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TECHNICAL NOTE

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THERMODYNAMIC CALCULATIONS OF CARBON MONOXIDE — AIR DETONATION PARAMETERS FOR INITIAL PRESSURES FROM 1 TO 100 ATMOSPHERES

By Loren E. Bollinger and Rudolph Edse

The Ohio State University
Rocket Research Laboratory
Columbus 10, Ohio

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
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ERRATA

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Correct the first paragraph on p 5 to read:

Instead of referring the reader to earlier papers on this subject (e.g., ref. 4), a brief presentation of the procedure used to calculate the detonation parameters of carbon monoxide - air mixtures is given here.

The correct list of references (p 14) is as follows:

REFERENCES

1. Edse, R.: Propagation of Shock Waves through Chemically Reacting Gas Mixtures. Proc. Propellant Thermodynamics and Handling Conference, July 20-21, 1959, Special Report 12, Engineering Experiment Station, Ohio State University, June 1960, pp. 247-258.

2. Bollinger, L. E., and Edse, R.: Thermodynamic Calculations of Hydrogen-Oxygen Detonation Parameters for Various Initial Pressures. ARS Journal, Vol. 31, No. 2, Feb. 1961, pp. 251-256.

3. Chu, S. T., and Edse, R.: Propagation of Sound Waves through Chemically Reacting Gas Mixtures. Proc. Propellant Thermodynamics and Handling Conference, July 20-21, 1959, Special Report 12, Engineering Experiment Station, Ohio State University, June 1960, pp. 235-246.

4. Edse, R.: Calculations of Detonation Velocities in Gases. Wright Air Development Center Technical Report 54-416, ASTIA No. AD 94173, March 1956.

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

TECHNICAL NOTE D-1667

THERMODYNAMIC CALCULATIONS OF CARBON MONOXIDE - AIR DETONATION PARAMETERS FOR INITIAL PRESSURES FROM 1 TO 100 ATMOSPHERES

By Loren E. Bollinger* and Rudolph Edse**

SUMMARY

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The composition, temperature, pressure and density behind a stable detonation wave and its propagation rate have been calculated for five mixtures of carbon monoxide and air at 1, 5, 25 and 100 atmospheres initial pressure, and at an initial temperature of 313.16°K. The results of these calculations show that the detonation velocities of stoichiometric carbon monoxide - air mixtures increase with increasing initial pressure whereas those of very rich and very lean mixtures are independent of the initial pressure.

The pressure ratios across the wave and the temperatures behind the wave increase with increasing pressure for near-stoichiometric mixtures, but they are unaffected by pressure for rather rich and lean mixtures.

INTRODUCTION

Complete thermodynamic and chemical equilibrium is assumed to exist behind the detonation wave. Dissipating effects such as heat transfer, viscosity, diffusion, and chemical reaction rates have been disregarded since it was not intended to determine the structure of the wave. Details of the method used for calculating the detonation parameters were pub-

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* Assistant Supervisor, Rocket Research Laboratory; Assistant Professor of Aeronautical and Astronautical Engineering, The Ohio State University.

** Director, Rocket Research Laboratory; Professor of Aeronautical and Astronautical Engineering, The Ohio State University.

lished previously (ref. 1), and calculations for various hydrogen-oxygen mixtures over the same range of initial pressures can be found in reference 2.

The detonation parameters have been derived from the Hugoniot equation for the reacted gas mixture in equilibrium, and from the Chapman-Jouguet condition that the detonation velocity is the minimum wave velocity. Therefore, the results are based on the Chapman-Jouguet point at which the velocity of the reacted gas (relative to the detonation wave) is equal to the equilibrium sonic speed (ref. 3).

Besides being of fundamental interest, the theoretical detonation parameters, particularly the detonation velocity, is of importance in the study of the formation of detonation waves. These values are used to determine the detonation induction distance. Results from these experiments will be published separately.

