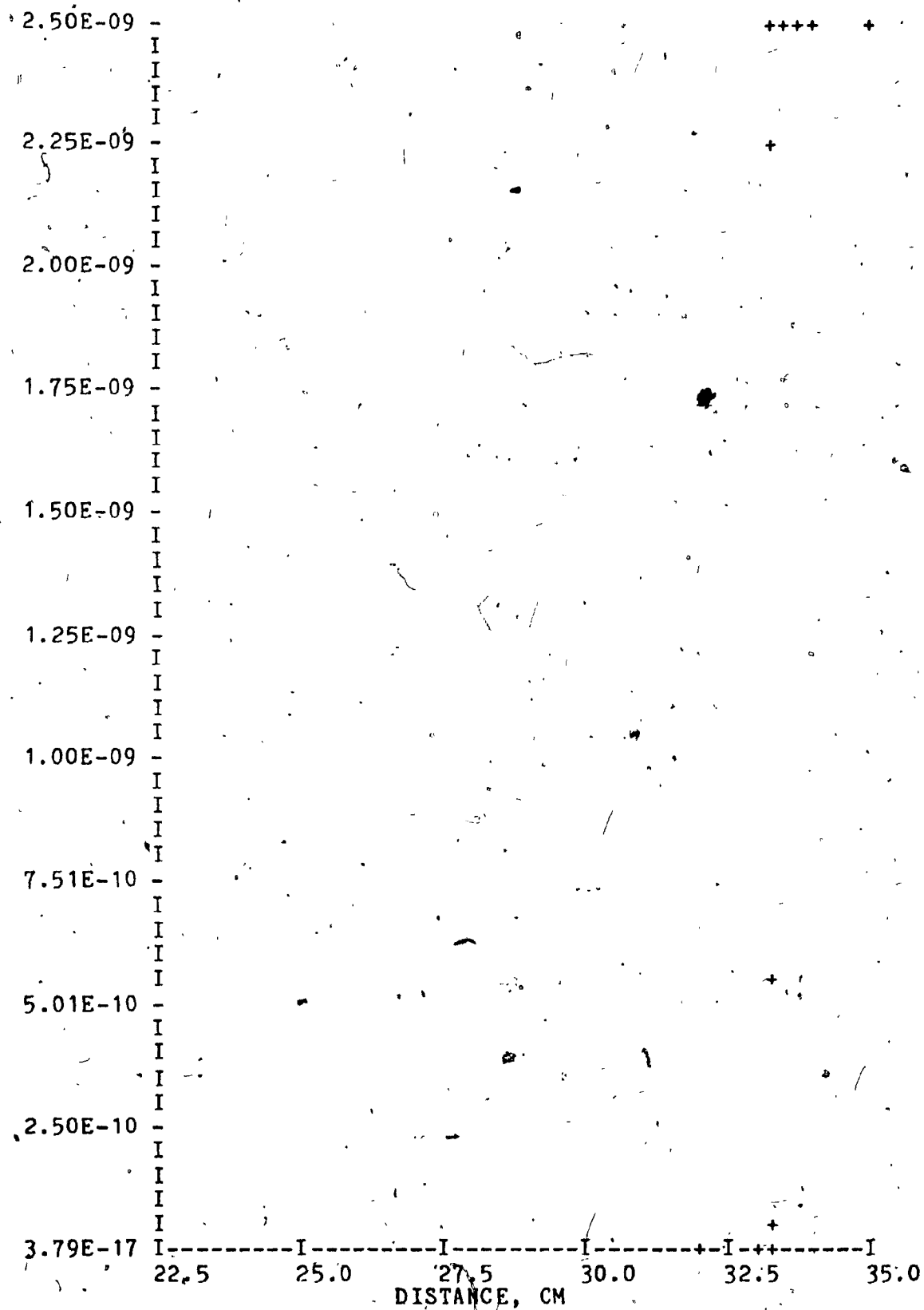


FIGURE B-16

NAME COP

CONCENTRATION (MOLES/CM**3) VS DISTANCE

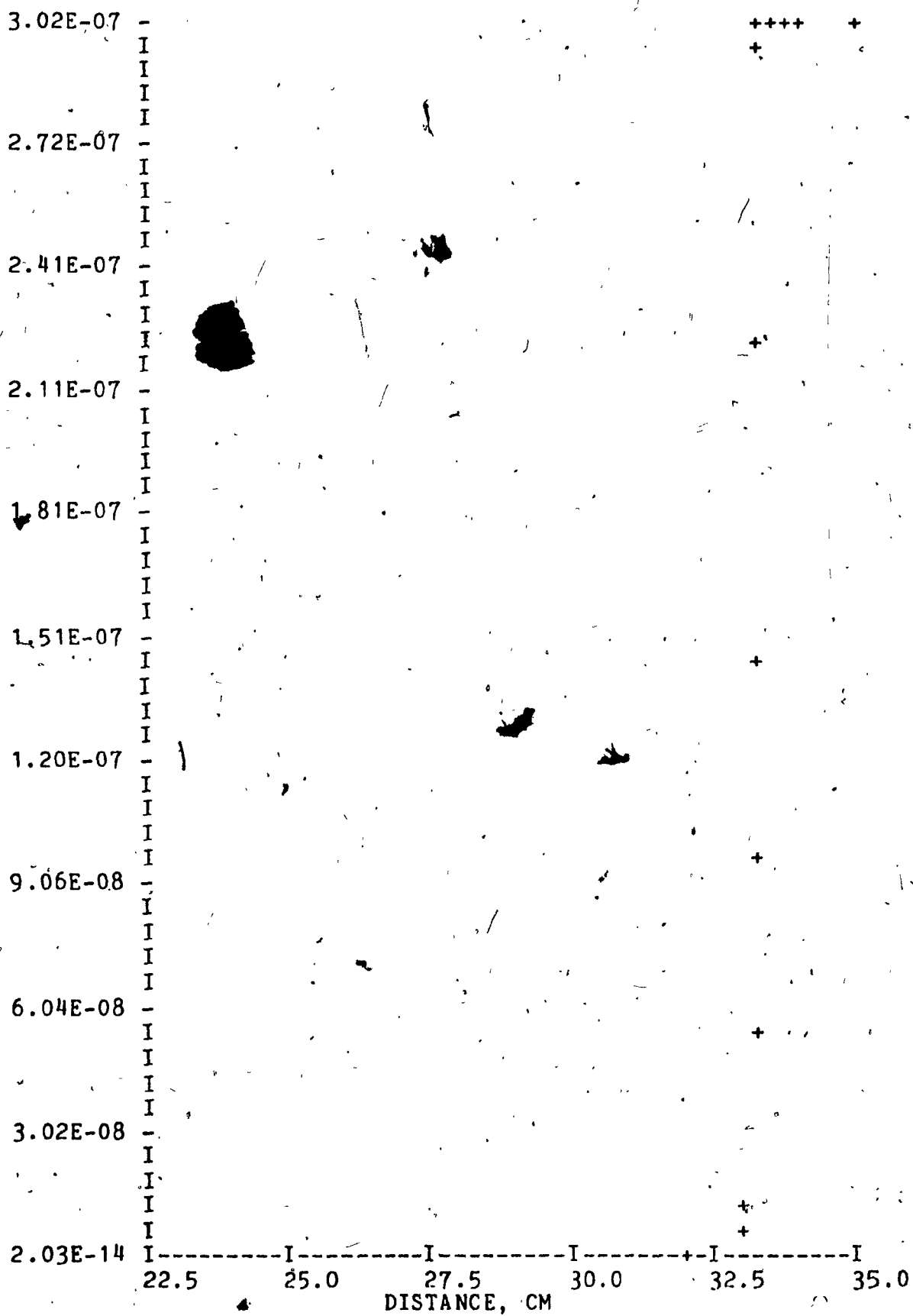


FIGURE B-17

NAME 02

CONCENTRATION (MOLES/CM**3) VS TIME

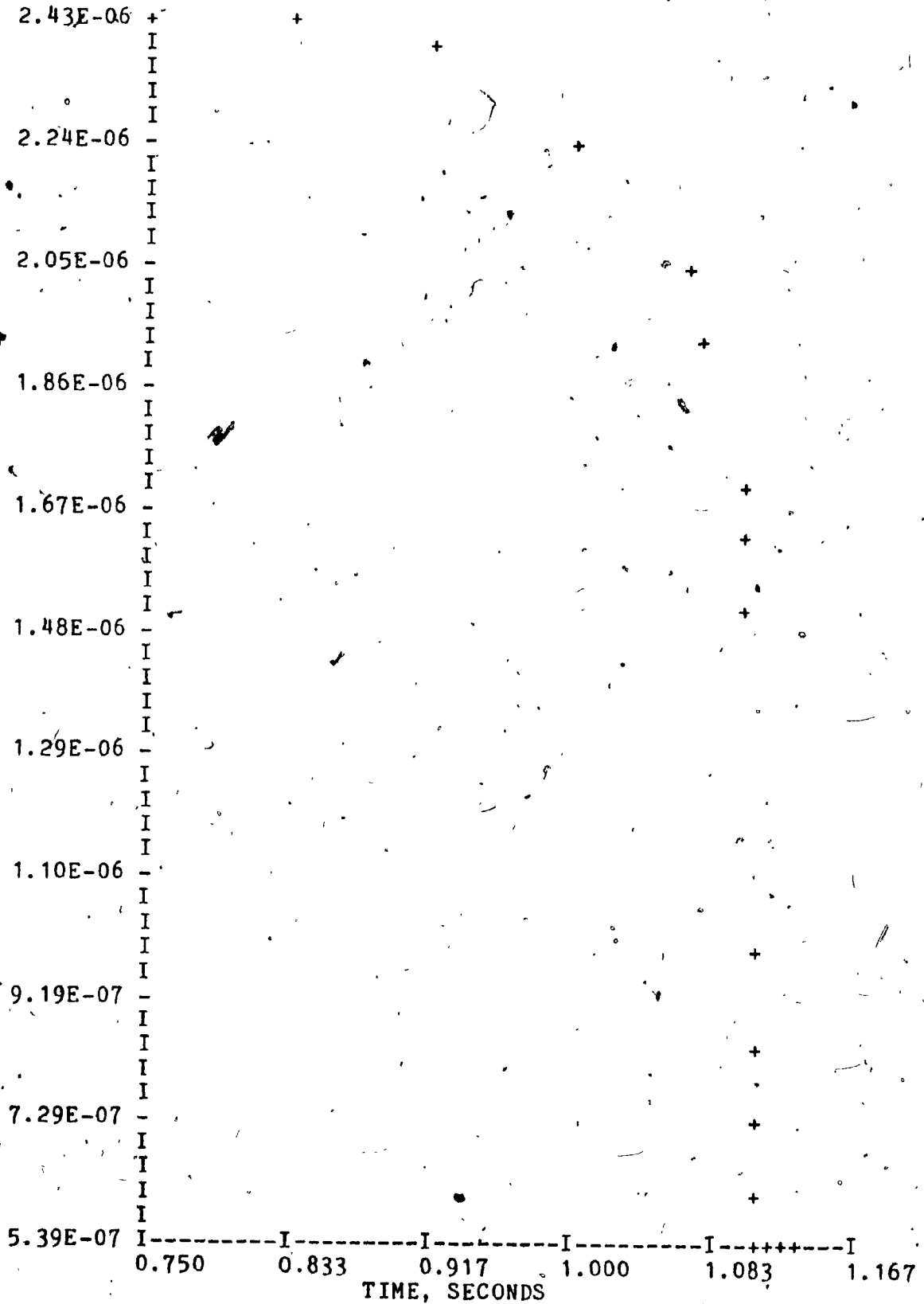


FIGURE B-18

NAME O2

CONCENTRATION (MOLES/CM**3) VS DISTANCE

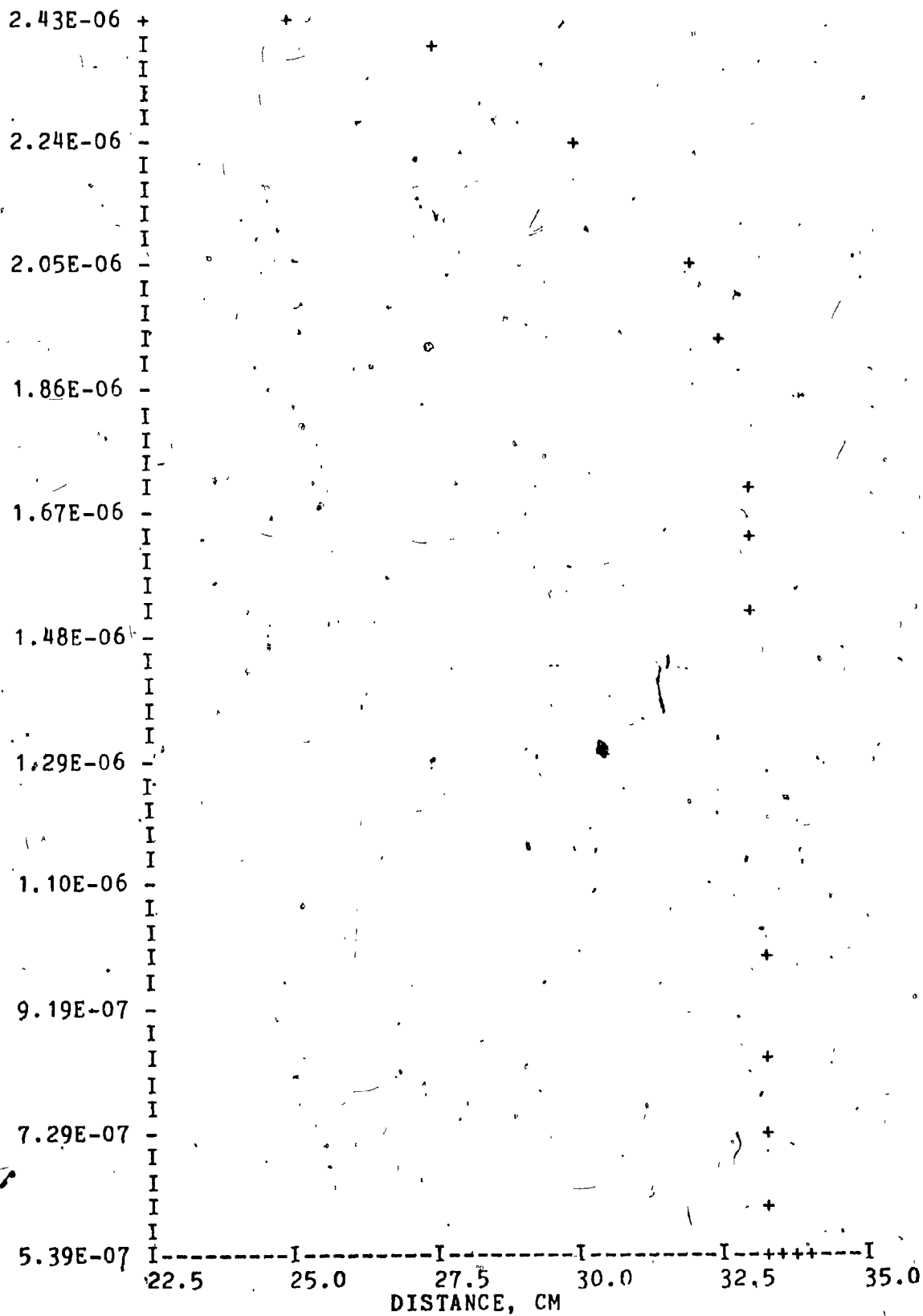


FIGURE B-19 NAME CH20
CONCENTRATION (MOLES/CM**3) VS TIME

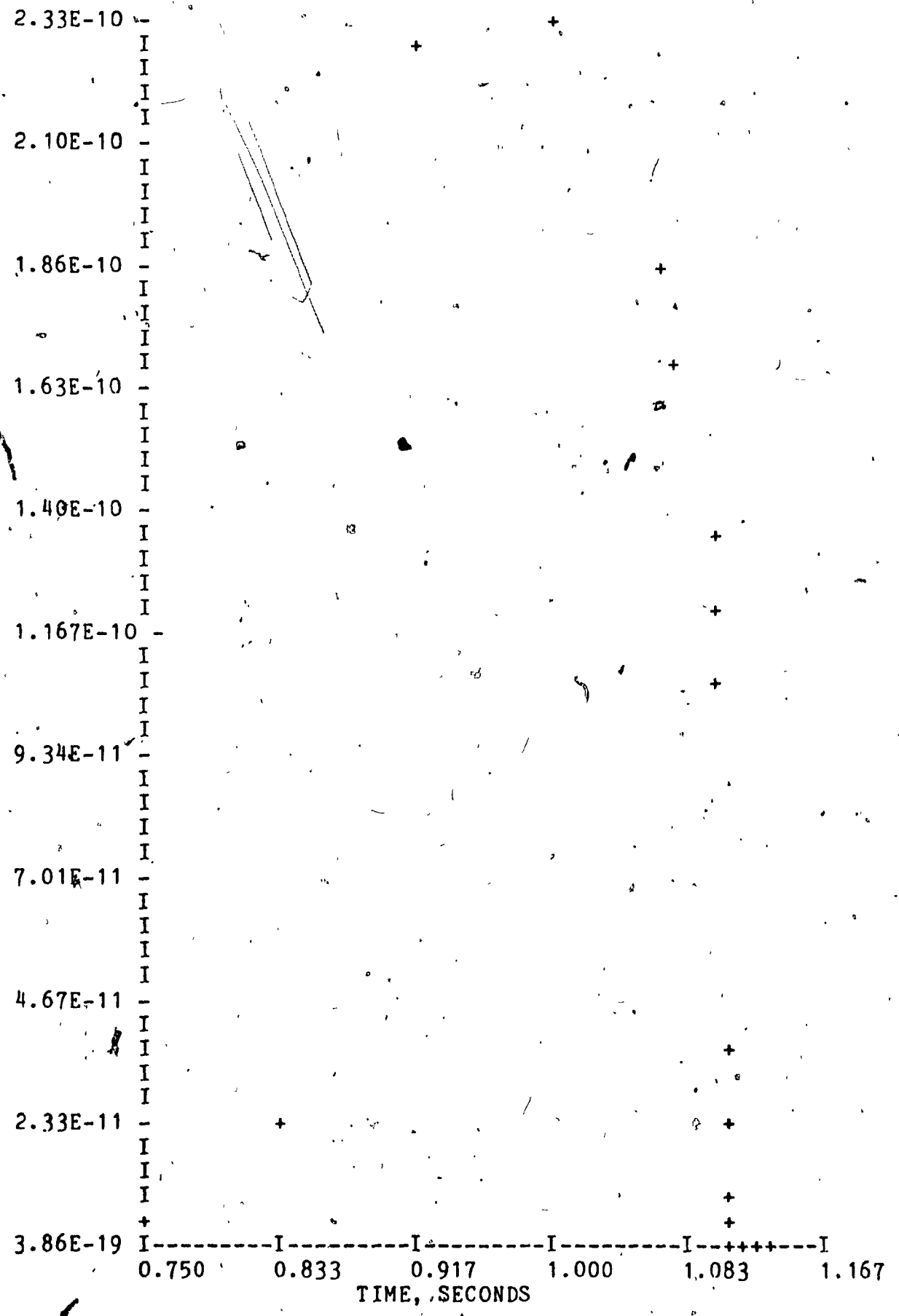


FIGURE B-20

NAME CH2O

CONCENTRATION (MOLES/CM**3) VS DISTANCE

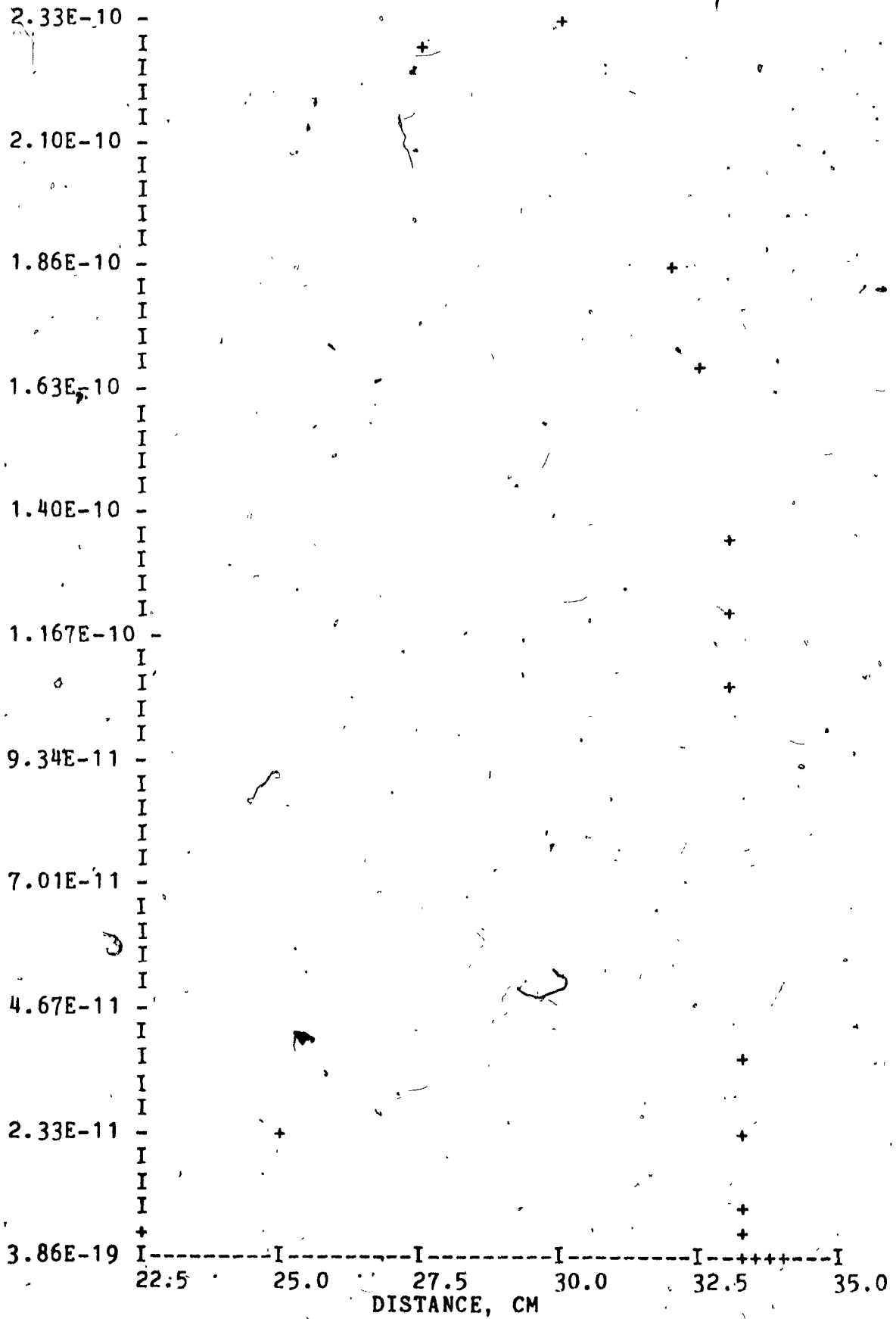


FIGURE B-21

NAME H2

CONCENTRATION (MOLES/CM**3) VS TIME

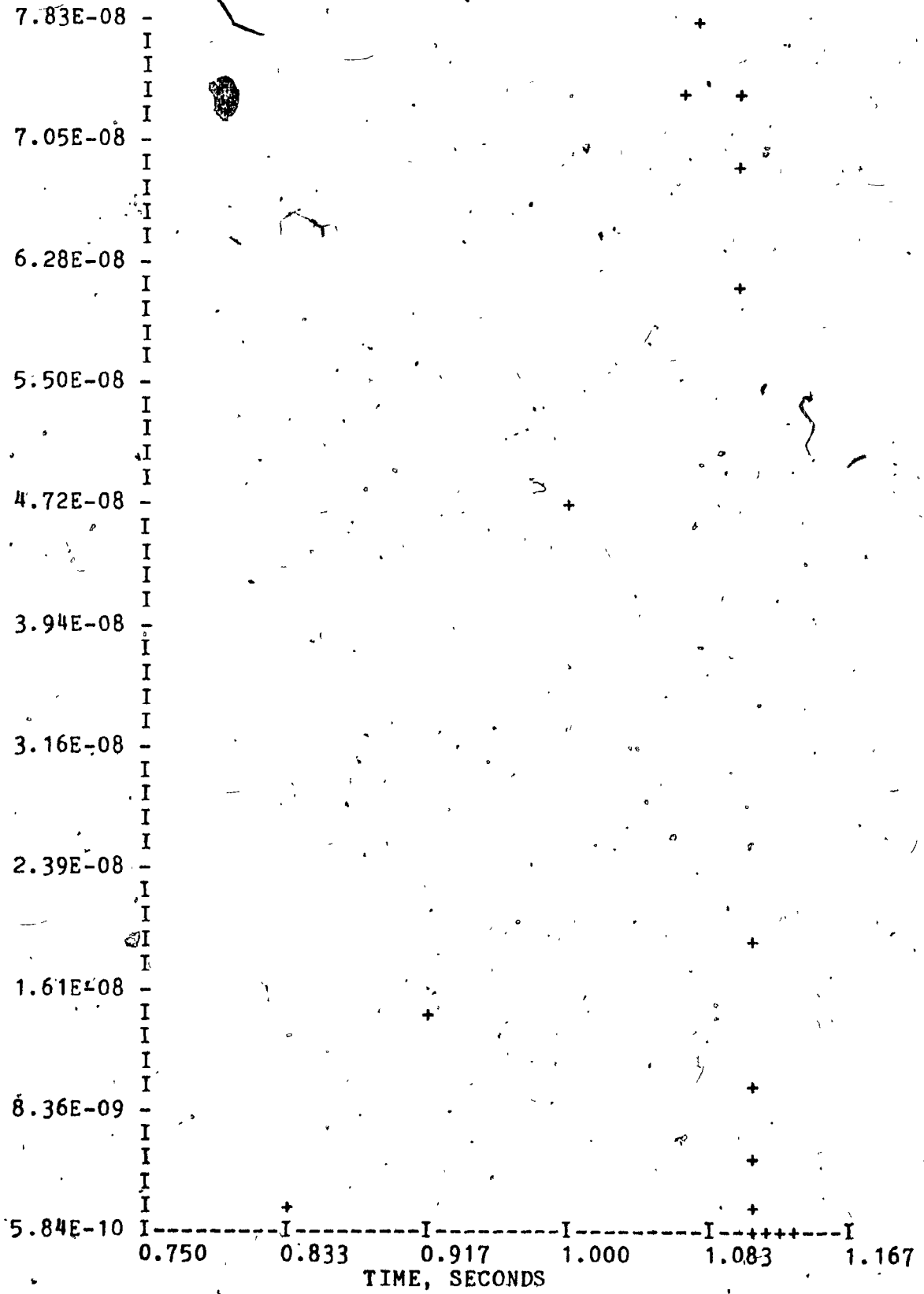


FIGURE R-22 NAME H2

CONCENTRATION (MOLES/CM**3) VS DISTANCE

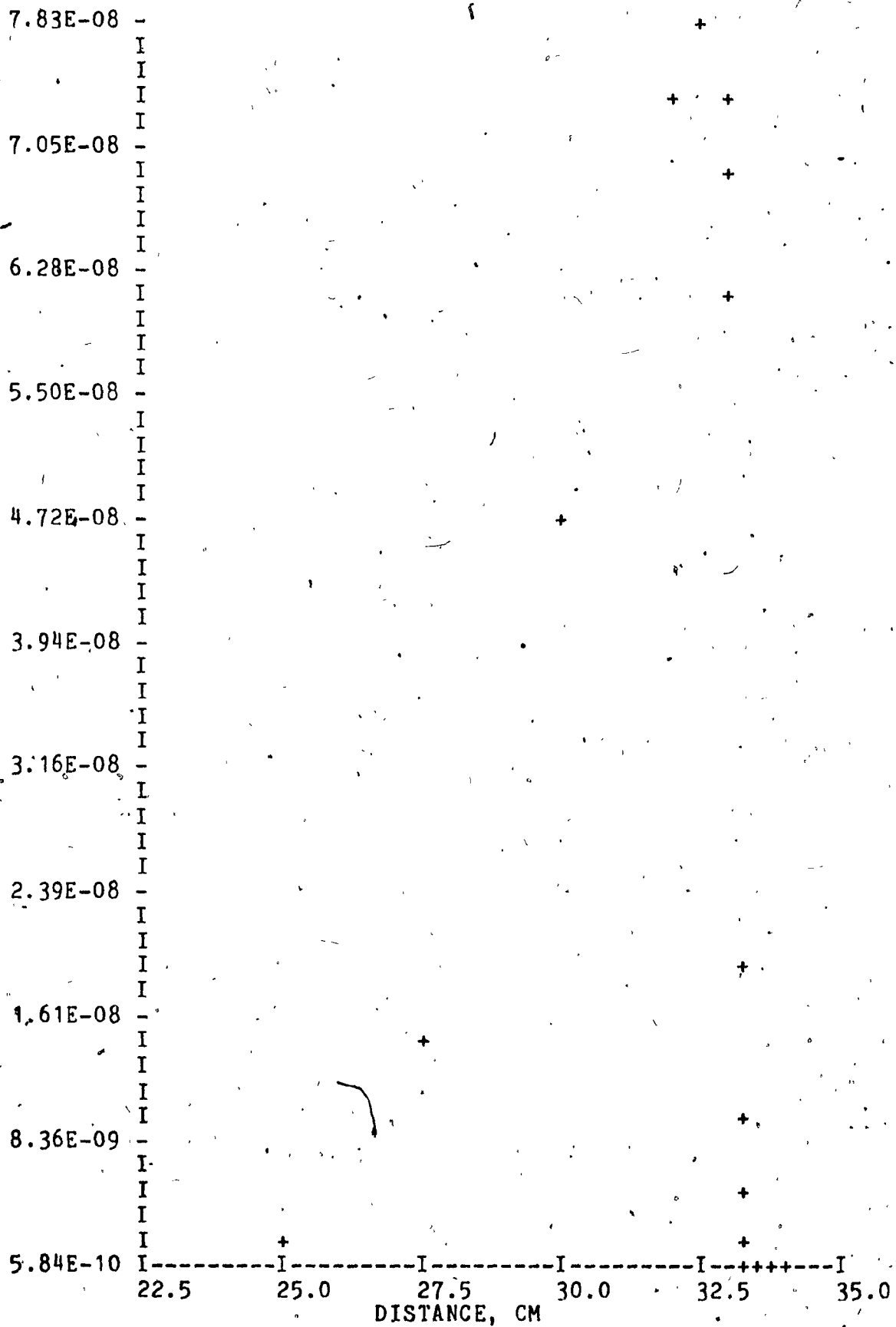


FIGURE D-23

NAME HO2

CONCENTRATION (MOLES/CM**3) VS TIME

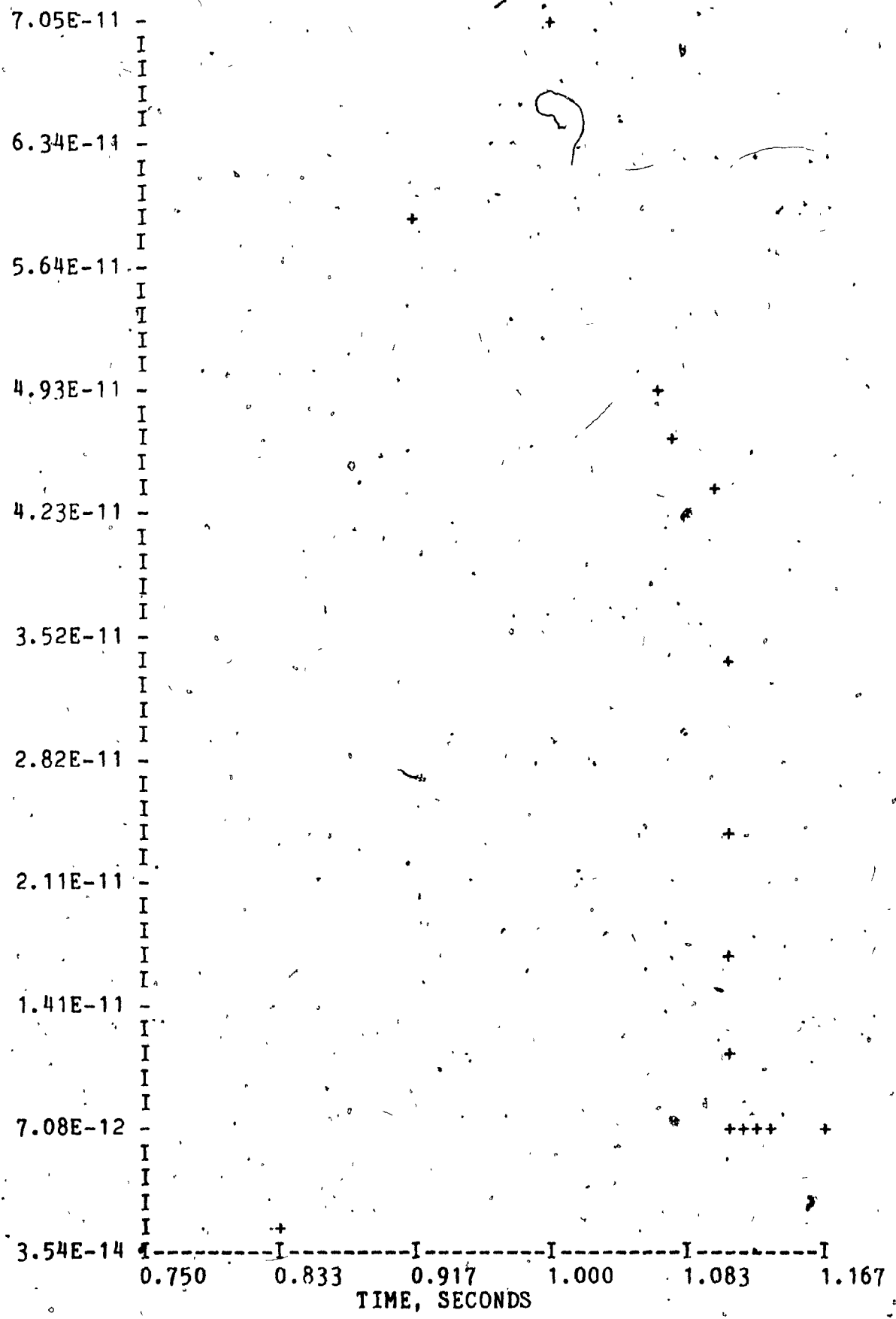


FIGURE B-24

NAME HO2

CONCENTRATION (MOLES/CM**3) VS DISTANCE

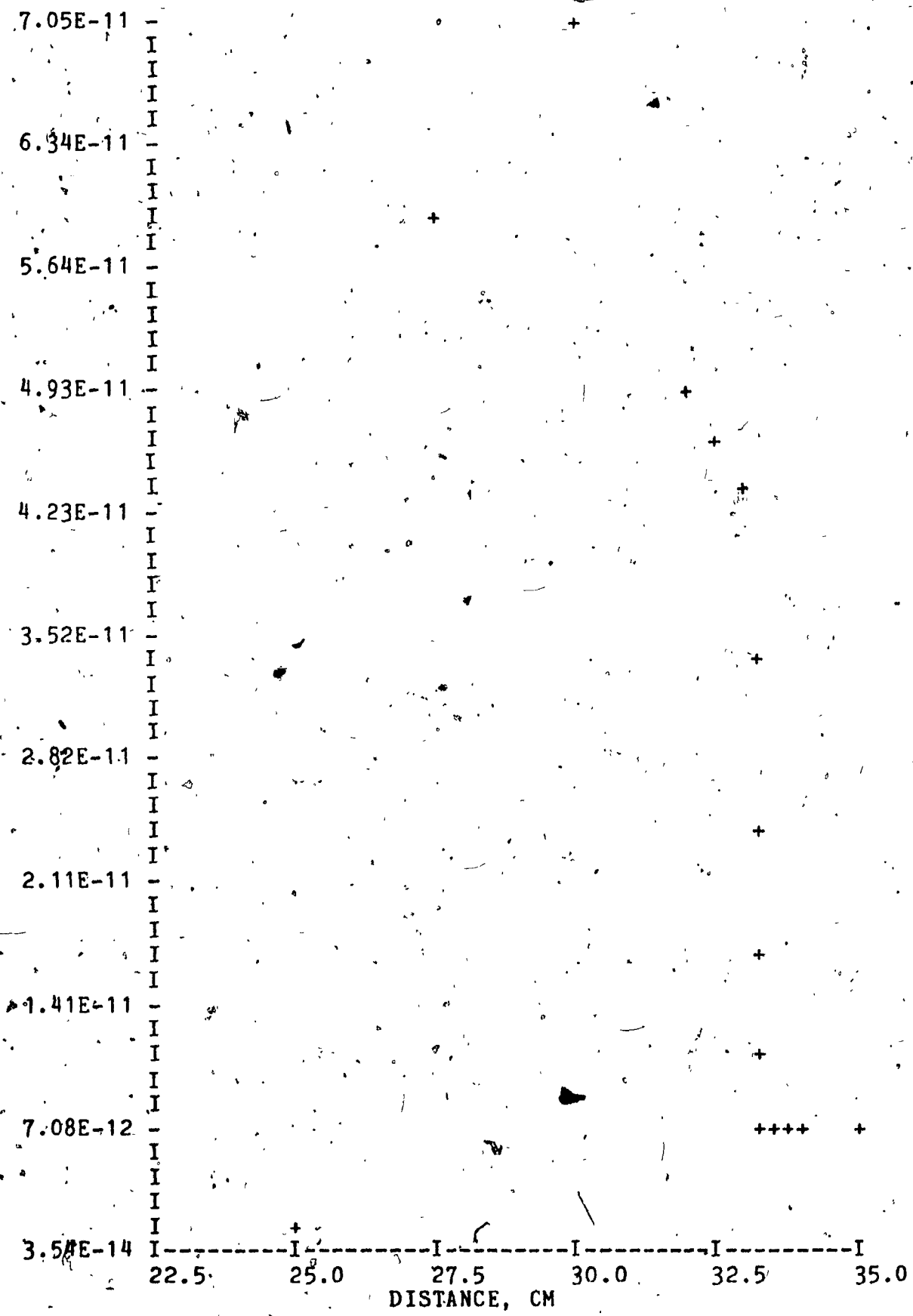
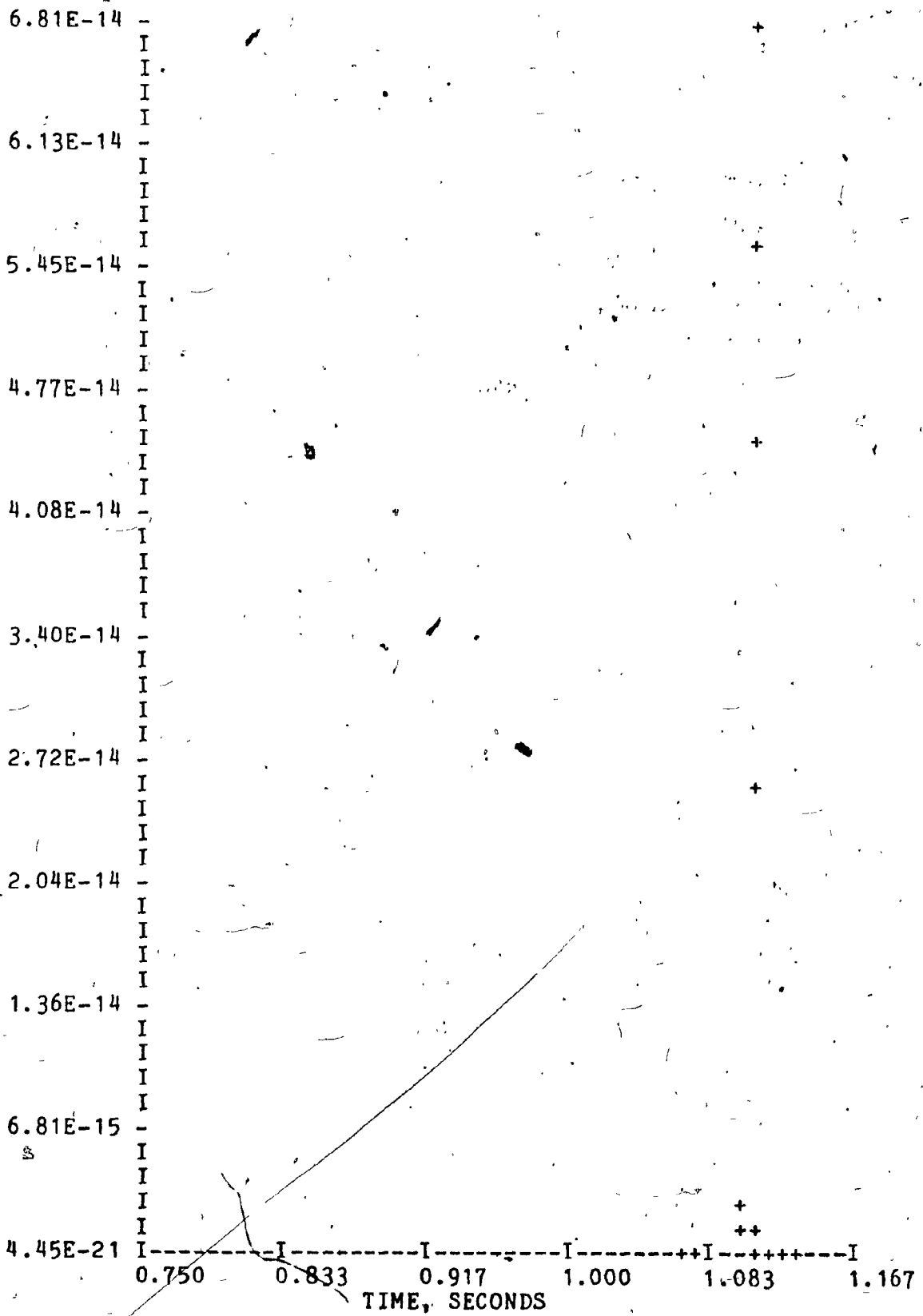


