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ANALYTICAL CHEMICAL KINETIC STUDY OF THE EFFECT OF CARBON DIOXIDE AND WATER VAPOR ON HYDROGEN-AIR CONSTANT-PRESSURE COMBUSTION

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16. Abstract

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SUMMARY

Numerical solutions have been obtained for the finite-rate constant-pressure combustion of stoichiometric hydrogen-air mixtures in the presence of small to moderate amounts of carbon dioxide (CO_2) and water vapor (H_2O). Computations have been carried out for initial mixture temperatures of 1150 K, 1250 K, and 1500 K at a pressure of 1 atm, with additional computations for pressures of 0.5 atm and 2 atm at an initial mixture temperature of 1250 K. The results show that the influence of CO_2 and H_2O on the induction time, for the condition of no free radicals (O, H, and OH) initially present, is quite small (an increase up to about 16 percent) for initial temperatures of 1250 K or higher at pressures of 1 atm or less. For an initial mixture temperature of 1150 K at 1 atm or 1250 K at 2 atm, the induction time without initial free radicals is increased considerably (nearly 60 percent) by the presence of moderate quantities of CO_2 and H_2O. These increases in induction times due to the presence of initial amounts of CO_2 and H_2O are offset somewhat when initial small amounts of free radicals (O, H, and OH) are included in the calculations. In some cases the inclusion of initial quantities of free radicals causes a reduction in induction time due to initial amounts of CO_2 and H_2O. The reaction time was measurably increased by the presence of CO_2 and H_2O for all test cases, but a large fraction of this increased time can be accounted for by the reduction in temperature due to the added CO_2 and H_2O. This study suggests that although all the conditions for hydrogen-burning hypersonic ramjet engine tests in a combustion-heated wind tunnel cannot be matched to clean-air flight conditions, the chemical kinetic effects of CO_2 and H_2O are small enough to allow useful interpretation of test results for initial temperatures of 1250 K or higher and pressures near 1 atm or less.

INTRODUCTION

A proposal has been made to carry out hydrogen-burning hypersonic ramjet engine tests in a combustion-heated wind tunnel in which the test stream is composed of the combustion products formed by burning a hydrocarbon fuel in oxygen-enriched air. The

Langley 8-foot high-temperature structures tunnel, if modified to include an oxygen-enrichment system, would be a facility of this kind. The use of such a simulated test stream raises the question of the influence of the tunnel-heater combustion products, mainly carbon dioxide (CO_2) and water vapor (H_2O), on the chemical kinetic processes in the test engine.

There have been, of course, many analytical and numerical studies of hydrogen-oxygen (H_2-O_2) combustion processes. Some of the more recent are listed as references 1 to 5. The effects of vitiation have also been the subject of studies such as references 6 to 9. It may be noted, however, that these studies have emphasized the ignition phase of the combustion process and do not generally consider the overall process which includes that final approach toward equilibrium. The gas temperature range considered in these previous studies are also generally higher than would apply to a tunnel such as the Langley 8-foot high-temperature structures tunnel, which is heated by methane combustion.

The purpose of this paper is to examine the influence of small to moderate amounts of CO_2 and H_2O on the induction time and reaction time for hydrogen-air combustion under constant pressure. The amounts of CO_2 and H_2O chosen for these calculations are representative of the concentrations of these two species in a tunnel test stream generated by oxygen-enriched methane-air combustion. For comparison, computations are also made for cases with no CO_2 and H_2O initially present. The calculations are based on the assumption that the hydrogen and oxidizer streams are completely mixed at the entrance of the combustor.

SYMBOLS

A_j	preexponential reaction rate coefficient
$a_{i,j}$	relative third-body efficiency of species i in reaction j
B_j	power on T in equation (8)
c_i	mass fraction of species i
E_j	activation energy of reaction j
h	static enthalpy (including enthalpy of formation)
h_i	static enthalpy of species i

h_o	static enthalpy at entrance of combustor
I,J	number of chemical species and finite-rate reactions, respectively
i,j	specific chemical species and finite-rate reaction, respectively
K_j	equilibrium constant in terms of molar concentrations for reaction j
k_j	reaction rate constant for reaction j
k_{-j}	reaction rate constant for reverse of reaction j
M	third-body species
M'	specific third-body species
p	pressure (1 atm = 101.325 kN/m^2)
R	universal gas constant
T	temperature
T_e	equilibrium adiabatic flame temperature
T_m	mean temperature, $\frac{1}{2}(T_o + T_e)$
T_o	initial temperature at entrance of combustor
t	time (t = 0 at entrance of combustor)
u	velocity
W_i	molecular weight of species i
X_i	general symbol for chemical species i
x	distance along combustor, measured from entrance
θ	fractional temperature rise (see eq. (12))

τ	induction time without initial quantities of free radicals O, H, and OH (time at which $\theta = 0.05$)
$\Delta\tau$	difference in induction time with and without free radicals
τ_r	reaction time (the total reaction time to $\theta = 0.95$ less the induction time at which $\theta = 0.05$)
$\nu_{i,j}$	stoichiometric coefficient of reactant species i in reaction j
$\nu'_{i,j}$	stoichiometric coefficient of product species i in reaction j
$\nu_{I+1,j}$	index in equation (9) which is unity for all three-body reactions and zero for all bimolecular reactions
ρ	gas density

ANALYSIS

The assumptions and equations for computing the supersonic flow properties along a constant-pressure combustion chamber are outlined in this section. It is assumed that the flow is quasi-one-dimensional, inviscid, and adiabatic. The hydrogen and test stream are assumed to be completely mixed just prior to the beginning of the combustion process.

Thermodynamic Relations

On the basis of the foregoing assumptions, the conservation of momentum

$$\rho u \frac{du}{dx} + \frac{dp}{dx} = 0 \tag{1}$$

and the conservation of energy

$$\frac{d}{dx}\left(h + \frac{u^2}{2}\right) = 0 \tag{2}$$

combine to show that, when $\frac{dp}{dx} = 0$ in equation (1), the static enthalpy along the combustor is constant – that is,

$$\frac{dh}{dx} = 0 \tag{3}$$

It also follows that the flow velocity along the combustor is constant – that is,

$$\frac{du}{dx} = 0 \tag{4}$$

and therefore the dwell time t of a given mass of reacting gas mixture is directly proportional to x, the distance from the entrance of the combustor. Since the static enthalpy of the reacting gas mixture, composed of I chemical species, in the combustor is independent of time, one equation which must be satisfied at every point in the combustor is

$$\sum_{i=1}^{I} c_i h_i(T) = h_o \tag{5}$$

where h_o is the static enthalpy at the entrance of the combustor. Equation (5) applies to any point in the combustor and indicates how the temperature relates to a particular chemical composition expressed by a set of mass fractions. The expression which relates the gas density to the temperature and chemical composition at a particular pressure is the equation of state

$$p = \rho RT \sum_{i=1}^{I} \frac{c_i}{W_i} \tag{6}$$

which must be solved along with equation (5).

For finite-rate combustion the differential equations which represent the various chemical reactions must be solved simultaneously in a stepwise manner along with equations (5) and (6). These differential rate equations are discussed in the next section.

Chemical Kinetic Relations

The reacting gas system is assumed to contain J finite-rate reactions, all of which may be expressed as

$$\sum_{i=1}^{I} \nu_{i,j} X_i \underset{k_{-j}}{\overset{k_j}{\rightleftharpoons}} \sum_{i=1}^{I} \nu'_{i,j} X_i \qquad (j = 1, 2, \ldots J) \tag{7}$$

where the rate constant k_j for the jth reaction is represented by

$$k_j = A_j T^{B_j} \exp\left(\frac{-E_j}{RT}\right) \qquad (j = 1, 2, \ldots J) \tag{8}$$

The rate of change of the mass fraction of the ith chemical species in the jth reaction, represented by equation (7), can be expressed as

$$\left(\frac{dc_i}{dt}\right)_j = k_j \frac{W_i}{\rho}\left(\nu'_{i,j} - \nu_{i,j}\right) \prod_{i=1}^{I} \left(\frac{c_i \rho}{W_i}\right)^{\nu_{i,j}} \left(\rho \sum_{i=1}^{I} \frac{a_{i,j} c_i}{W_i}\right)^{\nu_{I+1,j}} \qquad (j = 1, 2, \ldots J) \tag{9}$$

The last term in this equation accounts for the homogeneous catalysts, say M, in three-body reactions. The index $a_{i,j}$ is the relative third-body efficiency of species i in reaction j if the ith species is to be included as a third-body catalyst in the jth reaction, but is zero if that species is to be excluded. The quantity $\nu_{I+1,j}$ is also an index and is equal to unity for all three-body reactions. For bimolecular reactions, $\nu_{I+1,j}$ is zero with all values of $a_{i,j}$ set equal to unity.

The total rate of change of the mass fraction of the ith species in the reacting gas mixture is obtained by summation over all J reactions; that is,

$$\frac{dc_i}{dt} = \sum_{j=1}^{J} \left(\frac{dc_i}{dt}\right)_j \qquad (i = 1, 2, \ldots I) \qquad (10)$$

where the summation includes both forward and reverse reactions. The set of equations to be solved includes the I differential equations indicated by equation (10), along with equations (5), (6), (8), and (9). The unknowns are reduced to $c_1, c_2, \ldots c_I$ and T, after equations (6) and (8) are used to eliminate ρ and k_j. The initial values of the mass fractions and temperature are specified at the entrance of the combustor so that a forward integration of this set of equations can be carried out along the length of the combustor by use of a modified Runge-Kutta scheme.

Chemical Kinetic Scheme

The chemical kinetic scheme used in this investigation included the following reactions:

(1) $OH + H_2 \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} H_2O + H$

(2) $H + O_2 \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} OH + O$

(3) $O + H_2 \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} OH + H$

(4) $OH + OH \underset{k_{-4}}{\overset{k_4}{\rightleftarrows}} H_2O + O$

(5) $H + H + M \underset{k_{-5}}{\overset{k_5}{\rightleftarrows}} H_2 + M$

(6) $O + O + M \underset{k_{-6}}{\overset{k_6}{\rightleftarrows}} O_2 + M$

(7) $O + H + M \underset{k_{-7}}{\overset{k_7}{\rightleftarrows}} OH + M$

(8) $H + OH + M \underset{k_{-8}}{\overset{k_8}{\rightleftarrows}} H_2O + M$

(9) $CO + OH \underset{k_{-9}}{\overset{k_9}{\rightleftarrows}} CO_2 + H$

(10) $H + O_2 + M \underset{k_{-10}}{\overset{k_{10}}{\rightleftarrows}} HO_2 + M$

(11) $HO_2 + H_2 \underset{k_{-11}}{\overset{k_{11}}{\rightleftharpoons}} H_2O_2 + H$

(13) $H_2 + O_2 \underset{k_{-13}}{\overset{k_{13}}{\rightleftharpoons}} OH + OH$

(12) $H_2O_2 + M \underset{k_{-12}}{\overset{k_{12}}{\rightleftharpoons}} OH + OH + M$

The values of the reaction rate constant k_j (for $j = 1, 2, \ldots 13$) used in this study are listed in table 1 along with the sources (refs. 10 to 18). The reverse reaction rate constants, not shown in table 1, were calculated from the equation

$$k_{-j} = \frac{k_j}{K_j} \tag{11}$$

where the equilibrium constant for the jth reaction K_j was derived from thermochemical data of reference 19. For the three-body reactions the values of k_j are indicated in table 1 for a specific species, say M', and the relative third-body efficiencies of the remaining species are shown in table 2, along with the sources (refs. 15, 17, and 20 to 24).

CALCULATIONS

Three test-gas mixture compositions were chosen in order to determine the influence of moderate amounts of CO_2 and H_2O on the rate of H_2-air combustion. Table 3 lists these three combustion-chamber-inlet mixtures which include added H_2. All mixtures are stoichiometric with respect to H_2 and the amount of O_2 to form H_2O. The nitrogen (N_2) is assumed chemically inert. Mixture R is a reference mixture which contains no CO_2 or H_2O. The relative amounts of CO_2 and H_2O in mixtures A and B are based on complete stoichiometric combustion of CH_4 and air (in the heater section of the test facility) with O_2 added to bring the stream O_2 mole fraction to 0.2 before H_2 addition. The species included in mixtures A and B simulate products of combustion with tunnel stagnation temperatures of 1390 K and 2200 K, respectively, which are approximately the lower and upper limits for methane-air combustion-heated tunnels.

The three mixtures were used as the basis for calculating the finite-rate process along a combustion chamber for various combinations of initial temperature and pressure. The cases calculated are listed in table 4. For each of these 15 test cases the equilibrium adiabatic flame temperature was also computed. The finite-rate calculations were allowed to proceed in time for each case until at least 95 percent of the maximum possible temperature rise (the equilibrium adiabatic flame temperature less the initial temperature) was achieved. The foregoing set of calculations were first carried out with the assumption of no initial free radicals (O, H, and OH). The same set of calculations were then performed with the assumption of an equilibrium amount of free radicals in the separate hydrogen- and oxygen-containing streams at the initial temperature T_o and pressure p in the combustor prior to mixing. The sums of the free radicals in the two streams were added together to give the initial mole fractions of free radicals at the entrance of the combustor. These quantities are listed in table 5. The results of these calculations without and with initial free radicals are shown and discussed in the next section.