SYMBOLS

a_b	sonic velocity in gas entering shock wave
ΔE_o	heat of reaction at absolute zero temperature
h_a	absolute enthalpy of gas mixture per unit mass leaving shock wave
h_b	absolute enthalpy of gas mixture per unit mass entering shock wave
$\left(\Delta H_f\right)_i^{T_a}$	heat of formation of species i at temperature T_a formed from elements, making species i, in the standard state ($p = 1$ atm, $T = 298.16\ ^{\circ}K$)
$\left(\Delta H_f\right)_i^{T_b}$	heat of formation of species i at temperature T_b formed from elements, making species i, in the standard state ($p = 1$ atm, $T = 298.16\ ^{\circ}K$)

$\left(\frac{\Delta H_f}{\mathcal{R}\, T}\right)_i^{T}$	dimensionless heat of formation of species i at temperature T formed from elements, making species i, at standard state (p = 1 atm, T = 298.16 °K)
$\left(\frac{\Delta H_f}{\mathcal{R}\, T}\right)_i^{T_a}$	dimensionless heat of formation of species i at T_a formed from the elements, making species i, at standard state (p = 1 atm, T = 298.16 °K)
$\left(\frac{\Delta H_f}{\mathcal{R}\, T}\right)_i^{T_b}$	dimensionless heat of formation of species i at T_b formed from elements, making species i, at standard state (p = 1 atm, T = 298.16 °K)
K_j	equilibrium constant of reaction j based on partial pressures
M_b	Mach number of gas mixture entering shock wave
M_D	Mach number of stable detonation wave. $M_D = \frac{U_D}{a_b}$
n_b	mole number of gas mixture, per unit mass of mixture, entering shock wave
$n_{i,b}$	mole number of species i, per unit mass of mixture, entering shock wave
N_k	total mole number of element k in unit mass of mixture
p_a	absolute pressure of gas behind shock wave
$p_{a,D}$	absolute pressure of gas behind stable detonation wave
$p_{a,N.S.}$	absolute pressure of gas behind normal shock wave without chemical reactions

$p_{i,a}$	absolute partial pressure of species i behind shock wave
p_b	absolute pressure of gas entering shock wave
p_{imp}	absolute impact pressure of detonation wave
$\mathbb{P}_k$	total quantity of element k, in atomic state, in reacted mixture in terms of pressure units. $\mathbb{P}_k = N_k \frac{\mathcal{R} T_a}{v_a}$
$\mathcal{R}$	universal gas constant
T_a	absolute temperature of gas behind shock wave
$T_{a,D}$	absolute temperature of gas behind detonation wave
$T_{a,N.S.}$	absolute temperature of gas behind normal shock wave without chemical reactions
T_b	absolute temperature of gas entering shock wave
ΔT	temperature difference between estimated temperatures
U_a	linear velocity of gas leaving detonation or shock wave
U_b	linear velocity of gas entering shock wave
U_D	linear velocity of detonation wave relative to unreacted gas
$U_{a,D}$	linear velocity of detonation wave relative to reacted gas
v	specific volume. $v = \frac{1}{\rho}$
γ_b	isentropic coefficient (ratio of specific heats) of unreacted gas mixture
$\rho_{a,D}$	density of gas mixture behind detonation wave
ρ_b	density of gas mixture entering shock wave

METHOD OF CALCULATION

Instead of referring the reader to earlier papers on this subject, a brief presentation of the procedure used to calculate the detonation parameters of carbon monoxide - air mixtures is given here.

It has been assumed that only CO_2, CO, O_2, O, N_2 and NO occur to an appreciable extent in the detonation wave of carbon monoxide - air (0.79 mole N_2 plus 0.21 mole O_2) mixtures ranging in fuel concentration from 10 per cent CO to 50 per cent CO. The presence of atomic nitrogen, higher oxides of nitrogen, free carbon, and electrically charged species has been ignored because of the extremely low concentrations found for these species in the mixtures considered during the present study. Thus the composition of the detonated gas is governed by the following six equations:

$$\frac{p_{CO}\sqrt{p_{O_2}}}{p_{CO_2}} = K_{CO_2} \qquad (CO_2 \rightleftharpoons CO + \tfrac{1}{2} O_2 \quad j = CO_2) \tag{1}$$

$$\frac{p_O}{\sqrt{p_{O_2}}} = K_{O_2} \qquad (\tfrac{1}{2} O_2 \rightleftharpoons O \quad j = O_2) \tag{2}$$