FIGURE B-25

NAME HCO

CONCENTRATION (MOLES/CM**3) VS TIME



CONCENTRATION (MOLES/CM**3) VS DISTANCE

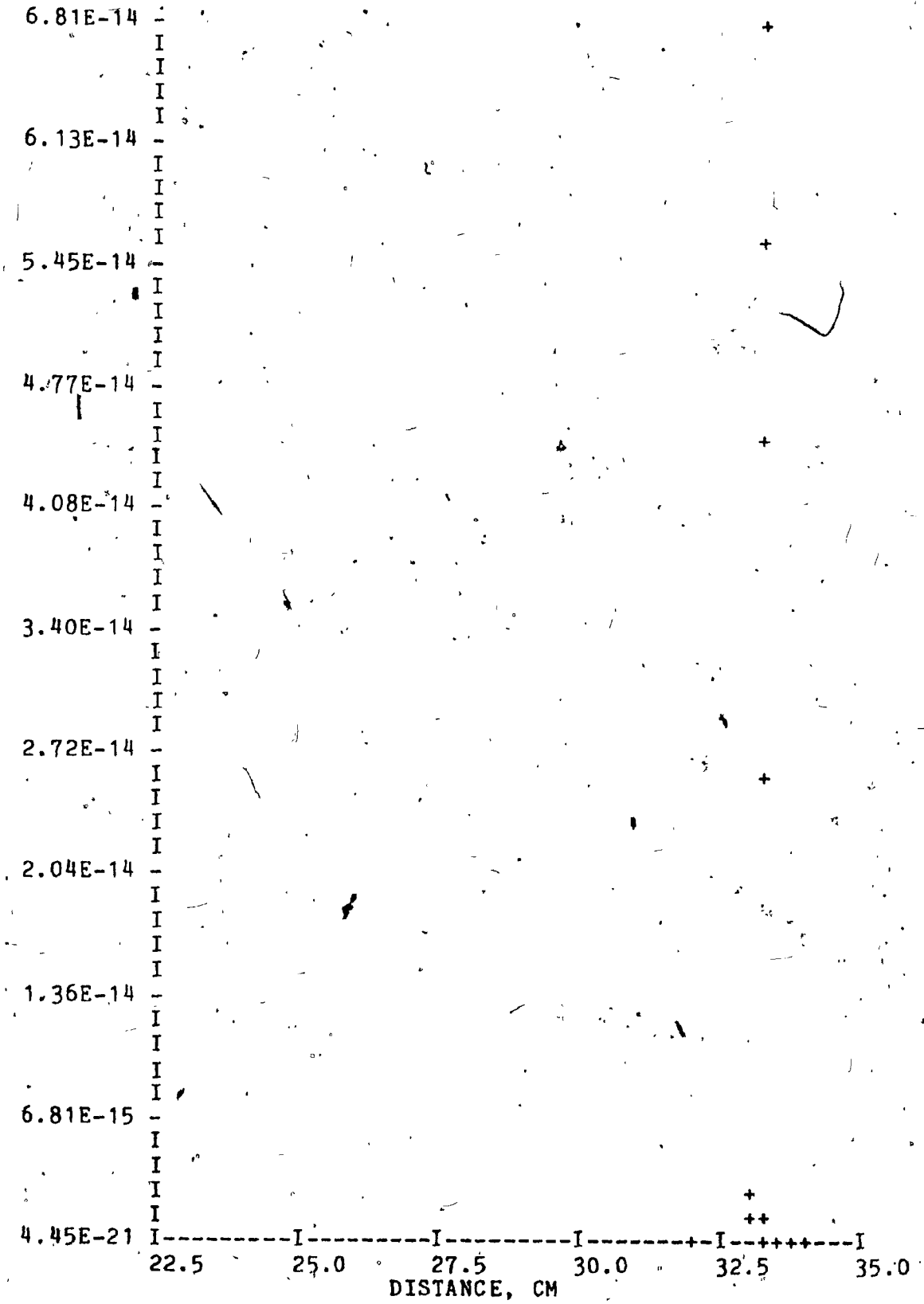


FIGURE B-27

NAME N2

CONCENTRATION (MOLES/CM**3) VS TIME

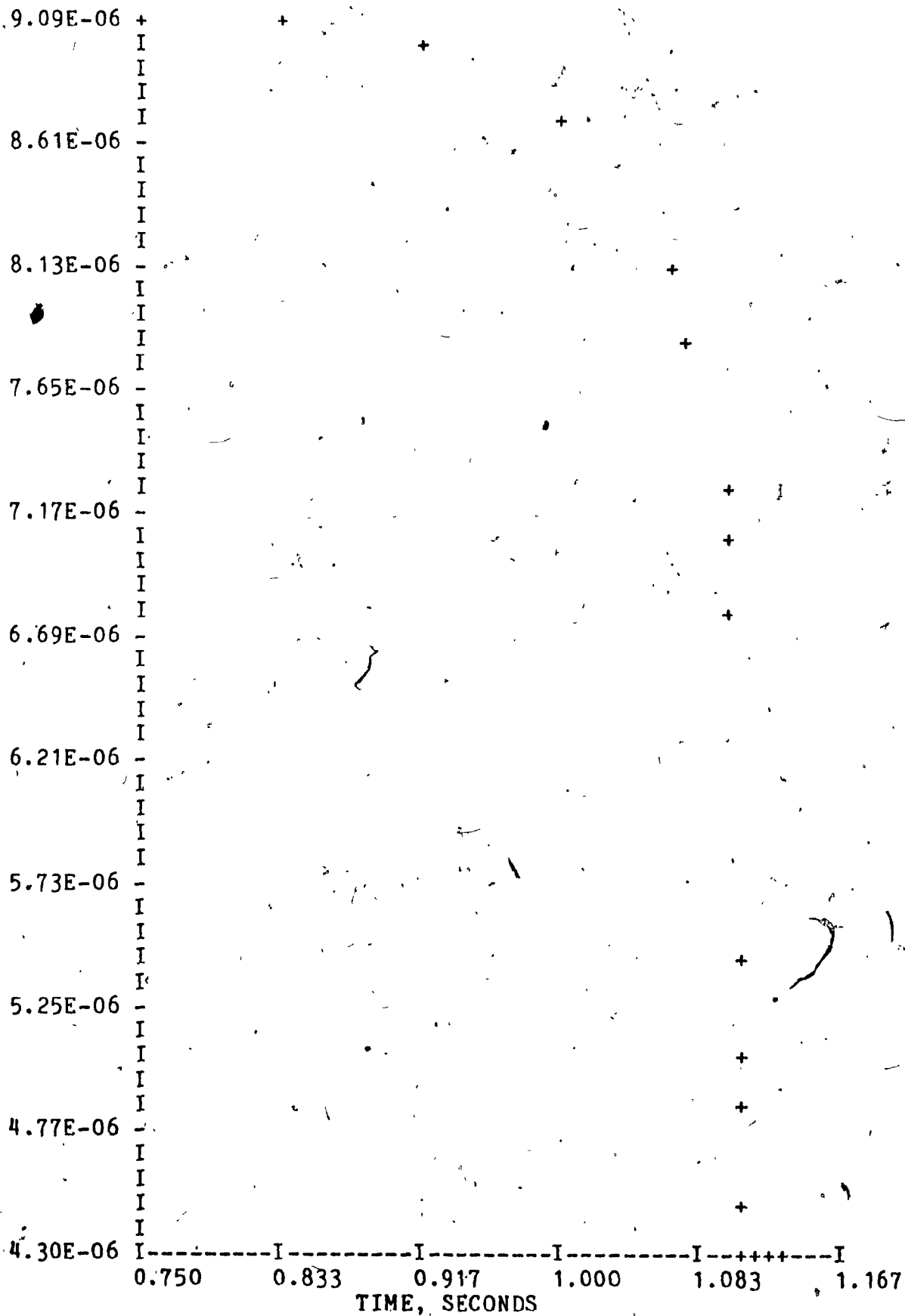


FIGURE B-28 NAME N2
CONCENTRATION (MOLES/CM**3) VS DISTANCE

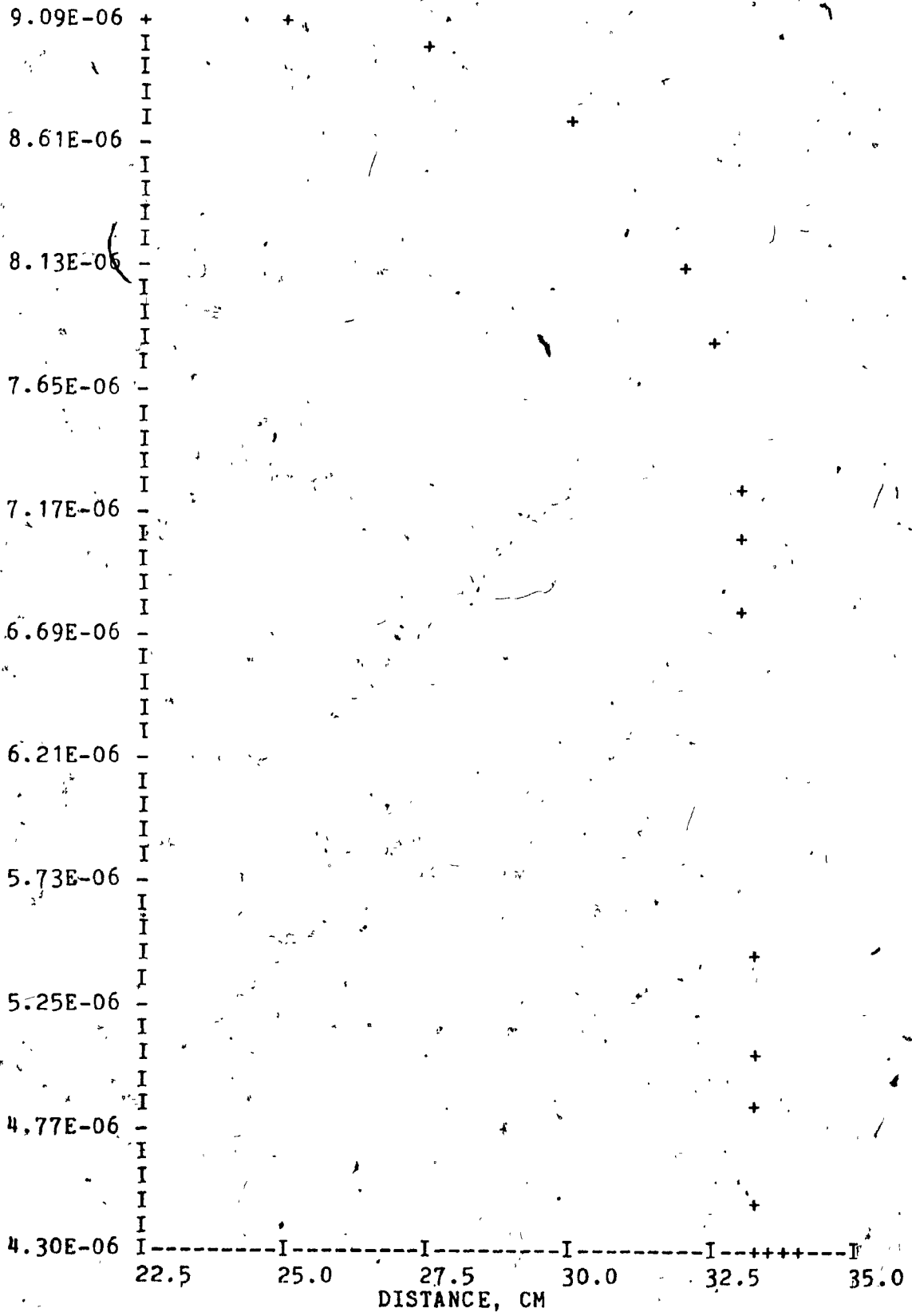


FIGURE B-29 NAME CH4

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

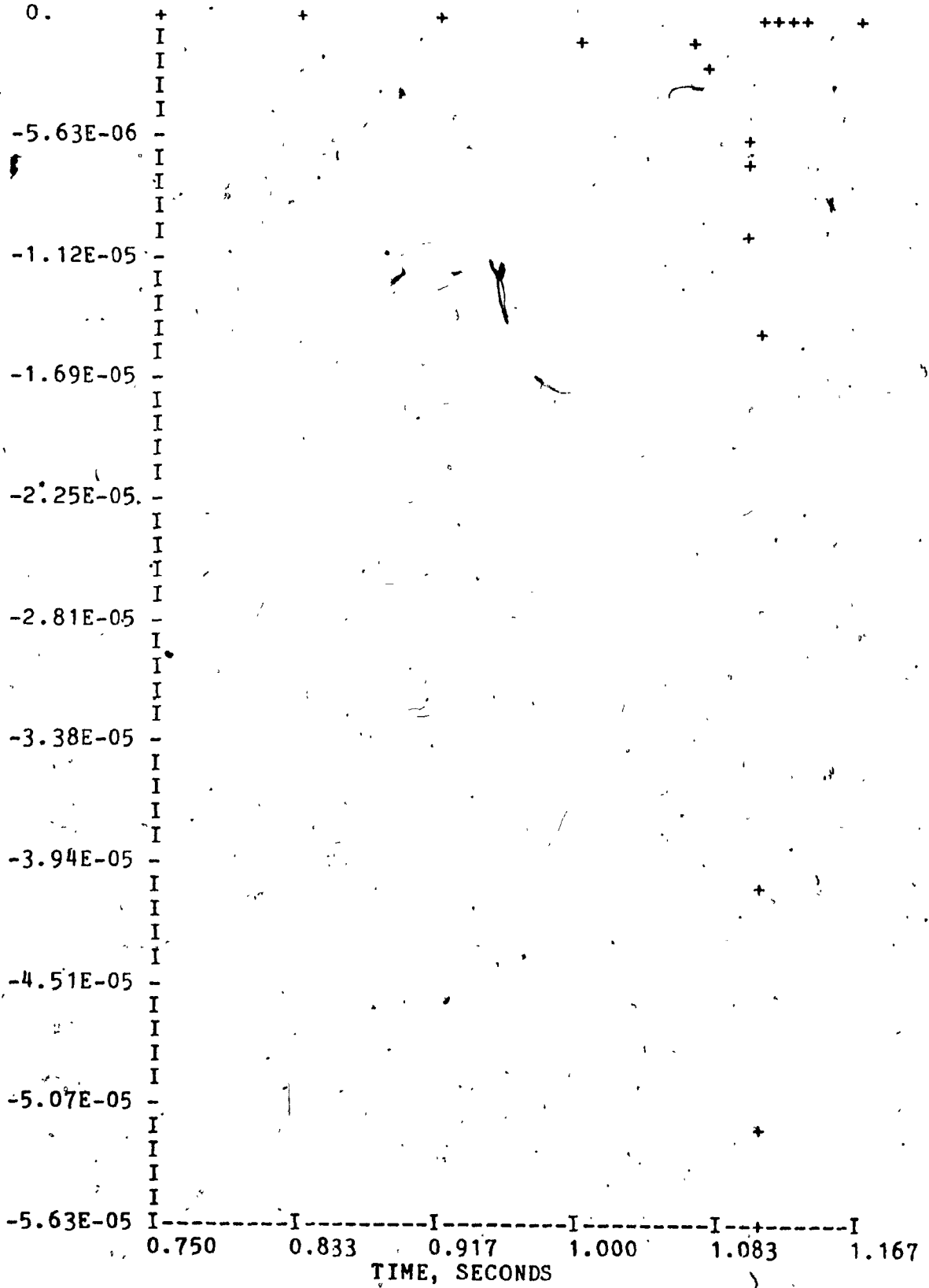


FIGURE B-30

NAME: G114

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

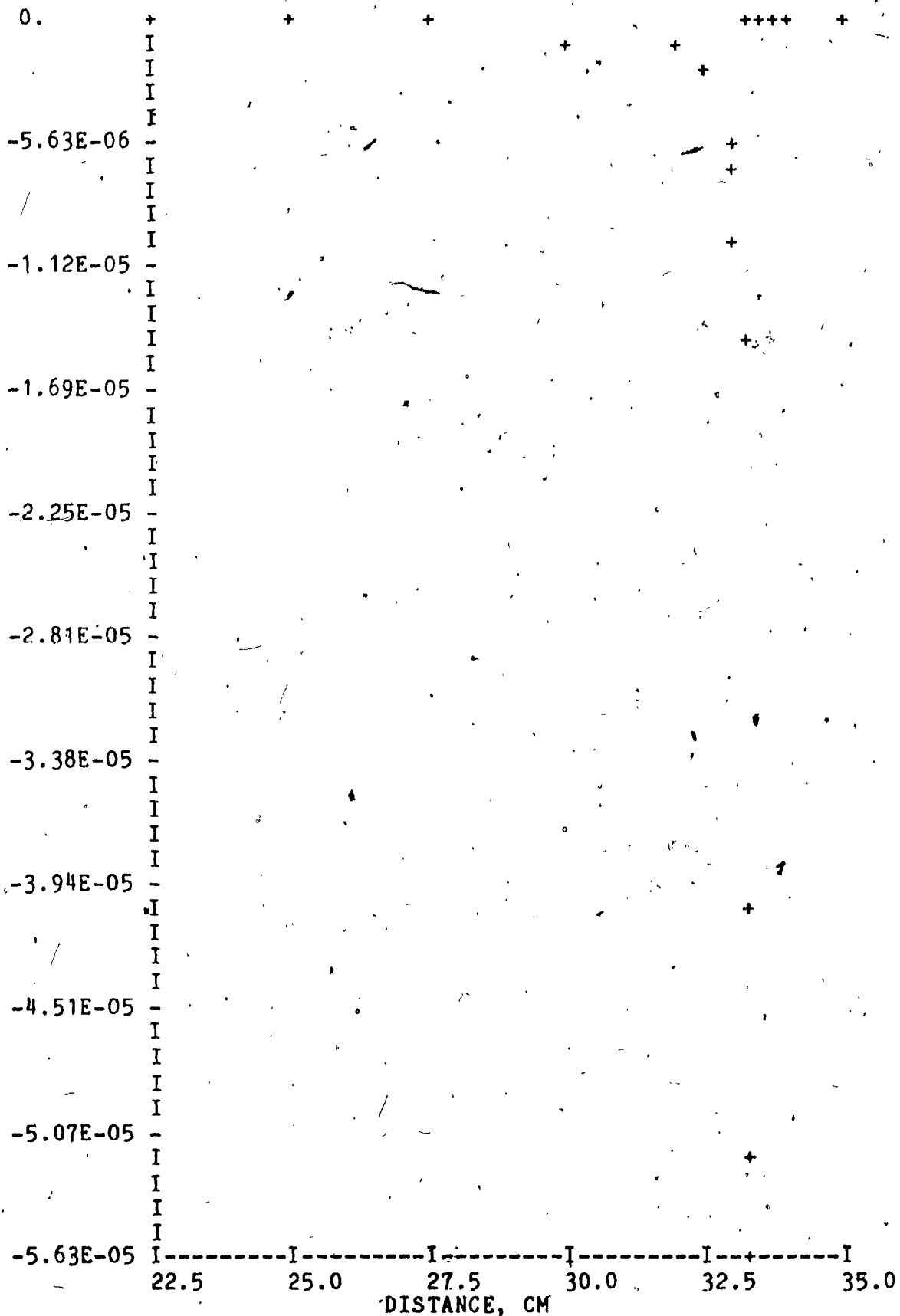


FIGURE B-31

NAME CH3

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

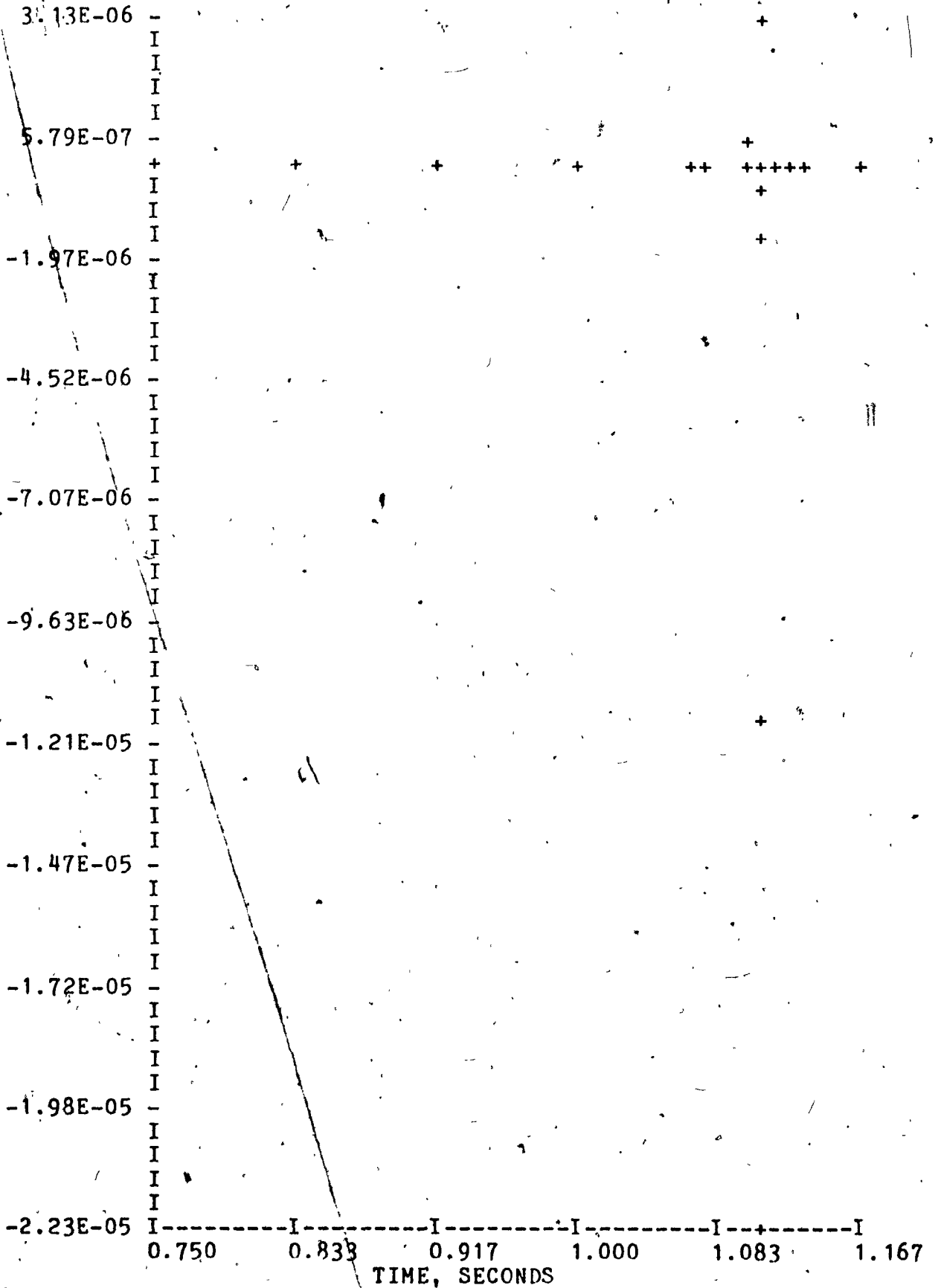


FIGURE R-32 NAME CH3

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

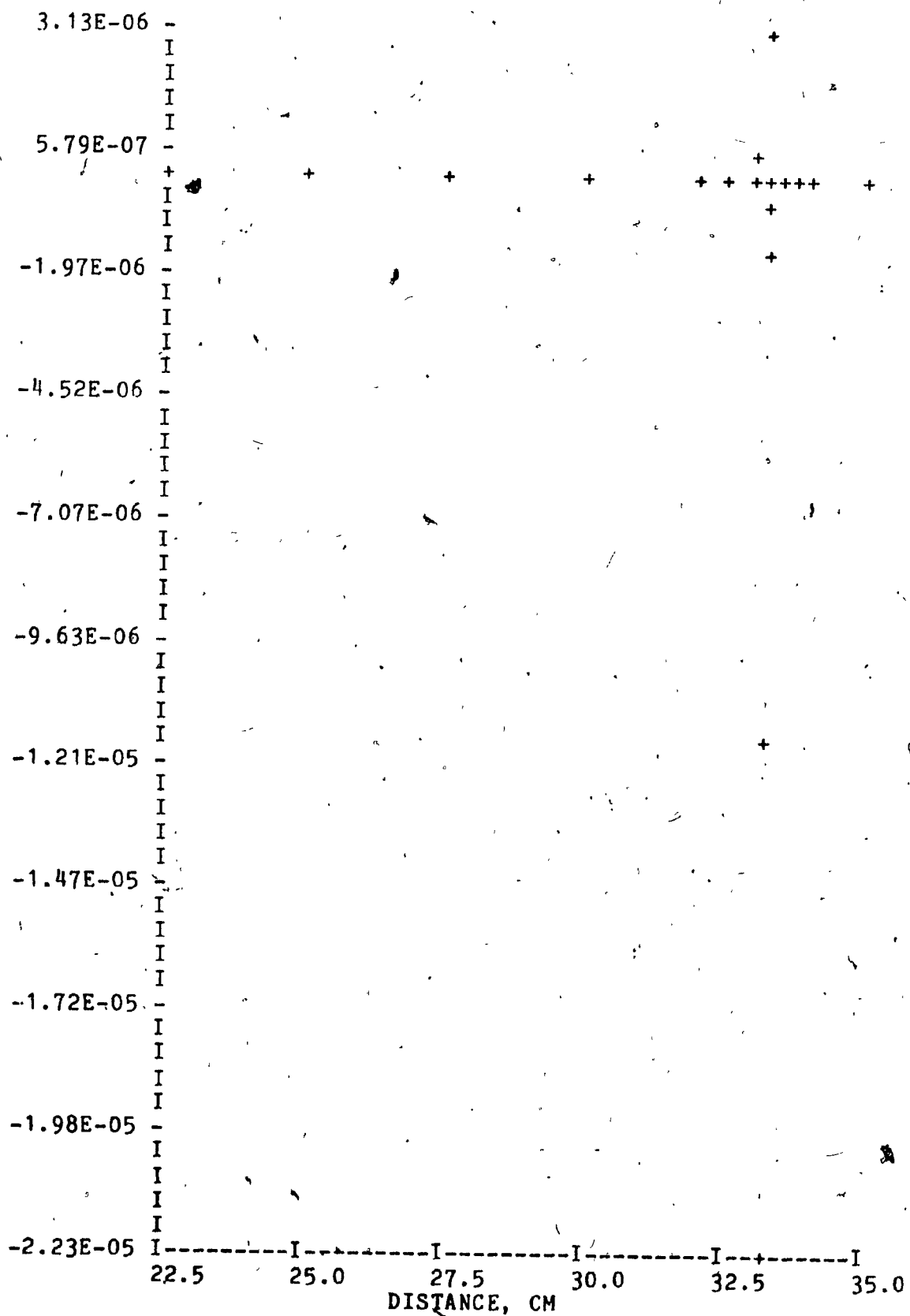


FIGURE B-33 NAME H

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

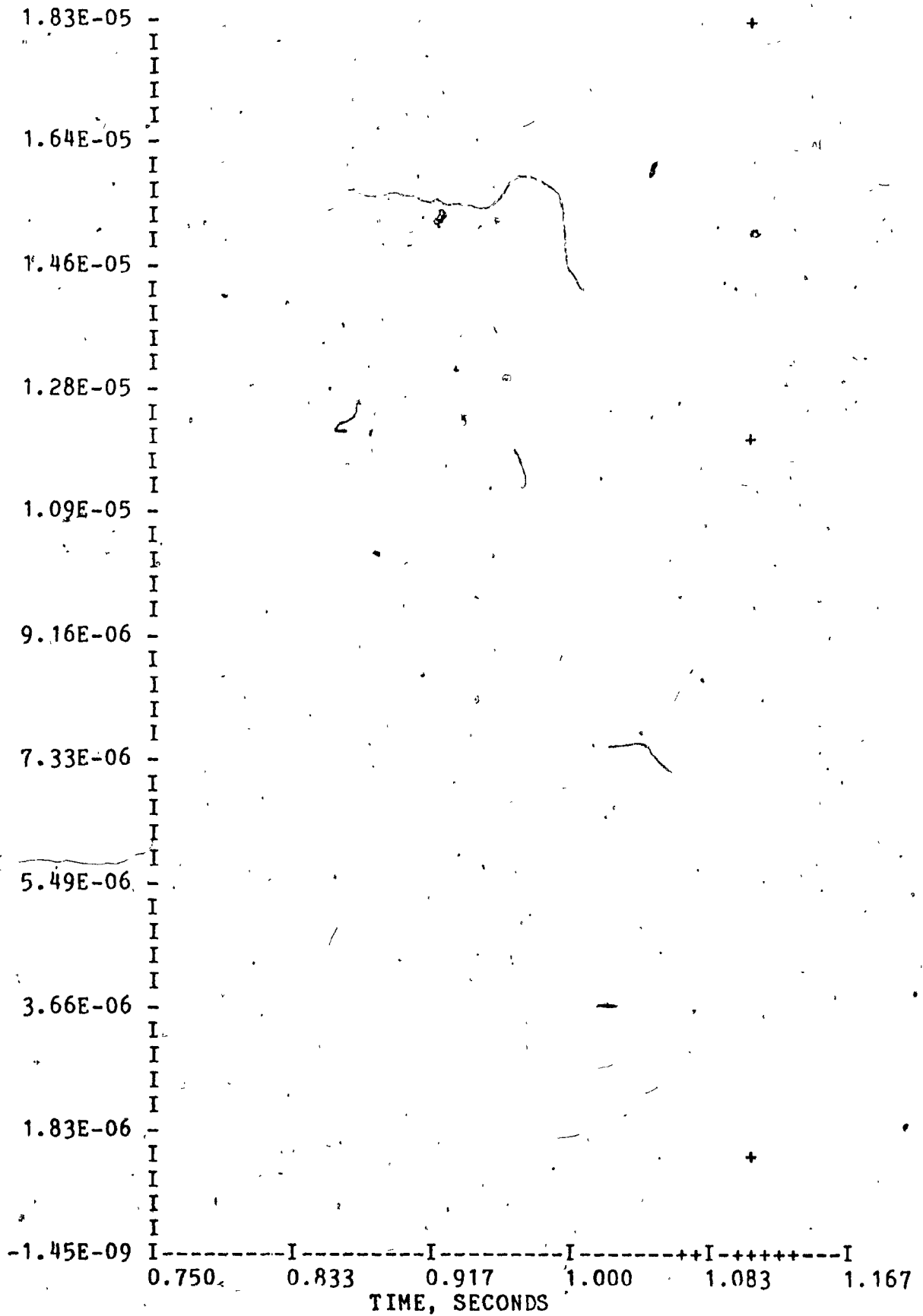
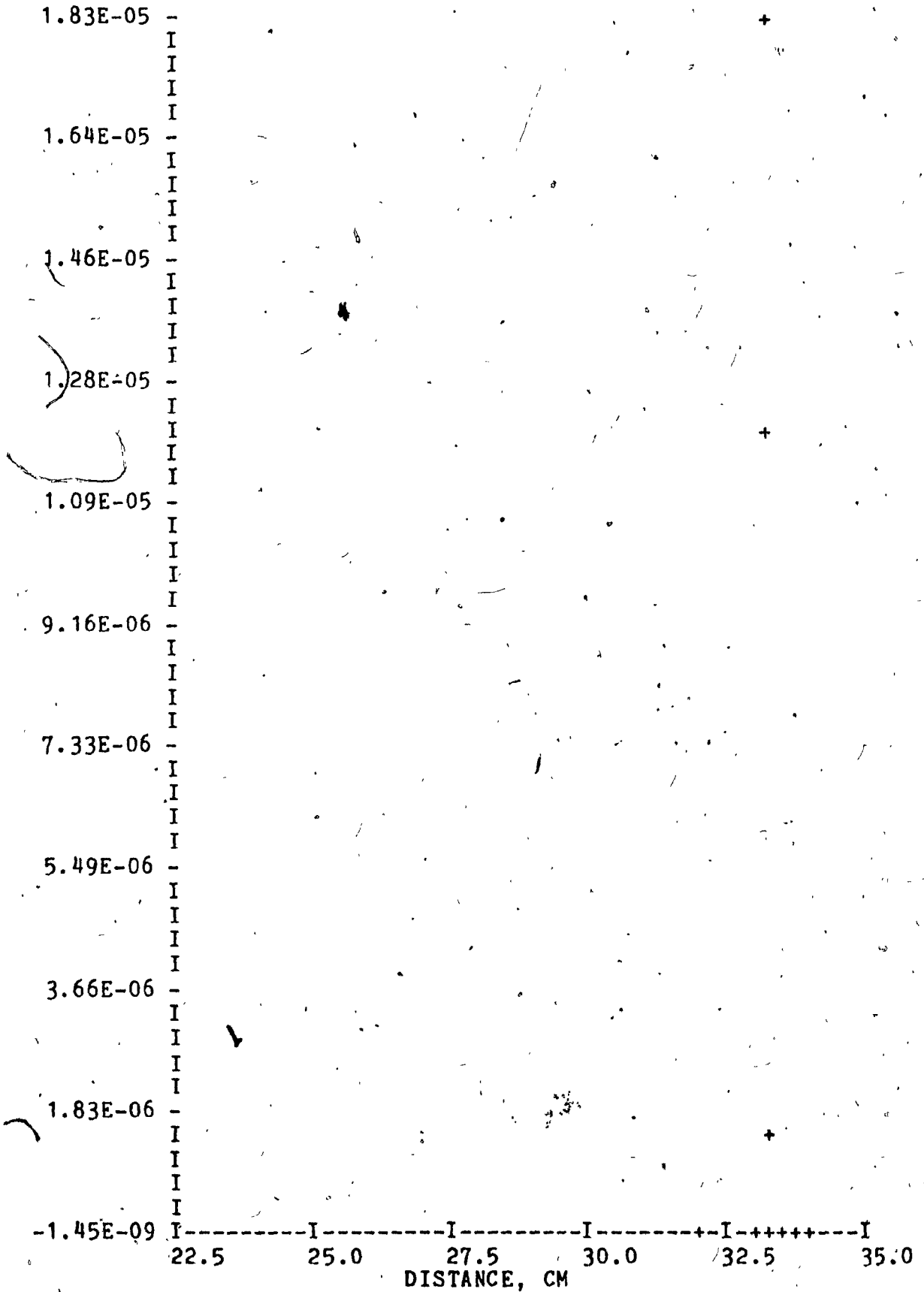