RESULTS AND DISCUSSION

Calculations have been made for the 15 cases indicated in table 4. Figures 1 to 15 show the time variation of the species mass fraction. In addition, the equilibrium condition in terms of mass fractions is also shown on the far right of these figures.

Figure 1 shows the detailed behavior of each reactant and product species for case 1, which was computed for an initial temperature of 1250 K, a pressure of 1 atm, and mixture R containing no initial CO_2 or H_2O and no initial free radicals. The attainment of maximum levels and subsequent decay toward equilibrium is observed for the intermediate species (OH, O, H, HO_2, and H_2O_2), while H_2O grows at the expense of depleting O_2 and H_2. The level of N_2 is fixed since it is inert. Figures 2 and 3 are based on the same initial temperature and pressure, but are for successively larger initial amounts of CO_2 and H_2O. These two figures include the variation of CO_2 and CO and indicate an initial concentration of H_2O.

Figures 4 to 6 represent similar results but for a pressure of 0.5 atm, with correspondingly longer times, whereas figures 7 to 9 are for a pressure of 2 atm. The reaction times for the 2-atm cases are, as expected, considerably shorter than for the lower pressure cases. Figures 10 to 15 show the effect of different initial temperatures (1500 K and 1150 K) on the species time histories.

In order to obtain a quantitative assessment of the influence of the addition of CO_2 and H_2O on the induction time and reaction time, the degree of reaction is defined by the equation

$$\theta = \frac{T - T_o}{T_e - T_o} \tag{12}$$

where θ ranges from zero at the entrance of the combustor toward unity as equilibrium is approached. The time variations of the fractional temperature rise θ for the 15 cases are shown in figures 16 and 17.

In this study the induction time is defined as the time at which $\theta = 0.05$, and the total reaction time is defined by $\theta = 0.95$. The induction times calculated for the reference mixture R for pressures of 0.5 and 1 atm have been compared with experimental and calculated results presented in references 1 and 25. It was found that the present calculations agree within the range of uncertainty of the reported induction times.

Table 6 lists the calculated induction times for various initial temperatures, pressures, and amounts of CO_2 and H_2O when (1) there are no initial free radicals (O, H, and OH) and when (2) the initial free radical concentration is based on the sum of the equilibrium amounts in the two separate streams (hydrogen- and oxygen-containing streams) prior to mixing. It is noted from table 6 that, with no initial free radicals, the addition of CO_2 and H_2O causes an increase in induction time of no more than 16 percent for initial temperatures of 1250 K or higher at pressures of 1 atm or less. However, as the pressure is increased to 2 atm at 1250 K, it is seen that the induction time increases by almost 60 percent for mixture B, and an even larger increase in induction time due to CO_2 and H_2O addition is noted for the 1150-K, 1-atm case (without initial free radicals).

An attempt to indicate the influence of an initial concentration of free radicals was made by calculating the induction times for the initial free radical concentrations listed in table 5. These results are presented in table 6 along with the results for no initial free radicals. It is noted that the increases in induction time in all cases just discussed are offset to some degree by an initial free radical concentration. In some cases the effect of an initial free radical concentration causes the induction time to be less for the mixtures containing initial quantities of CO_2 and H_2O than for the reference mixtures.

In an actual test, it is difficult to determine the amount of free radicals initially present. Figure 18 was therefore prepared in order to correlate the relative reduction in induction time $-\frac{\Delta\tau}{\tau}$ as a function of the total mole fraction of initial free radicals. The sums of the mole fractions of O, H, and OH are used because the growth for each free-radical species is strongly coupled to the other free radicals. It can be seen from figure 18 that the correlation of $-\frac{\Delta\tau}{\tau}$ as a function of the sum of the initial mole fractions O, H, and OH is very good for $T_0 = 1250$ K where a number of results have been obtained. The results for $T_0 = 1150$ K and $T_0 = 1500$ K are rather limited but suggest a reasonable correlation also.

The total reaction time required to achieve a 95-percent temperature rise ($\theta = 0.95$) less the induction time (at which $\theta = 0.05$) for each of the 15 cases is given in table 7(a) as reaction time τ_r. Calculations with and without initial free radicals show that this reaction time is independent of the initial free radical concentration. The reaction time is, however, influenced by the presence of initial quantities of CO_2 and H_2O. An examination of the calculated equilibrium temperatures as shown in table 7(b) suggests that the increases in τ_r due to initial amounts of CO_2 and H_2O may result to a large measure from the reduction in an average reaction temperature. Figure 19 shows the reaction time including a pressure-dependent term $\tau_r p^{1.6}$ as a function of the reciprocal of a mean temperature $1/T_m$. It can be seen that the expression $\log \tau_r p^{1.6} = \frac{3480}{T_m} + 0.040$ correlates the results to within ±10 percent. This figure does suggest that a large part of the increase in τ_r is due to the reduction in the mean reaction temperature T_m.

CONCLUDING REMARKS

Numerical solutions have been obtained which show the chemical kinetic effect of small to moderate amounts of carbon dioxide (CO_2) and water vapor (H_2O) on hydrogen-air combustion under constant pressure. These results were obtained for mixtures which cover a range of temperature, pressure, and chemical composition in an oxygen-enriched methane-heated wind tunnel which might be used for a hydrogen-burning ramjet engine test.

The results of this study for initially uniformly mixed systems show that the induction time is increased by no more than 16 percent by the presence of moderate amounts of CO_2 and H_2O for initial temperatures of 1250 K or higher at pressures of 1 atm or less when no free radicals are initially present. The initial presence of CO_2 and H_2O at lower initial temperatures or higher pressures causes rather large increases in induction time for no initial free radicals. However, the initial presence of rather small quantities of free radicals offsets to some degree these increases in induction times. In some cases an allowance for the initial presence of free radicals causes a net reduction in induction time for mixtures containing CO_2 and H_2O relative to the reference mixtures. The increase in reaction time (total reaction time less induction time) due to the presence of CO_2 and H_2O appears to result primarily from the diluting effect which reduces the mean reaction temperature.

On the basis of this limited set of calculations, it appears, from a purely chemical kinetic point of view, that results from hydrogen-burning ramjet engine tests in an oxygen-enriched methane-heated wind tunnel would not be grossly different from clean-air tests provided the combustion inlet temperature is 1250 K or higher and the pressure is 1 atm or less. Additional calculations, however, would be required to show more precisely the temperature and pressure limitations and allow interpretation of engine test results. The influence of the mixing process, which was not studied herein, must of course also be examined. Another point to be noted is that the values of the reaction rate constants used in the present kinetic scheme are of course subject to improved accuracy, but it is expected that the trends and approximate level of the results that are presented are correct.

Langley Research Center,
National Aeronautics and Space Administration,
Langley Station, Hampton, Va., February 10, 1970.

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TABLE 1.- REACTION RATE CONSTANTS

j	Reaction	Reaction rate constant (a)	Source
1	$OH + H_2 \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} H_2O + H$	$k_1 = 2.3 \times 10^{13} \exp(-5200/RT)$	Dixon-Lewis, Wilson, and Westenberg (ref. 10)
2	$H + O_2 \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} OH + O$	$k_2 = 1.0 \times 10^{14} \exp(-16\,000/RT)$	Recommendation by Richard S. Brokaw, NASA Lewis Research Center (1967)
3	$O + H_2 \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} OH + H$	$k_3 = 4.3 \times 10^{13} \exp(-10\,200/RT)$	Wong and Potter (ref. 11)
4	$OH + OH \underset{k_{-4}}{\overset{k_4}{\rightleftarrows}} H_2O + O$	$k_4 = 7.6 \times 10^{12} \exp(-1000/RT)$	Kaufman and Del Greco (ref. 12)
[b]5	$H + H + M \underset{k_{-5}}{\overset{k_5}{\rightleftarrows}} H_2 + M$	$k_{-5,Ar} = 1.18 \times 10^{12} T^{0.50} \exp(-94\,500/RT)$	Myerson, Watt, and Joseph (ref. 13)
[b]6	$O + O + M \underset{k_{-6}}{\overset{k_6}{\rightleftarrows}} O_2 + M$	$k_{6,O_2} = 8.2 \times 10^{18} T^{-1.22}$	Kiefer and Lutz (ref. 14)
[b]7	$O + H + M \underset{k_{-7}}{\overset{k_7}{\rightleftarrows}} OH + M$	$k_{7,M} = 6.0 \times 10^{14}$	Kaskan and Browne (ref. 15)
[b]8	$H + OH + M \underset{k_{-8}}{\overset{k_8}{\rightleftarrows}} H_2O + M$	$k_{8,H_2O} = 1.8 \times 10^{22} T^{-1.5}$	Kaskan and Browne (ref. 15)
9	$CO + OH \underset{k_{-9}}{\overset{k_9}{\rightleftarrows}} CO_2 + H$	$k_9 = 3.1 \times 10^{11} \exp(-600/RT)$	Dixon-Lewis, Wilson, and Westenberg (ref. 10)
[b]10	$H + O_2 + M \underset{k_{-10}}{\overset{k_{10}}{\rightleftarrows}} HO_2 + M$	$k_{10,Ar} = 8.6 \times 10^{14} \exp(1280/RT)$	Getzinger and Schott (ref. 16)
11	$HO_2 + H_2 \underset{k_{-11}}{\overset{k_{11}}{\rightleftarrows}} H_2O_2 + H$	$k_{-11} = 1.0 \times 10^{14} \exp(-9800/RT)$	Recommendation by Richard S. Brokaw, NASA Lewis Research Center (1967)
[b]12	$H_2O_2 + M \underset{k_{-12}}{\overset{k_{12}}{\rightleftarrows}} OH + OH + M$	$k_{12,N_2} = 1.7 \times 10^{17} \exp(-46\,300/RT)$	Baldwin and Brattan (ref. 17)
13	$H_2 + O_2 \underset{k_{-13}}{\overset{k_{13}}{\rightleftarrows}} OH + H$	$k_{13} = 2.5 \times 10^{12} \exp(-39\,000/RT)$	Ripley and Gardiner (ref. 18)

[a]All reactions have units of cm^3/mole-sec except reactions 5 to 8, 10, and 12 have units of $cm^6/mole^2$-sec; activation energies are expressed in units of cal/mole (1 cal/mole = 4.184 joules/mole).

[b]See table 2 for relative third-body efficiencies.

TABLE 2.- RELATIVE THIRD-BODY EFFICIENCIES

j	M'	M	$a_{i,j} = \frac{k_{j,M}}{k_{j,M'}}$	Source
5	Ar	H	8	Kaskan and Browne (ref. 15)
		H_2	2	
		H_2O	6	
		Others	1	
6	O_2	O	2.78	Wray (ref. 20)
		Others	0.225	Bortner (ref. 21)
7		(All species assumed to have an efficiency of unity)		
8	H_2O	All others	0.25	Kaskan and Browne (ref. 15)
10	Ar	H_2O	32	Baldwin and Brooks (ref. 22)
		N_2	2.15	Lewis and von Elbe (ref. 23)
		O_2	1.75	
		H_2	5	
		CO_2	7.35	
		CO	3.8	
		Others	1	
12	N_2	CO_2	1.25	Hoare, Protheroe, and Walsh (ref. 24)
		H_2O_2	6.6	Baldwin and Brattan (ref. 17)
		H_2O	6	
		O_2	0.78	
		Others	1	

TABLE 3.- TEST-GAS MIXTURE COMPOSITIONS AT ENTRANCE OF COMBUSTION CHAMBER

Species	Mass fractions for –		
	Mixture R	Mixture A (a)	Mixture B (b)
N_2	0.7568	0.6191	0.4794
O_2	.2162	.2177	.2192
H_2	.0270	.0272	.0274
CO_2	0	.0748	.1507
H_2O	0	.0612	.1233

[a] Mixture A is based on a tunnel stagnation temperature of 1390 K.

[b] Mixture B is based on a tunnel stagnation temperature of 2200 K.

TABLE 4.- INITIAL CONDITIONS FOR CALCULATIONS

Test case	Mixture (a)	Initial temperature, $^{\circ}$K	Pressure, atm
1	R	1250	1
2	A	↓	↓
3	B	↓	↓
4	R	↓	0.5
5	A	↓	↓
6	B	↓	↓
7	R	↓	2
8	A	↓	↓
9	B	↓	↓
10	R	1500	1
11	A	↓	↓
12	B	↓	↓
13	R	1150	↓
14	A	↓	↓
15	B	↓	↓

[a] See table 3 for composition of mixtures R, A, and B.