$$\frac{p_{NO}}{\sqrt{p_{O_2} \cdot p_{N_2}}} = K_{NO} \qquad (\tfrac{1}{2} N_2 + \tfrac{1}{2} O_2 \rightleftharpoons NO \quad j = NO) \tag{3}$$

$$\frac{2\,p_{CO_2} + p_{CO} + 2\,p_{O_2} + p_O + p_{NO}}{p_{CO_2} + p_{CO}} \equiv \frac{\mathbb{P}_O}{\mathbb{P}_C} = \frac{N_O}{N_C} \tag{4}$$

$$\frac{2\ p_{N_2} + p_{NO}}{p_{CO_2} + p_{CO}} \equiv \frac{\mathbb{P}_N}{\mathbb{P}_C} = \frac{N_N}{N_C}$$

$$p_{CO_2} + p_{CO} + p_{O_2} + p_O + p_{N_2} + p_{NO} = \Sigma\ p_{i,a} = p_a \tag{6}$$

For a temperature, T_a, in the vicinity of the expected detonation temperature and for an arbitrarily assumed value of p_{O_2} the partial pressure of molecular nitrogen can be calculated by using equations (1) through (5).

$$\sqrt{p_{N_2}} = \frac{K_{NO}\sqrt{p_{O_2}}}{4} \cdot \frac{N_N\left(1 + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}\right)}{N_O - N_C + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}\ (N_O - 2\ N_C)}$$
$$+ \left[\left(\frac{K_{NO}\sqrt{p_{O_2}}}{4}\ \frac{N_N + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}}{N_O - N_C + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}\ (N_O - 2\ N_C)}\right)^2\right. \tag{7}$$
$$\left. + \frac{\left(p_{O_2} + \frac{\sqrt{p_{O_2}}}{2}\ K_{O_2}\right)\ N_N\left(1 + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}\right)}{N_O - N_C + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}\ (N_O - 2\ N_C)}\right]^{\frac{1}{2}}$$

The remaining partial pressures follow easily. From equation (2) $p_O = \sqrt{p_{O_2}} \cdot K_{O_2}$. From equation (3) $p_{NO} = \sqrt{p_{O_2} \cdot p_{N_2}} \cdot K_{NO}$. From equations (5) and (1)

$$p_{CO} = \frac{2\, p_{N_2} + p_{NO}}{\frac{N_N}{N_C}\left(1 + \frac{\sqrt{p_{O_2}}}{K_{CO_2}}\right)}$$

And from equation (1)

$$p_{CO_2} = p_{CO} \frac{\sqrt{p_{O_2}}}{K_{CO_2}}$$

For these partial pressures and with the first estimate of the detonation temperature we obtain from the Hugoniot equation

$$h_a - h_b \equiv \frac{N_C}{\mathbb{P}_C} \Sigma\, p_{i,a} \left(\Delta\, H_f\right)_i^{T_a} - \Sigma\, n_{i,b} \left(\Delta\, H_f\right)_i^{T_b} =$$

$$\frac{1}{2} n_b \mathcal{R}\, T_b \left(\frac{\Sigma\, p_{i,a}}{p_b} - 1\right) \cdot \left(\frac{T_a}{T_b} \cdot \frac{p_b}{n_b} \cdot \frac{N_C}{\mathbb{P}_C} + 1\right) \tag{8a}$$

$$\begin{aligned}\frac{\Sigma\, p_{i,a}}{p_b} &= 1 + \frac{\dfrac{N_C}{\mathbb{P}_C}\, \Sigma\, p_{i,a} \left(\Delta\, H_f\right)_i^{T_a} - \Sigma\, n_{i,b} \left(\Delta\, H_f\right)_i^{T_b}}{\frac{1}{2}\, n_b\, \mathcal{R}\, T_b \left(\dfrac{T_a}{T_b} \cdot \dfrac{p_b}{n_b} \cdot \dfrac{N_C}{\mathbb{P}_C} + 1\right)} = \\ &\quad 1 + \frac{2\left[\dfrac{T_a}{T_b} \cdot \dfrac{N_C}{\mathbb{P}_C} \cdot \dfrac{p_b}{n_b} \cdot \dfrac{\Sigma\, p_{i,a} \left(\dfrac{\Delta\, H_f}{\mathcal{R}\, T}\right)_i^{T_a}}{p_b} - \Sigma\, \dfrac{n_{i,b}}{n_b} \left(\dfrac{\Delta\, H_f}{\mathcal{R}\, T}\right)_i^{T_b}\right]}{\dfrac{T_a}{T_b} \cdot \dfrac{N_C}{\mathbb{P}_C} \cdot \dfrac{p_b}{n_b} + 1}\end{aligned} \tag{8b}$$