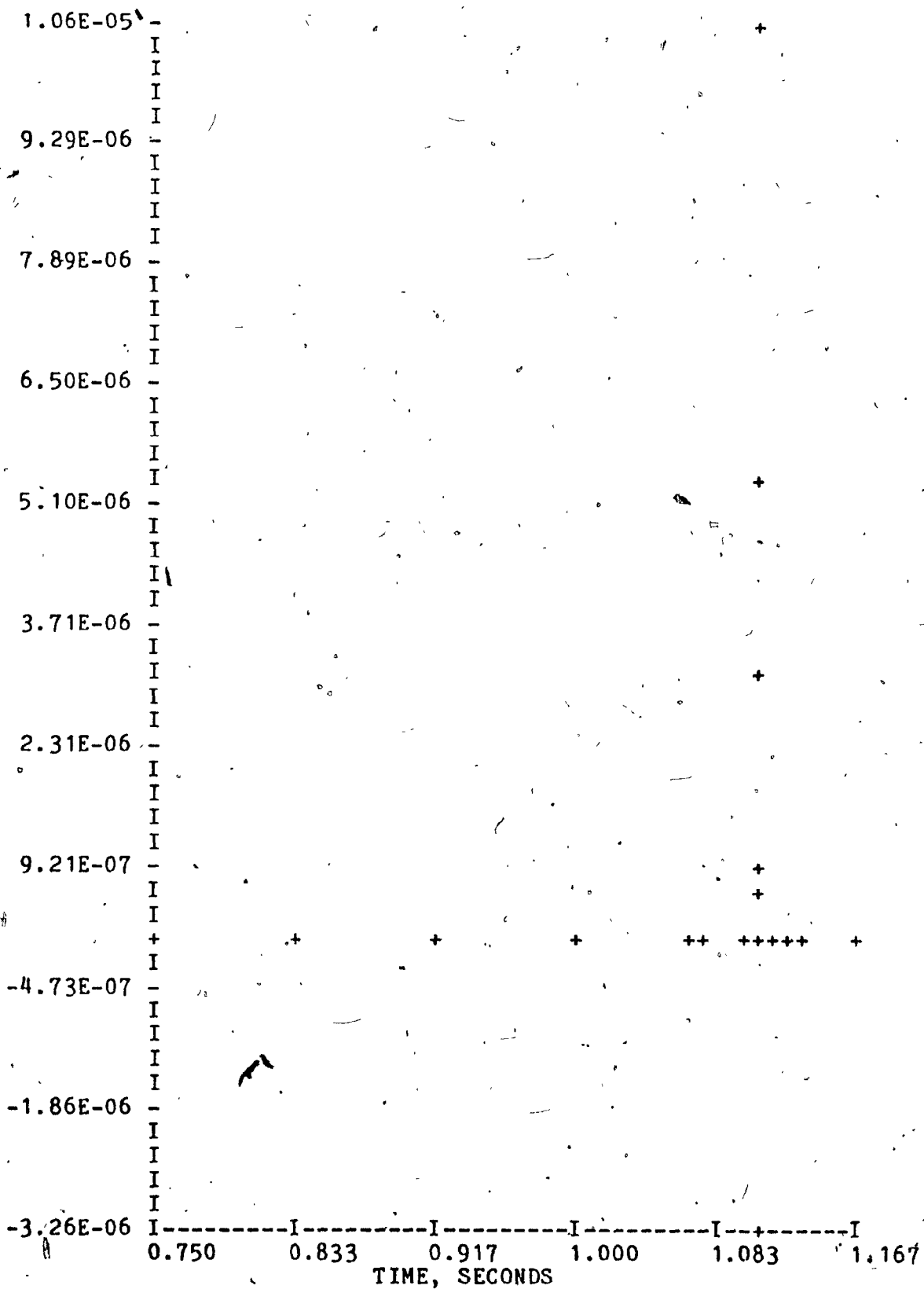


FIGURE B-34 NAME H

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)



NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)



NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

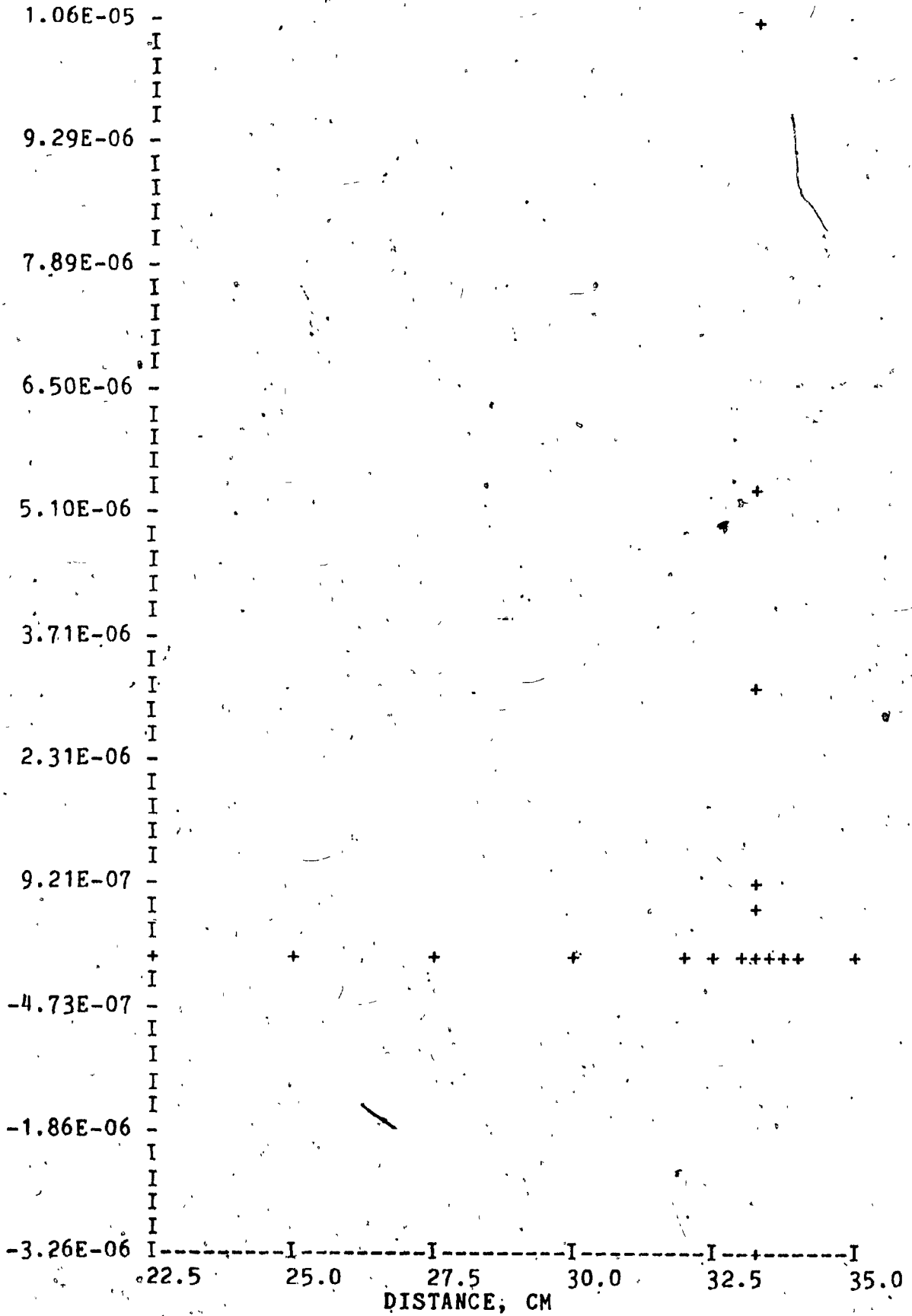
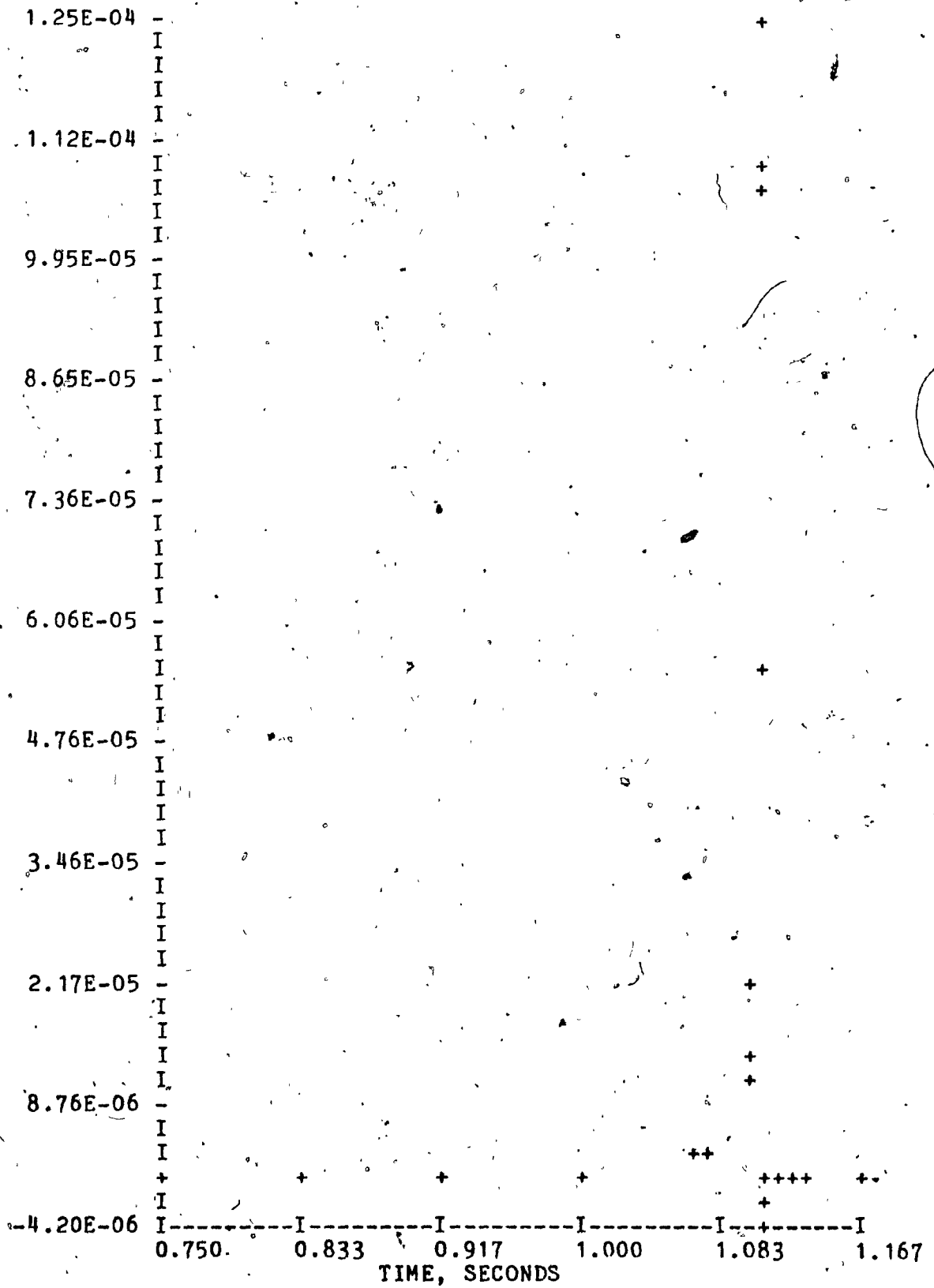


FIGURE D-37 NAME H2O

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)



NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

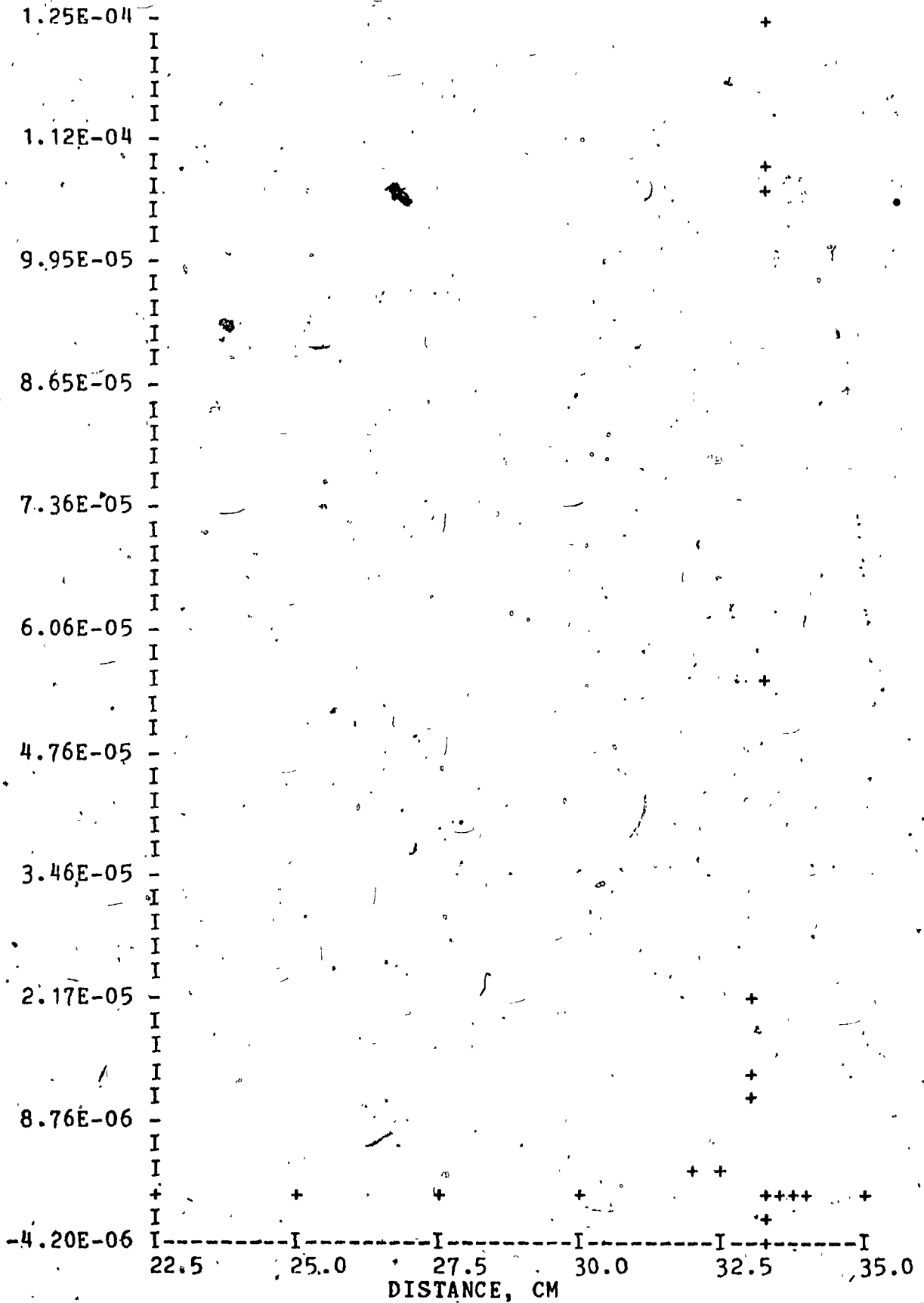
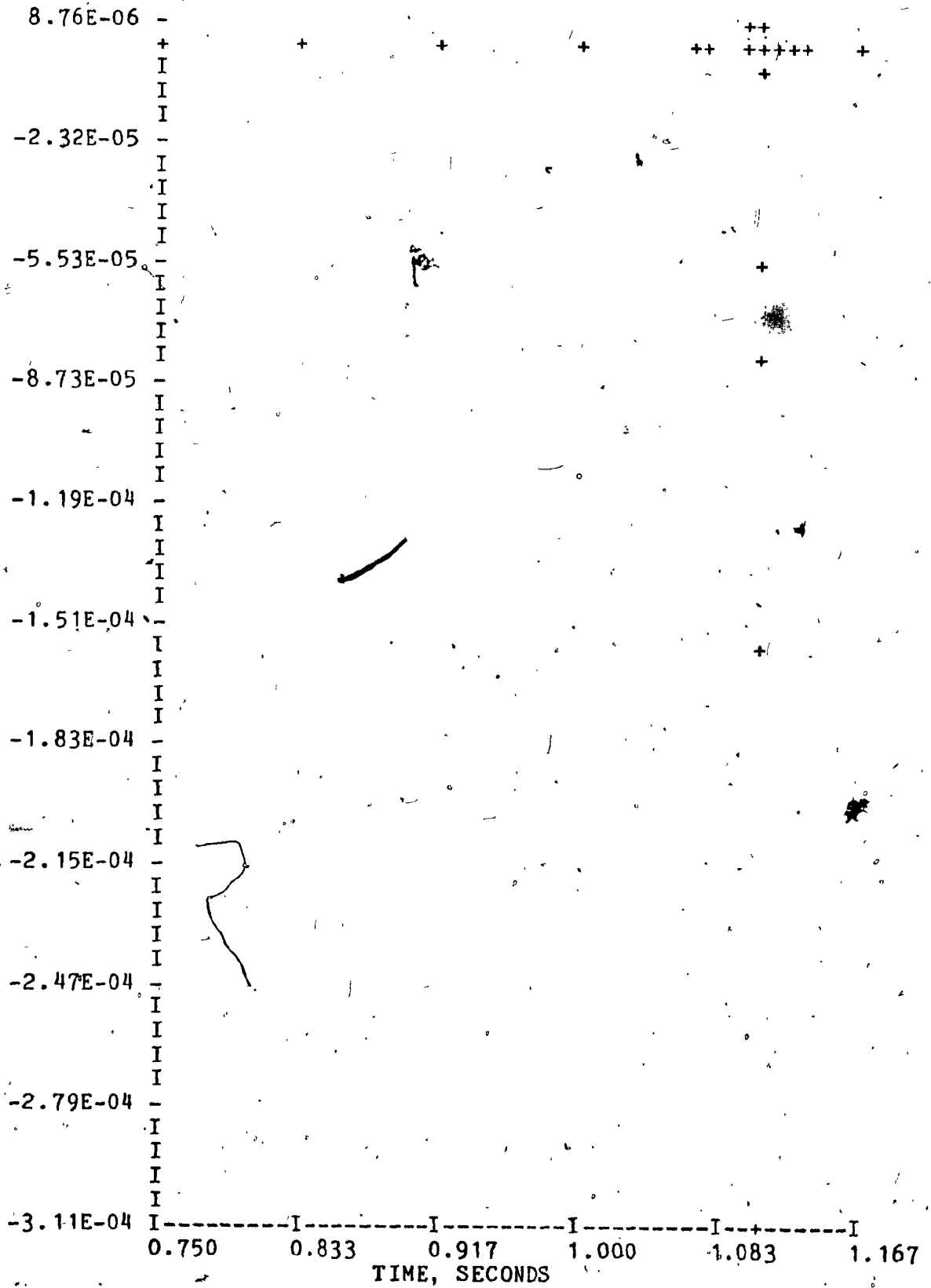


FIGURE B-19

NAME CO

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)



NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

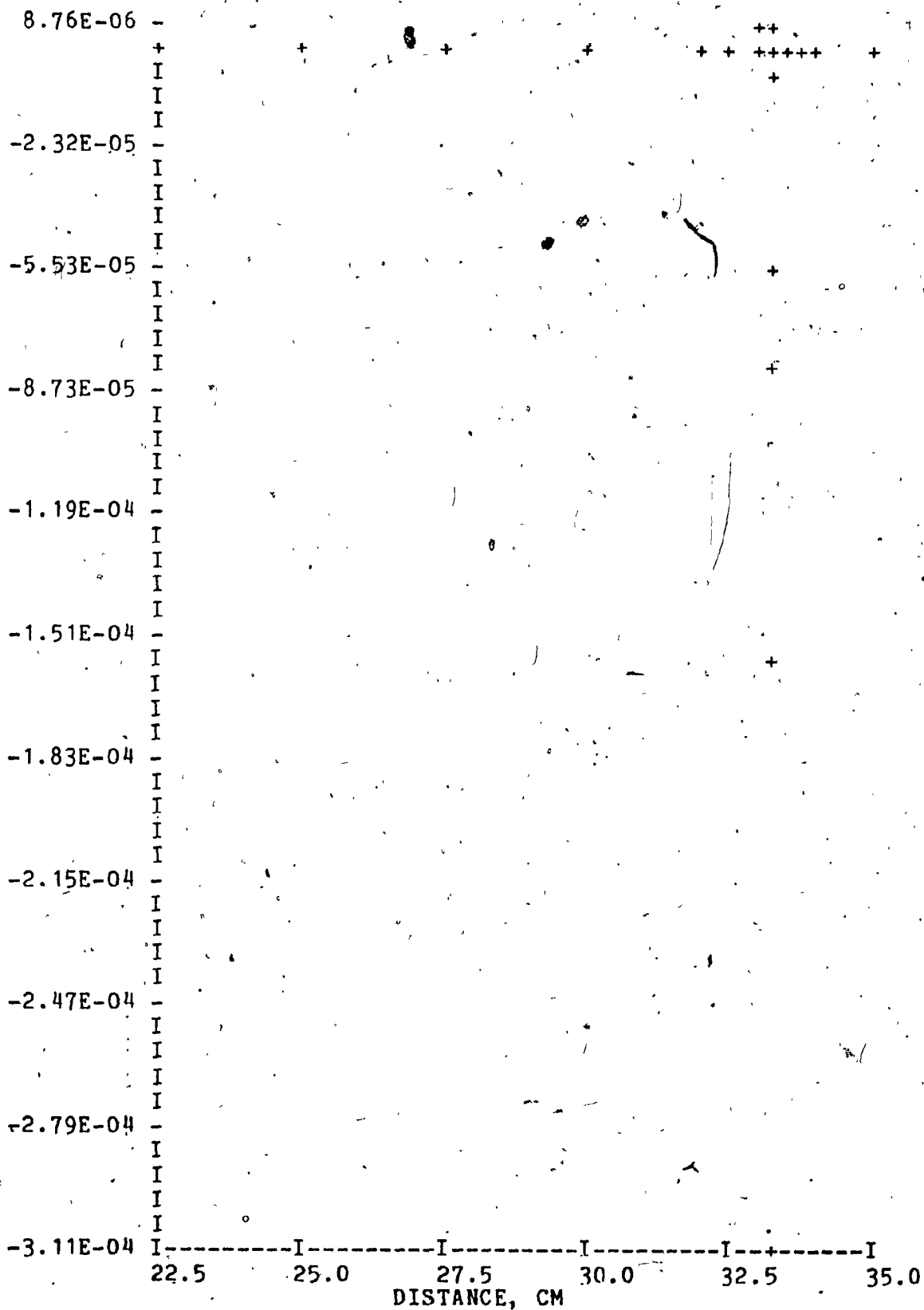


FIGURE R-41 NAME O

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

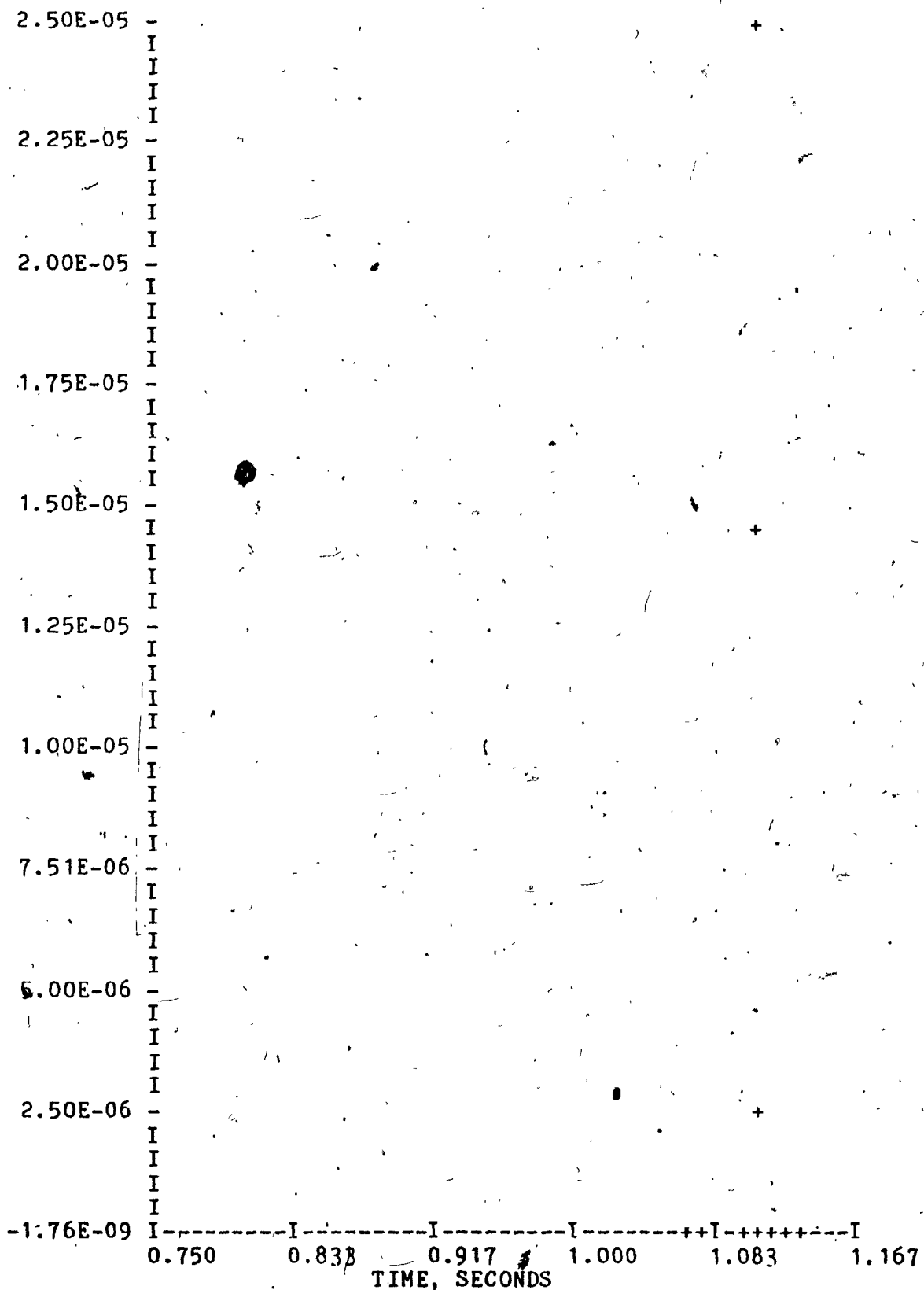
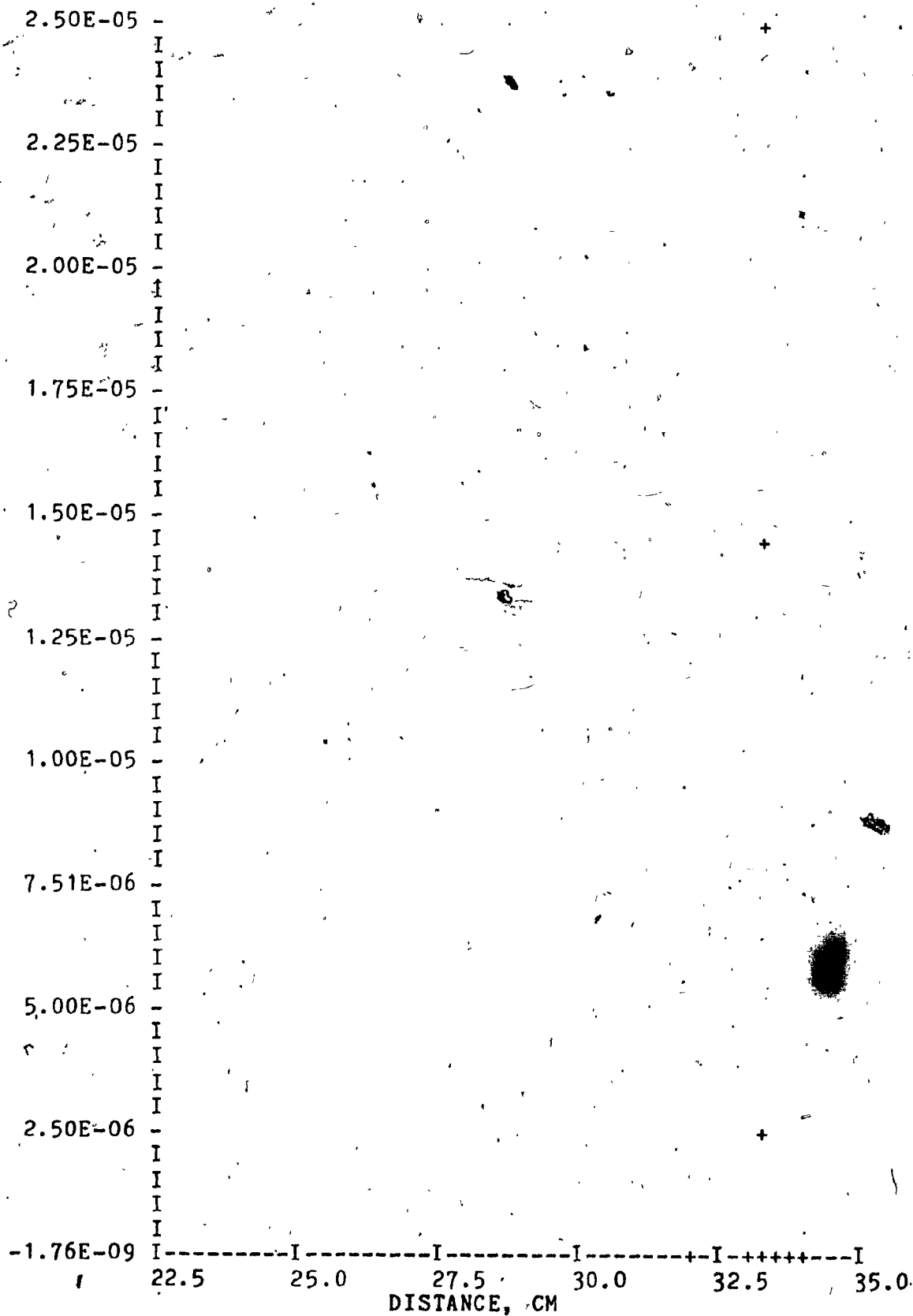


FIGURE B-12

NAME O

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)



NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

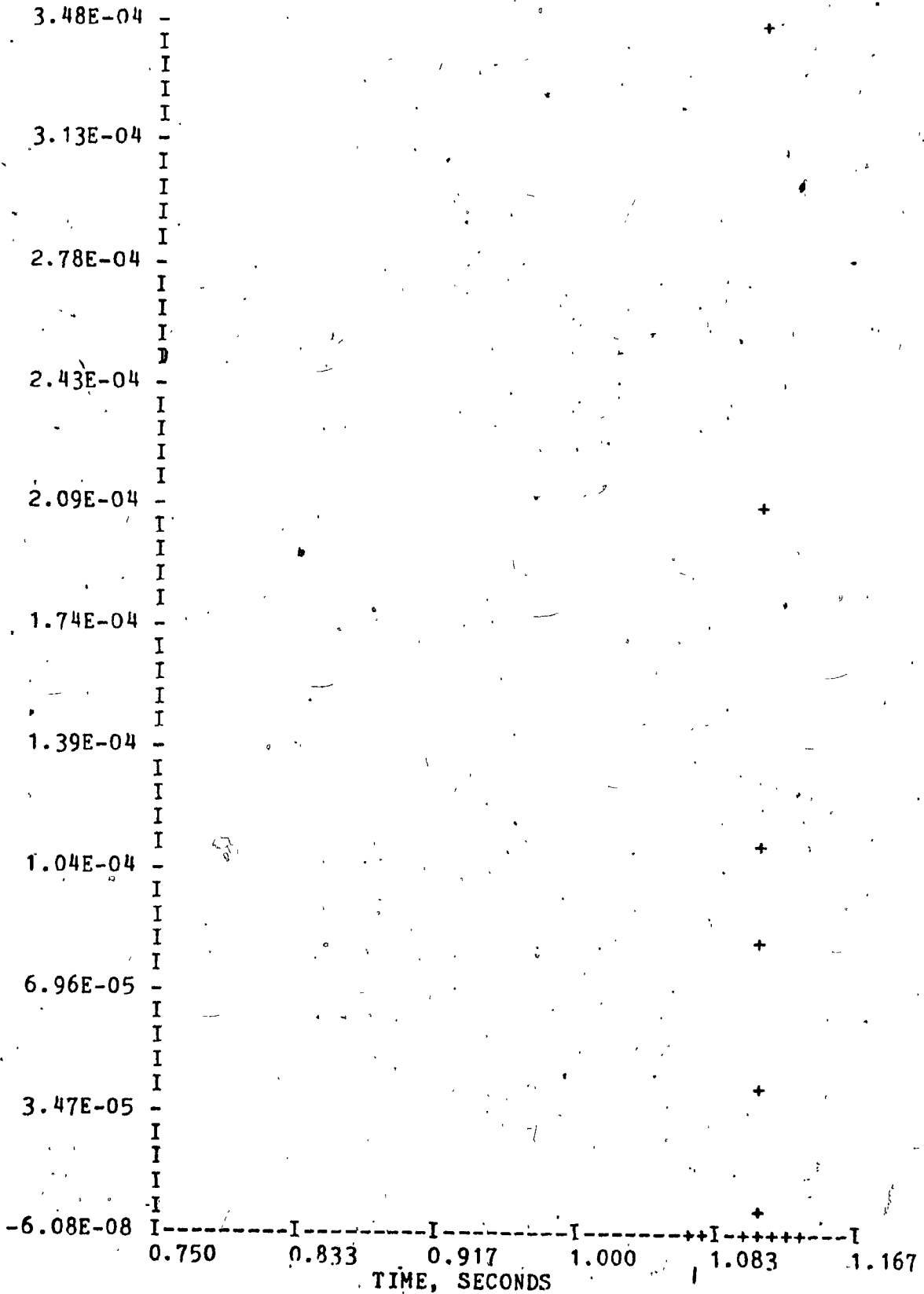


FIGURE B-44

NAME CO2

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

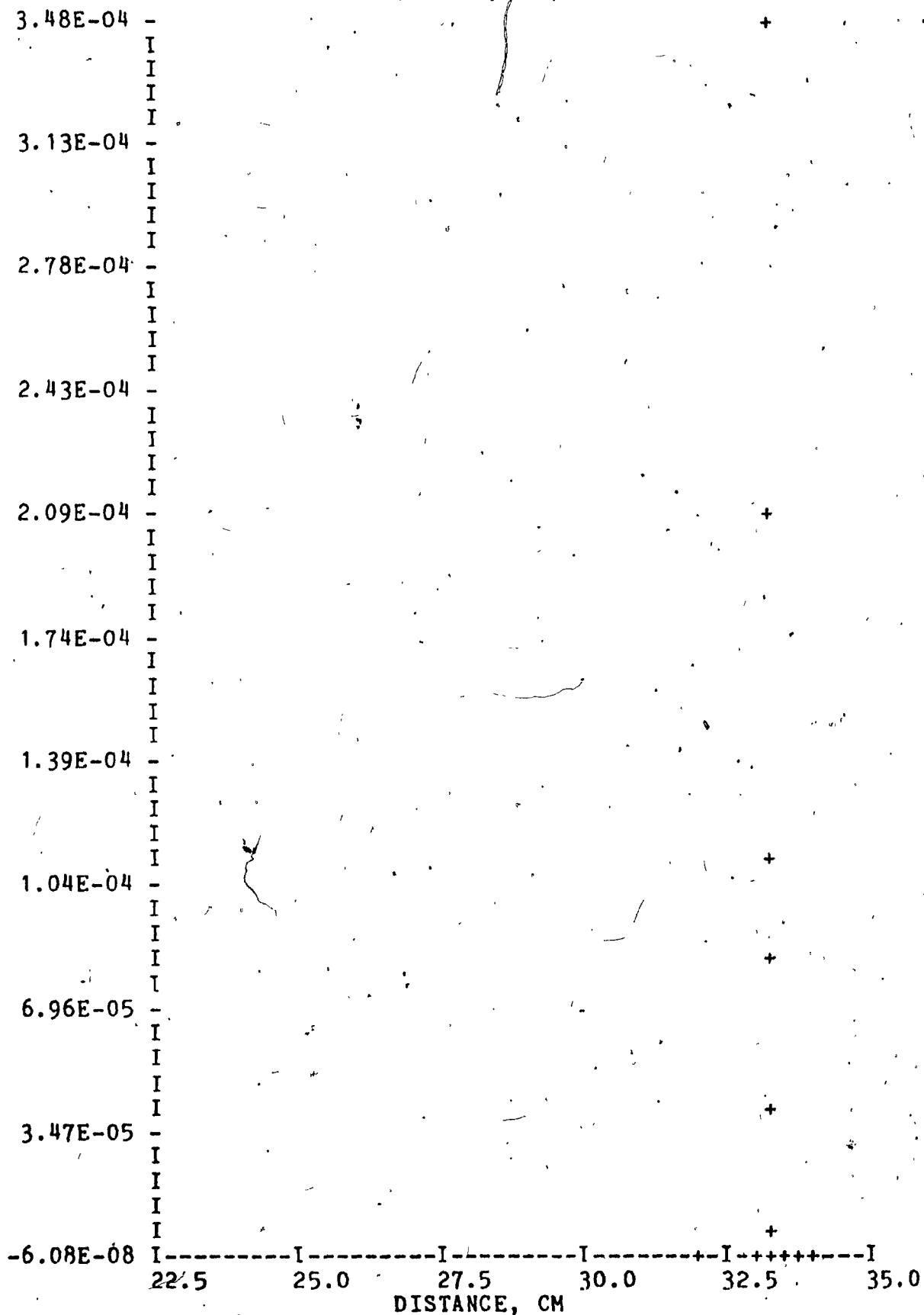
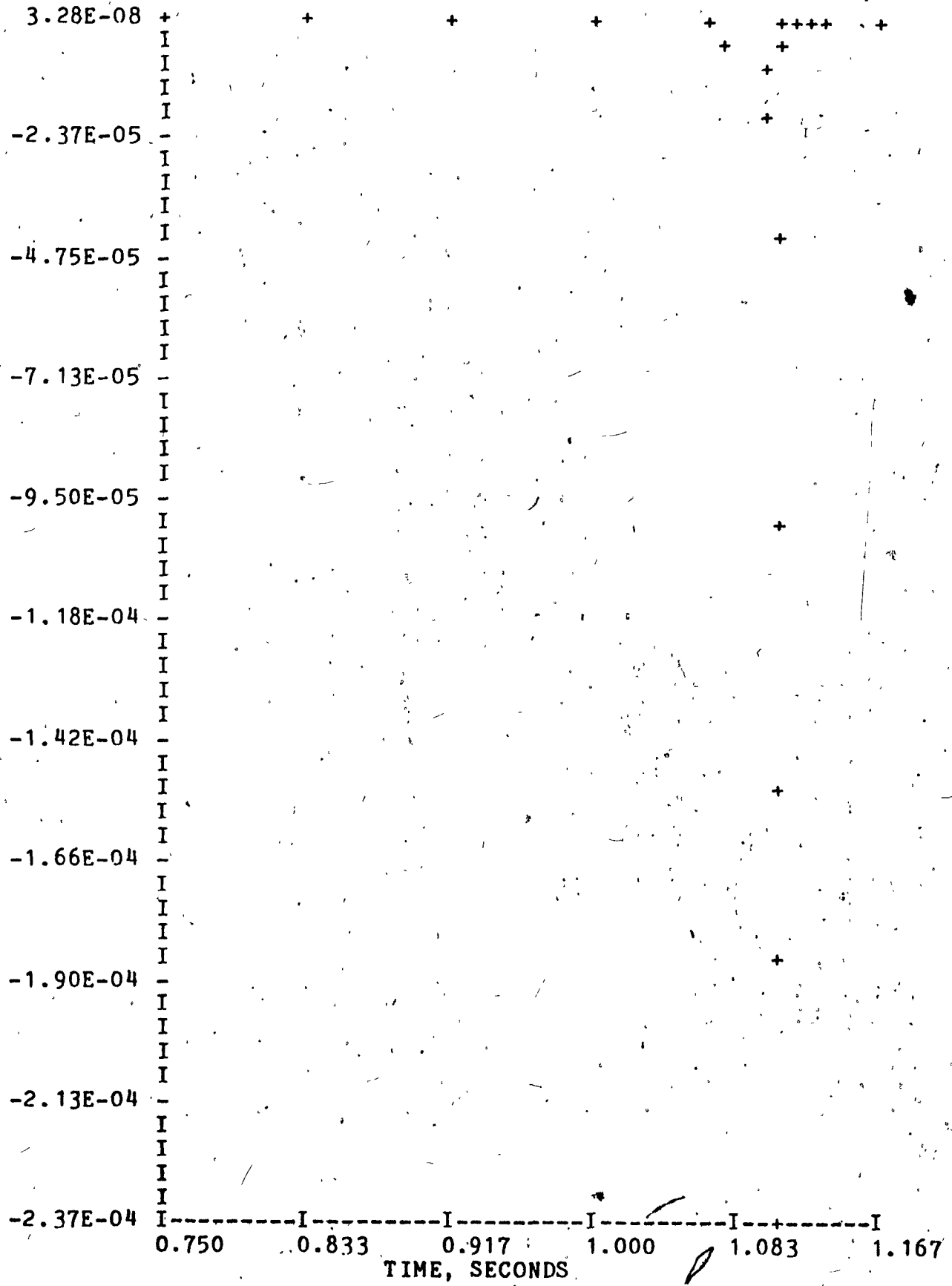


FIGURE B-45 NAME 02

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)



NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

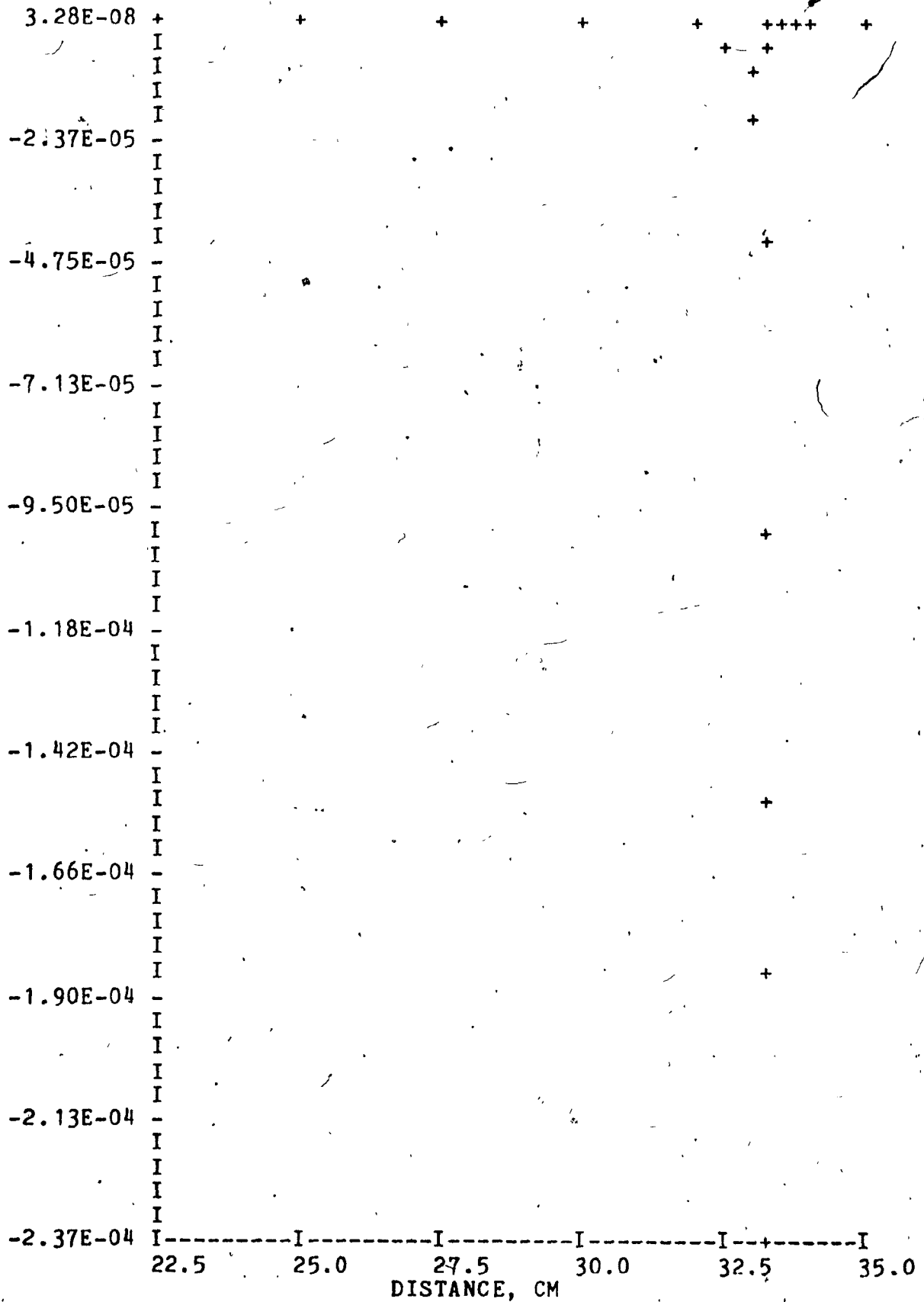


FIGURE B-17 NAME CH20

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

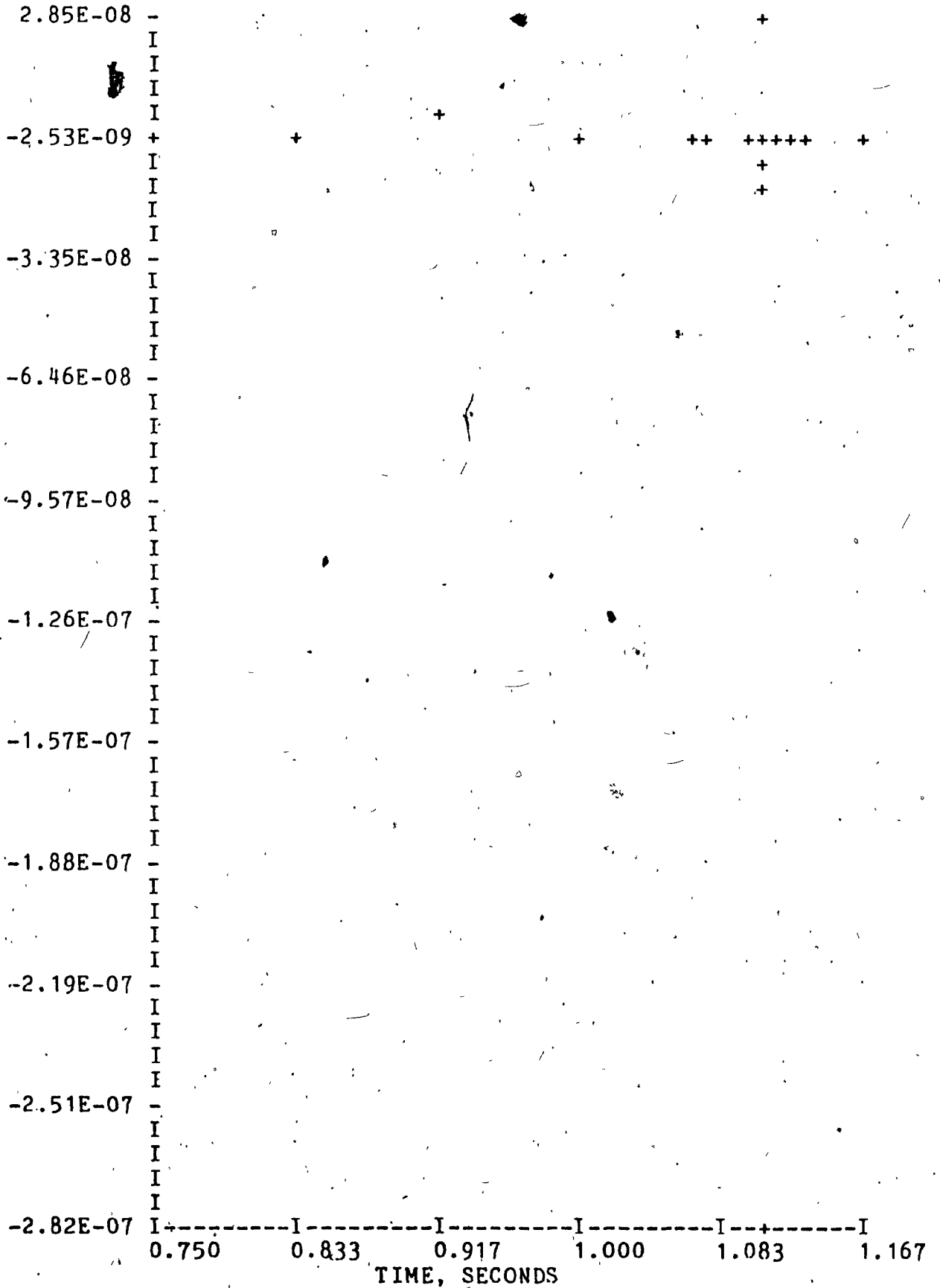


FIGURE B-48

NAME CH2O

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

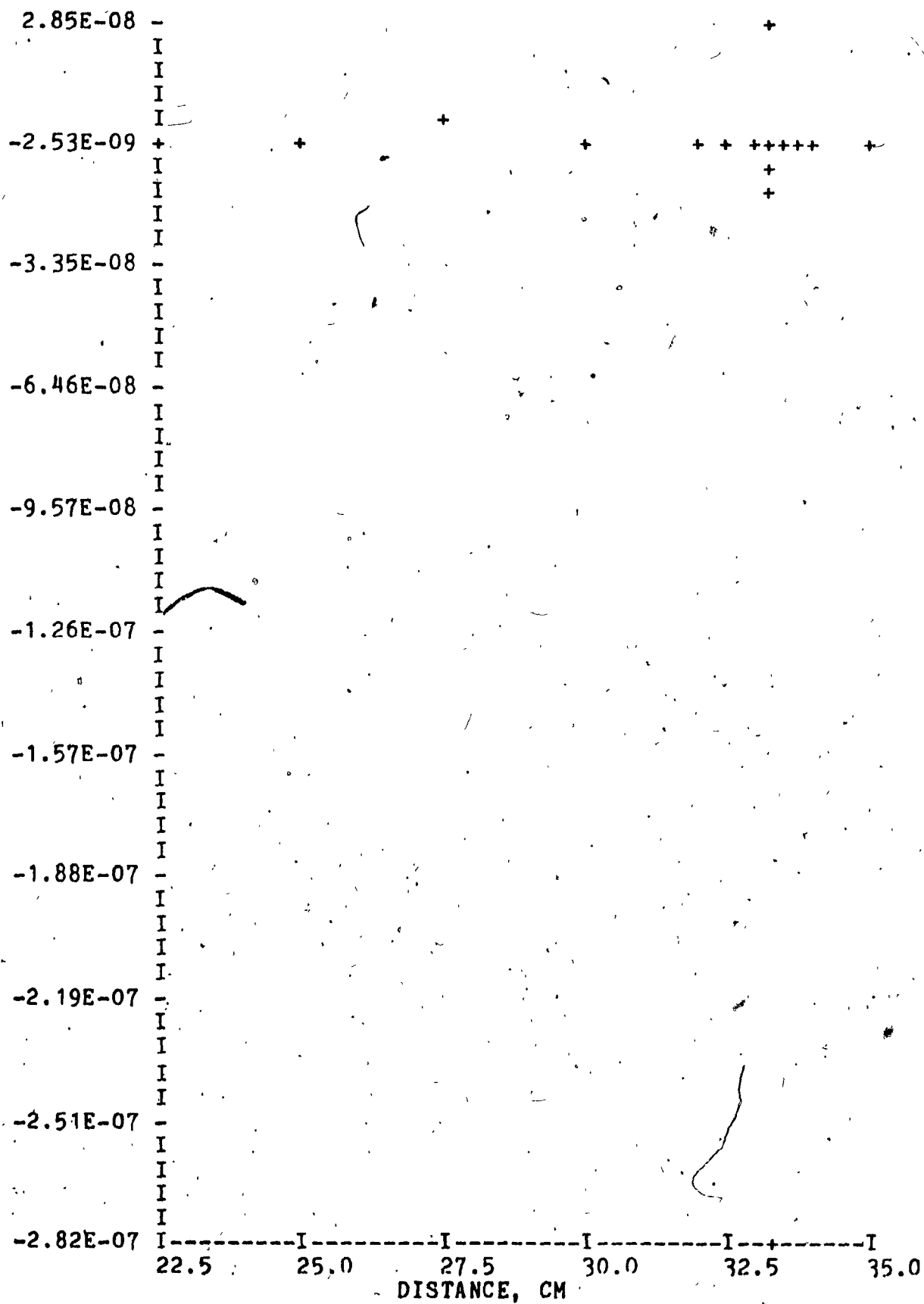
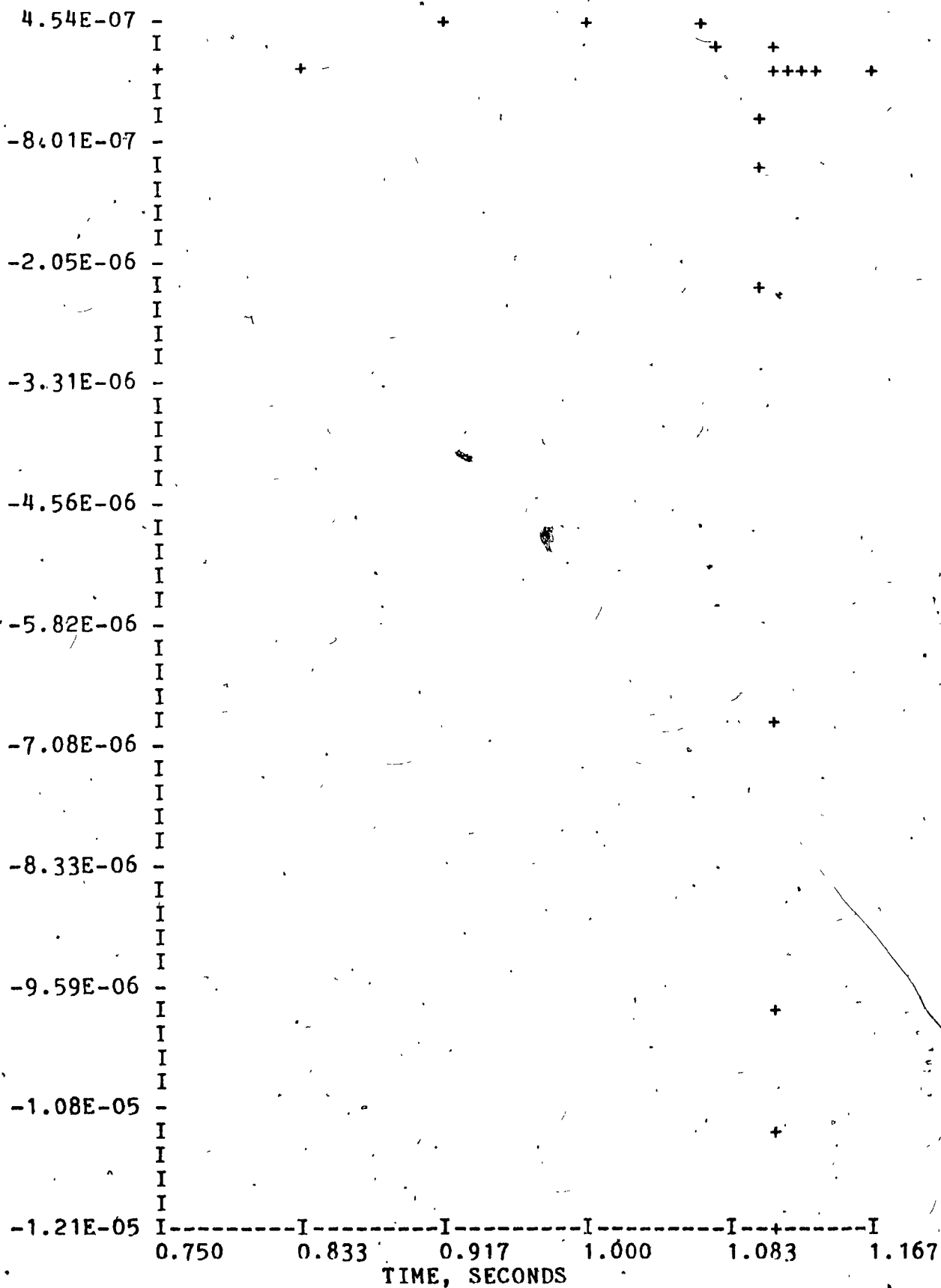


FIGURE B-49

NAME H2

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)



NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

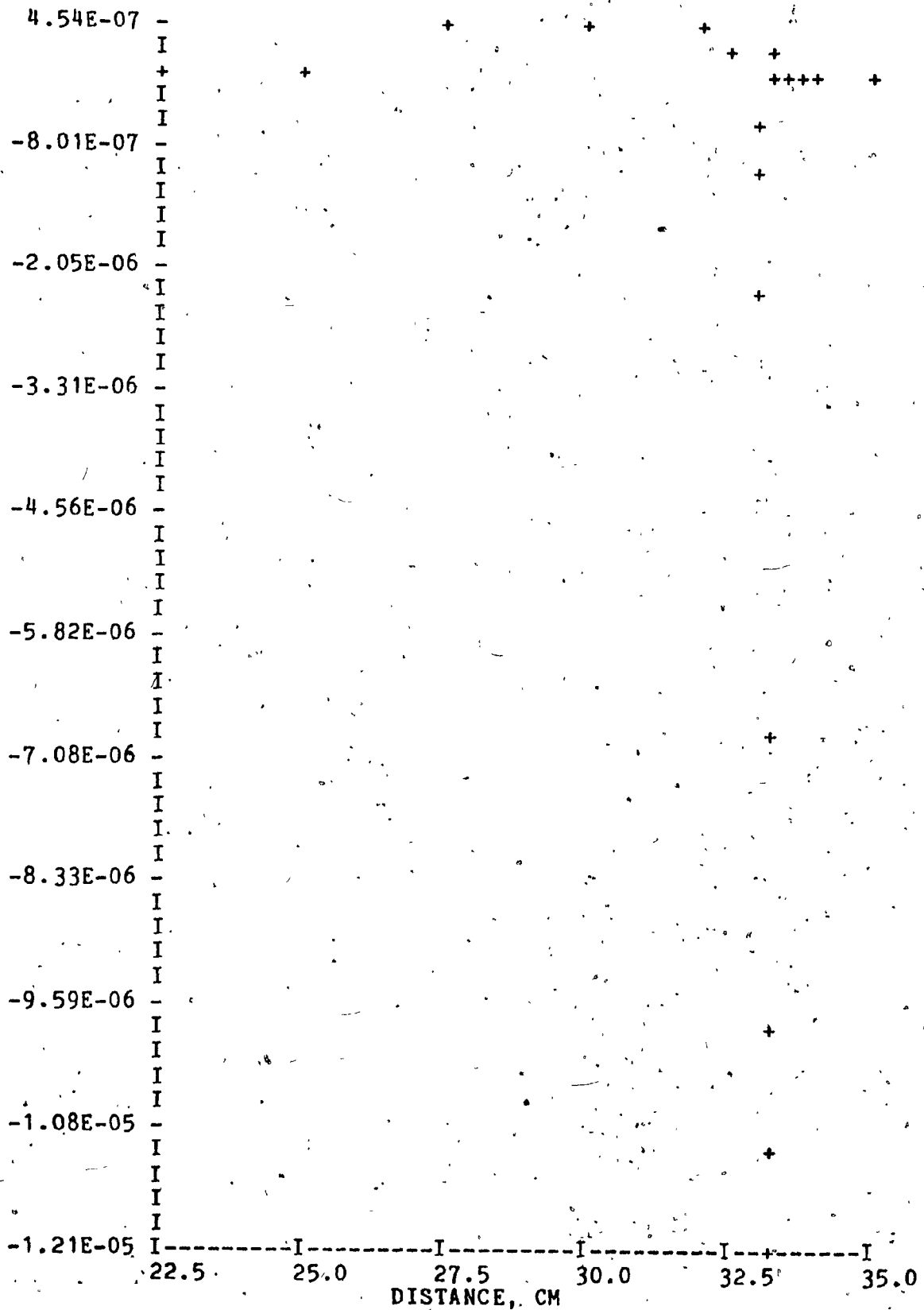


FIGURE B-51

NAME H02

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

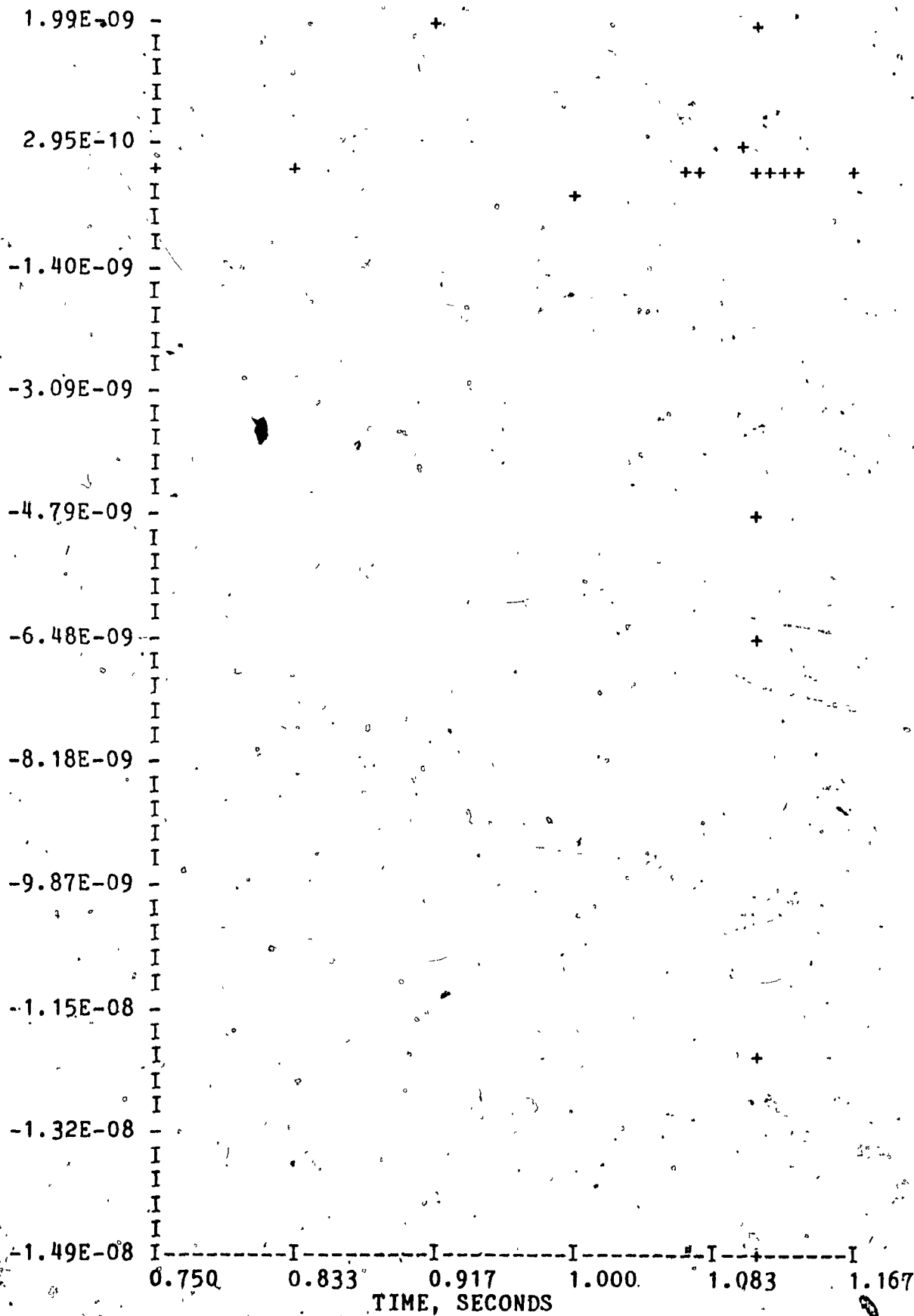


FIGURE B-52

NAME H02

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

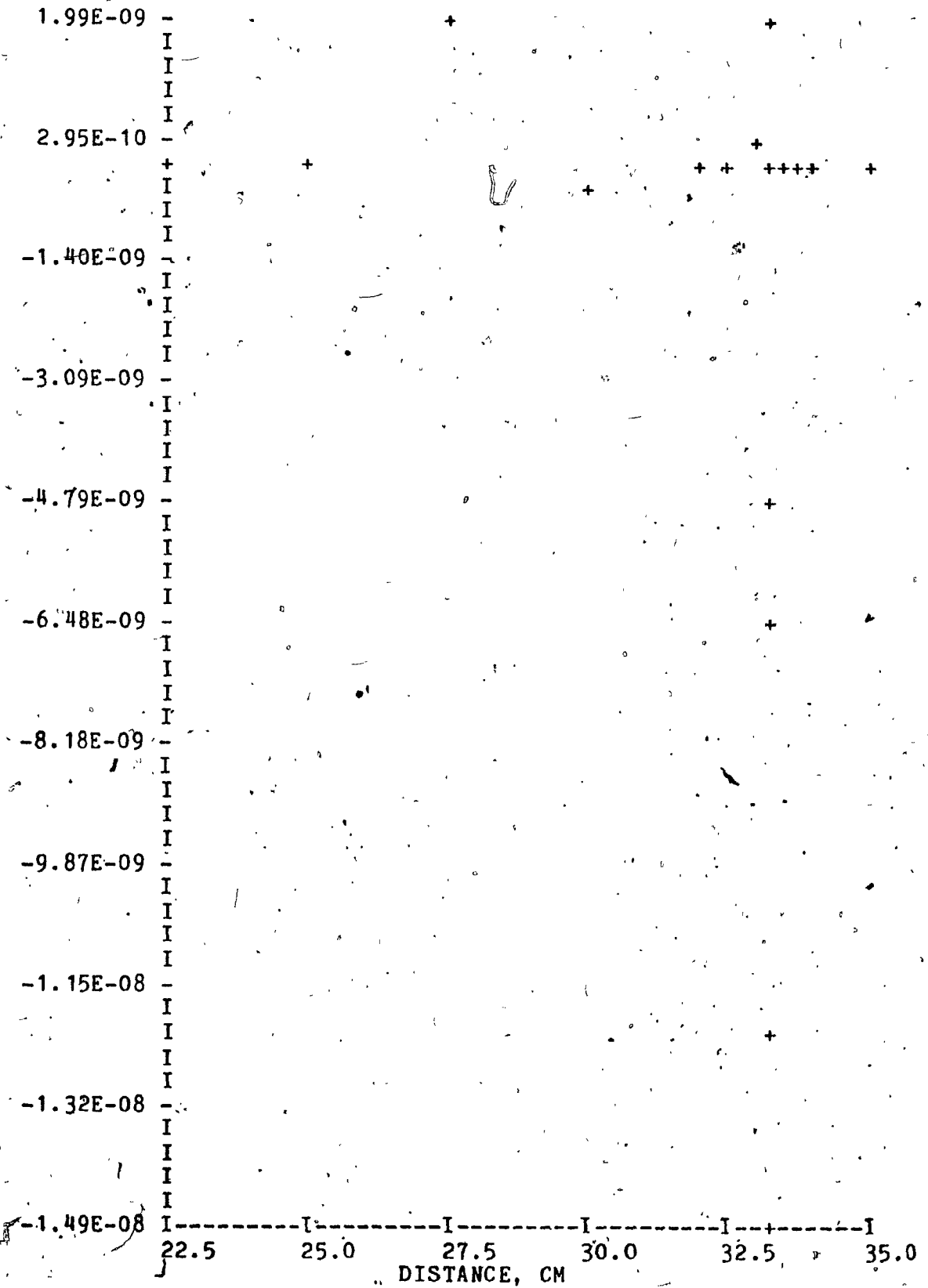


FIGURE R-5R

NAME HCO

NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

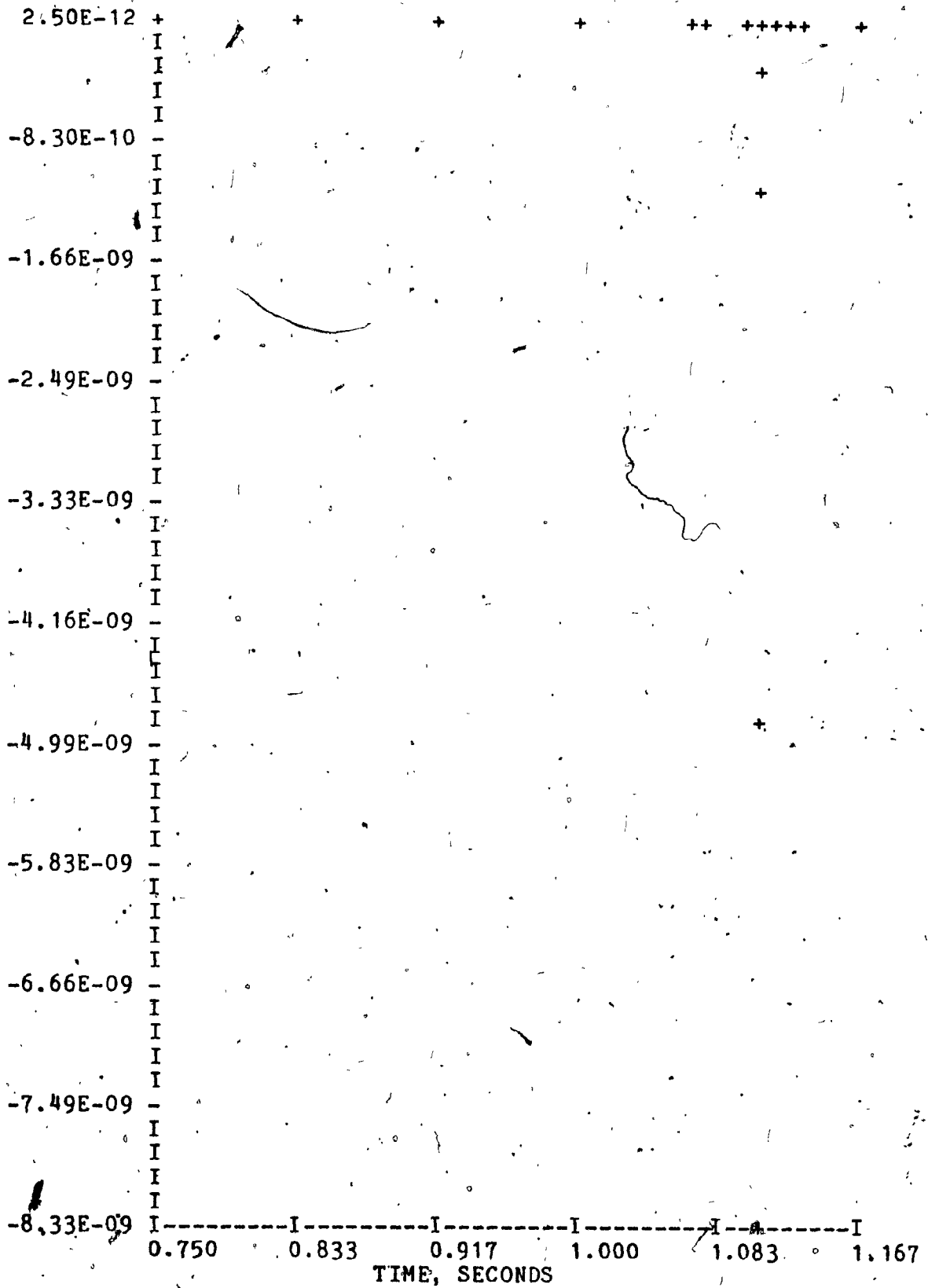
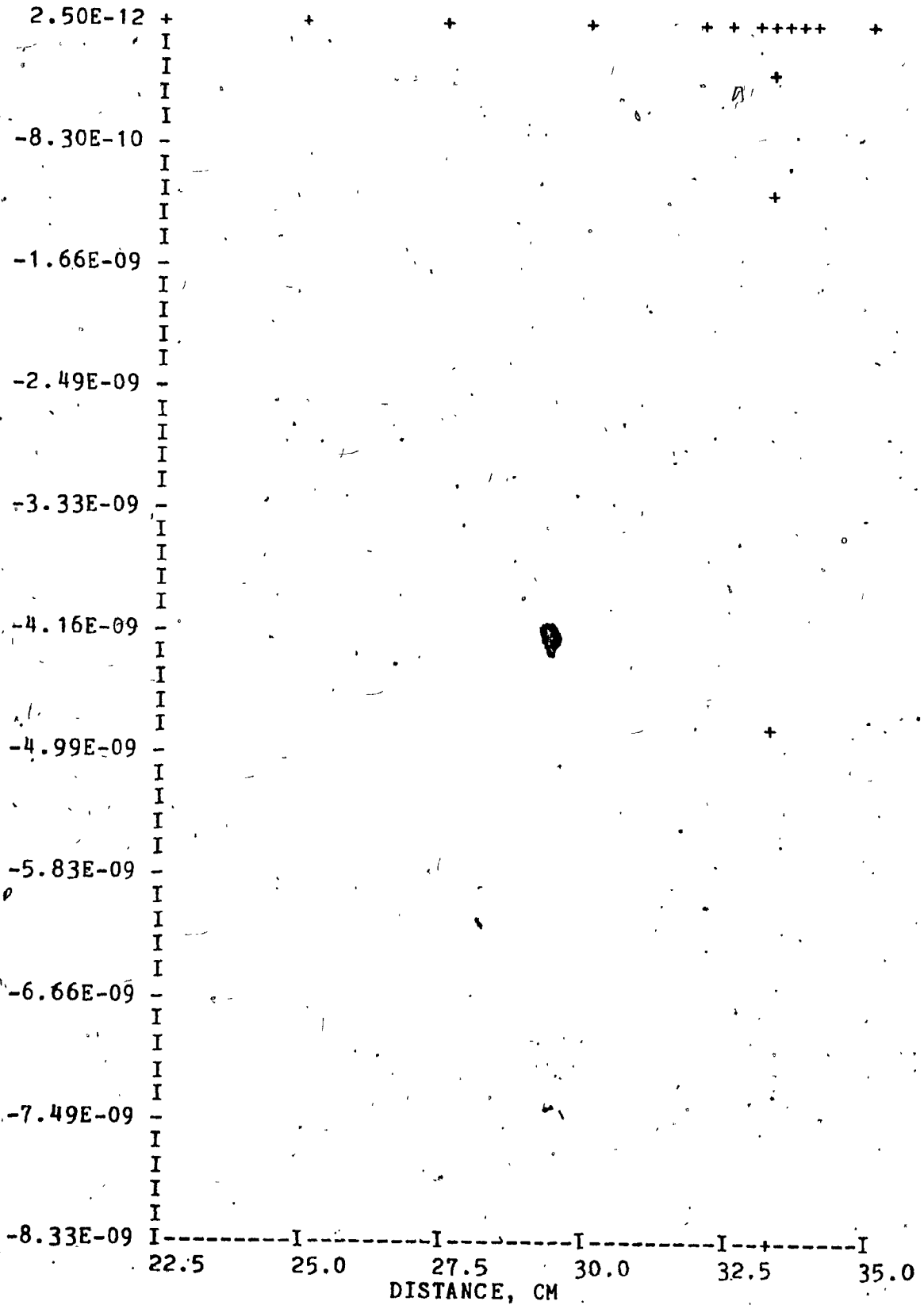


FIGURE B-54 NAME HCO

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)



NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)

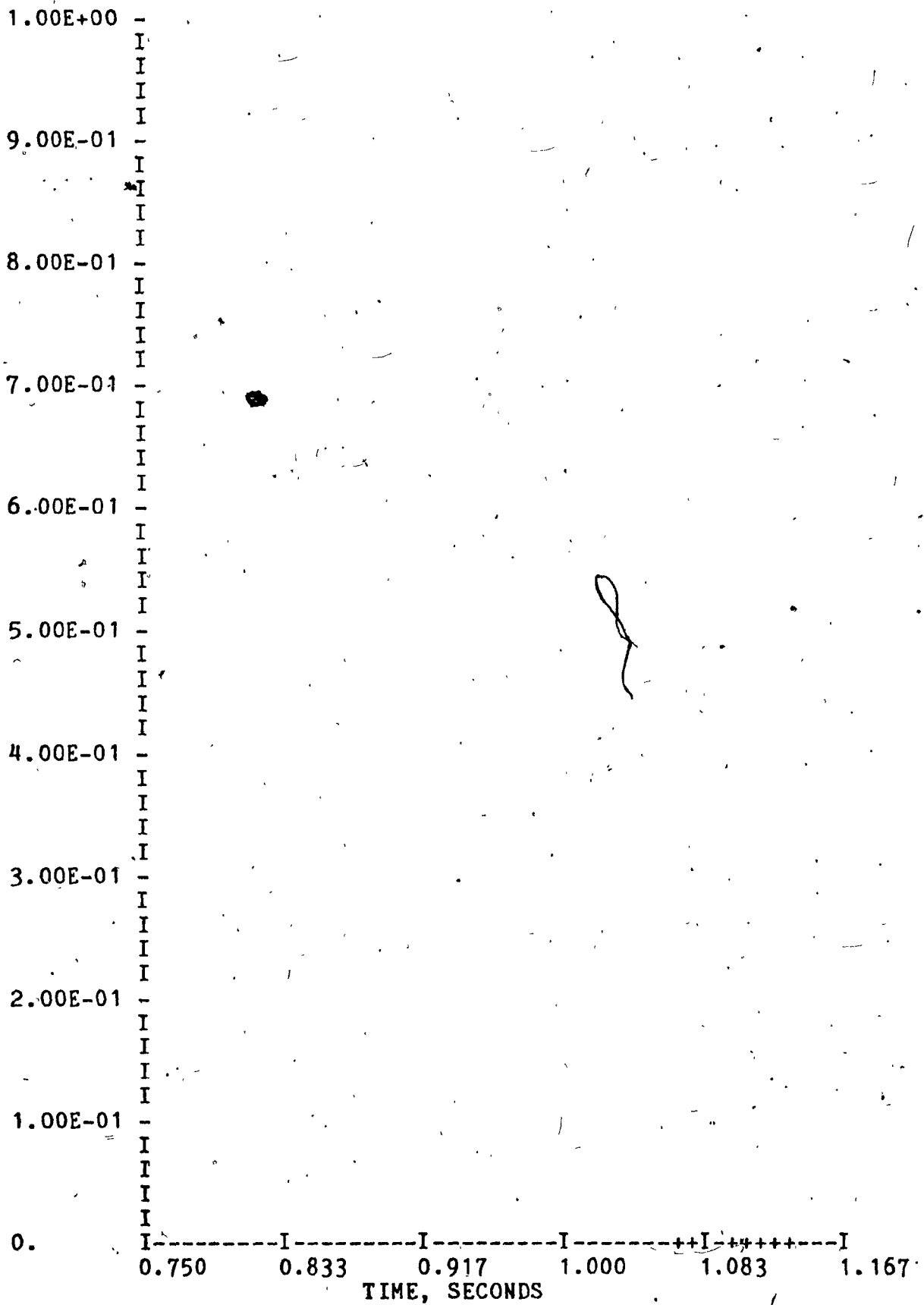


FIGURE B-56

NAME N2

NET SPECIES PRODUCTION RATE (IN MOLE/CM**3/SEC)