TABLE 5.- INITIAL MOLE FRACTIONS[a] OF O, H, AND OH

Free radicals	Initial mole fractions[a] for –				
	T_o = 1150 K; p = 1 atm	T_o = 1250 K; p = 0.5 atm	T_o = 1250 K; p = 1 atm	T_o = 1250 K; p = 2 atm	T_o = 1500 K; p = 1 atm
Mixture R:					
O	2.67×10^{-9}	3.13×10^{-8}	2.21×10^{-8}	1.56×10^{-8}	1.28×10^{-6}
H	2.12×10^{-8}	1.94×10^{-7}	1.38×10^{-7}	9.83×10^{-8}	5.04×10^{-6}
OH	0	0	0	0	0
Mixture A:					
O	2.67×10^{-9}	3.13×10^{-8}	2.21×10^{-8}	1.56×10^{-8}	1.28×10^{-6}
H	2.12×10^{-8}	1.94×10^{-7}	1.38×10^{-7}	9.83×10^{-8}	5.04×10^{-6}
OH	1.08×10^{-6}	4.96×10^{-6}	4.16×10^{-6}	3.54×10^{-6}	5.59×10^{-5}
Mixture B:					
O	2.67×10^{-9}	3.13×10^{-8}	2.21×10^{-8}	1.56×10^{-8}	1.28×10^{-6}
H	2.12×10^{-8}	1.94×10^{-7}	1.38×10^{-7}	9.83×10^{-8}	5.04×10^{-6}
OH	1.52×10^{-6}	7.04×10^{-6}	5.89×10^{-6}	4.97×10^{-6}	7.90×10^{-5}

[a] Based on equilibrium amounts in the two streams (hydrogen- and oxygen-containing streams) at the initial temperature T_o and pressure p in the combustor prior to mixing.

TABLE 6.- INDUCTION TIMES FOR VARIOUS INITIAL TEMPERATURES, PRESSURES, AND AMOUNTS OF CO_2 AND H_2O

Mixture	Induction time, μsec, for –				
	T_O = 1150 K; p = 1 atm	T_O = 1250 K; p = 0.5 atm	T_O = 1250 K; p = 1 atm	T_O = 1250 K; p = 2 atm	T_O = 1500 K; p = 1 atm
No initial O, H, and OH					
R	62.6	67.3	34.5	18.8	13.0
A	76.4	69.0	36.8	22.6	13.5
B	102.2	71.0	40.0	29.7	13.2
Initial amounts[a] of O, H, and OH					
R	62.3	65.9	33.9	18.5	12.2
A	68.7	57.0	30.8	19.6	9.7
B	90.8	56.8	32.7	25.1	9.2

[a] Based on equilibrium amounts in the two streams (hydrogen- and oxygen-containing streams) at the initial temperature and pressure in the combustor prior to mixing.

TABLE 7.- REACTION TIMES AND EQUILIBRIUM TEMPERATURES FOR VARIOUS INITIAL TEMPERATURES, PRESSURES, AND AMOUNTS OF CO_2 AND H_2O

(a) Reaction times

Mixture	τ_r, μsec, for –				
	T_o = 1150 K; p = 1 atm	T_o = 1250 K; p = 0.5 atm	T_o = 1250 K; p = 1 atm	T_o = 1250 K; p = 2 atm	T_o = 1500 K; p = 1 atm
R	65.4	177.7	56.5	18.3	43.0
A	77.6	200	67.2	22.4	47.5
B	91.8	226	73.0	26.5	54.8

(b) Equilibrium temperatures

Mixture	T_e, K, for –				
	T_o = 1150 K; p = 1 atm	T_o = 1250 K; p = 0.5 atm	T_o = 1250 K; p = 1 atm	T_o = 1250 K; p = 2 atm	T_o = 1500 K; p = 1 atm
R	2696	2682	2730	2778	2816
A	2588	2582	2625	2666	2712
B	2513	2513	2550	2588	2644

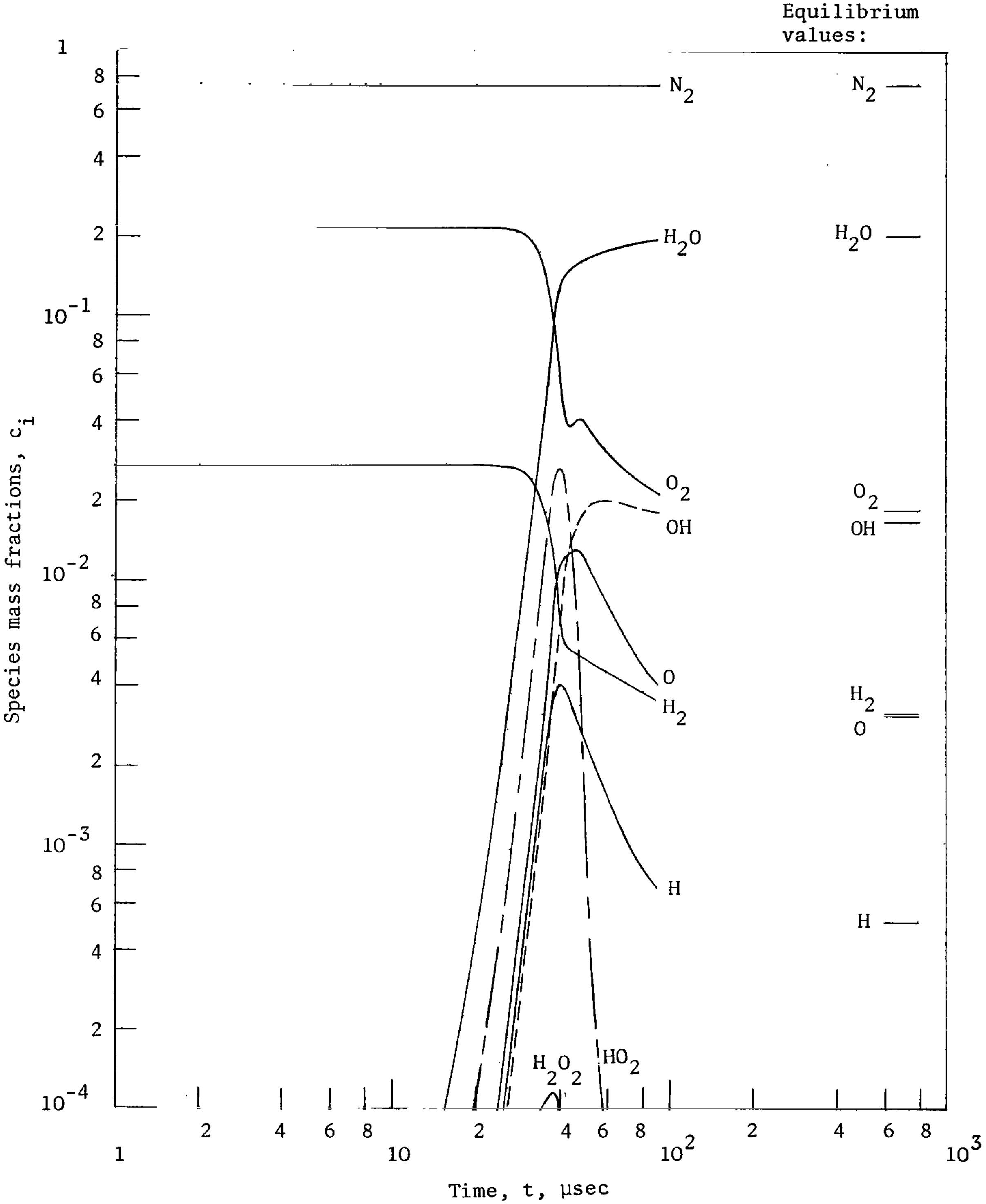

Figure 1.- Time variation of species mass fractions and equilibrium levels for case 1 (T_0 = 1250 K, p = 1 atm, mixture R).

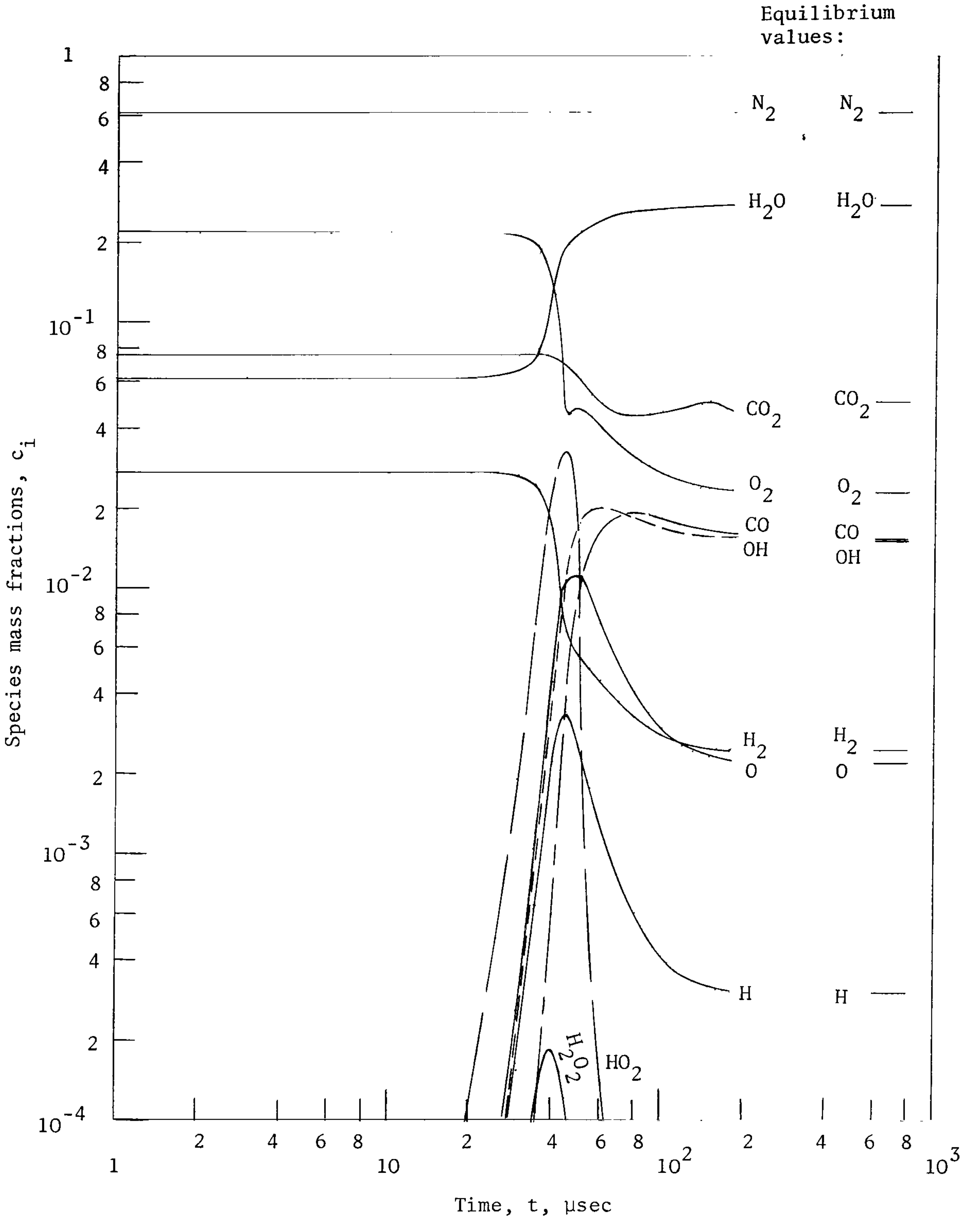

Figure 2.- Time variation of species mass fractions and equilibrium levels for case 2 (T_0 = 1250 K, p = 1 atm, mixture A).