and from equation (6) we also obtain a value for this pressure ratio

$$\frac{\Sigma\, p_{i,a}}{p_b} = \frac{p_{CO_2} + p_{CO} + p_{O_2} + p_{O} + p_{N_2} + p_{NO}}{p_b} \tag{6}$$

If the pressure ratios derived from equation (8b) and equation (6) differ, the calculations must be repeated with a new value of p_{O_2} for the same value of $T_{a,1}$ until agreement is obtained. These calculations are carried out for three values of T_a ($T_{a,1} < T_{a,2} < T_{a,3}$). The three corresponding Mach numbers (multiplied by the specific heat ratio γ_b) are calculated from the relationship

$$\frac{U_b^2}{n_b \mathcal{R} T_b} = \gamma_b M_b^2 = \frac{\dfrac{\Sigma p_{i,a}}{p_b} - 1}{1 - \dfrac{T_a}{T_b} \cdot \dfrac{N_C}{\mathbb{P}_C} \cdot \dfrac{p_b}{n_b}} \qquad (9)$$

The Mach number of the stable detonation wave is obtained by locating the minimum of the parabola which can be drawn when the three $\gamma_b M_b^2$ values are plotted versus the three assumed T_a values. To obtain maximum accuracy with this interpolation method, the temperatures $T_{a,1}$, $T_{a,2}$ and $T_{a,3}$ must be selected in such a fashion that

$$(\gamma_b M_b^2)_1 \quad > \quad (\gamma_b M_b^2)_2 \quad < \quad (\gamma_b M_b^2)_3 \qquad (10)$$

If equal temperature intervals between the three assumed temperatures are chosen so that

$$T_{a,3} - T_{a,2} = T_{a,2} - T_{a,1} = \frac{1}{2} (T_{a,3} - T_{a,1}) = \Delta T \qquad (11)$$

the parabolic interpolation method leads to

$$\gamma_b M_D^2 = (\gamma_b M_b^2)_2 - \frac{\frac{1}{8}\left[(\gamma_b M_b^2)_3 - (\gamma_b M_b^2)_1\right]^2}{\left[(\gamma_b M_b^2)_1 - (\gamma_b M_b^2)_2\right] + \left[(\gamma_b M_b^2)_3 - (\gamma_b M_b^2)_2\right]} \tag{12}$$

Then, according to equation (9), the detonation velocity becomes

$$U_D = \sqrt{\gamma_b M_D^2 \cdot n_b \mathcal{R} T_b} \tag{13}$$

For the temperature behind the detonation wave, the interpolation yields

$$T_{a,D} = T_{a,1} + \frac{\Delta T}{2} + \frac{\Delta T \left[(\gamma_b M_b^2)_1 - (\gamma_b M_b^2)_2\right]}{\left[(\gamma_b M_b^2)_1 - (\gamma_b M_b^2)_2\right] + \left[(\gamma_b M_b^2)_3 - (\gamma_b M_b^2)_2\right]} \tag{14}$$

Finally, values of $p_{a,D}$ and $\rho_{a,D}$ are obtained by linear interpolation between the respective values calculated for the three temperatures chosen. If the temperature intervals, ΔT, are sufficiently small (e.g., 10°K), the error due to this linear interpolation is negligible.

The impact pressures are calculated according to the relationship

$$p_{imp} = p_{a,D} - p_b + \rho_{a,D} (U_D - U_{a,D})^2 = \frac{\rho_{a,D}}{\rho_b} (p_{a,D} - p_b) \tag{15}$$

The pressure and temperature behind the normal shock which forms the front of the detonation wave have been calculated on the basis that no chemical reactions occur in the shock zone and that the vibrational degrees of freedom in the molecules of the initial gas are inactive. Thus the usual equations employing constant specific heats could be used for calculating the conditions behind the normal shock propagating at the same rate as the detonation velocity.