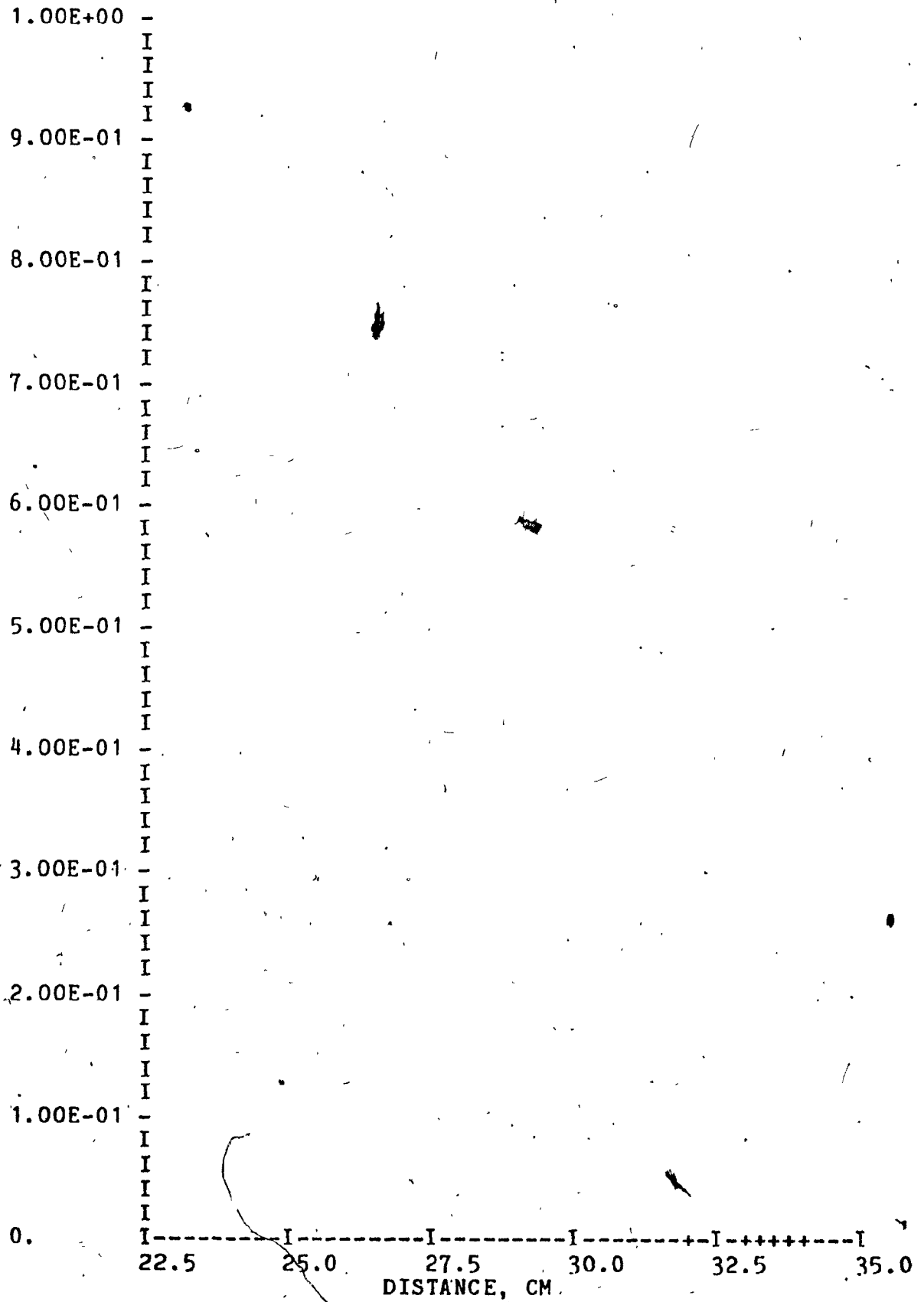


FIGURE R-57

TEMPERATURE (KELVIN) VS TIME

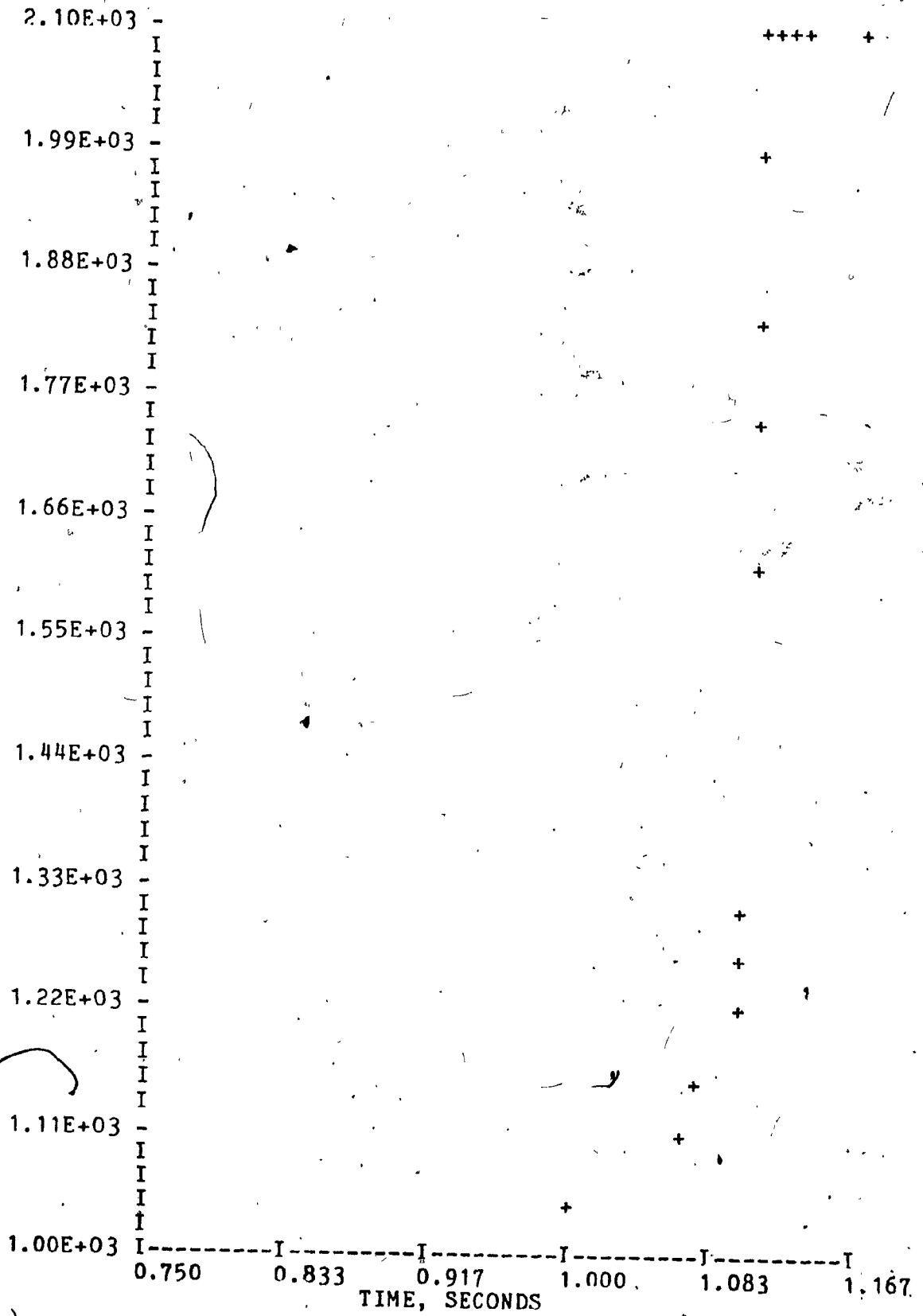


FIGURE B-58 TEMPERATURE (KELVIN) VS DISTANCE

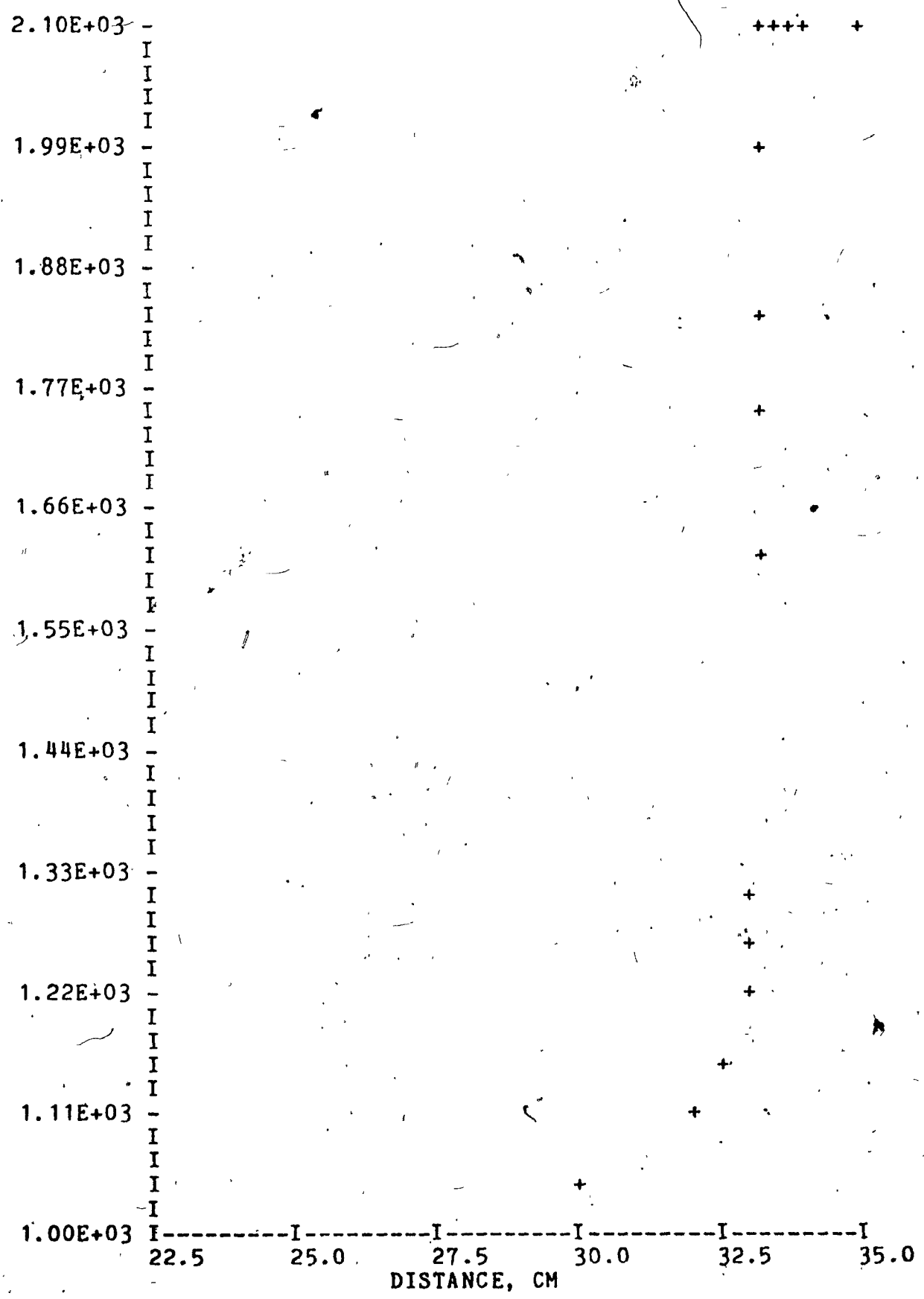


FIGURE B-59

ENTROPY (CAL/GM-K) VS TIME

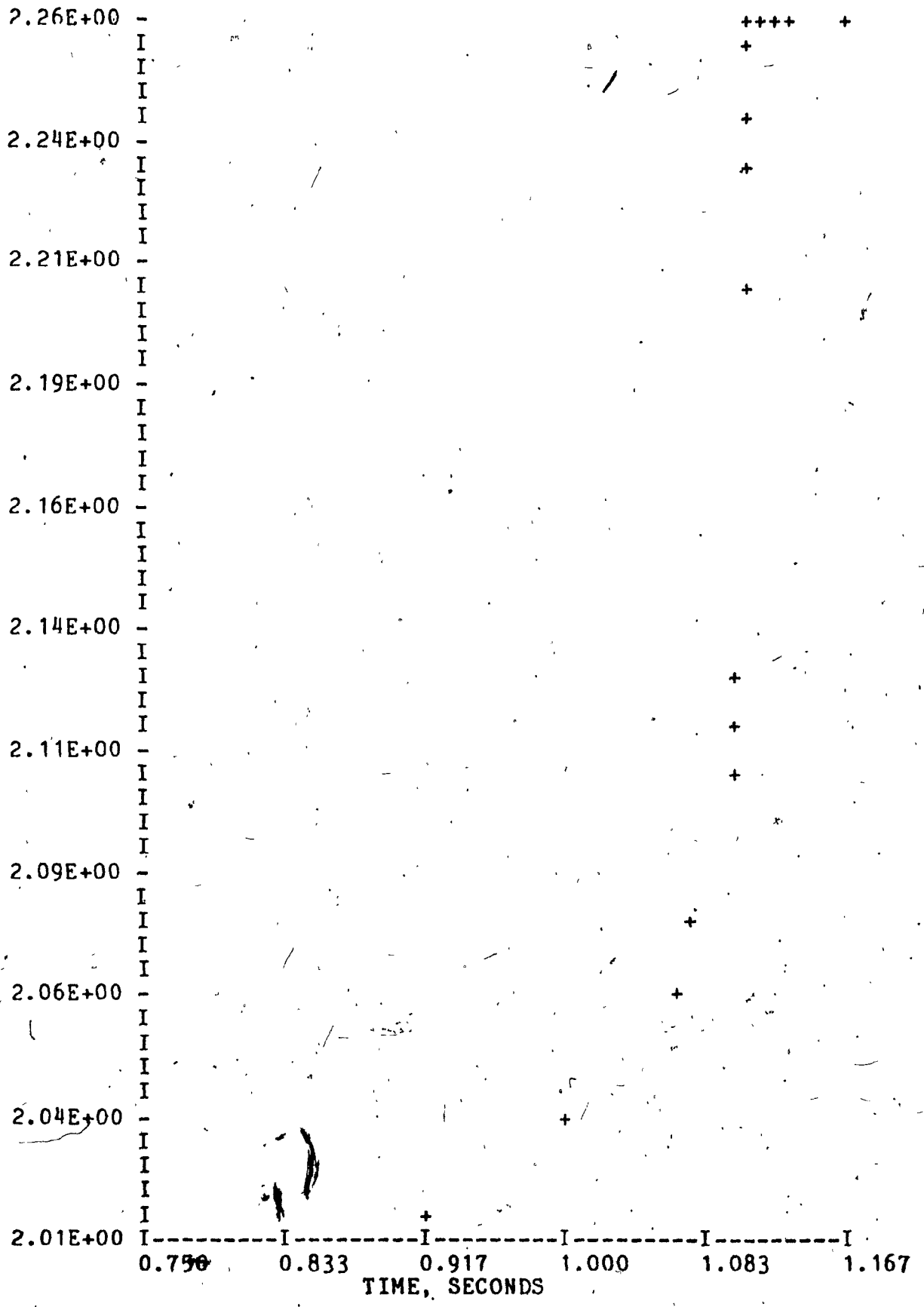


FIGURE B-60

ENTROPY (IN CAL/GM -K) VS DISTANCE

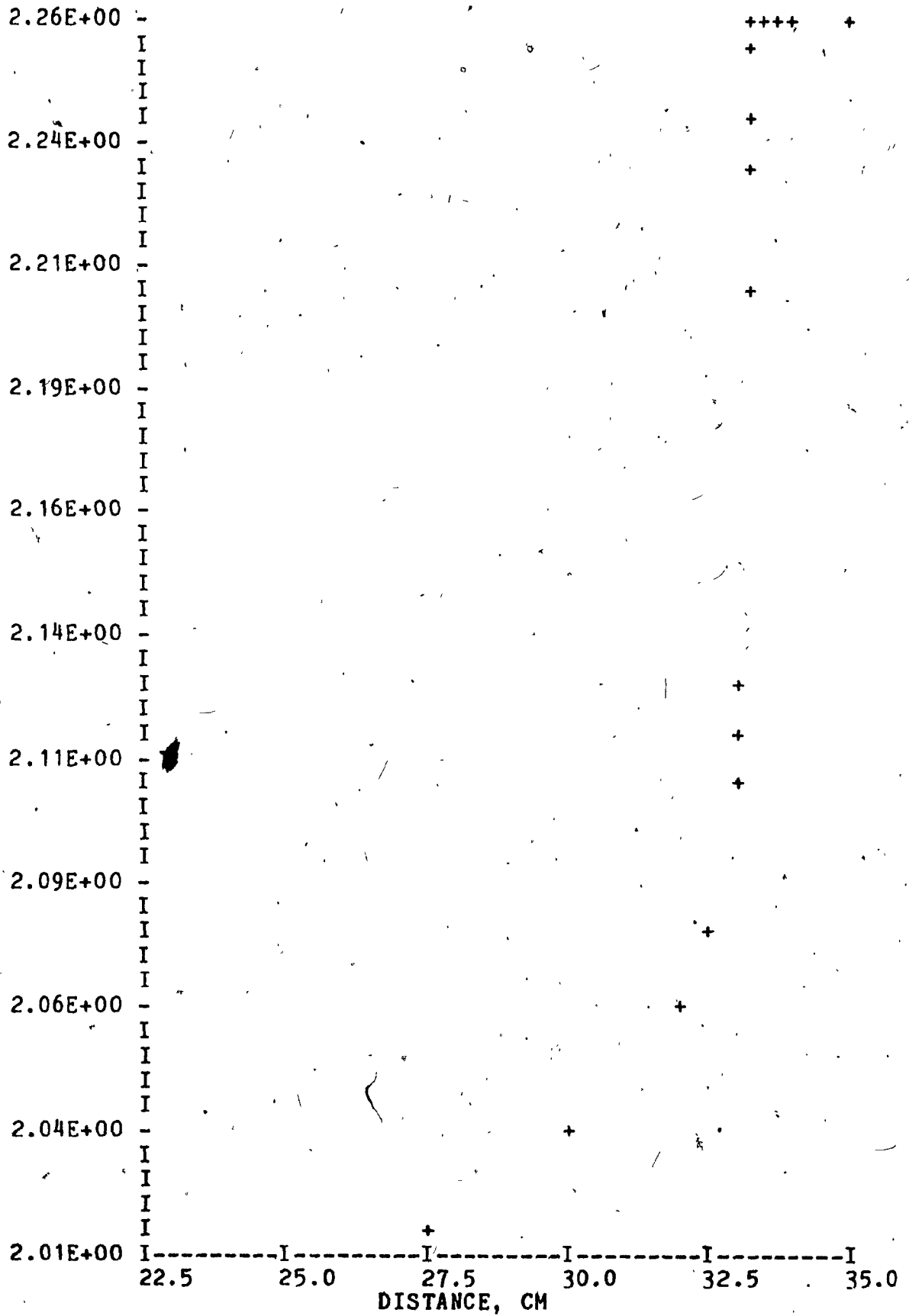


FIGURE R-61

ENTHALPY (CAL/GM) VS TIME

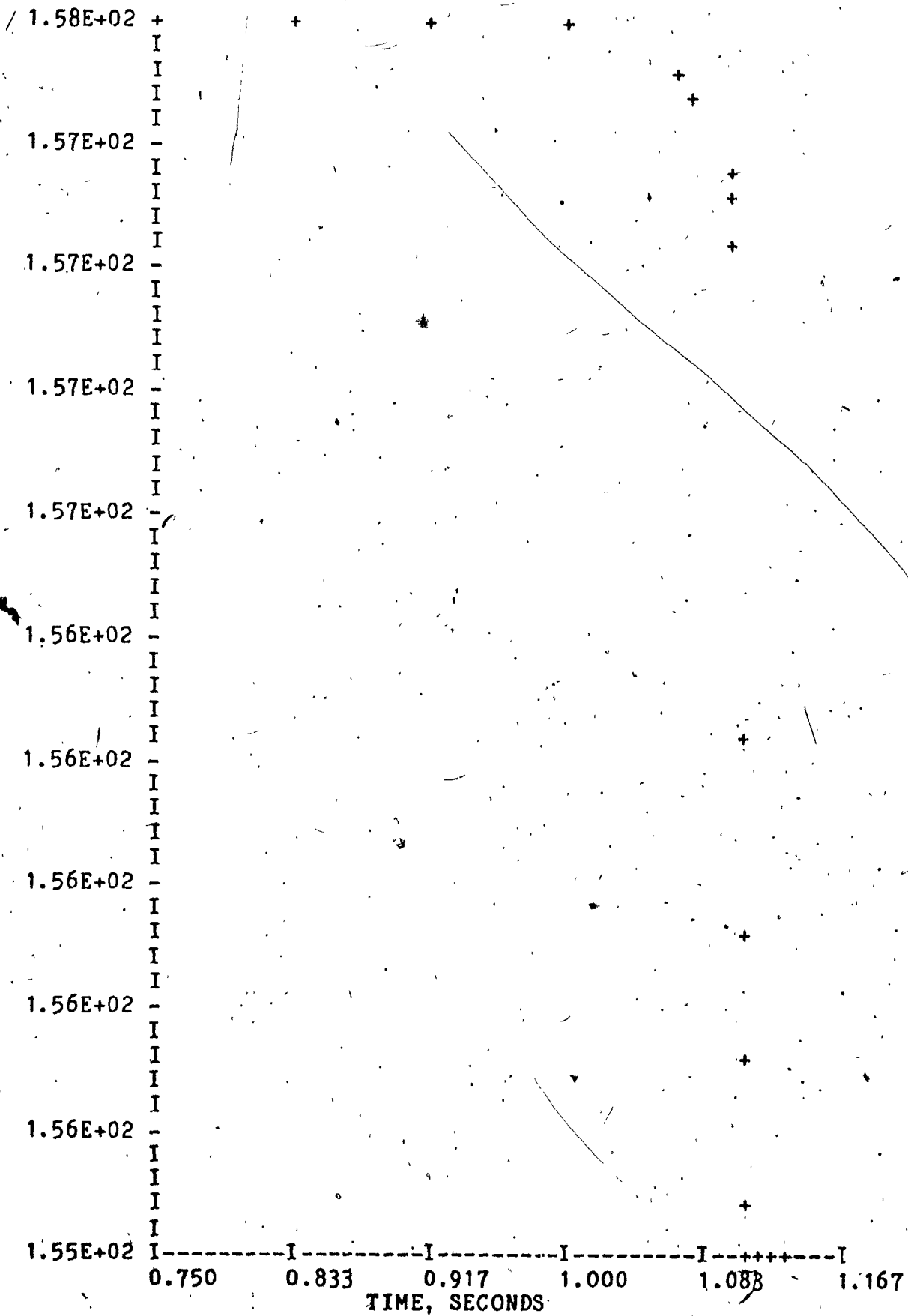


FIGURE H-63 GIBBS F E (CAL/GM) VS TIME

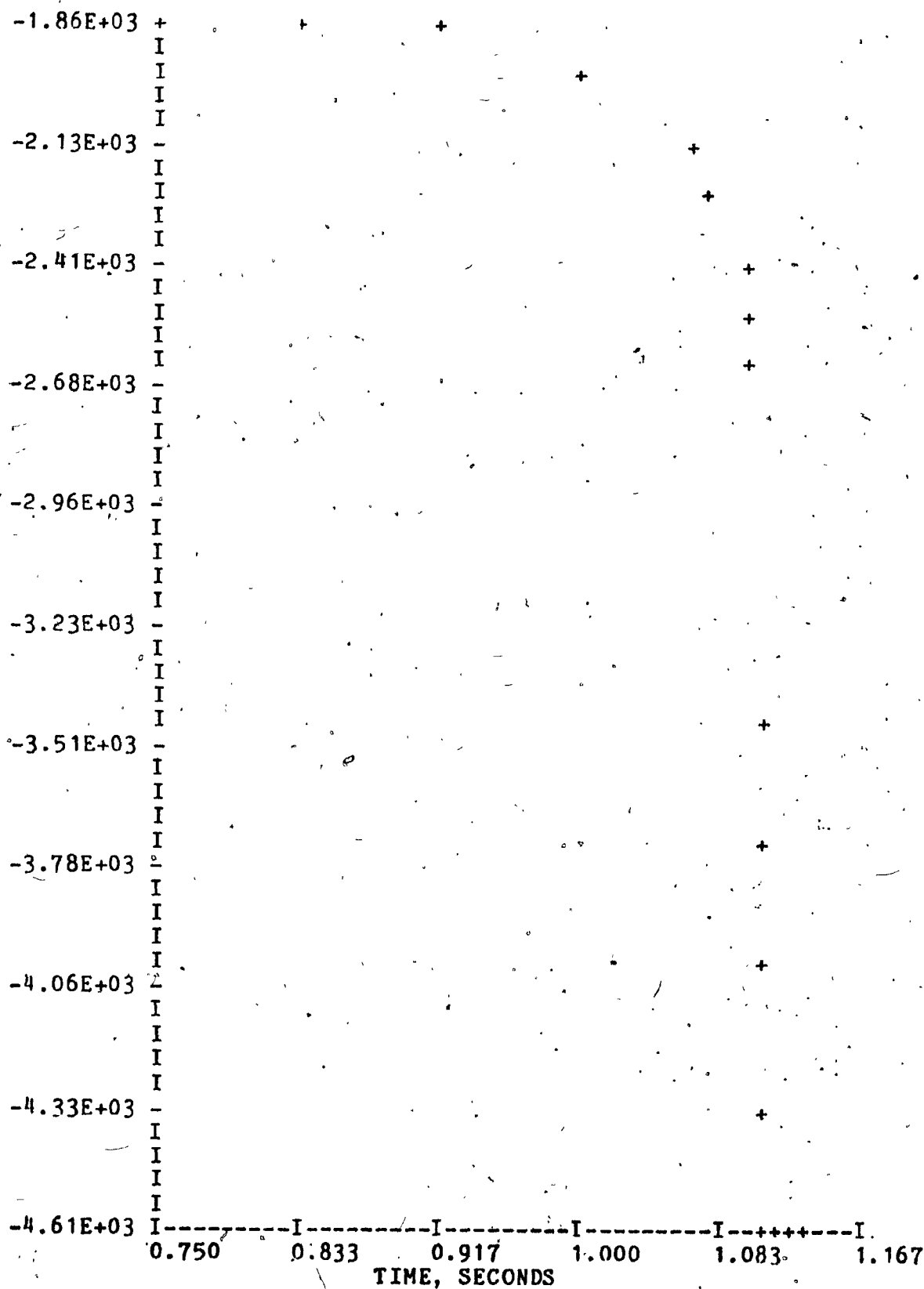
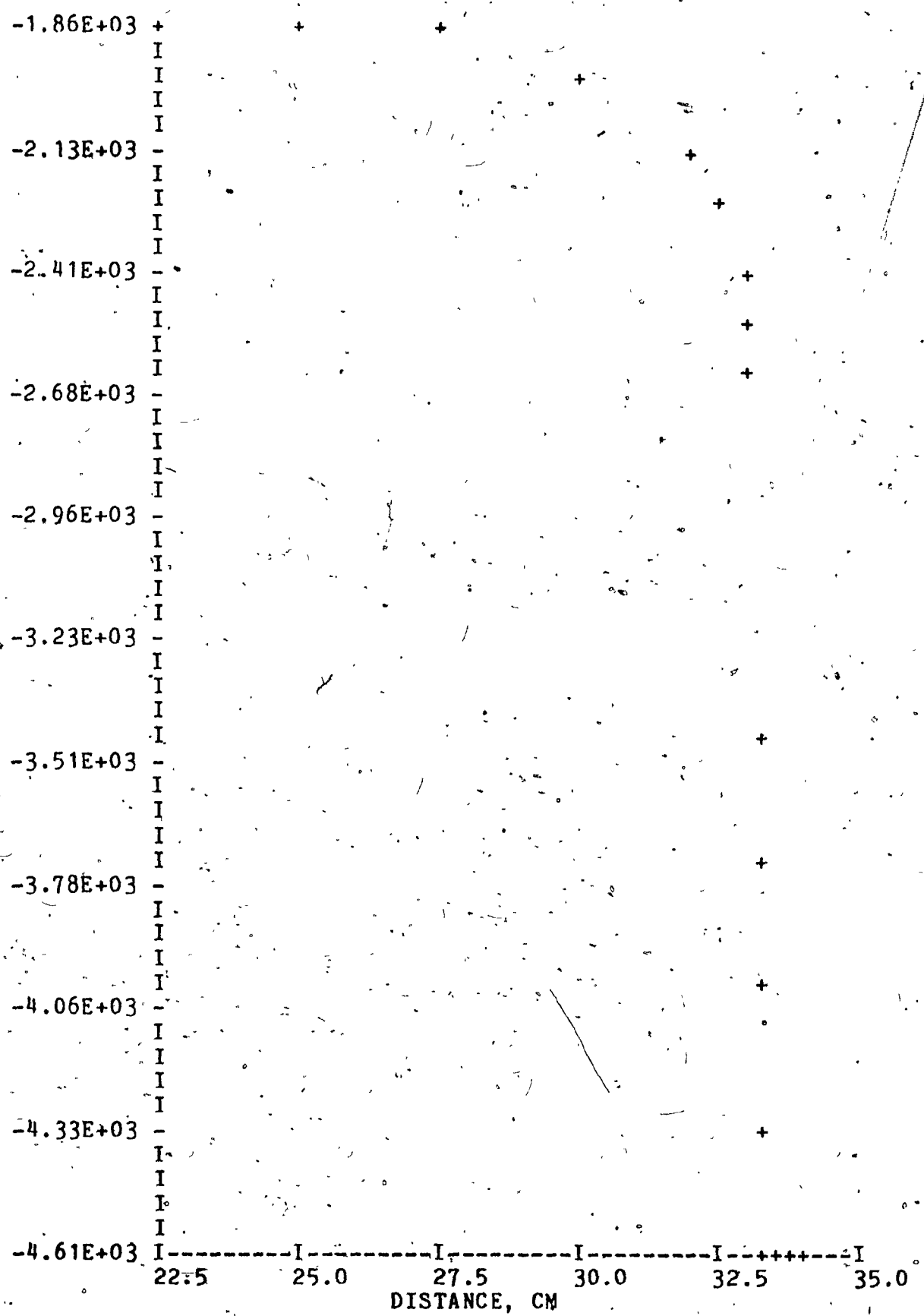


FIGURE B-64

GIBBS F E (CAL/GM) VS DISTANCE



APPENDIX C
DETAILED CALCULATIONS

Detailed Calculations

The combustion zone used in the kinetics scheme has been divided into forty elements. Each of these elements has associated with it the products of the reactions of the previous zone. In that way, using stiff kinetics, it has been possible to build up the species appearing in the entire flame.

These species have been shown as profiles in Appendix A, to show the trend involved. For convenience, the species are listed below:

CH₄

CH₃

H

OH

H₂O

CO

O

CO₂

O₂

CH₂O

H₂

HO₂

HCO

N₂

In the following, the magnitudes calculated in the chemical kinetic code are explicitly listed.

The thermodynamic and chemical quantities which appear are:

Pressure
Density
Temperature
Entropy
Ratio of Specific Heats (γ)
Enthalpy
Gibbs Free Energy

and

Species
Concentration
Mole Fraction
Net Species Production Rate

followed by

Reaction Number (as in the text)
Net Reaction Conversion Rate
Ratio of Net Reaction Rate to Forward Reaction Rate.

These quantities are traced from the time zero to approximately 1.333 second, when the reaction is essentially complete.

These data have been included in the belief that some of the information herein may be considered by other investigators, with a view to providing more detailed understanding of chemical kinetics in general, and kinetics mechanisms at the flammability limits in particular. Indeed, some focus is directed toward the understanding of the role of the Gibbs free energy in the understanding.

It should be noted that the units used in the following tables are cgs, except where explicitly stated otherwise, as is the case for pressure where the units are atmospheres."

Also, the form of floating point numbers is exponential to the base ten, i.e., in what may be termed "E - format."

Tables of Detailed Calculation Results.

TIME 01 SEC AREA 19.5 SQ CM POSITION 0. CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43382E-04
 TEMPERATURE, K 1000.00
 ENTROPY, CAL/GM-K 2.0185
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86046E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45900E-07	5.30000E-02	-3.73150E-13
CH3	0.	0.	3.73150E-13
H	0.	0.	3.73150E-13
OH	0.	0.	0.
H2O	0.	0.	0.
CO	0.	0.	0.
O	0.	0.	0.
CO2	0.	0.	0.
O2	2.44089E-06	2.00290E-01	0.
CH2O	0.	0.	0.
H2	0.	0.	0.
HO2	0.	0.	0.
HCO	0.	0.	0.
N2	9.10000E-06	7.46710E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.16467E-06	1.00000E+00
2	0.	0.
3	0.	0.
4	0.	0.
5	0.	0.
6	0.	0.
7	0.	0.
8	0.	0.
9	0.	0.
10	0.	0.
11	0.	0.

DETAILED KINETIC CALCULATION

12	0.	0.
13	0.	0.
14	0.	0.
15	0.	0.
16	0.	0.
17	0.	0.
18	0.	0.
19	0.	0.
20	0.	0.
21	0.	0.
22	0.	0.
23	0.	0.
24	0.	0.
25	0.	0.
26	0.	0.
27	0.	0.
28	0.	0.
29	0.	0.
30	0.	0.

DETAILED KINETIC CALCULATION

150

TIME 5.00000E-02 SEC AREA 19.5 SQ CM POSITION 1.50000E+00 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43381E-04
 TEMPERATURE, K 1000.00
 ENTROPY, CAL/GM-K 2.0185
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86046E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45897E-07	5.29998E-02	-8.70618E-11
CH3	5.22784E-14	4.28976E-09	1.04547E-12
H	1.25095E-18	1.02648E-13	5.02292E-16
OH	7.39680E-17	6.06953E-12	1.53569E-15
H2O	2.16496E-12	1.77648E-07	8.63171E-11
CO	2.08791E-12	1.71326E-07	8.48530E-11
O	7.48703E-19	6.14357E-14	1.11716E-16
CO2	2.43067E-19	1.99452E-14	2.12527E-17
O2	2.44089E-06	2.00290E-01	-8.61687E-11
CH2O	6.20363E-14	5.09046E-09	1.16336E-12
H2	2.09898E-12	1.72234E-07	8.50734E-11
HO2	4.75269E-17	3.89987E-12	1.13479E-15
HCO	2.67973E-24	2.19889E-19	2.44482E-17
N2	9.09999E-06	7.46710E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.16460E-06	9.99921E-01
2	7.3205E-04	1.00000E+00
3	1.58542E-16	1.00000E+00
4	1.28253E-06	1.00000E+00
5	1.80244E-10	1.00000E+00
6	7.29504E-04	1.00000E+00
7	1.87355E-06	9.93403E-01
8	1.28157E-06	1.00000E+00
9	7.27610E-09	9.98638E-01
10	-6.82352E-10	9.99984E-01
11	2.66523E-12	9.99926E-01

DETAILED KINETIC CALCULATION

12	2.15218E-09	9.99963E-01
13	-2.66813E-19	9.88021E-01
14	2.44259E-12	1.00000E+00
15	1.66140E-12	1.00000E+00
16	1.86800E-09	1.00000E+00
17	1.97515E-12	1.00000E+00
18	3.97507E-21	9.99986E-01
19	1.68104E-19	9.99993E-01
20	4.64516E-21	8.16943E-01
21	9.36725E-14	9.97807E-01
22	1.66420E-09	9.99997E-01
23	3.71021E-14	1.00000E+00
24	1.52883E-14	1.00000E+00
25	-6.38671E-14	7.79113E-01
26	-1.50300E-12	5.57577E-01
27	2.19285E-19	9.96922E-01
28	9.45347E-13	9.93835E-01
29	8.44513E-14	5.00733E-01
30	7.19636E-04	1.00000E+00

TIME 8.33333E-02 SEC AREA 1.95001E+01 SQ CM POSITION 2.50000E+00 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43380E-04
 TEMPERATURE, K 1000.00
 ENTROPY, CAL/GM-K 2.0185
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86047E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45892E-07	5.29995E-02	-1.44589E-10
CH3	8.72372E-14	7.15836E-09	1.05172E-12
H	1.27457E-18	1.04586E-13	3.35443E-18
OH	1.23264E-16	1.01146E-11	1.48335E-15
H2O	6.00019E-12	4.92353E-07	1.43843E-10
CO	5.87105E-12	4.81757E-07	1.42272E-10
O	7.63404E-19	6.26421E-14	6.16782E-19
CO2	2.04192E-18	1.67552E-13	9.95892E-17
O2	2.44088E-06	2.00289E-01	-1.43693E-10
CH2O	1.04011E-13	8.53476E-09	1.26475E-12
H2	5.88943E-12	4.83265E-07	1.42490E-10
HO2	9.46481E-17	7.76647E-12	1.71517E-15
HCO	8.41242E-24	6.90292E-19	8.84441E-20
N2	9.09997E-06	7.46710E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIONAL DIR RATE
1	3.16474E-06	9.99866E-01
2	1.21993E-03	9.99999E-01
3	4.54565E-16	1.00000E+00
4	1.30677E-06	1.00000E+00
5	8.44619E-10	1.00000E+00
6	1.21734E-03	1.00000E+00
7	1.86337E-06	9.69683E-01
8	1.30675E-06	9.99999E-01
9	7.40380E-09	9.97338E-01
10	-1.91473E-09	9.99988E-01
11	7.62547E-12	9.99956E-01

12	1.00634E-08	9.99978E-01
13	-7.54452E-19	9.95569E-01
14	4.15602E-12	1.00000E+00
15	2.83816E-12	1.00000E+00
16	5.21921E-09	1.00000E+00
17	3.37663E-12	1.00000E+00
18	1.27239E-20	9.99980E-01
19	8.79429E-19	9.99990E-01
20	9.97388E-21	5.48404E-01
21	2.94128E-13	9.97999E-01
22	5.22438E-09	9.99995E-01
23	7.52831E-14	1.00000E+00
24	3.10210E-14	1.00000E+00
25	-9.98470E-14	7.30866E-01
26	-3.51367E-12	4.70277E-01
27	3.71597E-19	9.94975E-01
28	9.78428E-13	9.90110E-01
29	2.30406E-13	4.91934E-01
30	1.20661E-03	1.00000E+00

DETAILED KINETIC CALCULATION

TIME 1.66667E-01 SEC AREA 1.95003E+01 SQ CM POSITION 5.00000E+00 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43376E-04
 TEMPERATURE, K 1000.02
 ENTROPY, CAL/GM-K 2.0185
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86050E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45865E-07	5.29979E-02	-2.91347E-10
CH3	1.76397E-13	1.44747E-08	1.09842E-12
H	1.47274E-18	1.20849E-13	2.45082E-17
OH	2.49022E-16	2.04340E-11	1.55211E-15
H2O	2.40577E-11	1.97411E-06	2.90602E-10
CO	2.37943E-11	1.95250E-06	2.88928E-10
O	8.82111E-19	7.23835E-14	2.49546E-18
CO2	3.36130E-17	2.75819E-12	8.15428E-16
O2	2.44083E-06	2.00288E-01	-2.90431E-10
CH2O	2.11183E-13	1.73291E-08	1.31962E-12
H2	2.38300E-11	1.95543E-06	2.89121E-10
HO2	3.37236E-16	2.76726E-11	4.44245E-15
HCO	3.44898E-23	2.83014E-18	3.98408E-19
N2	9.09985E-06	7.46709E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIONAL DIR RATE
1	3.16568E-06	9.99686E-01
2	2.46456E-03	9.99997E-01
3	2.12877E-15	1.00000E+00
4	1.51009E-06	1.00000E+00
5	6.91585E-09	1.00000E+00
6	2.46167E-03	1.00000E+00
7	1.74385E-06	7.85323E-01
8	1.51002E-06	9.99995E-01
9	8.50722E-09	9.91790E-01
10	-7.75011E-09	9.99988E-01
11	3.56561E-11	9.99978E-01

12	8.22674E-08	9.99987E-01
13	-3.06363E-18	9.98539E-01
14	9.71075E-12	1.00000E+00
15	6.65888E-12	1.00000E+00
16	2.14091E-08	1.00000E+00
17	7.92237E-12	1.00000E+00
18	6.02794E-20	9.99966E-01
19	7.28415E-18	9.99980E-01
20	-4.85980E-20	3.60632E-01
21	1.20569E-12	9.97714E-01
22	2.14191E-08	9.99981E-01
23	3.09953E-13	1.00000E+00
24	1.27718E-13	1.00000E+00
25	-1.24702E-13	4.51686E-01
26	-1.47957E-12	4.93694E-02
27	8.64276E-19	9.91363E-01
28	1.29965E-12	9.85026E-01
29	8.09021E-13	4.23210E-01
30	2.45046E-03	1.00000E+00

DETAILED KINETIC CALCULATION

156

TIME 2.50000E-01 SEC AREA 1.95008E+01 SQ CM POSITION 7.50000E+00 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43369E-04
 TEMPERATURE, K 1000.03
 ENTROPY, CAL/GM-K 2.0185
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86055E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45820E-07	5.29953E-02	-4.50019E-10
CH3	2.72731E-13	2.23800E-08	1.23322E-12
H	2.04082E-18	1.67467E-13	2.55117E-17
OH	3.84982E-16	3.15912E-11	1.74311E-15
H2O	5.47574E-11	4.49333E-06	4.49274E-10
CO	5.43439E-11	4.45940E-06	4.47303E-10
O	1.22242E-18	1.00310E-13	6.15287E-18
CO2	1.75048E-16	1.43643E-11	2.87933E-15
O2	2.44074E-06	2.00285E-01	-4.49042E-10
CH2O	3.26829E-13	2.68192E-08	1.47926E-12
H2	5.43933E-11	4.46345E-06	4.47428E-10
HO2	8.99264E-16	7.37926E-11	9.50279E-15
HCO	8.25287E-23	6.77221E-18	2.16080E-19
N2	9.09965E-06	7.46707E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.16712E-06	9.99329E-01
2	3.81023E-03	9.99994E-01
3	6.73777E-15	1.00000E+00
4	2.09294E-06	1.00000E+00
5	2.44213E-08	1.00000E+00
6	3.80643E-03	1.00000E+00
7	1.39483E-06	-4.53243E-01
8	2.09274E-06	9.99992E-01
9	1.16982E-08	9.84193E-01
10	-1.77002E-08	9.99981E-01
11	1.12803E-10	9.99985E-01

DETAILED KINETIC CALCULATION

12	2.90331E-07	9.99989E-01
13	-7.00163E-18	9.98772E-01
14	2.08074E-11	1.00000E+00
15	1.42818E-11	1.00000E+00
16	5.12250E-08	1.00000E+00
17	1.69922E-11	1.00000E+00
18	1.99898E-19	9.99964E-01
19	2.69471E-17	9.99972E-01
20	-4.17443E-19	5.93677E-01
21	2.88350E-12	9.96977E-01
22	5.12515E-08	9.99952E-01
23	1.14540E-12	1.00000E+00
24	4.71965E-13	1.00000E+00
25	1.32369E-13	2.36618E-01
26	4.91920E-11	4.18820E-01
27	1.85050E-18	9.90813E-01
28	2.50315E-12	9.87933E-01
29	1.09055E-12	2.38677E-01
30	3.79383E-03	1.00000E+00

DETAILED KINETIC CALCULATION

158

TIME 3.33333E-01 SEC AREA 1.95014E+01 SQ CM POSITION 1.00000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43358E-04
 TEMPERATURE, K 1000.06
 ENTROPY, CAL/GM-K 2.0185
 GAMMA- 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86063E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45755E-07	5.29914E-02	-6.37377E-10
CH3	3.86374E-13	3.17063E-08	1.53034E-12
H	3.29188E-18	2.70135E-13	1.13985E-16
OH	5.45512E-16	4.47653E-11	2.17446E-15
H2O	9.97197E-11	8.18311E-06	6.36633E-10
CO	9.91180E-11	8.13373E-06	6.34007E-10
O	1.97190E-18	1.61816E-13	1.27001E-17
CO2	5.81928E-16	4.77536E-11	7.44203E-15
O2	2.44062E-06	2.00280E-01	-6.36263E-10
CH2O	4.63012E-13	3.79953E-08	1.83217E-12
H2	9.91723E-11	8.13819E-06	6.33983E-10
HO2	2.01830E-15	1.65624E-10	1.81185E-14
HCO	1.65689E-22	1.35967E-17	1.14971E-18
N2	9.09936E-06	7.46704E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.16816E-06	9.98468E-01
2	5.39917E-03	9.99989E-01
3	1.98245E-14	1.00000E+00
4	3.37681E-06	1.00000E+00
5	6.31245E-08	1.00000E+00
6	5.39336E-03	1.00000E+00
7	6.17577E-07	1.24390E-01
8	3.37627E-06	9.99990E-01
9	1.87500E-08	9.77990E-01
10	-3.22989E-08	9.99961E-01
11	3.31838E-10	9.99988E-01

DETAILED KINETIC CALCULATION

12	7.50172E-07	9.99987E-01
13	-1.27780E-17	9.98250E-01
14	4.75552E-11	1.00000E+00
15	3.26403E-11	9.99999E-01
16	1.02836E-07	1.00000E+00
17	3.88368E-11	1.00000E+00
18	6.47454E-19	9.99971E-01
19	7.66640E-17	9.99968E-01
20	-1.41610E-18	6.04813E-01
21	5.78269E-12	9.95572E-01
22	1.02892E-07	9.99903E-01
23	4.14700E-12	1.00000E+00
24	1.70876E-12	1.00000E+00
25	1.41987E-12	7.01007E-01
26	2.49113E-10	6.66870E-01
27	4.23735E-18	9.92668E-01
28	6.54946E-12	9.93419E-01
29	-1.04752E-12	1.02474E-01
30	5.37771E-03	1.00000E+00

DETAILED KINETIC CALCULATION

160

TIME 4.16667E-01 SEC AREA 1.95022E+01 SQ CM POSITION 1.25000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43342E-04
 TEMPERATURE, K 1000.10
 ENTROPY, CAL/GM-K 2.0185
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86074E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45663E-07	5.29859E-02	-8.84870E-10
CH3	5.36325E-13	4.40132E-08	2.14133E-12
H	5.86598E-18	4.81388E-13	6.25432E-17
OH	7.57549E-16	6.21678E-11	3.03207E-15
H2O	1.62501E-10	1.33356E-05	8.84128E-10
CO	1.61631E-10	1.32642E-05	8.80154E-10
O	3.51414E-18	2.88385E-13	2.67304E-17
CO2	1.54735E-15	1.26983E-10	1.68547E-14
O2	2.44045E-06	2.00274E-01	-8.83472E-10
CH2O	6.42316E-13	5.27113E-08	2.55759E-12
H2	1.61673E-10	1.32676E-05	8.79824E-10
HO2	4.10034E-15	3.36492E-10	3.34121E-14
HCO	3.19331E-22	2.62057E-17	2.25634E-19
N2	9.09896E-06	7.46700E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.16628E-06	9.96217E-01
2	7.49809E-03	9.99982E-01
3	5.76151E-14	1.00000E+00
4	6.01942E-06	1.00000E+00
5	1.42977E-07	1.00000E+00
6	7.48812E-03	1.00000E+00
7	-9.91696E-07	1.00773E-01
8	6.01798E-06	9.99989E-01
9	3.33041E-08	9.74882E-01
10	-5.27147E-08	9.99915E-01
11	9.64361E-10	9.99990E-01

DETAILED KINETIC CALCULATION

12	1.69861E-06	9.99984E-01
13	-2.08398E-17	9.96598E-01
14	1.17654E-10	1.00000E+00
15	8.07030E-11	9.99999E-01
16	1.98128E-07	1.00000E+00
17	9.60311E-11	1.00000E+00
18	2.22410E-18	9.99981E-01
19	2.05203E-16	9.99968E-01
20	-3.05789E-18	4.90368E-01
21	1.11245E-11	9.93325E-01
22	1.98292E-07	9.99832E-01
23	1.50149E-11	1.00000E+00
24	6.18671E-12	1.00000E+00
25	6.49197E-12	8.85199E-01
26	8.50902E-10	8.07316E-01
27	1.05117E-17	9.95160E-01
28	2.08766E-11	9.97116E-01
29	-1.20048E-11	4.04202E-01
30	7.46622E-03	1.00000E+00

1

TIME 5.00000E-01 SEC AREA 1.95035E+01 SQ CM POSITION 1.50000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43321E-04
 TEMPERATURE, K 1000.16
 ENTROPY, CAL/GM-K 2.0186
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86089E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45535E-07	5.29783E-02	-1.25733E-09
CH3	7.61698E-13	6.25118E-08	3.43668E-12
H	1.13392E-17	9.30598E-13	3.44892E-16
OH	1.07662E-15	8.83571E-11	4.89978E-15
H2O	2.50463E-10	2.05552E-05	1.25659E-09
CO	2.49158E-10	2.04481E-05	1.24976E-09
O	6.79382E-18	5.57561E-13	5.79711E-17
CO2	3.67859E-15	3.01898E-10	3.69311E-14
O2	2.44021E-06	2.00265E-01	-1.25533E-09
CH2O	9.11138E-13	7.47761E-08	4.09425E-12
H2	2.49148E-10	2.04473E-05	1.24878E-09
HO2	7.99726E-15	6.56326E-10	6.39926E-14
HCO	6.44048E-22	5.28563E-17	3.49660E-18
N2	9.09839E-06	7.46695E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.15272E-06	9.89643E-01
2	1.06568E-02	9.99972E-01
3	1.71719E-13	1.00000E+00
4	1.16415E-05	1.00000E+00
5	3.13322E-07	1.00000E+00
6	1.06380E-02	1.00000E+00
7	-4.43739E-06	2.05920E-01
8	1.16375E-05	9.99989E-01
9	6.43576E-08	9.74621E-01
10	-8.13629E-08	9.99791E-01
11	2.87438E-09	9.99991E-01

DETAILED KINETIC CALCULATION

12	3.72119E-06	9.99978E-01
13	-3.20533E-17	9.91776E-01
14	3.23100E-10	1.00000E+00
15	2.21353E-10	9.99999E-01
16	3.99473E-07	1.00000E+00
17	2.63422E-10	1.00000E+00
18	8.67391E-18	9.99989E-01
19	5.88259E-16	9.99973E-01
20	-2.46089E-18	1.65688E-01
21	2.23782E-11	9.90143E-01
22	3.99906E-07	9.99750E-01
23	5.66192E-11	1.00000E+00
24	2.33287E-11	1.00000E+00
25	2.64586E-11	9.56668E-01
26	2.60823E-09	8.92652E-01
27	2.89383E-17	9.97276E-01
28	7.81612E-11	9.98900E-01
29	-5.28099E-11	5.96345E-01
30	1.06028E-02	1.00000E+00

DETAILED KINETIC CALCULATION

164

TIME 5.83333E-01 SEC AREA 1.95053E+01 SQ CM POSITION 1.75000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43289E-04
 TEMPERATURE, K 1000.24
 ENTROPY, CAL/GM-K 2.0186
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86111E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45347E-07	5.29672E-02	-1.91098E-09
CH3	1.15660E-12	9.49286E-08	6.51881E-12
H	2.44160E-17	2.00395E-12	2.80222E-16
OH	1.63653E-15	1.34319E-10	9.25674E-15
H2O	3.79493E-10	3.11471E-05	1.91028E-09
CO	3.77379E-10	3.09736E-05	1.89664E-09
O	1.46311E-17	1.20085E-12	1.61499E-16
CO2	8.44769E-15	6.93349E-10	8.50469E-14
O2	2.43986E-06	2.00253E-01	-1.90756E-09
CH2O	1.38073E-12	1.13324E-07	7.73762E-12
H2	3.77232E-10	3.09616E-05	1.89410E-09
HO2	1.59232E-14	1.30690E-09	1.38510E-13
HCO	1.48474E-21	1.21861E-16	1.99097E-19
N2	9.09756E-06	7.46687E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.08880E-06	9.66273E-01
2	1.62003E-02	9.99957E-01
3	5.60195E-13	1.00000E+00
4	2.50849E-05	1.00000E+00
5	7.21668E-07	1.00000E+00
6	1.61604E-02	1.00000E+00
7	-1.27155E-05	2.56470E-01
8	2.50717E-05	9.99988E-01
9	1.38830E-07	9.76484E-01
10	-1.23446E-07	9.99410E-01
11	9.37842E-09	9.99991E-01

DETAILED KINETIC CALCULATION

12	8.56766E-06	9.99968E-01
13	-4.79109E-17	9.74923E-01
14	1.05685E-09	1.00000E+00
15	7.22554E-10	9.99999E-01
16	9.20350E-07	1.00000E+00
17	8.60002E-10	1.00000E+00
18	4.30761E-17	9.99995E-01
19	2.06180E-15	9.99982E-01
20	2.73313E-17	4.44248E-01
21	5.14219E-11	9.86063E-01
22	9.21880E-07	9.99672E-01
23	2.42805E-10	1.00000E+00
24	1.00038E-10	1.00000E+00
25	1.16788E-10	9.84607E-01
26	8.36824E-09	9.46108E-01
27	9.48492E-17	9.98733E-01
28	3.62734E-10	9.99638E-01
29	-2.06620E-10	7.14371E-01
30	1.60938E-02	1.00000E+00

TIME 6.66667E-01 SEC AREA 1.95081E+01 SQ CM POSITION 2.00000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43239E-04
 TEMPERATURE, K 1000.37
 ENTROPY, CAL/GM-K 2.0187
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86147E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.45042E-07	5.29491E-02	-3.31637E-09
CH3	2.00374E-12	1.64480E-07	1.56079E-11
H	6.32994E-17	5.19601E-12	2.34884E-15
OH	2.84021E-15	2.33143E-10	2.23851E-14
H2O	5.88715E-10	4.83254E-05	3.31585E-09
CO	5.84792E-10	4.80034E-05	3.28211E-09
O	3.79412E-17	3.11446E-12	5.06949E-16
CO2	2.03268E-14	1.66855E-09	2.28810E-13
O2	2.43929E-06	2.00232E-01	-3.30882E-09
CH2O	2.38365E-12	1.95665E-07	1.84308E-11
H2	5.84276E-10	4.79611E-05	3.27484E-09
HO2	3.54937E-14	2.91354E-09	3.86602E-13
HCO	4.45304E-21	3.65533E-16	3.66992E-17
N2	9.09621E-06	7.46674E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.73058E-06	8.49498E-01
2	2.81193E-02	9.99934E-01
3	2.25158E-12	1.00000E+00
4	6.51095E-05	1.00000E+00
5	1.94214E-06	1.00000E+00
6	2.80171E-02	1.00000E+00
7	-3.75467E-05	2.81897E-01
8	6.50554E-05	9.99986E-01
9	3.61064E-07	9.79713E-01
10	-1.91653E-07	9.97807E-01
11	3.77065E-08	9.99990E-01

12	2.30445E-05	9.99952E-01
13	-6.83605E-17	8.91924E-01
14	4.74999E-09	1.00000E+00
15	3.23599E-09	9.99999E-01
16	2.75831E-06	1.00000E+00
17	3.85237E-09	1.00000E+00
18	3.35180E-16	9.99998E-01
19	1.07352E-14	9.99992E-01
20	3.95940E-16	8.27438E-01
21	1.53706E-10	9.81350E-01
22	2.76493E-06	9.99622E-01
23	1.40375E-09	1.00000E+00
24	5.78322E-10	1.00000E+00
25	6.82657E-10	9.95363E-01
26	3.34840E-08	9.78290E-01
27	4.27074E-16	9.99560E-01
28	2.43951E-09	9.99906E-01
29	-9.16399E-10	7.86392E-01
30	2.78579E-02	1.00000E+00

TIME 7.50000E-01 SEC AREA 1.95139E+01 SQ CM POSITION 2.25000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.43138E-04
 TEMPERATURE, K 1000.63
 ENTROPY, CAL/GM-K 2.0189
 GAMMA 1.3092
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86217E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.44439E-07	5.29133E-02	-7.49628E-09
CH3	4.51318E-12	3.70566E-07	5.55096E-11
H	2.37471E-16	1.94982E-11	4.37457E-14
OH	6.41966E-15	5.27103E-10	8.36118E-14
H2O	1.00269E-09	8.23281E-05	7.49745E-09
CO	9.93268E-10	8.15549E-05	7.37498E-09
O	1.42393E-16	1.16916E-11	2.81146E-15
CO2	5.88986E-14	4.83602E-09	8.79078E-13
O2	2.43816E-06	2.00191E-01	-7.47141E-09
CH2O	5.33081E-12	4.37700E-07	6.49044E-11
H2	9.91499E-10	8.14096E-05	7.34596E-09
HO2	1.08029E-13	8.87003E-09	1.81505E-12
HCO	2.25403E-20	1.85073E-15	1.51141E-15
N2	9.09354E-06	7.46649E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-8.30365E-07	2.03521E-01
2	6.35733E-02	9.99887E-01
3	1.43584E-11	1.00000E+00
4	2.44824E-04	1.00000E+00
5	7.46601E-06	1.00000E+00
6	6.31946E-02	1.00000E+00
7	-1.50900E-04	2.95717E-01
8	2.44446E-04	9.99981E-01
9	1.35933E-06	9.83433E-01
10	-3.23702E-07	9.85350E-01
11	2.40624E-07	9.99986E-01

DETAILED KINETIC CALCULATION

12	8.84986E-05	9.99921E-01
13	-1.52624E-17	1.15755E-01
14	4.01863E-08	1.00000E+00
15	2.71841E-08	9.99999E-01
16	1.39511E-05	1.00000E+00
17	3.23720E-08	1.00000E+00
18	6.37314E-15	1.00000E+00
19	1.22895E-13	9.99998E-01
20	8.85113E-15	9.73501E-01
21	7.76415E-10	9.76569E-01
22	1.39970E-05	9.99612E-01
23	1.60420E-08	1.00000E+00
24	6.60819E-09	1.00000E+00
25	7.83146E-09	9.99076E-01
26	2.34322E-07	9.94576E-01
27	3.62197E-15	9.99910E-01
28	3.43558E-08	9.99985E-01
29	-6.19854E-09	8.29661E-01
30	6.26294E-02	1.00000E+00