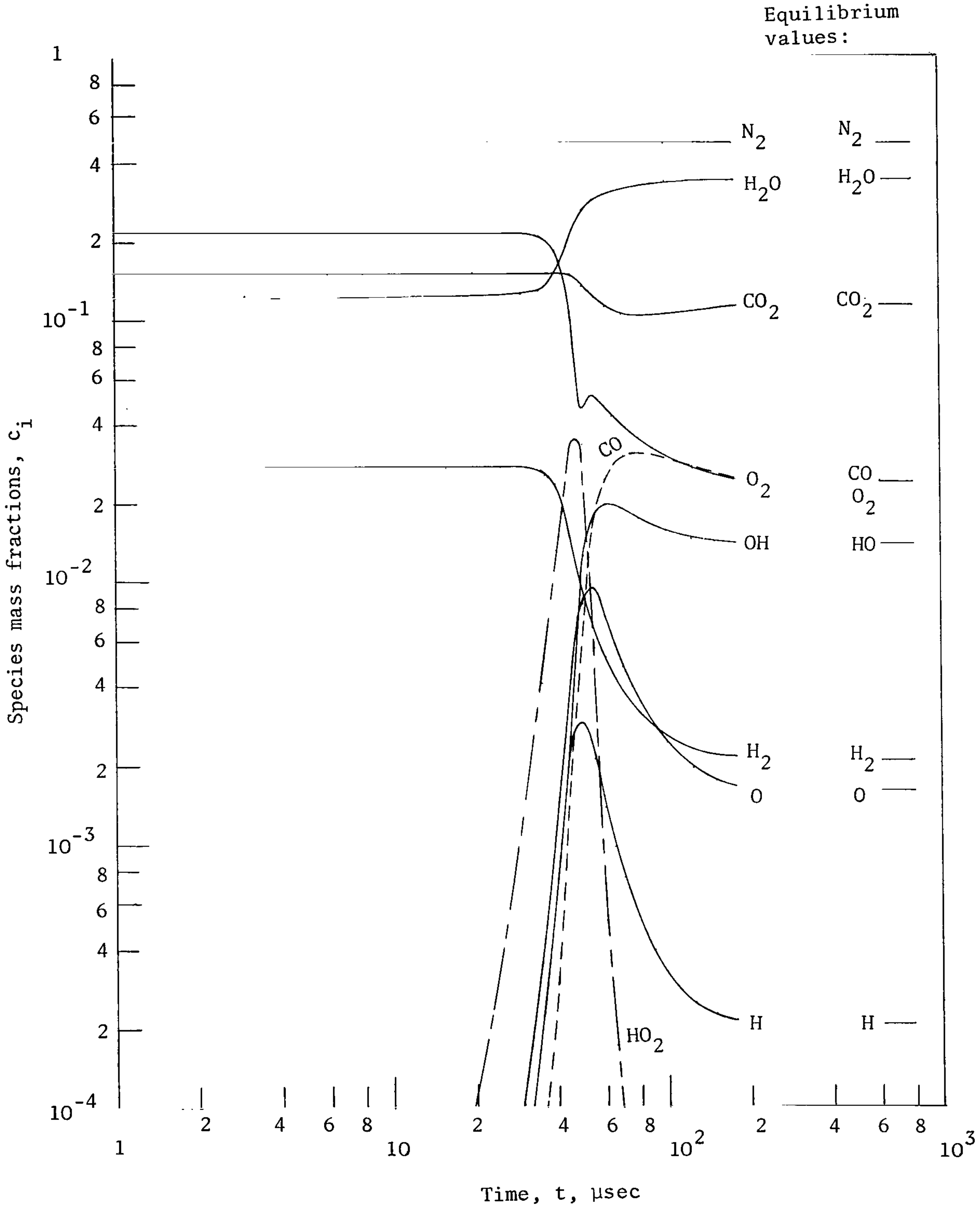

Figure 3.- Time variation of species mass fractions and equilibrium levels for case 3 (T_0 = 1250 K, p = 1 atm, mixture B).

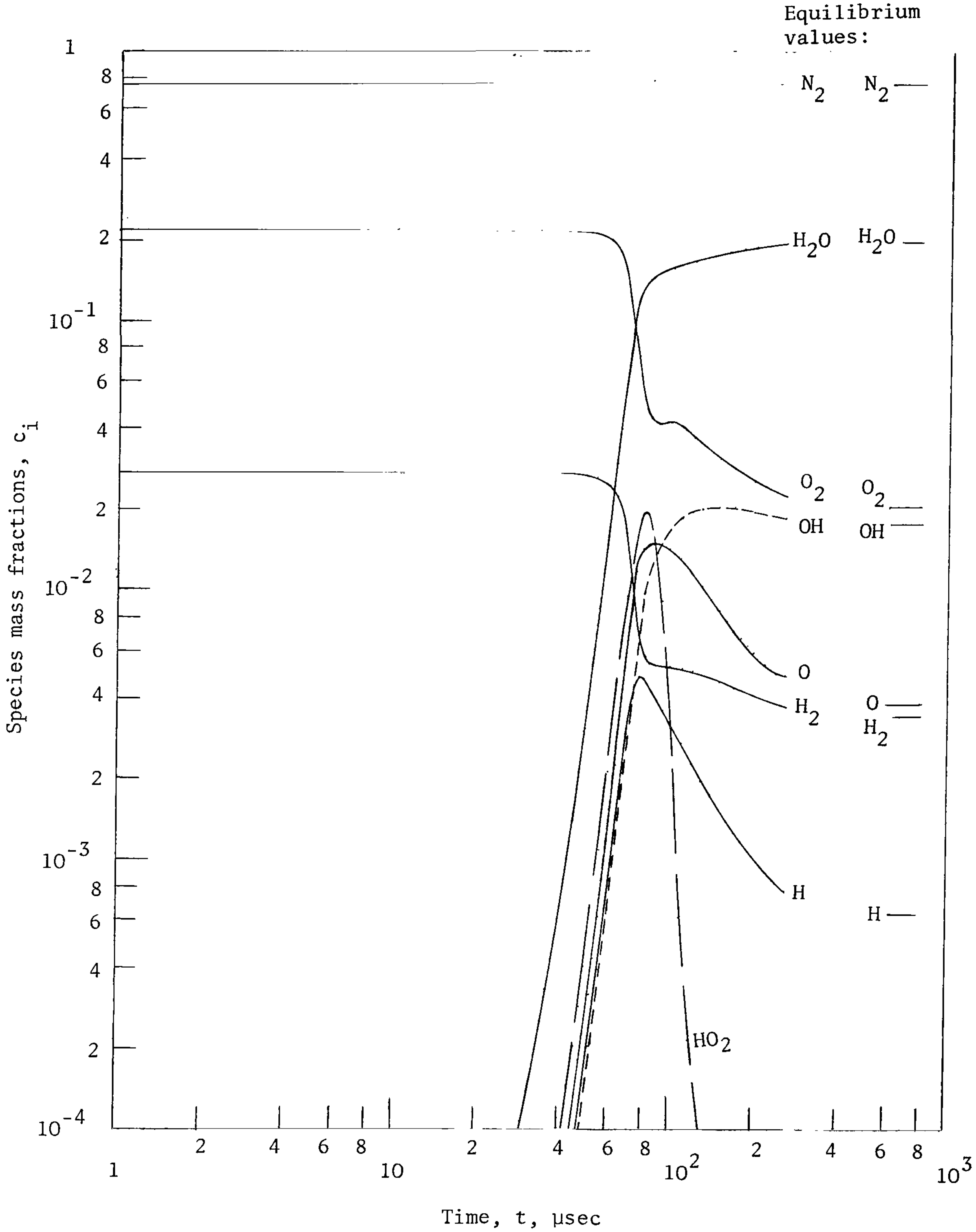

Figure 4.- Time variation of species mass fractions and equilibrium levels for case 4 (T_0 = 1250 K, p = 0.5 atm, mixture R).

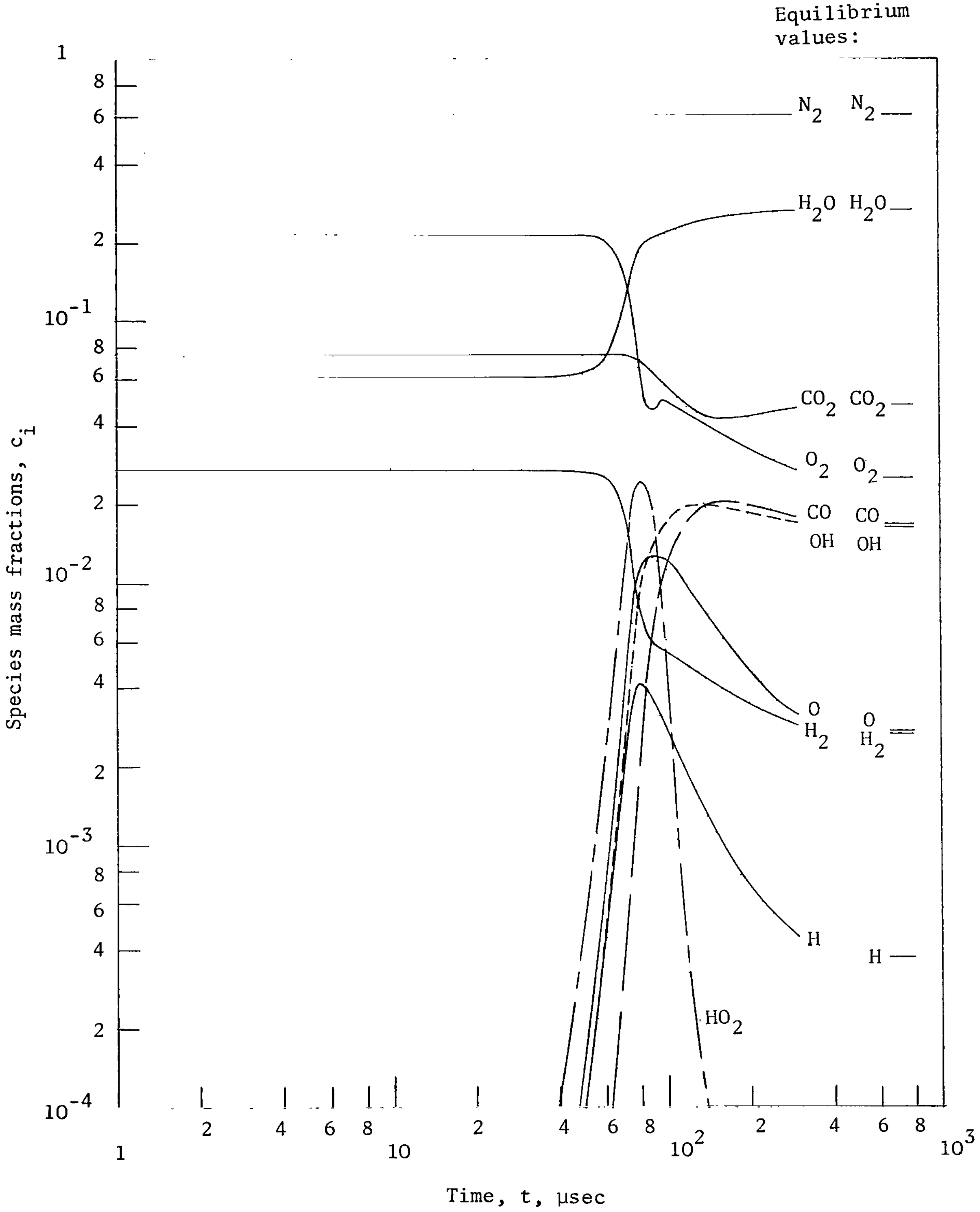

Figure 5.- Time variation of species mass fractions and equilibrium levels for case 5 (T_0 = 1250 K, p = 0.5 atm, mixture A).

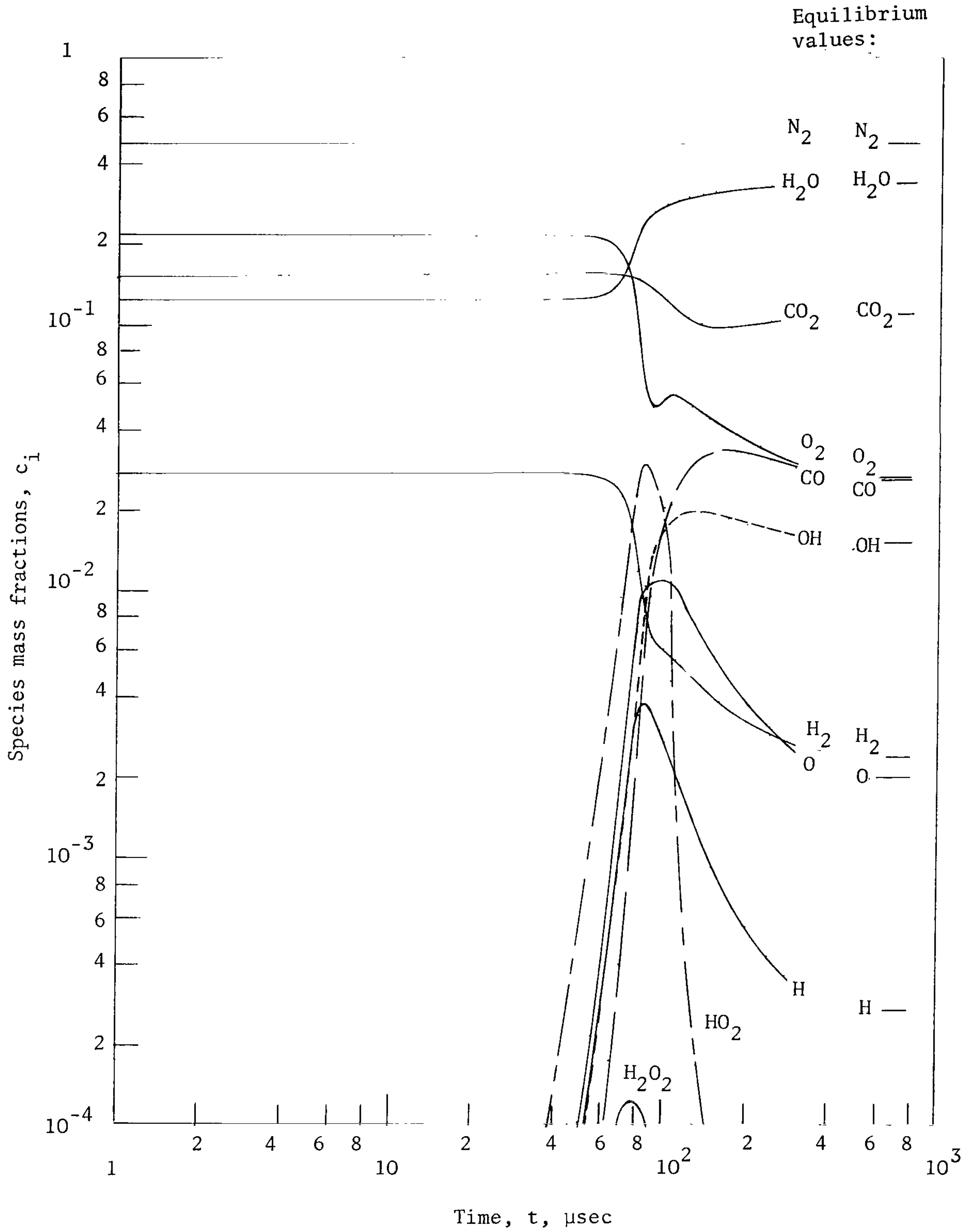

Figure 6.- Time variation of species mass fractions and equilibrium levels for case 6 (T_0 = 1250 K, p = 0.5 atm, mixture B).