DISCUSSION OF RESULTS

The results of the calculations are compiled in tables 1 through 5 and they are depicted graphically in figures 1 through 6. Values of the equilibrium constants used for the calculations are given in table 6 and the dimensionless heats of formation are listed in table 7. Both thermodynamic functions have been tabulated only for large temperature intervals to save space. These data represent carefully checked and, in some instances, recalculated values of the statistical calculations of several authors (refs. 5-14). A method to correct old values with respect to new data on atomic and molecular constants has been described in reference 15. Values for 10°K intervals were obtained by interpolation.

From figure 1 it can be seen that the detonation velocity increases only slightly when the initial gas pressure of the combustible mixture is raised. For example, consider a carbon monoxide - air mixture containing 29.6 per cent carbon monoxide. For this mixture the detonation velocity increases only from 1668 m/sec to 1744 m/sec for a rise in the initial pressure from 1 to 100 atmospheres. The maximum of the curves depicting the velocity as a function of the initial gas composition occurs in the region of rich mixtures at low initial pressures. As the initial pressure is increased the maxima of these curves approach the stoichiometric fuel concentration because at the higher pressures less dissociation occurs in the reacted gas of the wave. In the case of carbon monoxide - air mixtures the sonic speed in the initial gas is practically independent of its composition. However, in hydrogen-oxygen mixtures the sonic speed increases rather markedly when the concentration of hydrogen is increased. Therefore, the maximum detonation velocity of hydrogen-oxygen mixtures (ref. 2) occurs in rather rich mixtures even at very high pressures. The small reduction of the degree of dissociation in this range of fuel concentrations is not as effective as the increase in the speed of sound in the initial gas mixture. As a result of this condition the maximum of the curves representing the detonation velocity as a function of the hydrogen concentration for hydrogen-oxygen mixtures shifts only very slightly towards the stoichiometric fuel concentration as the initial gas pressure is increased (see fig. 3, ref. 2). That the detonation velocity of a combustible gas mixture is proportional to the speed of sound in the unburned gas is indicated by equation (13).

Figure 2 illustrates the effect of initial pressure on the pressure ratio across the detonation wave. For a mixture containing 29.6 per cent carbon monoxide, this ratio increases by about 10 per cent when the pressure of the initial gas is increased from 1 to 100 atmospheres. Following the behavior of the detonation velocity, the pressure ratio as a function of the fuel concentration also has a maximum in the region where the mixtures are rich in fuel and, with increasing initial pressure, this maximum also moves toward the stoichiometric fuel concentration. According to these calculations, the pressure behind the detonation wave of carbon monoxide - air mixtures is only 20 per cent lower than that of hydrogen-oxygen mixtures having the same equivalence ratio. The pressure ratios across the normal shock preceding the detonation wave, figure 6, are approximately 80 per cent greater than the detonation pressure ratios.

The curves representing the gas temperature behind the detonation, figure 3, are quite similar in shape to those depicting the detonation velocity, figure 1. When the initial pressure is increased from 1 to 100 atmospheres, the detonation wave temperature of a mixture containing 29.6 per cent carbon monoxide increases from $2864^{\circ}K$ to $3173^{\circ}K$. This temperature increment amounts to almost 11 per cent of the lower temperature. Again, at the lower initial pressures the maximum temperature is produced by rather fuel-rich mixtures and this maximum approaches the stoichiometric fuel concentration as the initial pressure is raised. The temperature behind the normal shock preceding the detonation wave, figure 5, is approximately 45 per cent lower than the temperature in the fully detonated gas.

The mole fractions of the various species occurring in the detonation wave are graphically represented in figures 7 through 10 for each of the four initial pressures of 1, 5, 25 and 100 atmospheres.

These curves demonstrate clearly the well-known fact that the degree of dissociation is less at the higher pressures whereas the absolute concentration of free radicals increases with increasing pressure. As anticipated, the mole fraction of molecular oxygen decreases with increasing carbon monoxide content in the mixtures. However, the mole fraction of atomic oxygen attains a maximum in nearly stoichiometric mixtures.