TIME 8.33333E-01 SEC AREA 1.95317E+01 SQ CM POSITION 2.50000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.42824E-04
 TEMPERATURE, K 1001.44
 ENTROPY, CAL/GM-K 2.0194
 GAMMA 1.3091
 ENTHALPY, CAL/GM 1.58006E+02
 GIBBS F E, CAL/GM -1.86434E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.42551E-07	5.28011E-02	-3.21619E-08
CH3	1.91701E-11	1.57529E-06	4.74133E-10
H	2.23461E-15	1.83627E-10	2.35672E-13
OH	2.75520E-14	2.26406E-09	7.02360E-13
H2O	2.30183E-09	1.89151E-04	3.22238E-08
CO	2.25950E-09	1.85673E-04	3.11424E-08
O	1.33980E-15	1.10097E-10	5.43282E-14
CO2	3.08872E-13	2.53813E-08	8.60271E-12
O2	2.43464E-06	2.00064E-01	-3.19904E-08
CH2O	2.21722E-11	1.82198E-06	5.36726E-10
H2	2.24912E-09	1.84820E-04	3.08366E-08
HO2	8.28125E-13	6.80505E-08	2.99677E-11
HCO	4.05196E-19	3.32967E-14	1.20643E-14
N2	9.08523E-06	7.46571E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.58750E-04	9.79259E-01
2	2.73056E-01	9.99741E-01
3	3.07714E-10	1.00000E+00
4	2.32041E-03	9.99998E-01
5	7.31964E-05	1.00000E+00
6	2.69616E-01	1.00000E+00
7	-1.55443E-03	3.13847E-01
8	2.30863E-03	9.99963E-01
9	1.28170E-05	9.86223E-01
10	-4.15637E-07	5.44233E-01
11	5.16813E-06	9.99974E-01

DETAILED KINETIC CALCULATION

12	8.64897E-04	9.99823E-01
13	1.00138E-14	9.69772E-01
14	1.61033E-06	1.00000E+00
15	1.06815E-06	9.99999E-01
16	2.49494E-04	1.00000E+00
17	1.27156E-06	1.00000E+00
18	1.08105E-12	1.00000E+00
19	9.49895E-12	1.00000E+00
20	1.53954E-12	9.99162E-01
21	1.40185E-08	9.72268E-01
22	2.51717E-04	9.99618E-01
23	1.16025E-06	1.00000E+00
24	4.77747E-07	1.00000E+00
25	5.66393E-07	9.99944E-01
26	7.76242E-06	9.99611E-01
27	1.46201E-13	9.99995E-01
28	3.04353E-06	9.99999E-01
29	-1.39406E-07	8.55772E-01
30	2.64799E-01	1.00000E+00

TIME 9.16667E-01, SEC. AREA 1.97135E+01 SQ CM POSITION 2.75000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.39662E-04
 TEMPERATURE, K 1009.74
 ENTROPY, CAL/GM-K 2.0244
 GAMMA 1.3089
 ENTHALPY, CAL/GM 1.58005E+02
 GIBBS F E, CAL/GM -1.88616E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.23822E-07	5.16873E-02	-3.79007E-07
CH3	2.21682E-10	1.83676E-05	2.65738E-09
H	1.26736E-13	1.05008E-08	4.94401E-11
OH	3.44220E-13	2.85206E-08	2.75487E-11
H2O	1.55582E-08	1.28909E-03	4.09596E-07
CO	1.46189E-08	1.21126E-03	3.73623E-07
O	7.17190E-14	5.94234E-09	-7.83405E-13
CO2	1.36969E-11	1.13487E-06	7.12144E-10
O2	2.39918E-06	1.98786E-01	-3.95333E-07
CH2O	2.27650E-10	1.88621E-05	2.01160E-09
H2	1.40159E-08	1.16130E-03	3.41386E-07
HO2	5.87963E-11	4.87162E-06	1.99095E-09
HCO	5.45039E-17	4.51597E-12	2.50128E-12
N2	9.00143E-06	7.45822E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.00103E-01	9.99953E-01
2	3.43871E+00	9.98233E-01
3	1.07933E-07	1.00000E+00
4	1.41543E-01	9.99980E-01
5	6.17256E-03	9.99999E-01
6	3.26107E+00	1.00000E+00
7	-1.81866E-01	4.73044E-01
8	1.28387E-01	9.99898E-01
9	7.15294E-04	9.78750E-01
10	1.43348E-03	9.95760E-01
11	1.83742E-03	9.99946E-01

DETAILED KINETIC CALCULATION

12	7.00241E-02	9.99069E-01
13	3.32781E-11	9.99910E-01
14	1.02384E-03	1.00000E+00
15	6.47334E-04	9.99999E-01
16	3.26024E-02	1.00000E+00
17	7.25510E-04	1.00000E+00
18	8.01178E-09	1.00000E+00
19	1.62618E-08	1.00000E+00
20	1.19745E-08	9.99994E-01
21	1.96941E-06	9.28884E-01
22	3.39516E-02	9.98489E-01
23	4.79863E-03	1.00000E+00
24	1.96781E-03	1.00000E+00
25	2.19301E-03	1.00000E+00
26	7.01697E-03	9.99996E-01
27	1.02949E-10	1.00000E+00
28	9.28922E-03	1.00000E+00
29	-6.10755E-05	9.42113E-01
30	3.21069E+00	1.00000E+00

TIME 1.00000E+00 SEC AREA 2.04373E+01 SQ CM POSITION 3.00000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.27634E-04
 TEMPERATURE, K 1043.36
 ENTROPY, CAL/GM-K 2.0416
 GAMMA 1.3079
 ENTHALPY, CAL/GM 1.57994E+02
 GIBBS F E, CAL/GM -1.97218E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.58859E-07	4.78483E-02	-6.86296E-07
CH3	3.63107E-10	3.10884E-05	2.34119E-09
H	7.19120E-13	6.15695E-08	1.28163E-11
OH	7.54680E-13	6.46140E-08	1.13513E-11
H2O	6.68936E-08	5.72728E-03	9.15152E-07
CO	5.65735E-08	4.84369E-03	6.77663E-07
O	3.56662E-13	3.05366E-08	5.22688E-12
CO2	2.48751E-10	2.12975E-05	6.62798E-09
O2	2.26678E-06	1.94077E-01	-8.02440E-07
CH2O	2.33749E-10	2.00130E-05	-3.36493E-10
H2	4.71301E-08	4.03518E-03	4.54470E-07
HO2	7.05376E-11	6.03927E-06	-4.35108E-10
HCO	1.38907E-16	1.18929E-11	-7.64687E-15
N2	8.68266E-06	7.43390E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-7.35884E-01	9.99975E-01
2	7.81304E+00	9.92040E-01
3	2.17943E-06	1.00000E+00
4	1.06623E+00	9.99969E-01
5	6.17431E-02	9.99990E-01
6	6.36236E+00	1.00000E+00
7	-1.42822E-01	5.04068E-01
8	7.44494E-01	9.99922E-01
9	3.97000E-01	9.89892E-01
10	1.08199E-02	9.95034E-01
11	3.93933E-02	9.99961E-01

DETAILED KINETIC CALCULATION

12	6.01015E-01	9.96052E-01
13	1.07853E-09	9.99950E-01
14	9.25410E-03	1.00000E+00
15	4.40783E-03	9.99997E-01
16	7.88815E-02	1.00000E+00
17	4.28487E-03	1.00000E+00
18	1.13672E-07	1.00000E+00
19	9.76580E-08	1.00000E+00
20	1.86108E-07	9.99976E-01
21	3.95493E-06	5.18032E-01
22	8.75699E-02	9.95128E-01
23	3.62464E-02	1.00000E+00
24	1.46287E-02	1.00000E+00
25	1.40621E-02	1.00000E+00
26	1.98361E-02	9.99980E-01
27	1.24761E-09	1.00000E+00
28	2.67330E-01	1.00000E+00
29	-1.98718E-03	9.90169E-01
30	6.28718E+00	9.99999E-01

TIME 1.06667E+00 SEC AREA 2.18250E+01 SQ CM POSITION 3.20000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 3.06802E-04
 TEMPERATURE, K 1109.33
 ENTROPY, CAL/GM-K 2.0695
 GAMMA 1.3055
 ENTHALPY, CAL/GM 1.57942E+02
 GIBBS F E, CAL/GM -2.13785E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	4.59583E-07	4.18429E-02	-1.53358E-06
CH3	6.73788E-10	6.13453E-05	9.91757E-09
H	2.39405E-12	2.17967E-07	6.21350E-10
OH	2.15742E-12	1.96396E-07	1.39110E-09
H2O	1.59406E-07	1.45132E-02	2.59992E-06
CO	1.15220E-07	1.04903E-02	1.47913E-06
O	1.03291E-12	9.40421E-08	3.72416E-11
CO2	1.43016E-09	1.30209E-04	4.55146E-08
O2	2.04198E-06	1.85913E-01	-2.08513E-06
CH2O	1.87416E-10	1.70633E-05	-9.82661E-10
H2	7.43921E-08	6.77306E-03	4.52404E-07
HO2	4.91210E-11	4.47224E-06	-1.29744E-10
HCO	3.63389E-16	3.30849E-11	-4.54998E-12
N2	8.13061E-06	7.40254E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-2.99046E+00	9.99932E-01
2	2.37954E+01	9.77467E-01
3	1.39631E-05	1.00000E+00
4	5.88516E+00	9.99947E-01
5	4.83527E-01	9.99935E-01
6	1.61271E+01	1.00000E+00
7	-7.35851E+00	5.20625E-01
8	2.84610E+00	9.99841E-01
9	1.24231E-02	9.90977E-01
10	2.99550E-02	9.84227E-01
11	2.82165E-01	9.99924E-01

DETAILED KINETIC CALCULATION

12	3.56149E+00	9.89198E-01
13	1.20559E-08	9.99858E-01
14	6.00399E-02	1.00000E+00
15	1.56276E-02	9.99994E-01
16	2.06160E-01	1.00000E+00
17	1.29355E-02	1.00000E+00
18	1.05922E-06	1.00000E+00
19	8.32776E-07	9.99999E-01
20	1.84828E-06	9.99884E-01
21	6.87069E-06	1.85616E-01
22	2.34761E-01	9.92652E-01
23	1.01450E-01	1.00000E+00
24	3.97946E-02	1.00000E+00
25	3.23419E-02	9.99999E-01
26	4.50205E-02	9.99830E-01
27	1.12626E-08	9.99998E-01
28	2.66427E+00	1.00000E+00
29	-2.66928E-02	9.92944E-01
30	1.59629E+01	9.99995E-01

DETAILED KINETIC CALCULATION

TIME 1.08333E+00 SEC AREA 2.26210E+01 SQ CM POSITION 3.25000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 2.96006E-04
 TEMPERATURE, K 1147.63
 ENTROPY, CAL/GM-K 2.0837
 GAMMA 1.3040
 ENTHALPY, CAL/GM 1.57882E+02
 GIBBS F E, CAL/GM -2.23349E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	4.12532E-07	3.88626E-02	-2.34685E-06
CH3	9.35887E-10	8.81653E-05	2.21740E-08
H	3.75323E-12	3.53574E-07	9.58617E-10
OH	3.68151E-12	3.46817E-07	4.13394E-09
H2O	2.08554E-07	1.96468E-02	4.34284E-06
CO	1.40643E-07	1.32493E-02	2.22311E-06
O	1.54298E-12	1.45357E-07	1.81439E-10
CO2	2.50845E-09	2.36309E-04	1.03455E-07
O2	1.92689E-06	1.81523E-01	-3.38758E-06
CH2O	1.67105E-10	1.57421E-05	-1.87550E-09
H2	7.83579E-08	7.38171E-03	3.16963E-07
HO2	4.59059E-11	4.32458E-06	-6.02794E-11
HCO	5.84917E-16	5.51021E-11	-1.19155E-11
N2	7.84449E-06	7.38991E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-5.22499E+00	9.99861E-01
2	4.17595E+01	9.66819E-01
3	2.65710E-05	1.00000E+00
4	1.20414E+01	9.99929E-01
5	1.18070E+00	9.99878E-01
6	2.63936E+01	1.00000E+00
7	-1.46601E+01	5.31053E-01
8	4.91014E+00	9.99732E-01
9	1.87474E-02	9.88399E-01
10	4.81069E-02	9.74492E-01
11	5.64915E-01	9.99874E-01

DETAILED KINETIC CALCULATION

12	7.40164E+00	9.84440E-01
13	2.97328E-08	9.99704E-01
14	1.37916E-01	1.00000E+00
15	2.54745E-02	9.99991E-01
16	3.37020E-01	1.00000E+00
17	1.98347E-02	1.00000E+00
18	2.85187E-06	1.00000E+00
19	2.45764E-06	9.99996E-01
20	5.00990E-06	9.99771E-01
21	1.87480E-05	2.27055E-01
22	5.82436E-01	9.91033E-01
23	1.64554E-01	1.00000E+00
24	6.35843E-02	1.00000E+00
25	4.85040E-02	9.99997E-01
26	7.71226E-02	9.99603E-01
27	2.92334E-08	9.99995E-01
28	6.34747E+00	1.00000E+00
29	-7.41136E-02	9.91923E-01
30	2.61705E+01	9.99993E-01

DETAILED KINETIC CALCULATION

180

TIME 1.10000E+00 SEC AREA 2.42968E+01 SQ CM POSITION 3.30000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 2.75589E-04
 TEMPERATURE, K 1228.98
 ENTROPY, CAL/GM-K 2.1110
 GAMMA 1.3008
 ENTHALPY, CAL/GM 1.57755E+02
 GIBBS F E, CAL/GM -2.43657E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION/	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	3.28858E-07	3.31880E-02	-5.29767E-06
CH3	1.75520E-09	1.77133E-04	1.13394E-07
H	7.66549E-12	7.73594E-07	-1.86070E-10
OH	1.01072E-11	1.02001E-06	3.40569E-09
H2O	3.02779E-07	3.05561E-02	1.09460E-05
CO	1.81894E-07	1.83566E-02	4.75254E-06
O	2.98240E-12	3.00981E-07	2.71951E-10
CO2	5.74262E-09	5.79539E-04	4.34110E-07
O2	1.71080E-06	1.72653E-01	-8.28425E-06
CH2O	1.33469E-10	1.34696E-05	-2.37079E-09
H2	7.34750E-08	7.41503E-03	-5.20299E-07
HO2	4.36117E-11	4.40125E-06	2.01865E-10
HCO	1.42281E-15	1.43588E-10	-4.73925E-12
N2	7.30343E-06	7.37055E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.31585E+01	9.99384E-01
2	1.18085E+02	9.37433E-01
3	7.19961E-05	1.00000E+00
4	4.08878E+01	9.99871E-01
5	5.71570E+00	9.99684E-01
6	6.76485E+01	1.00000E+00
7	-4.75041E+01	5.52431E-01
8	1.23302E+01	9.99181E-01
9	3.51321E-02	9.76272E-01
10	1.10278E-01	9.42036E-01
11	1.63938E+00	9.99634E-01

12	2.52152E+01	9.71997E-01
13	1.24586E-07	9.98625E-01
14	6.11012E-01	1.00000E+00
15	5.63016E-02	9.99981E-01
16	8.52567E-01	9.99999E-01
17	4.03375E-02	1.00000E+00
18	1.68063E-05	1.00000E+00
19	1.89340E-05	9.99979E-01
20	2.86989E-05	9.99249E-01
21	1.70930E-04	4.54268E-01
22	9.49033E-01	9.87051E-01
23	3.90210E-01	1.00000E+00
24	1.46495E-01	1.00000E+00
25	1.02751E-01	9.99979E-01
26	2.31773E-01	9.98377E-01
27	1.53920E-07	9.99961E-01
28	2.58984E+01	9.99999E-01
29	-4.08541E-01	9.86916E-01
30	6.73415E+01	9.99990E-01

TIME 1.10333E+00 SEC AREA 2.49603E+01 SQ CM POSITION 3.31000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 2.68264E-04
 TEMPERATURE, K 1261.40
 ENTROPY, CAL/GM-K 2.1210
 GAMMA 1.2996
 ENTHALPY, CAL/GM 1.57716E+02
 GIBBS F E, CAL/GM -2.51766E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	3.00016E-07	3.10792E-02	-7.06572E-06
CH3	2.19612E-09	2.27500E-04	1.77178E-07
H	9.58965E-12	9.93410E-07	-1.45048E-09
OH	1.45087E-11	1.50299E-06	1.80715E-08
H2O	3.36781E-07	3.48877E-02	1.49595E-05
CO	1.94853E-07	2.01851E-02	6.18450E-06
O	3.70276E-12	3.83576E-07	1.32486E-09
CO2	7.41639E-09	7.68278E-04	7.09209E-07
O2	1.63358E-06	1.69225E-01	-1.12887E-05
CH2O	1.22419E-10	1.26816E-05	-5.13764E-09
H2	6.89442E-08	7.14205E-03	-1.09715E-06
HO2	4.33876E-11	4.49460E-06	3.16931E-10
HCO	1.94933E-15	2.01935E-10	-2.99383E-11
N2	7.10929E-06	7.36465E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.77094E+01	9.98913E-01
2	1.69250E+02	9.22651E-01
3	9.85603E-05	1.00000E+00
4	6.14426E+01	9.99838E-01
5	9.85476E+00	9.99577E-01
6	9.46974E+01	1.00000E+00
7	-7.00608E+01	5.60422E-01
8	1.67021E+01	9.98743E-01
9	4.23202E-02	9.67625E-01
10	1.45013E-01	9.23588E-01
11	2.27247E+00	9.99447E-01

DETAILED KINETIC CALCULATION

12	3.76135E+01	9.65999E-01
13	1.95100E-07	9.97526E-01
14	1.02287E+00	1.00000E+00
15	7.23581E-02	9.99975E-01
16	1.18466E+00	9.99999E-01
17	5.08655E-02	1.00000E+00
18	3.11280E-05	9.99999E-01
19	3.92983E-05	9.99962E-01
20	5.18923E-05	9.98870E-01
21	3.51845E-04	5.43089E-01
22	1.30783E+00	9.85207E-01
23	5.23368E-01	1.00000E+00
24	1.94444E-01	1.00000E+00
25	1.33937E-01	9.99958E-01
26	3.48980E-01	9.97402E-01
27	2.69753E-07	9.99916E-01
28	4.07153E+01	9.99999E-01
29	-7.21013E-01	9.83743E-01
30	9.44837E+01	9.99989E-01

DETAILED KINETIC CALCULATION

184

TIME 1.10667E+00 SEC AREA 2.59484E+01 SQ CM POSITION 3.32000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 2.58049E-04
 TEMPERATURE, K 1309.71
 ENTROPY, CAL/GM-K 2.1352
 GAMMA 1.2978
 ENTHALPY, CAL/GM 1.57636E+02
 GIBBS F E, CAL/GM -2.63881E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.60476E-07	2.80223E-02	-1.05194E-05
CH3	2.98352E-09	3.20970E-04	3.71379E-07
H	1.27889E-11	1.37584E-06	4.87086E-10
OH	2.40841E-11	2.59100E-06	9.08454E-09
H2O	3.84108E-07	4.13228E-02	2.26975E-05
CO	2.11438E-07	2.27468E-02	8.76271E-06
O	4.94558E-12	5.32052E-07	6.76363E-10
CO2	1.03841E-08	1.11714E-03	1.39025E-06
O2	1.52604E-06	1.64174E-01	-1.71232E-05
CH2O	1.07463E-10	1.15610E-05	-4.92021E-09
H2	6.10958E-08	6.57277E-03	-2.21584E-06
HO2	4.32445E-11	4.65230E-06	4.52146E-10
HCO	3.01076E-15	3.23902E-10	-9.01503E-12
N2	6.83858E-06	7.35703E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-2.60000E+01	9.97545E-01
2	2.75786E+02	8.97204E-01
3	1.48719E-04	1.00000E+00
4	1.05751E+02	9.99773E-01
5	2.08779E+01	9.99385E-01
6	1.50332E+02	1.00000E+00
7	-1.16730E+02	5.71449E-01
8	2.49188E+01	9.97659E-01
9	5.29942E-02	9.48360E-01
10	2.06479E-01	8.89061E-01
11	3.44112E+00	9.98997E-01

DETAILED KINETIC CALCULATION

12	6.38488E+01	9.55947E-01
13	3.46644E-07	9.94271E-01
14	2.06540E+00	1.00000E+00
15	9.96059E-02	9.99965E-01
16	1.86564E+00	9.99998E-01
17	6.89374E-02	1.00000E+00
18	7.25861E-05	9.99998E-01
19	1.08885E-04	9.99913E-01
20	1.15419E-04	9.98026E-01
21	9.03632E-04	6.55394E-01
22	2.03312E+00	9.82205E-01
23	7.74146E-01	1.00000E+00
24	2.83441E-01	9.99999E-01
25	1.92685E-01	9.99889E-01
26	6.22575E-01	9.95113E-01
27	5.76356E-07	9.99748E-01
28	7.37894E+01	9.99994E-01
29	-1.54763E+00	9.77231E-01
30	1.50438E+02	9.99988E-01

DETAILED KINETIC CALCULATION

186

TIME 1.11333E+00 SEC AREA 3.24163E+01 SQ CM POSITION 3.34000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 2.06561E-04
 TEMPERATURE, K 1626.87
 ENTROPY, CAL/GM-K 2.2128
 GAMMA 1.2880
 ENTHALPY, CAL/GM 1.56751E+02
 GIBBS F E, CAL/GM -3.44324E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	7.11362E-08	9.52452E-03	-5.21976E-05
CH3	1.02785E-08	1.37621E-03	3.13195E-06
H	4.27506E-11	5.72393E-06	6.67445E-09
OH	3.90221E-10	5.22471E-05	7.90097E-07
H2O	6.00593E-07	8.04142E-02	1.09268E-04
CO	2.51634E-07	3.36916E-02	7.90621E-06
O	1.92786E-11	2.58123E-06	1.89941E-08
CO2	5.54542E-08	7.42484E-03	4.11743E-05
O2	9.86494E-07	1.32083E-01	-1.00152E-04
CH2O	3.81705E-11	5.11070E-06	-1.45927E-08
H2	1.85275E-08	2.48066E-03	-9.95064E-06
HO2	3.36841E-11	4.51001E-06	-6.53366E-09
HCO	2.56157E-14	3.42972E-09	-2.57851E-10
N2	5.47411E-06	7.32935E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-9.11968E+01	8.46912E-01
2	1.93194E+03	6.27369E-01
3	8.45141E-04	9.99953E-01
4	-1.24280E+03	9.98022E-01
5	9.65001E+02	9.96922E-01
6	1.09972E+03	1.00000E+00
7	-7.08615E+02	6.06317E-01
8	9.12316E+01	9.00085E-01
9	5.34509E-02	3.80285E-01
10	4.07976E-01	3.72515E-01
11	1.48163E+01	9.60665E-01

DETAILED KINETIC CALCULATION

12	6.43523E+02	8.53302E-01
13	2.40354E-06	6.11138E-01
14	5.02353E+01	1.00000E+00
15	2.90854E-01	9.99772E-01
16	1.67559E+01	9.99967E-01
17	2.09772E-01	9.99991E-01
18	4.83983E-03	9.99172E-01
19	2.33547E-02	9.96912E-01
20	5.02504E-03	9.78947E-01
21	5.80707E-02	9.45859E-01
22	1.71713E+01	9.66448E-01
23	3.65047E+00	9.99951E-01
24	1.24059E+00	9.99818E-01
25	8.90635E-01	9.75318E-01
26	1.11882E+01	9.07949E-01
27	2.39286E-05	9.42955E-01
28	1.04245E+03	9.84704E-01
29	-4.37635E+01	7.31866E-01
30	1.13304E+03	9.99988E-01

DETAILED KINETIC CALCULATION

TIME 1.11400E+00 SEC AREA 3.48596E+01 SQ CM POSITION 3.34200E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.92084E-04
 TEMPERATURE, K 1750.38
 ENTROPY, CAL/GM-K 2.2348
 GAMMA 1.2839
 ENTHALPY, CAL/GM 1.56410E+02
 GIBBS F E, CAL/GM -3.75531E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.97390E-08	4.28682E-03	-5.63792E-05
CH3	1.11382E-08	1.60555E-03	-1.48906E-06
H	6.39111E-11	9.21266E-06	4.24175E-08
OH	1.07708E-09	1.55260E-04	3.21180E-06
H2O	6.35727E-07	9.16389E-04	1.25488E-04
CO	2.24016E-07	3.22915E-02	-5.66032E-05
O	3.32281E-11	4.78977E-06	1.64559E-07
CO2	9.63940E-08	1.38950E-02	1.14484E-04
O2	8.38549E-07	1.20875E-01	-1.50593E-04
CH2O	2.11665E-11	3.05112E-06	-1.16995E-08
H2	1.01005E-08	1.45596E-03	-1.21031E-05
HO2	2.44685E-11	3.52709E-06	-1.49665E-08
HCO	4.52216E-14	6.51861E-09	-1.14576E-09
N2	5.09043E-06	7.33775E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIONAL DIR RATE
1	-8.00937E+01	6.10986E-01
2	2.23641E+03	4.88322E-01
3	1.36870E-03	9.99196E-01
4	2.62049E+03	9.94777E-01
5	3.10288E+03	9.94747E-01
6	1.45510E+03	1.00000E+00
7	-6.94698E+02	5.80879E-01
8	6.64352E+01	6.06375E-01
9	3.65339E-03	1.94600E-02
10	7.67220E-02	5.34144E-02
11	1.83013E+01	8.35023E-01

12	1.15394E+03	7.85545E-01
13	6.30374E-07	7.18350E-02
14	1.13312E+02	1.00000E+00
15	3.21516E-01	9.99633E-01
16	2.96570E+01	9.99921E-01
17	2.56162E-01	9.99940E-01
18	1.84535E-02	9.95424E-01
19	1.31227E-01	9.94051E-01
20	1.52320E-02	9.72262E-01
21	1.71266E-01	9.70115E-01
22	2.99295E+01	9.70697E-01
23	4.78394E+00	9.99184E-01
24	1.59076E+00	9.98940E-01
25	1.11569E+00	8.43835E-01
26	2.27717E+01	7.97000E-01
27	7.78229E-05	8.00950E-01
28	2.37479E+03	8.46874E-01
29	-4.33892E+01	2.30717E-01
30	1.53850E+03	9.99989E-01

TIME 1.11433E+00 SEC AREA 3.67423E+01 SQ CM POSITION 3.34300E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.82241E-04
 TEMPERATURE, K 1849.48
 ENTROPY, CAL/GM-K 2.2480
 GAMMA 1.2801
 ENTHALPY, CAL/GM 1.56210E+02
 GIBBS F E, CAL/GM -4.00144E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	1.17040E-08	1.78324E-03	-4.05122E-05
CH3	8.91839E-09	1.35882E-03	-1.15397E-05
H	8.32386E-11	1.26824E-05	1.40799E-06
OH	2.23673E-09	3.40793E-04	5.34021E-06
H2O	6.41972E-07	9.78122E-02	1.06136E-04
CO	1.79566E-07	2.73591E-02	-1.55555E-04
O	7.49812E-11	1.14243E-05	2.31328E-06
CO2	1.42594E-07	2.17260E-02	2.07583E-04
O2	7.40897E-07	1.12885E-01	-1.86700E-04
CH2O	1.11925E-11	1.70532E-06	2.85278E-08
H2	5.65131E-09	8.61045E-04	-1.11958E-05
HO2	1.72880E-11	2.63404E-06	-1.21931E-08
HCO	5.54956E-14	8.45543E-09	-4.84515E-09
N2	4.82958E-06	7.35846E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-2.96399E+01	2.64639E-01
2	1.62911E+03	3.62922E-01
3	2.55328E-03	9.95555E-01
4	4.28247E+03	9.83352E-01
5	6.25030E+03	9.91515E-01
6	1.33276E+03	1.00000E+00
7	-4.17017E+02	5.19802E-01
8	3.73661E+01	2.87684E-01
9	-5.22001E-02	1.89257E-01
10	-3.65707E-01	1.94554E-01
11	2.45280E+01	6.57947E-01

DETAILED KINETIC CALCULATION

12	1.42510E+03	6.94076E-01
13	-7.86792E-06	3.46990E-01
14	2.34519E+02	1.00000E+00
15	2.72938E-01	9.99539E-01
16	3.61769E+01	9.99859E-01
17	3.64303E-01	9.99842E-01
18	6.00737E-02	9.89288E-01
19	3.70170E-01	9.90420E-01
20	2.69466E-02	9.68684E-01
21	2.99245E-01	9.79553E-01
22	3.62036E+01	9.74776E-01
23	5.01103E+00	9.92930E-01
24	1.64261E+00	9.93677E-01
25	1.34732E+00	5.75325E-01
26	2.88833E+01	6.20181E-01
27	1.31497E-04	5.31517E-01
28	3.99072E+03	4.76190E-01
29	7.44534E+01	1.05625E-01
30	1.52960E+03	9.99991E-01

DETAILED KINETIC CALCULATION

TIME 1.11467E+00 SEC AREA 3.92951E+01 SQ CM POSITION 3.34400E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.70401E-04
 TEMPERATURE, K 1989.68
 ENTROPY, CAL/GM-K 2.2611
 GAMMA 1.2740
 ENTHALPY, CAL/GM 1.55950E+02
 GIBBS F E, CAL/GM -4.34284E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	1.51837E-09	2.48993E-04	-1.41881E-05
CH3	3.16364E-09	5.18797E-04	-2.23975E-05
H	1.35455E-10	2.22129E-05	1.83285E-05
OH	6.58228E-09	1.07941E-03	1.06879E-05
H2O	6.27661E-07	1.02929E-01	5.46997E-05
CO	9.29345E-08	1.52401E-02	-3.11638E-04
O	5.37460E-10	8.81368E-05	2.50543E-05
CO2	2.22904E-07	3.65535E-02	3.48514E-04
O2	6.24506E-07	1.02411E-01	-2.37766E-04
CH2O	4.08603E-12	6.70058E-07	-2.82081E-07
H2	2.23755E-09	3.66930E-04	-6.94673E-06
HO2	1.10386E-11	1.81019E-06	-4.89734E-09
HCO	6.81610E-14	1.11775E-08	-8.33203E-09
N2	4.51583E-06	7.40540E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.12506E+01	1.81862E-01
2	4.90594E+02	2.27550E-01
3	9.67743E-03	9.79932E-01
4	7.63001E+03	8.10908E-01
5	1.20025E+04	9.78662E-01
6	5.51444E+02	1.00000E+00
7	-5.32470E+01	2.79944E-01
8	4.00306E+01	2.30556E-01
9	-1.27676E-01	2.85322E-01
10	-3.98435E-01	1.75705E-01
11	6.89158E+01	4.45957E-01

DETAILED KINETIC CALCULATION

12	1.34080E+03	4.43792E-01
13	-2.70157E-05	4.10895E-01
14	7.08535E+02	1.00000E+00
15	2.12050E-01	9.99494E-01
16	4.44478E+01	9.99719E-01
17	1.19007E+00	9.99720E-01
18	6.57423E-01	9.89909E-01
19	1.52948E+00	9.89870E-01
20	6.24355E-02	9.81787E-01
21	5.68640E-01	9.89271E-01
22	4.33189E+01	9.84987E-01
23	5.43878E+00	8.72903E-01
24	1.74690E+00	8.72407E-01
25	4.01929E+00	3.27858E-01
26	3.25534E+01	3.25232E-01
27	6.07502E-05	5.58437E-02
28	5.91769E+03	5.95178E-02
29	-2.78545E+01	3.89145E-03
30	1.22384E+03	9.99995E-01

DETAILED KINETIC CALCULATION

194

TIME 1.1500E+00 SEC AREA 4.11049E+01 SQ CM POSITION 3.34500E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62899E-04
 TEMPERATURE, K 2094.17
 ENTROPY, CAL/GM-K 2.2664
 GAMMA 1.2691
 ENTHALPY, CAL/GM 1.55860E+02
 GIBBS F E, CAL/GM -4.59044E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	1.87021E-12	3.22850E-07	-4.78379E-08
CH3	7.70332E-12	1.32980E-06	-2.07123E-07
H	2.46883E-10	4.26187E-05	1.21222E-05
OH	1.47485E-08	2.54599E-03	-3.26380E-06
H2O	6.04133E-07	1.04290E-01	-4.20936E-06
CO	1.17206E-08	2.02329E-03	-8.22826E-05
O	2.26276E-09	3.90615E-04	1.44661E-05
CO2	2.94682E-07	5.08703E-02	8.25438E-05
O2	5.46828E-07	9.43976E-02	-4.48977E-05
CH2O	1.85650E-14	3.20482E-09	-5.89155E-09
H2	1.17523E-09	2.02877E-04	1.91647E-07
HO2	7.01087E-12	1.21027E-06	1.84905E-09
HCO	8.72103E-16	1.50549E-10	-3.50188E-10
N2	4.31700E-06	7.45234E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	5.01789E-02	2.07587E-01
2	1.42377E+00	2.05389E-01
3	4.08241E-03	7.63044E-01
4	1.68954E+03	8.32971E-02
5	3.11062E+03	7.62743E-01
6	1.45835E+00	1.00000E+00
7	8.99358E-02	2.05320E-01
8	2.38870E-01	2.08590E-01
9	2.93654E-04	5.60504E-04
10	-8.30860E-03	3.41062E-03
11	1.81254E+00	4.11413E-03

12	3.57017E-01	8.59734E-05
13	-3.63412E-07	2.85171E-03
14	8.14975E+00	1.00000E+00
15	2.10517E-03	9.99500E-01
16	4.95027E-01	9.99501E-01
17	2.63827E-02	9.99503E-01
18	3.47526E-02	8.38210E-01
19	4.05968E-02	8.37556E-01
20	1.35912E-03	8.37542E-01
21	8.14980E-03	8.38005E-01
22	4.51853E-01	8.38096E-01
23	6.79330E-01	8.39442E-02
24	2.06085E-01	8.02389E-02
25	2.53212E-02	7.05926E-04
26	-5.19962E-01	3.32493E-03
27	-1.15624E-05	2.76597E-03
28	9.73673E+02	1.26603E-03
29	-1.60631E+02	4.02851E-03
30	9.30661E+00	9.99919E-01

TIME 1.11527E+00 SEC AREA 4.12558E+01 SQ CM POSITION 3.34581E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62303E-04
 TEMPERATURE, K 2103.20
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2687
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61111E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	4.61067E-20	7.99364E-15	-4.73080E-15
CH3	5.73539E-20	9.94359E-15	2.66870E-15
H	2.63527E-10	4.56884E-05	5.71885E-08
OH	1.55971E-08	2.70411E-03	6.13130E-07
H2O	6.01451E-07	1.04275E-01	-3.59776E-07
CO	3.53975E-09	6.13694E-04	-5.92330E-06
O	2.48850E-09	4.31438E-04	2.17682E-07
CO2	3.01752E-07	5.23155E-02	5.92330E-06
O2	5.40417E-07	9.36935E-02	-3.19724E-06
CH2O	4.63908E-19	8.04288E-14	-9.16818E-16
H2	1.19875E-09	2.07831E-04	2.45822E-08
HO2	7.05339E-12	1.22286E-06	6.84150E-11
HCO	4.49035E-17	7.78503E-12	-1.13012E-13
N2	4.30121E-06	7.45712E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIONAL DIR RATE
1	5.04575E-09	7.70543E-01
2	1.40999E-07	7.70504E-01
3	3.03306E-04	1.70447E-01
4	1.21308E+02	5.53192E-03
5	2.24859E+02	1.70355E-01
6	1.09210E-08	9.99999E-01
7	9.14571E-09	7.70553E-01
8	2.43993E-08	7.70569E-01
9	1.07321E-04	1.93796E-04
10	-3.98653E-04	1.51455E-04
11	3.47169E-02	6.87963E-05