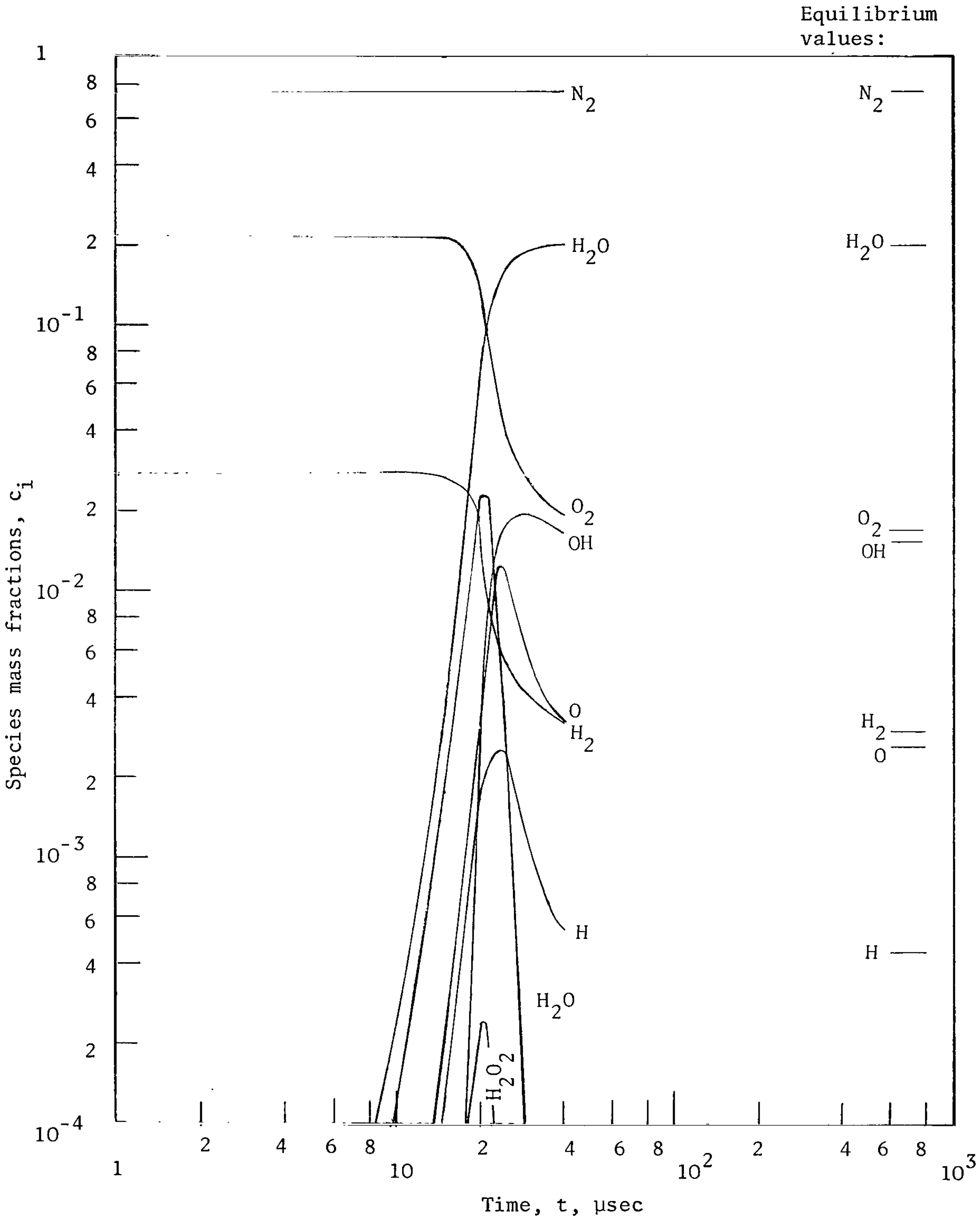

Figure 7.- Time variation of species mass fractions and equilibrium levels for case 7 (T_0 = 1250 K, p = 2 atm, mixture R).

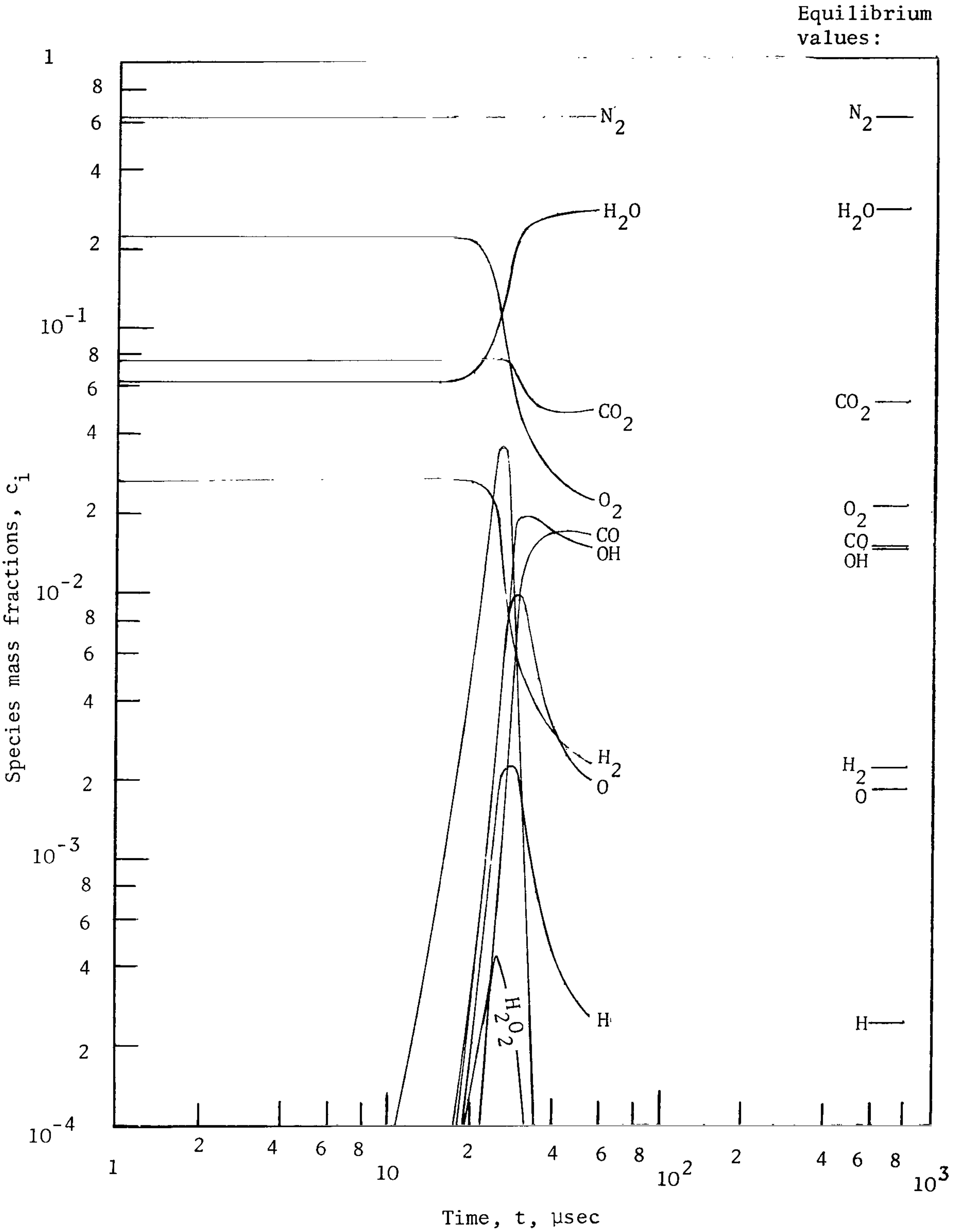

Figure 8.- Time variation of species mass fractions and equilibrium levels for case 8 (T_0 = 1250 K, p = 2 atm, mixture A).

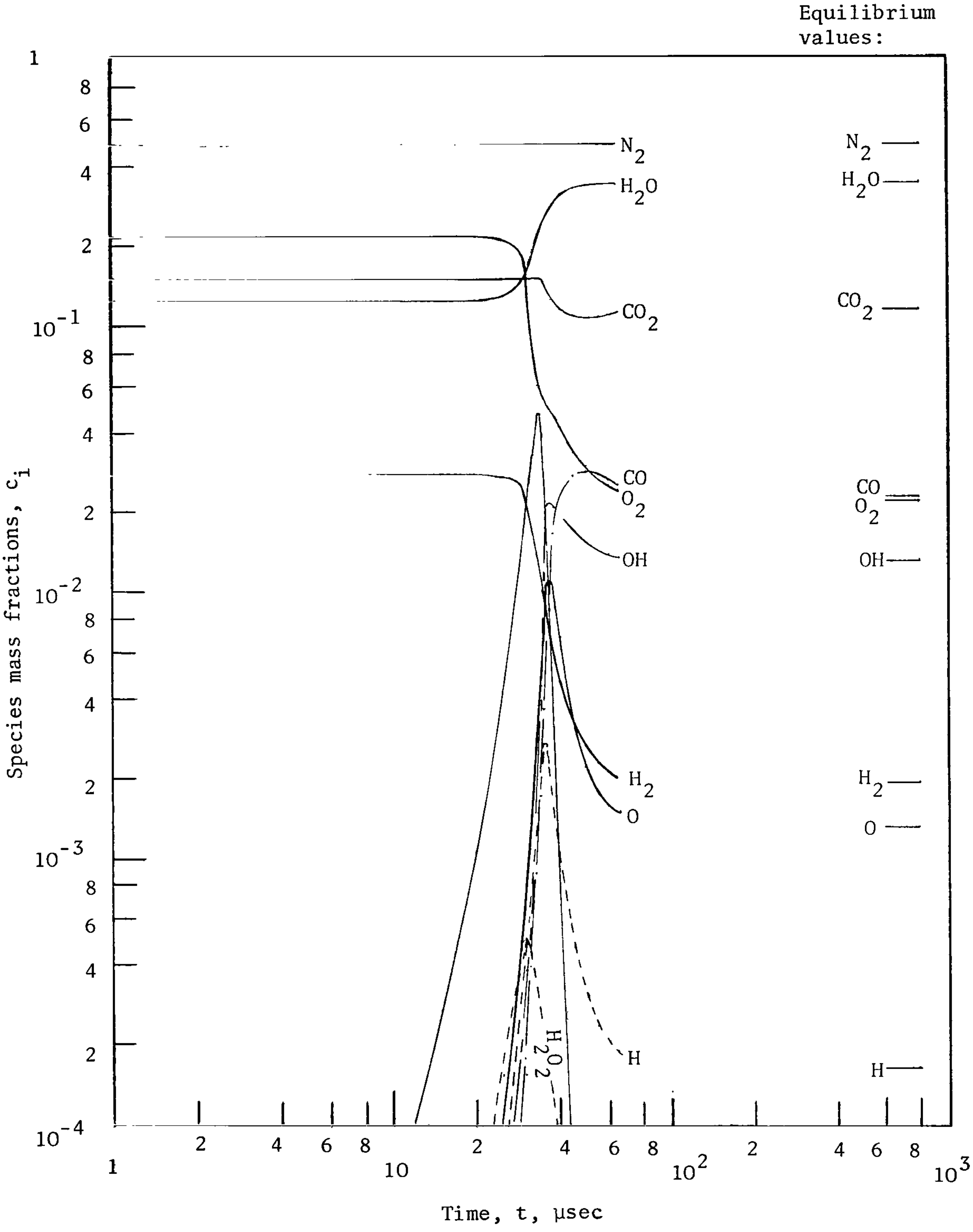

Figure 9.- Time variation of species mass fractions and equilibrium levels for case 9 (T_0 = 1250 K, p = 2 atm, mixture B).

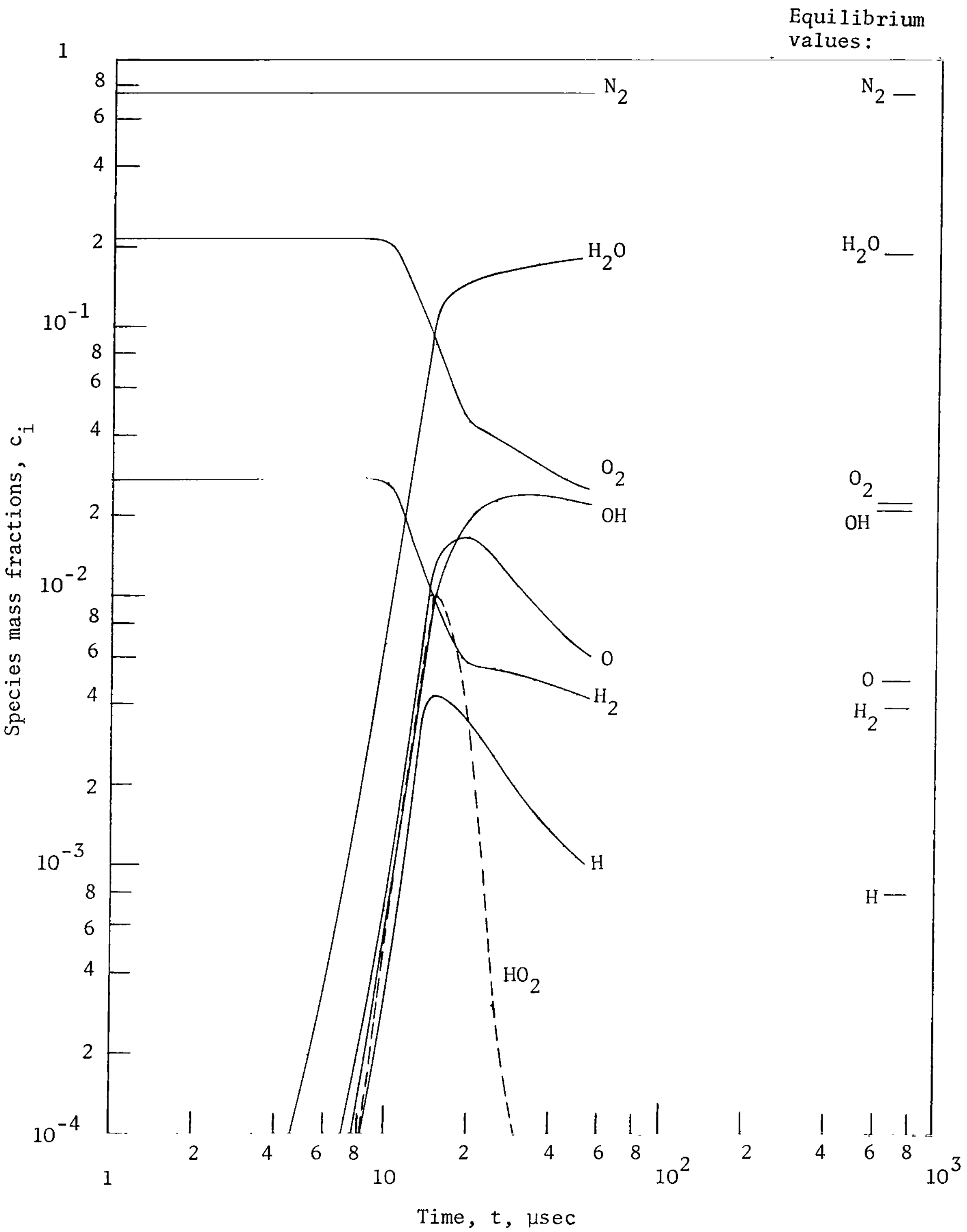

Figure 10.- Time variation of species mass fractions and equilibrium levels for case 10 (T_0 = 1500 K, p = 1 atm, mixture R).

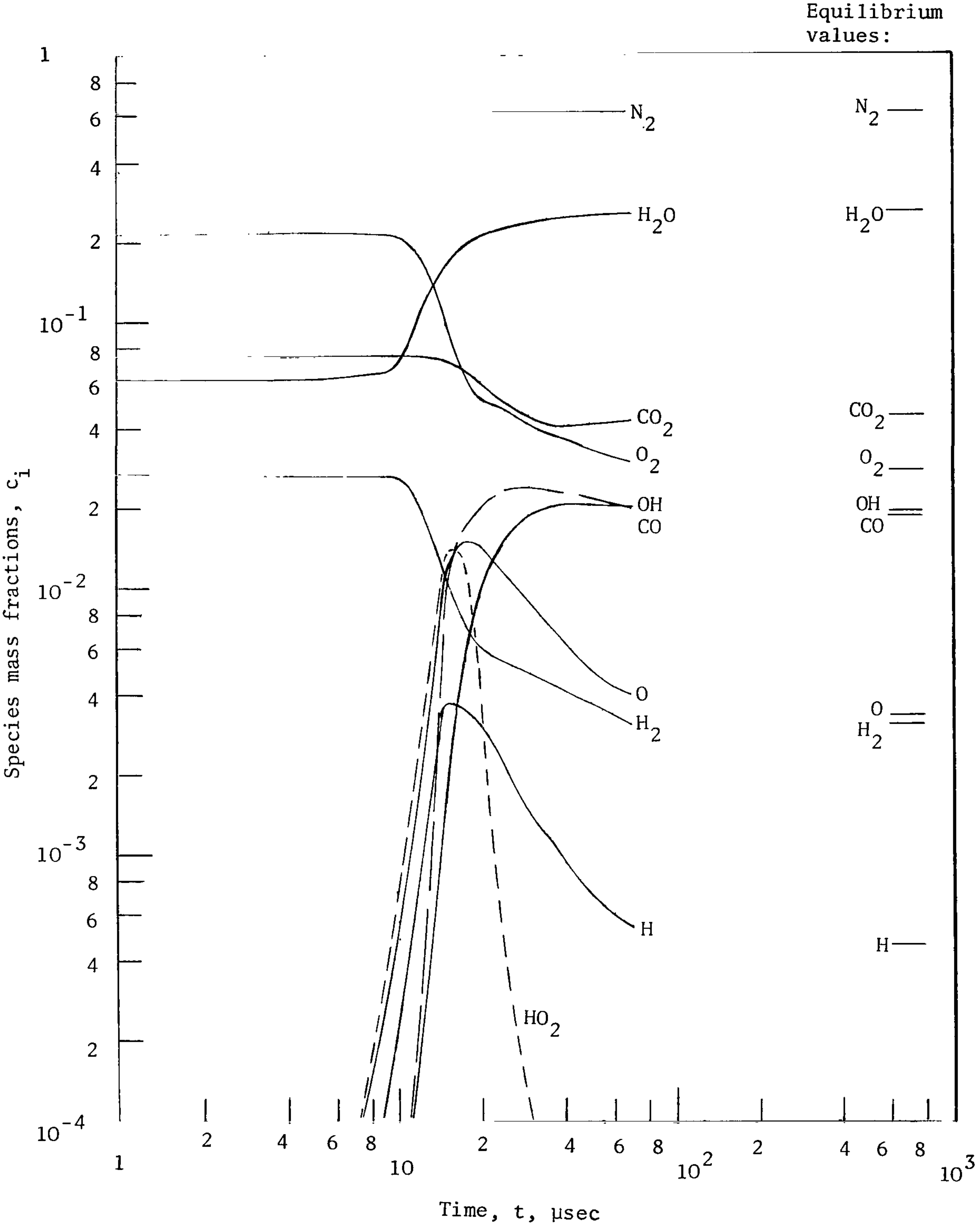

Figure 11.- Time variation of species mass fractions and equilibrium levels for case 11 (T_0 = 1500 K, p = 1 atm, mixture A).

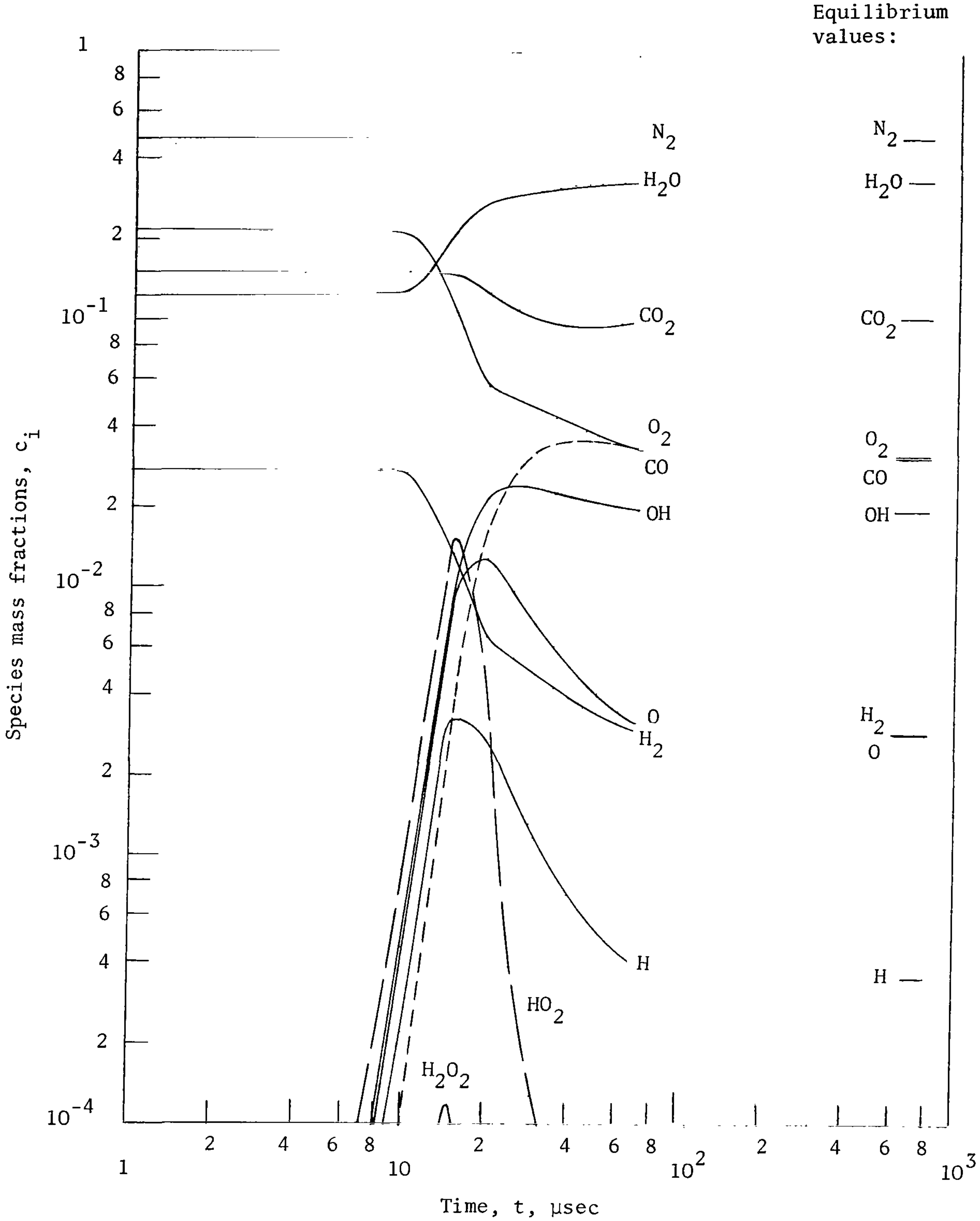

Figure 12.- Time variation of species mass fractions and equilibrium levels for case 12 (T_0 = 1500 K, p = 1 atm, mixture B).