12	-9.68298E-01	2.13397E-04
13	6.12335E-09	4.23469E-05
14	6.73600E-08	9.99999E-01
15	2.71693E-11	4.76458E-04
16	3.46906E-09	2.63117E-04
17	4.00291E-10	5.45222E-04
18	2.01635E-07	8.48485E-05
19	-5.24791E-07	1.97347E-04
20	1.44227E-09	1.60533E-05
21	-1.34692E-08	2.62940E-05
22	4.62922E-06	1.67506E-04
23	4.78076E-02	5.44971E-03
24	1.43766E-02	5.16899E-03
25	-3.30514E-03	8.26646E-05
26	-6.09656E-02	3.64820E-04
27	-8.00608E-07	1.71057E-04
28	1.00384E+02	1.11140E-04
29	-1.26428E+01	2.82179E-04
30	1.09188E-07	4.50176E-04



DETAILED KINETIC CALCULATION

198

TIME 1.11543E+00 SEC AREA 4.12645E+01 SQ CM POSITION 3.34629E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62269E-04
 TEMPERATURE, K 2103.72
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61230E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	1.83111E-24	3.17544E-19	-1.08505E-19
CH3	5.53992E-24	9.60708E-19	-9.04078E-20
H	2.64531E-10	4.58738E-05	4.29099E-09
OH	1.56464E-08	2.71333E-03	1.29393E-07
H2O	6.01295E-07	1.04274E-01	-7.17891E-08
CO	3.06580E-09	5.31657E-04	-1.17823E-06
O	2.50183E-09	4.33857E-04	3.62103E-08
CO2	3.02161E-07	5.23995E-02	1.17823E-06
O2	5.40048E-07	9.36527E-02	-6.36037E-07
CH2O	4.02247E-19	6.97560E-14	-1.58282E-16
H2	1.20048E-09	2.08181E-04	4.94071E-09
HO2	7.05709E-12	1.22381E-06	1.31049E-11
HCO	3.90083E-17	6.76465E-12	-1.61793E-14
N2	4.30031E-06	7.45740E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	1.15901E-13	4.43251E-01
2	3.23374E-12	4.43232E-01
3	6.04485E-05	3.90093E-02
4	2.41424E+01	1.09597E-03
5	4.47466E+01	3.89880E-02
6	1.04887E-12	9.93982E-01
7	2.10089E-13	4.43256E-01
8	5.61035E-13	4.43263E-01
9	2.14010E-05	3.85204E-05
10	-7.83105E-05	2.96106E-05
11	6.76315E-03	1.32956E-05

DETAILED KINETIC CALCULATION

12	-1.94479E-01	4.26397E-05
13	1.29813E-09	8.91003E-06
14	6.50538E-12	9.93976E-01
15	1.90060E-12	3.82606E-05
16	-5.02446E-11	4.37933E-06
17	3.30189E-11	5.15556E-05
18	2.61010E-08	1.25671E-05
19	-1.00529E-07	4.33682E-05
20	-5.70994E-11	7.28513E-07
21	-4.29470E-09	9.63854E-06
22	6.93218E-07	2.88821E-05
23	9.51765E-03	1.07967E-03
24	2.86122E-03	1.02379E-03
25	-6.56396E-04	1.63153E-05
26	-1.21198E-02	7.22491E-05
27	-1.58898E-07	3.37300E-05
28	2.02412E+01	2.22055E-05
29	-2.52265E+00	5.59348E-05
30	6.03407E-09	2.86223E-05

DETAILED KINETIC CALCULATION

200

TIME 1.11600E+00 SEC AREA 4.12668E+01 SQ CM POSITION 3.34800E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61261E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	6.24585E-27	1.08320E-21	-4.93054E-24
CH3	3.37612E-26	5.85510E-21	-5.63388E-23
H	2.64793E-10	4.59222E-05	-1.18811E-10
OH	1.56593E-08	2.71573E-03	-6.79037E-09
H2O	6.01254E-07	1.04274E-01	3.71020E-09
CO	2.94259E-09	5.10323E-04	6.08685E-08
O	2.50530E-09	4.34487E-04	-1.76629E-09
CO2	3.02268E-07	5.24213E-02	-6.08685E-08
O2	5.39952E-07	9.36421E-02	3.28582E-08
CH2O	3.86227E-19	6.69820E-14	7.85474E-18
H2	1.20093E-09	2.08273E-04	-2.55276E-10
HO2	7.05805E-12	1.22406E-06	-6.68010E-13
HCO	3.74702E-17	6.49833E-12	7.43022E-16
N2	4.30007E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	5.26746E-18	5.89761E-03
2	1.46957E-16	5.89934E-03
3	-3.12438E-06	2.09334E-03
4	-1.24735E+00	5.65550E-05
5	-2.31190E+00	2.09220E-03
6	3.22411E-16	5.01318E-02
7	9.54747E-18	5.89715E-03
8	2.54992E-17	5.89647E-03
9	-1.10656E-06	1.99005E-06
10	4.04361E-06	1.52707E-06
11	-3.49598E-04	6.85846E-07

12	1.00495E-02	2.20042E-06
13	-6.75853E-11	4.62981E-07
14	2.00472E-15	5.01855E-02
15	-9.80012E-14	2.05218E-06
16	1.63450E-12	1.48236E-07
17	-1.68637E-12	2.73802E-06
18	-1.13660E-09	5.68822E-07
19	5.16467E-09	2.31744E-06
20	8.82010E-12	1.17024E-07
21	2.48327E-10	5.80004E-07
22	-3.25068E-08	1.41005E-06
23	-4.91785E-04	5.57138E-05
24	-1.47831E-04	5.28277E-05
25	3.38991E-05	8.41228E-07
26	6.25907E-04	3.72749E-06
27	18.19869E-09	1.73744E-06
28	-1.04970E+00	1.14883E-06
29	1.30393E-01	2.88626E-06
30	-2.98186E-10	1.47218E-06

TIME 1.11633E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.34900E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61260E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.96848E-27	1.03509E-21	-2.81283E-24
CH3	3.23385E-26	5.60835E-21	-5.66409E-24
H	2.64786E-10	4.59208E-05	-3.45844E-11
OH	1.56589E-08	2.71567E-03	-2.88785E-09
H2O	6.01256E-07	1.04274E-01	1.56962E-09
CO*	2.94608E-09	5.10927E-04	2.57335E-08
O	2.50521E-09	4.34469E-04	-7.31672E-10
CO2	3.02265E-07	5.24207E-02	-2.57335E-08
O2	5.39955E-07	9.36424E-02	1.38920E-08
CH2O	3.86681E-19	6.70606E-14	3.27620E-18
H2	1.20092E-09	2.08270E-04	-1.08265E-10
HO2	7.05803E-12	1.22405E-06	-2.82053E-13
HCO	3.75138E-17	6.50588E-12	3.00863E-16
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	3.00518E-18	3.52120E-03
2	8.38357E-17	3.52194E-03
3	-1.32088E-06	8.85052E-04
4	-5.27362E-01	2.39122E-05
5	-9.77405E-01	8.84566E-04
6	4.45238E-17	7.22762E-03
7	5.44713E-18	3.52101E-03
8	1.45485E-17	3.52072E-03
9	-4.67903E-07	8.41506E-07
10	1.70298E-06	6.43153E-07
11	-1.46787E-04	2.87986E-07

12	4.26058E-03	9.32922E-07
13	-2.89538E-11	1.98353E-07
14	2.77445E-16	7.25136E-03
15	-4.19265E-14	8.76955E-07
16	6.17822E-13	5.59671E-08
17	-7.18308E-13	1.16494E-06
18	-4.44740E-10	2.22325E-07
19	2.22798E-09	9.98583E-07
20	4.95447E-12	6.56608E-08
21	1.13167E-10	2.64014E-07
22	-1.33288E-08	5.77493E-07
23	-2.07923E-04	2.35570E-05
24	-6.25006E-05	2.23361E-05
25	1.43116E-05	3.55168E-07
26	2.64641E-04	1.57607E-06
27	3.46615E-09	7.34569E-07
28	-4.44346E-01	4.86340E-07
29	5.51544E-02	1.22091E-06
30	-1.24294E-10	6.12941E-07

DETAILED KINETIC CALCULATION

204

TIME 1.11667E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.35000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61260E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.95004E-27	1.03189E-21	-2.61490E-24
CH3	3.22462E-26	5.59234E-21	-2.34965E-24
H	2.64785E-10	4.59207E-05	-1.80278E-11
OH	1.56588E-08	2.71566E-03	-2.38425E-09
H2O	6.01256E-07	1.04274E-01	1.29030E-09
CO	2.94653E-09	5.11006E-04	2.11491E-08
O	2.50519E-09	4.34466E-04	-5.90927E-10
CO2	3.02264E-07	5.24206E-02	-2.11491E-08
O2	5.39955E-07	9.36424E-02	1.14172E-08
CH2O	3.86740E-19	6.70709E-14	2.66074E-18
H2	1.20091E-09	2.08270E-04	-8.90407E-11
HO2	7.05802E-12	1.22405E-06	-2.31084E-13
HCO	3.75195E-17	6.50686E-12	2.38032E-16
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	2.79377E-18	3.28365E-03
2	7.79360E-17	3.28425E-03
3	-1.08557E-06	7.27386E-04
4	-4.33416E-01	1.96526E-05
5	-8.03281E-01	7.26987E-04
6	2.60460E-17	4.24019E-03
7	5.06395E-18	3.28348E-03
8	1.35252E-17	3.28325E-03
9	-3.84636E-07	6.91755E-07
10	1.39812E-06	5.28021E-07
11	-1.20490E-04	2.36394E-07

12	3.50382E-03	7.67220E-07
13	-2.39003E-11	1.63735E-07
14	1.62517E-16	4.25976E-03
15	-3.47713E-14	7.27186E-07
16	4.42001E-13	4.00339E-08
17	-5.94235E-13	9.63580E-07
18	-3.40736E-10	1.70309E-07
19	1.85950E-09	8.33305E-07
20	4.98721E-12	6.60849E-08
21	9.85250E-11	2.29819E-07
22	-1.06633E-08	4.67936E-07
23	-1.70886E-04	1.93609E-05
24	-5.13668E-05	1.83574E-05
25	1.17511E-05	2.91627E-07
26	2.17485E-04	1.29524E-06
27	2.84760E-09	6.03485E-07
28	-3.65575E-01	4.00128E-07
29	4.53378E-02	1.00361E-06
30	-1.00872E-10	4.97367E-07

TIME 1.11700E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.35100E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90351E-27	1.02382E-21	9.96919E-26
CH3	3.21032E-26	5.56754E-21	8.07773E-25
H	2.64781E-10	4.59199E-05	8.20389E-13
OH	1.56587E-08	2.71562E-03	-3.08237E-10
H2O	6.01256E-07	1.04274E-01	1.65104E-10
CO	2.94836E-09	5.11324E-04	2.70598E-09
O	2.50514E-09	4.34457E-04	-7.23970E-11
CO2	3.02263E-07	5.24203E-02	-2.70598E-09
O2	5.39956E-07	9.36426E-02	1.46078E-09
CH2O	3.86978E-19	6.71121E-14	3.30391E-19
H2	1.20091E-09	2.08269E-04	-1.13807E-11
HO2	7.05801E-12	1.22404E-06	-2.92435E-14
HCO	3.75423E-17	6.51083E-12	2.75897E-17
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.06568E-19	1.26228E-04
2	-2.97051E-18	1.26151E-04
3	-1.38895E-07	9.30699E-05
4	-5.54536E-02	2.51454E-06
5	-1.02778E-01	9.30186E-05
6	-4.79317E-18	7.83172E-04
7	-1.93205E-19	1.26249E-04
8	-5.16187E-19	1.26279E-04
9	-4.92452E-08	8.85672E-08
10	1.78972E-07	6.75928E-08
11	-1.54710E-05	3.03542E-08

DETAILED KINETIC CALCULATION

12	4.47908E-04	9.80791E-08
13	-3.06155E-12	2.09745E-08
14	-2.96740E-17	7.80660E-04
15	-4.54560E-15	9.50071E-08
16	3.39388E-14	3.07213E-09
17	-7.73554E-14	1.25361E-07
18	-3.58764E-11	1.79214E-08
19	2.46751E-10	1.10512E-07
20	9.38799E-13	1.24325E-08
21	1.43303E-11	3.34068E-08
22	-1.27410E-09	5.51603E-08
23	-2.18647E-05	2.47730E-06
24	-6.57228E-06	2.34887E-06
25	1.50050E-06	3.72387E-08
26	2.78177E-05	1.65672E-07
27	3.63814E-10	7.71044E-08
28	-4.68945E-02	5.13286E-08
29	5.80178E-03	1.28433E-07
30	-1.25009E-11	6.16004E-08

TIME 1.11733E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.35200E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.89969E-27	1.02316E-21	2.26128E-25
CH3	3.20875E-26	5.56482E-21	1.35166E-24
H	2.64780E-10	4.59198E-05	8.92399E-12
OH	1.56586E-08	2.71562E-03	-9.23377E-12
H2O	6.01256E-07	1.04274E-01	1.64957E-13
CO	2.94863E-09	5.11370E-04	2.82171E-13
O	2.50513E-09	4.34456E-04	9.02417E-12
CO2	3.02263E-07	5.24203E-02	-2.82163E-13
O2	5.39957E-07	9.36426E-02	1.62659E-13
CH2O	3.87013E-19	6.71182E-14	-2.78620E-20
H2	1.20091E-09	2.08268E-04	-1.04320E-14
HO2	7.05801E-12	1.22404E-06	7.44506E-16
HCO	3.75457E-17	6.51141E-12	-8.03198E-18
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIONAL DIR RATE
1	-2.41624E-19	2.86340E-04
2	-6.73924E-18	2.86340E-04
3	-1.50355E-11	1.00749E-08
4	-6.20098E-06	2.81185E-10
5	-1.07170E-05	9.69945E-09
6	-8.31076E-18	1.35781E-03
7	-4.37986E-19	2.86341E-04
8	-1.16989E-18	2.86341E-04
9	-9.08735E-11	1.63436E-10
10	-4.58087E-10	1.73008E-10
11	-1.98033E-08	3.88544E-11

12	4.15574E-07	9.09990E-11
13	-4.91303E-14	3.36591E-10
14	-5.16165E-17	1.35781E-03
15	-2.68257E-16	5.60631E-09
16	-6.09352E-14	5.51534E-09
17	-3.48365E-15	5.64506E-09
18	2.15495E-11	1.07638E-08
19	2.43253E-11	1.08935E-08
20	8.15788E-13	1.08026E-08
21	4.77866E-12	1.11390E-08
22	2.53535E-10	1.09754E-08
23	-4.35119E-09	4.93000E-10
24	-1.01696E-09	4.63452E-10
25	-8.52538E-09	2.11580E-10
26	-1.37634E-08	8.19699E-11
27	-1.15980E-12	2.45802E-10
28	-3.43063E-04	3.75503E-10
29	5.86454E-06	1.29823E-10
30	1.12288E-12	5.53267E-09

DETAILED KINETIC CALCULATION

TIME 1.11800E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.35400E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.89612E-27	1.02254E-21	3.41962E-25
CH3	3.20728E-26	5.56225E-21	1.86591E-24
H	2.64780E-10	4.59197E-05	1.67203E-11
OH	1.56586E-08	2.71561E-03	2.69181E-10
H2O	6.01257E-07	1.04274E-01	-1.53551E-10
CO	2.94888E-09	5.11413E-04	-2.52138E-09
O	2.50513E-09	4.34454E-04	8.51543E-11
CO2	3.02262E-07	5.24202E-02	2.52138E-09
O2	5.39957E-07	9.36426E-02	-1.36111E-09
CH2O	3.87046E-19	6.71238E-14	-3.62484E-19
H2	1.20090E-09	2.08268E-04	1.05862E-11
HO2	7.05801E-12	1.22404E-06	2.87176E-14
HCO	3.75488E-17	6.51195E-12	-4.14427E-17
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-3.65354E-19	4.33168E-04
2	-1.01920E-17	4.33241E-04
3	1.29419E-07	8.67133E-05
4	5.16698E-02	2.34298E-06
5	9.57663E-02	8.66662E-05
6	-1.16173E-17	1.89787E-03
7	-6.62239E-19	4.33150E-04
8	-1.76876E-18	4.33121E-04
9	4.57180E-08	8.22238E-08
10	-1.67697E-07	6.33352E-08
11	1.43800E-05	2.82138E-08

DETAILED KINETIC CALCULATION

12	-4.16631E-04	9.12308E-08
13	2.75703E-12	1.88885E-08
14	-7.22416E-17	1.90021E-03
15	3.71167E-15	7.75641E-08
16	-1.51007E-13	1.36668E-08
17	6.52824E-14	1.05778E-07
18	7.56304E-11	3.77736E-08
19	-1.82387E-10	8.16712E-08
20	7.21976E-13	9.55953E-09
21	-4.00256E-12	9.32913E-09
22	1.68402E-09	7.28947E-08
23	2.03690E-05	2.30786E-06
24	6.12328E-06	2.18842E-06
25	-1.41516E-06	3.51212E-08
26	-2.59528E-05	1.54566E-07
27	-3.41343E-10	7.23425E-08
28	4.30328E-02	4.71023E-08
29	-5.39568E-03	1.19445E-07
30	1.38497E-11	6.82350E-08

DETAILED KINETIC CALCULATION

212

TIME 1.11867E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.35600E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90714E-27	1.02445E-21	7.24499E-26
CH3	3.21218E-26	5.57076E-21	3.16869E-25
H	2.64780E-10	4.59198E-05	3.05132E-12
OH	1.56586E-08	2.71561E-03	1.46709E-10
H2O	6.01257E-07	1.04274E-01	-8.04326E-11
CO	2.94876E-09	5.11393E-04	-1.31917E-09
O	2.50513E-09	4.34455E-04	3.87900E-11
CO2	3.02263E-07	5.24202E-02	1.31917E-09
O2	5.39957E-07	9.36426E-02	-7.12133E-10
CH2O	3.87030E-19	6.71211E-14	-1.71854E-19
H2	1.20091E-09	2.08268E-04	5.54501E-12
HO2	7.05801E-12	1.22404E-06	1.45499E-14
HCO	3.75473E-17	6.51169E-12	-1.65560E-17
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-7.73929E-20	9.16181E-05
2	-2.15949E-18	9.16558E-05
3	6.77114E-08	4.53699E-05
4	2.70337E-02	1.22585E-06
5	5.01043E-02	4.53450E-05
6	-2.04421E-18	3.33968E-04
7	-1.40273E-19	9.16080E-05
8	-3.74617E-19	9.15932E-05
9	2.39743E-08	4.31177E-08
10	-8.74265E-08	3.30188E-08
11	7.53374E-06	1.47813E-08

DETAILED KINETIC CALCULATION

12	-2.18230E-04	4.77864E-08
13	1.47404E-12	1.00986E-08
14	-1.27428E-17	3.35193E-04
15	2.11276E-15	4.41528E-08
16	-4.01502E-14	3.63391E-09
17	3.63706E-14	5.89341E-08
18	2.58186E-11	1.28956E-08
19	-1.10923E-10	4.98722E-08
20	-1.42401E-13	1.88558E-09
21	-5.14162E-12	1.19845E-08
22	7.19214E-10	3.11332E-08
23	1.06583E-05	1.20761E-06
24	3.20388E-06	1.14504E-06
25	-7.34856E-07	1.82374E-08
26	-1.35678E-05	8.08053E-08
27	-1.77829E-10	3.76881E-08
28	2.27303E-02	2.48798E-08
29	-2.82638E-03	6.25676E-08
30	6.52896E-12	3.21683E-08

DETAILED KINETIC CALCULATION

214

TIME 1.11933E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.35800E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90855E-27	1.02470E-21	3.04605E-26
CH3	3.21277E-26	5.57179E-21	1.24263E-25
H	2.64780E-10	4.59198E-05	1.94101E-12
OH	1.56586E-08	2.71561E-03	8.97725E-11
H2O	6.01256E-07	1.04274E-01	-4.92568E-11
CO	2.94871E-09	5.11384E-04	-8.07892E-10
O	2.50513E-09	4.34455E-04	2.38283E-11
CO2	3.02263E-07	5.24202E-02	8.07892E-10
O2	5.39957E-07	9.36426E-02	-4.36127E-10
CH2O	3.87024E-19	6.71200E-14	-1.05477E-19
H2	1.20091E-09	2.08268E-04	3.39563E-12
HO2	7.05801E-12	1.22404E-06	8.91532E-15
HCO	3.75467E-17	6.51158E-12	-1.02060E-17
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-3.25346E-20	3.85074E-05
2	-9.07980E-19	3.85305E-05
3	4.14681E-08	2.77861E-05
4	1.65560E-02	7.50737E-07
5	3.06851E-02	2.77708E-05
6	-8.11023E-19	1.32501E-04
7	-5.89652E-20	3.85012E-05
8	-1.57462E-19	3.84922E-05
9	1.46817E-08	2.64051E-08
10	-5.35486E-08	2.02240E-08
11	4.61416E-06	9.05306E-09

DETAILED KINETIC CALCULATION

12	-1.33640E-04	2.22634E-08
13	9.02179E-13	6.18081E-09
14	-5.06564E-18	1.33252E-04
15	1.29166E-15	2.69938E-08
16	-2.50782E-14	2.26981E-09
17	2.22456E-14	3.60469E-08
18	1.59910E-11	7.98713E-09
19	-6.77269E-11	3.03292E-08
20	-8.05120E-14	1.06610E-09
21	-3.10902E-12	7.24689E-09
22	4.42567E-10	1.91581E-08
23	6.52736E-06	7.39566E-07
24	1.96213E-06	7.01250E-07
25	-4.50116E-07	1.11708E-08
26	-8.30932E-06	4.94874E-08
27	-1.08914E-10	2.30827E-08
28	1.39179E-02	1.52340E-08
29	-1.73087E-03	3.83164E-08
30	4.00774E-12	1.97465E-08

TIME 1.12000E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.36000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90870E-27	1.02472E-21	2.68104E-26
CH3	3.21284E-26	5.57191E-21	1.04065E-25
H	2.64780E-10	4.59198E-05	1.98770E-12
OH	1.56586E-08	2.71561E-03	9.22982E-11
H2O	6.01256E-07	1.04274E-01	-5.06383E-11
CO	2.94872E-09	5.11384E-04	-8.30551E-10
O	2.50513E-09	4.34455E-04	2.44884E-11
CO2	3.02263E-07	5.24202E-02	8.30551E-10
O2	5.39957E-07	9.36426E-02	-4.48359E-10
CH2O	3.87024E-19	6.71201E-14	-1.08416E-19
H2	1.20091E-09	2.08268E-04	3.49082E-12
HO2	7.05801E-12	1.22404E-06	9.16524E-15
HCO	3.75467E-17	6.51159E-12	-1.04868E-17
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-2.86340E-20	3.38900E-05
2	-7.99202E-19	3.39137E-05
3	4.26311E-08	2.85654E-05
4	1.70204E-02	7.71793E-07
5	3.15457E-02	2.85497E-05
6	-6.85299E-19	1.11961E-04
7	-5.18944E-20	3.38836E-05
8	-1.38575E-19	3.38743E-05
9	1.50936E-08	2.71458E-08
-10	-5.50516E-08	2.07916E-08
11	4.74375E-06	9.30732E-09

DETAILED KINETIC CALCULATION

12	-1.37386E-04	3.00838E-08
13	9.27477E-13	6.35413E-09
14	-4.28560E-18	1.12732E-04
15	1.32806E-15	2.77544E-08
16	-2.57375E-14	2.32948E-09
17	2.28719E-14	3.70618E-08
18	1.64251E-11	8.20398E-09
19	-6.96436E-11	3.11875E-08
20	-8.33426E-14	1.10358E-09
21	-3.19956E-12	7.45793E-09
22	4.54809E-10	1.96880E-08
23	6.71044E-06	7.60309E-07
24	2.01716E-06	7.20917E-07
25	-4.62738E-07	1.14841E-08
26	-8.54237E-06	5.08754E-08
27	-1.11969E-10	2.37300E-08
28	1.43085E-02	1.56616E-08
29	-1.77942E-03	3.93911E-08
30	4.11936E-12	2.02965E-08

DETAILED KINETIC CALCULATION

218

TIME 1.12667E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.38000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90957E-27	1.02487E-21	-5.25883E-27
CH3	3.21319E-26	5.57251E-21	-2.32312E-26
H	2.64780E-10	4.59198E-05	-1.55483E-13
OH	1.56586E-08	2.71562E-03	-8.40952E-12
H2O	6.01256E-07	1.04274E-01	4.60001E-12
CO	2.94863E-09	5.11369E-04	7.54321E-11
O	2.50513E-09	4.34456E-04	-2.19829E-12
CO2	3.02263E-07	5.24203E-02	-7.54321E-11
O2	5.39957E-07	9.36426E-02	4.07208E-11
CH2O	3.87012E-19	6.71180E-14	9.76604E-21
H2	1.20091E-09	2.08268E-04	-3.17099E-13
HO2	7.05801E-12	1.22404E-06	-8.30738E-16
HCO	3.75456E-17	6.51139E-12	9.28434E-19
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	5.61796E-21	6.64843E-06
2	1.56744E-19	6.65058E-06
3	-3.87184E-09	2.59443E-06
4	-1.54582E-03	7.00956E-08
5	-2.86504E-03	2.59300E-06
6	1.49697E-19	2.44569E-05
7	1.01827E-20	6.64785E-06
8	2.71950E-20	6.64700E-06
9	-1.37091E-09	2.46558E-09
10	4.99847E-09	1.88779E-09
11	-4.30909E-07	8.45450E-10

DETAILED KINETIC CALCULATION

12	1.24799E-05	2.73275E-09
13	-8.43797E-14	5.78084E-10
14	9.32405E-19	2.45270E-05
15	-1.21418E-16	2.53753E-09
16	2.15778E-15	1.95305E-10
17	-2.08760E-15	3.38286E-09
18	-1.42707E-12	7.12808E-10
19	6.39773E-12	2.86509E-09
20	9.99721E-15	1.32382E-10
21	3.04653E-13	7.10143E-10
22	-4.05489E-11	1.75535E-09
23	-6.09460E-07	6.90532E-08
24	-1.83203E-07	6.54752E-08
25	4.20057E-08	1.04248E-09
26	7.75800E-07	4.62039E-09
27	1.01660E-11	2.15452E-09
28	-1.30047E-03	1.42345E-09
29	1.61644E-04	3.57831E-09
30	-3.70879E-13	1.82741E-09

DETAILED KINETIC CALCULATION

220

TIME 1.13333E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.40000E+01 CM.

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90960E-27	1.02488E-21	-6.13417E-27
CH3	3.21320E-26	5.57252E-21	-2.70269E-26
H	2.64780E-10	4.59198E-05	-2.16225E-13
OH	1.56586E-08	2.71562E-03	-1.13588E-11
H2O	6.01256E-07	1.04274E-01	6.21661E-12
CO	2.94862E-09	5.11368E-04	1.01951E-10
O	2.50513E-09	4.34456E-04	-2.97746E-12
CO2	3.02263E-07	5.24203E-02	-1.01951E-10
O2	5.39957E-07	9.36426E-02	5.50362E-11
CH2O	3.87012E-19	6.71180E-14	1.32110E-20
H2	1.20091E-09	2.08268E-04	-4.28517E-13
HO2	7.05801E-12	1.22404E-06	-1.12222E-15
HCO	3.75456E-17	6.51138E-12	1.25892E-18
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	6.55285E-21	7.75476E-06
2	1.82837E-19	7.75768E-06
3	-5.23300E-09	3.50651E-06
4	-2.08926E-03	9.47379E-08
5	-3.87226E-03	3.50459E-06
6	1.74171E-19	2.84553E-05
7	1.18770E-20	7.75398E-06
8	3.17195E-20	7.75284E-06
9	-1.85281E-09	3.33227E-09
10	6.75666E-09	2.55182E-09
11	-5.82428E-07	1.14273E-09

12	1.68650E-05	3.69296E-09
13	-1.13964E-13	7.80765E-10
14	1.08535E-18	2.85500E-05
15	-1.63956E-16	3.42654E-09
16	2.94421E-15	2.66486E-10
17	-2.81973E-15	4.56923E-09
18	-1.93967E-12	9.68850E-10
19	8.63445E-12	3.86676E-09
20	1.31145E-14	1.73661E-10
21	4.09421E-13	9.54356E-10
22	-5.49332E-11	2.37805E-09
23	-8.23716E-07	9.33289E-08
24	-2.47609E-07	8.84933E-08
25	5.67784E-08	1.40911E-09
26	1.04851E-06	6.24453E-09
27	1.37403E-11	2.91205E-09
28	-1.75743E-03	1.92362E-09
29	2.18452E-04	4.83587E-09
30	-5.01737E-13	2.47218E-09

DETAILED KINETIC CALCULATION

222

TIME 1.16667E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.50000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90940E-27	1.02485E-21	9.64657E-30
CH3	3.21312E-26	5.57238E-21	4.03216E-29
H	2.64780E-10	4.59198E-05	-6.29493E-15
OH	1.56586E-08	2.71562E-03	5.60348E-14
H2O	6.01256E-07	1.04274E-01	-2.67551E-14
CO	2.94863E-09	5.11370E-04	-4.40331E-13
O	2.50513E-09	4.34456E-04	5.94577E-15
CO2	3.02263E-07	5.24203E-02	4.40331E-13
O2	5.39957E-07	9.36426E-02	-2.37784E-13
CH2O	3.87013E-19	6.71182E-14	-5.64870E-23
H2	1.20091E-09	2.08268E-04	1.88252E-15
HO2	7.05801E-12	1.22404E-06	5.30845E-18
HCO	3.75457E-17	6.51141E-12	-5.48750E-21
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.03007E-23	1.21904E-08
2	-2.87589E-22	1.22026E-08
3	2.26021E-11	1.51451E-08
4	9.02661E-06	4.09314E-10
5	1.67245E-05	1.51365E-08
6	-2.61042E-22	4.26488E-08
7	-1.86660E-23	1.21866E-08
8	-4.98379E-23	1.21817E-08
9	8.38816E-12	1.50861E-11
10	-2.85070E-11	1.07664E-11
11	2.42289E-09	4.75375E-12

12	-7.39528E-08	1.61936E-11
13	5.40160E-16	3.70063E-12
14	-1.63684E-21	4.30581E-08
15	7.17649E-19	1.49982E-11
16	-1.11673E-17	1.01077E-12
17	1.23260E-17	1.99737E-11
18	8.96505E-15	4.47796E-12
19	-3.70537E-14	1.65937E-11
20	-3.07913E-17	4.07735E-13
21	-1.92989E-15	4.49855E-12
22	2.38476E-13	1.03236E-11
23	3.55908E-09	4.03252E-10
24	1.06901E-09	3.82056E-10
25	-2.43290E-10	6.03788E-12
26	-4.54929E-09	2.70940E-11
27	-5.89457E-14	1.24926E-11
28	7.86087E-06	8.60421E-12
29	-9.38773E-07	2.07816E-11
30	2.14360E-15	1.05620E-11

DETAILED KINETIC CALCULATION

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TIME 1.20000E+00 SEC AREA 4.12667E+01 SQ CM POSITION 3.60000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90941E-27	1.02485E-21	3.18567E-32
CH3	3.21312E-26	5.57238E-21	1.13746E-31
H	2.64780E-10	4.59198E-05	-1.08296E-14
OH	1.56586E-08	2.71562E-03	1.19596E-14
H2O	6.01256E-07	1.04274E-01	-6.44464E-16
CO	2.94863E-09	5.11370E-04	-9.72919E-15
O	2.50513E-09	4.34456E-04	-1.03296E-14
CO2	3.02263E-07	5.24203E-02	9.72919E-15
O2	5.39957E-07	9.36426E-02	-5.35759E-15
CH2O	3.87013E-19	6.71182E-14	-6.37000E-25
H2	1.20091E-09	2.08268E-04	7.93481E-17
HO2	7.05801E-12	1.22404E-06	2.27335E-19
HCO	3.75457E-17	6.51141E-12	-2.73749E-22
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-3.41172E-26	4.03763E-11
2	-9.52187E-25	4.04021E-11
3	5.00168E-13	3.35151E-10
4	2.03378E-07	9.22220E-12
5	3.69531E-07	3.34444E-10
6	-7.18002E-25	1.17307E-10
7	-6.10263E-26	3.98427E-11
8	-1.62644E-25	3.97546E-11
9	3.67855E-13	6.61585E-13
10	-2.84217E-13	1.07342E-13
11	-4.54747E-11	8.92221E-14

DETAILED KINETIC CALCULATION

12	-2.96859E-09	6.50039E-13
13	7.93197E-17	5.43417E-13
14	-4.81223E-24	1.26589E-10
15	2.60463E-20	5.44343E-13
16	-1.13841E-18	1.03040E-13
17	3.96411E-19	6.42363E-13
18	4.16334E-16	2.07955E-13
19	-1.11022E-16	4.97189E-14
20	2.94903E-17	3.90507E-13
21	-1.52084E-16	3.54505E-13
22	1.02141E-14	4.42163E-13
23	8.04334E-11	9.11329E-12
24	2.39169E-11	8.54770E-12
25	4.54747E-13	1.12858E-14
26	-1.12777E-10	6.71662E-13
27	-5.45405E-16	1.15590E-13
28	5.74362E-07	6.28674E-13
29	-2.14204E-08	4.74184E-13
30	2.49103E-17	1.22739E-13

DETAILED KINETIC CALCULATION

TIME 1.33333E+00 SEC AREA 4.12667E+01 SQ CM POSITION 4.00000E+01 CM

PRESSURE, ATM 1.00000
 DENSITY, GM/CM**3 1.62260E-04
 TEMPERATURE, K 2103.85
 ENTROPY, CAL/GM-K 2.2665
 GAMMA 1.2686
 ENTHALPY, CAL/GM 1.55859E+02
 GIBBS F E, CAL/GM -4.61259E+03

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	5.90941E-27	1.02485E-21	-1.63998E-34
CH3	3.21312E-26	5.57238E-21	2.83630E-34
H	2.64780E-10	4.59198E-05	-5.40494E-15
OH	1.56586E-08	2.71562E-03	4.12908E-15
H2O	6.01256E-07	1.04274E-01	7.04374E-16
CO	2.94863E-09	5.11370E-04	-5.55529E-18
O	2.50513E-09	4.34456E-04	-4.85752E-15
CO2	3.02263E-07	5.24203E-02	5.55539E-18
O2	5.39957E-07	9.36426E-02	7.07306E-17
CH2O	3.87013E-19	6.71182E-14	-4.29680E-25
H2	1.20091E-09	2.08268E-04	-6.57093E-17
HO2	7.05801E-12	1.22404E-06	-1.47566E-18
HCO	3.75457E-17	6.51141E-12	-1.01871E-22
N2	4.30008E-06	7.45747E-01	0.

REACTION NUMBER	NET REACTION CONVERSION RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
1	-1.95555E-28	2.31481E-13
2	6.26040E-27	2.65634E-13
3	8.07619E-16	5.41166E-13
4	-3.49246E-10	1.58366E-14
5	2.11003E-10	1.90968E-13
6	-1.00974E-28	1.64971E-14
7	1.26218E-29	8.24048E-15
8	1.51461E-28	3.70212E-14
9	2.38971E-13	4.29789E-13
10	-9.94760E-14	3.75695E-14
11	2.18279E-11	4.28266E-14

DETAILED KINETIC CALCULATION

12	2.47383E-09	5.41699E-13
13	2.42548E-17	1.66169E-13
14	-4.44286E-27	1.16872E-13
15	2.39287E-20	5.00087E-13
16	8.13152E-18	7.35997E-13
17	2.98156E-19	4.83145E-13
18	2.91434E-16	1.45568E-13
19	1.45717E-15	6.52560E-13
20	3.03577E-18	4.01992E-14
21	-9.43970E-17	2.20038E-13
22	2.22045E-15	9.61225E-14
23	-2.84217E-12	3.22025E-13
24	5.68434E-13	2.03154E-13
25	-5.91172E-12	1.46715E-13
26	6.45741E-11	3.84581E-13
27	2.13966E-15	4.53468E-13
28	2.08347E-07	2.28048E-13
29	2.42144E-08	5.36034E-13
30	7.86641E-18	3.87596E-14

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