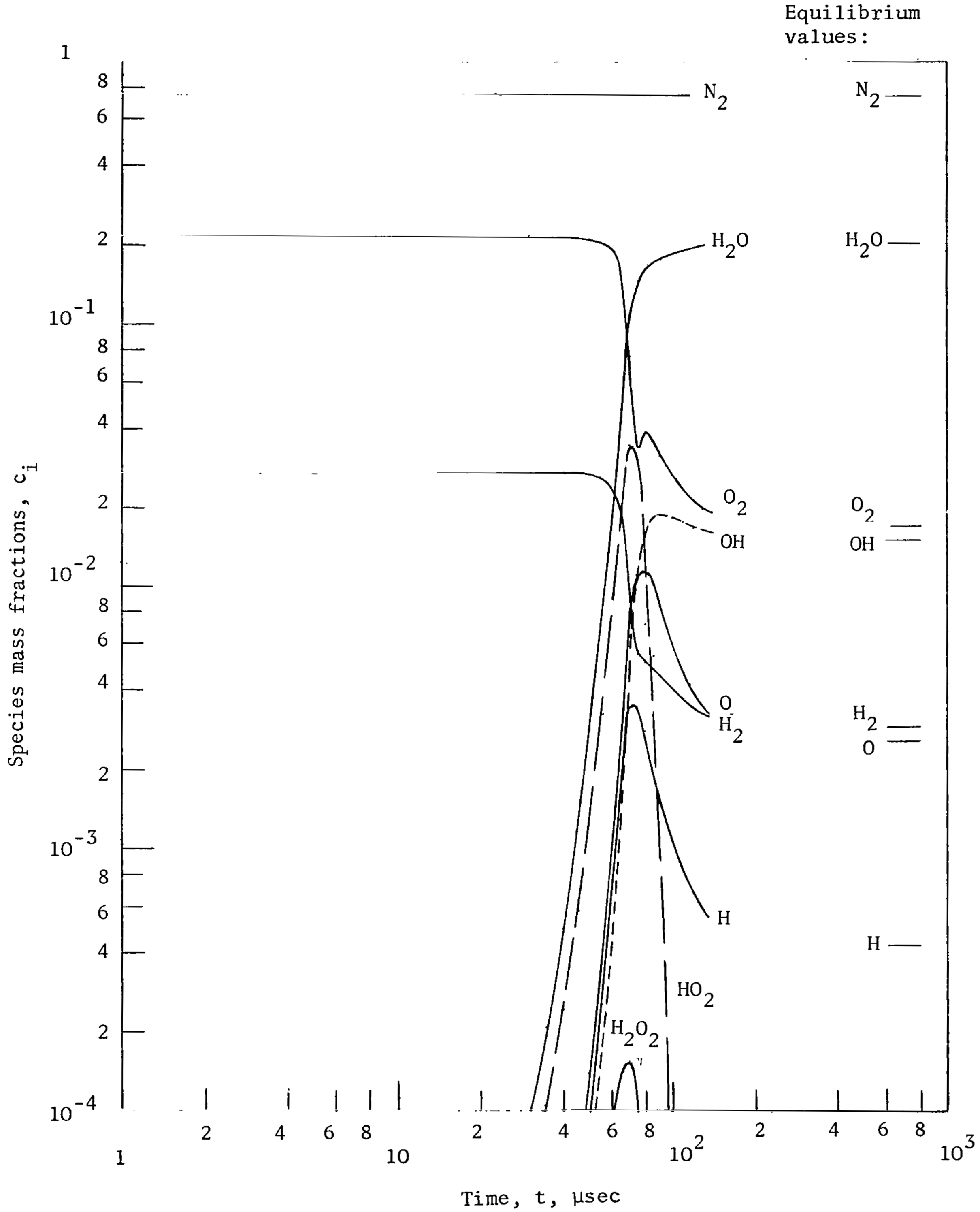

Figure 13.- Time variation of species mass fractions and equilibrium levels for case 13 (T_0 = 1150 K, p = 1 atm, mixture R).

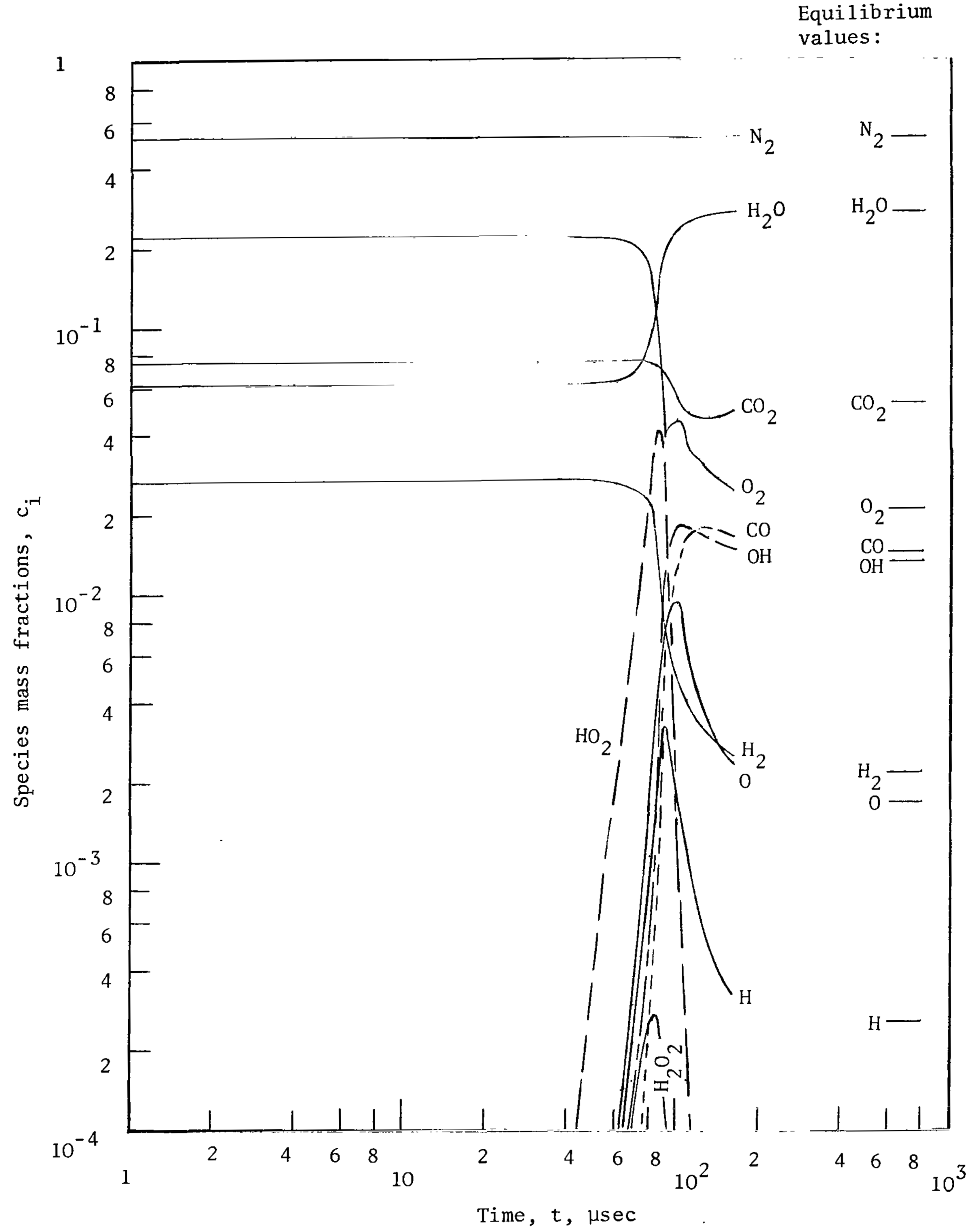

Figure 14.- Time variation of species mass fractions and equilibrium levels for case 14 (T_0 = 1150 K, p = 1 atm, mixture A).

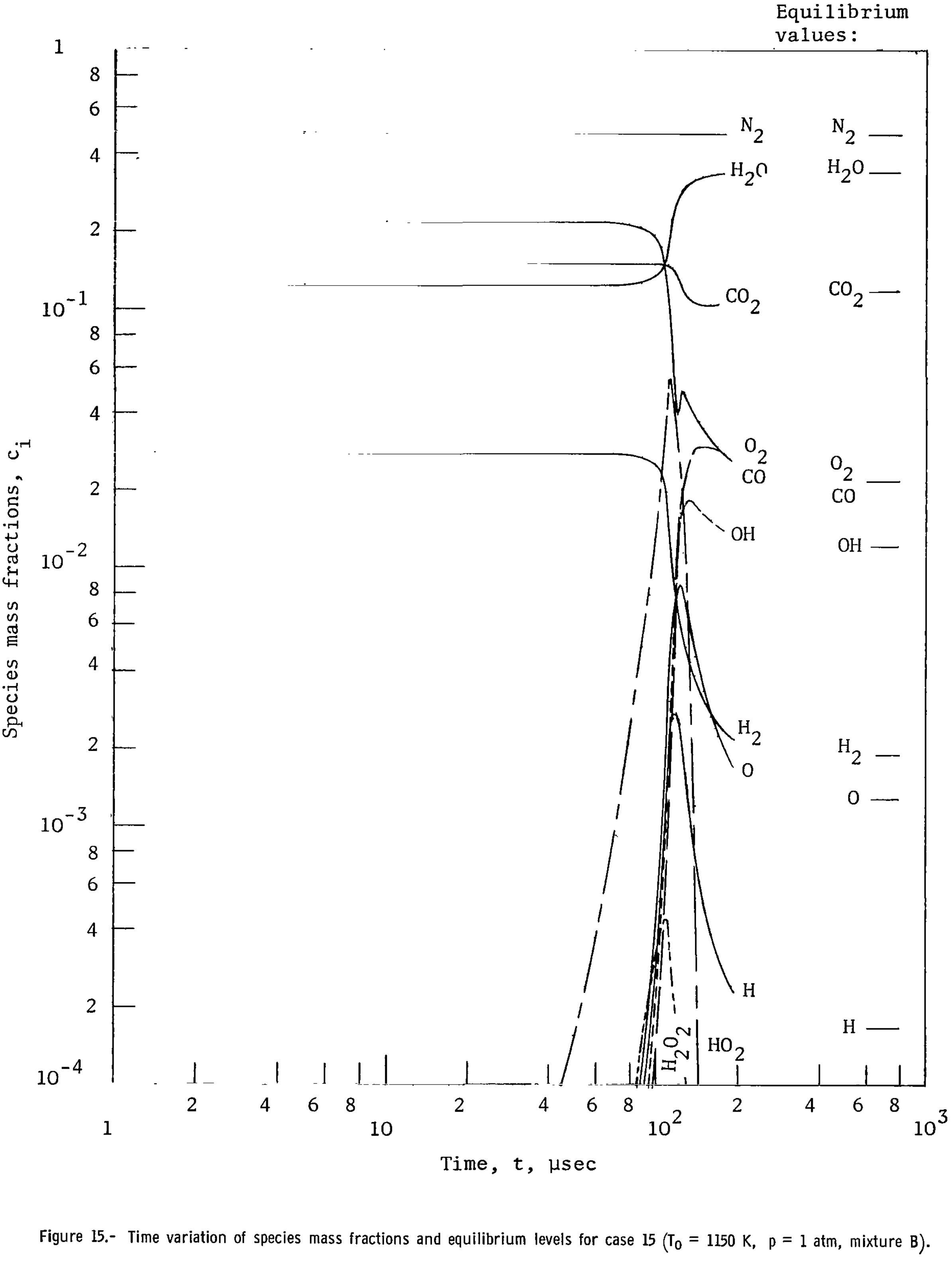

Figure 15.- Time variation of species mass fractions and equilibrium levels for case 15 (T_0 = 1150 K, p = 1 atm, mixture B).

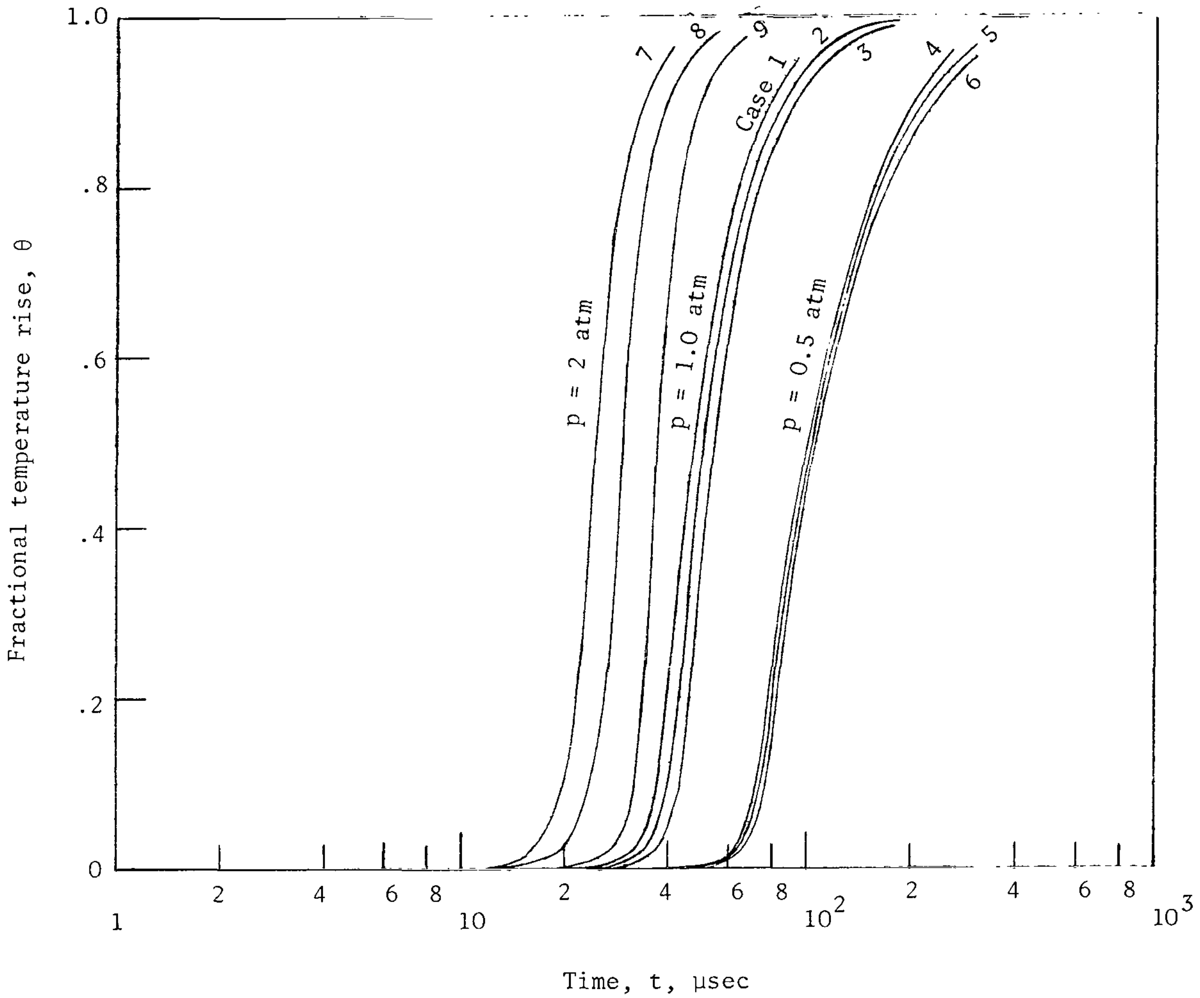

Figure 16.- Time variation of fractional temperature rise for cases 1 to 9. T_0 = 1250 K.

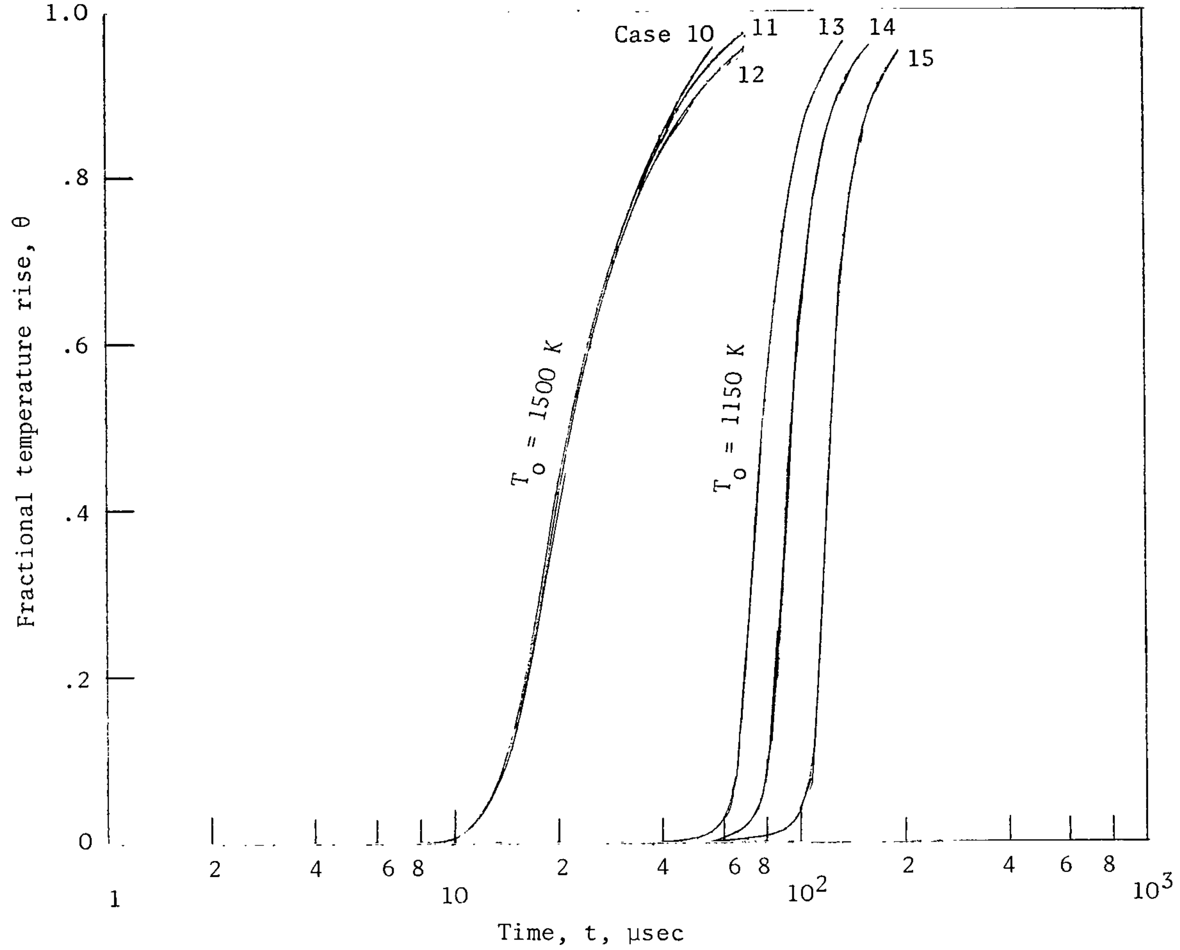

Figure 17.- Time variation of fractional temperature rise for cases 10 to 15. p = 1 atm.

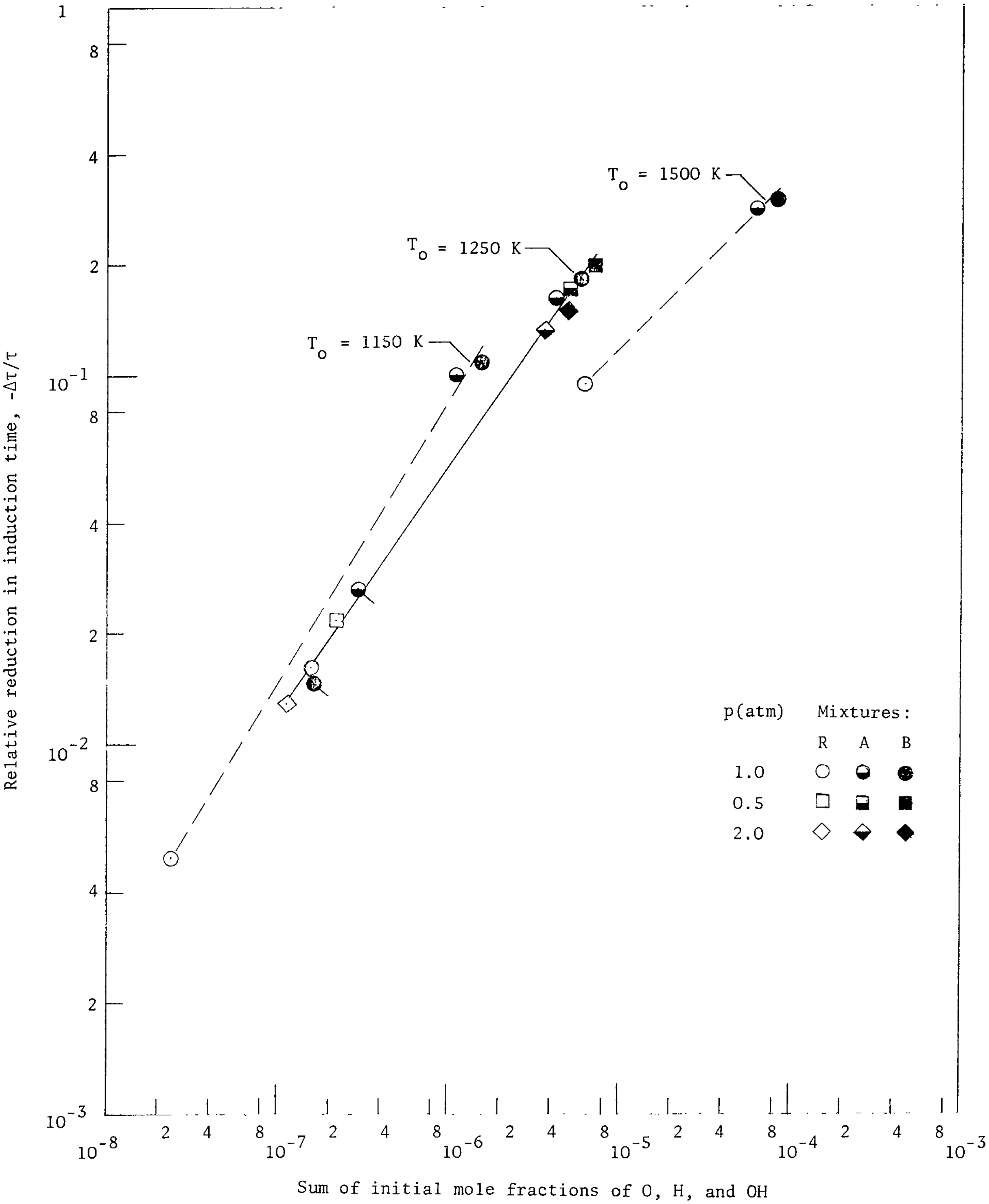

Figure 18.- Relative reduction in induction time as a function of the sum of initial mole fractions of O, H, and OH. (Flagged symbols are for a set of initial mole fractions taken to be less than equilibrium amount.)

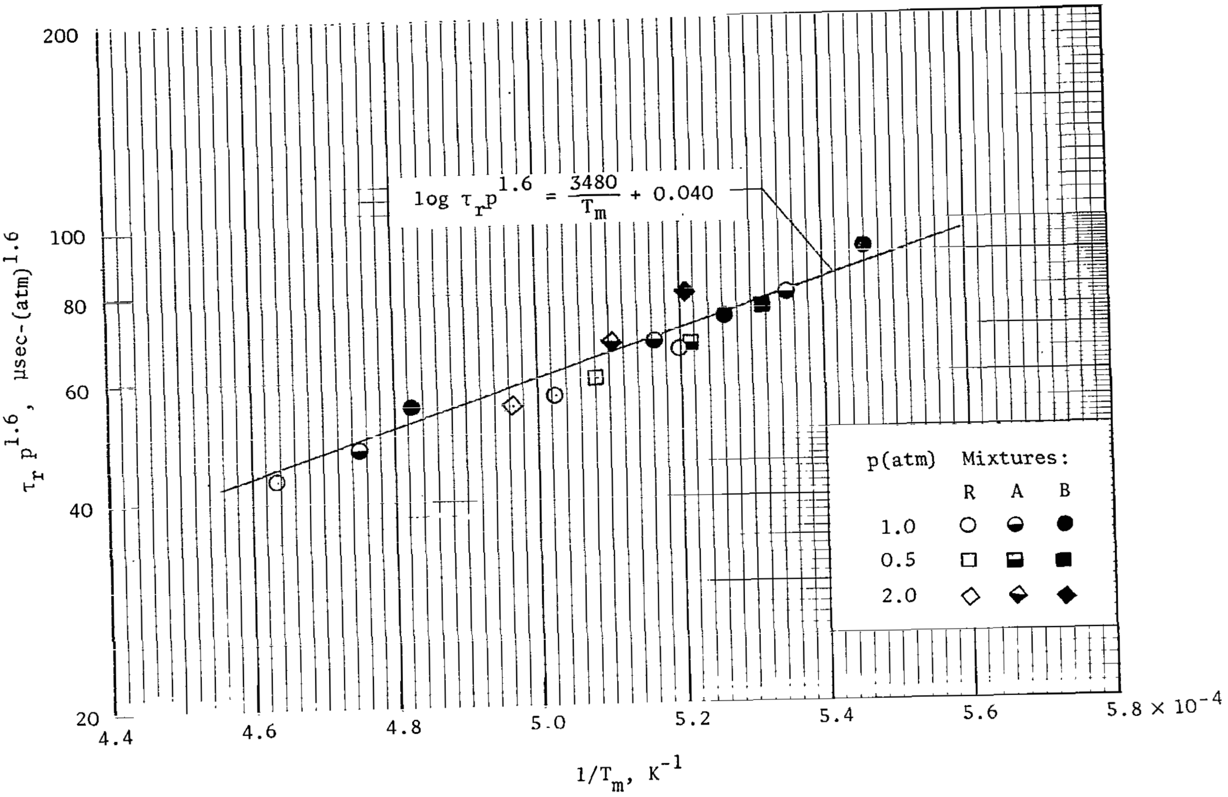

Figure 19.- Reaction-time parameter $\tau_r p^{1.6}$ as a function of the reciprocal of a mean reaction temperature $1/T_m$.

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