The precision of the calculations is about equal to the accuracy of the thermodynamic data used. Because of the somewhat large temperature intervals used in the present calculations, the estimated precision attained is about 0.1 per cent of the value of the calculated parameters.

CONCLUSIONS

Although the present method of calculating detonation parameters is intended primarily for use with desk calculators, it is too slow when very many calculations are to be made. However, the method can be adapted for electronic computing machines quite easily.

The detonation parameters of carbon monoxide - air mixtures are affected less by changes in the initial pressure than those of corresponding hydrogen-oxygen mixtures because of the lower degree of dissociation of the former.

The Ohio State University
Rocket Research Laboratory
Columbus 10, Ohio May 15, 1962

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TABLE 1. COMPOSITION OF COMBUSTION GAS IN DETONATION WAVE*

Molar per cent fuel in mixture	p_b atm	$\frac{p_{CO_2}}{p_{a,D}}$	$\frac{p_{CO}}{p_{a,D}}$	$\frac{p_{O_2}}{p_{a,D}}$	$\frac{p_{O}}{p_{a,D}}$	$\frac{p_{N_2}}{p_{a,D}}$	$\frac{p_{NO}}{p_{a,D}}$
10	1	0.1051	0.0000	0.1456	0.0000	0.7475	0.0018
	5	0.1051	0.0000	0.1456	0.0000	0.7475	0.0018
	25	0.1051	0.0000	0.1456	0.0000	0.7475	0.0018
	100	0.1051	0.0000	0.1456	0.0000	0.7475	0.0018
20	1	0.2121	0.0090	0.0724	0.0013	0.6918	0.0134
	5	0.2165	0.0050	0.0706	0.0007	0.6930	0.0141
	25	0.2194	0.0025	0.0694	0.0003	0.6938	0.0145
	100	0.2207	0.0013	0.0689	0.0002	0.6943	0.0146
29.6	1	0.2578	0.0757	0.0294	0.0033	0.6202	0.0135
	5	0.2735	0.0625	0.0232	0.0020	0.6247	0.0140
	25	0.2890	0.0495	0.0173	0.0011	0.6294	0.0138
	100	0.3011	0.0392	0.0128	0.0006	0.6333	0.0130
40	1	0.2615	0.1904	0.0073	0.0020	0.5322	0.0067
	5	0.2737	0.1809	0.0034	0.0008	0.5361	0.0051
	25	0.2817	0.1746	0.0011	0.0003	0.5391	0.0032
	100	0.2853	0.1718	0.0004	0.0001	0.5407	0.0019
50	1	0.2324	0.3257	0.0004	0.0002	0.4403	0.0011
	5	0.2339	0.3246	0.0001	0.0001	0.4409	0.0005
	25	0.2344	0.3242	0.0000	0.0000	0.4411	0.0002
	100	0.2346	0.3240	0.0000	0.0000	0.4412	0.0001

* Initial temperature = 313.16°K

TABLE 2. PROPERTIES OF A CARBON MONOXIDE - AIR DETONATION WAVE, $p_b = 1$ atm

Molar per cent fuel in mixture	T_b °K	$T_{a,D}$ °K	$T_{a,N.S.}$ °K	$p_{a,D}$ atm	$p_{a,N.S.}$ atm	p_{imp} atm	U_a m/sec	U_D m/sec	$\frac{\rho_{a,D}}{\rho_b}$	$M_D = \frac{U_D}{a_b}$
10	313.16	1632	1077	8.415	14.87	12.60	751	1277	1.700	3.59
20	313.16	2524	1485	12.96	22.65	21.25	887	1575	1.777	4.42
29.6	313.16	2864	1625	14.72	25.34	24.89	919	1668	1.814	4.68
40	313.16	2919	1650	14.96	25.82	25.26	931	1686	1.811	4.72
50	313.16	2717	1573	13.68	24.34	22.31	932	1640	1.760	4.58

TABLE 3. PROPERTIES OF A CARBON MONOXIDE - AIR DETONATION WAVE, $p_b = 5$ atm

Molar per cent fuel in mixture	T_b °K	$T_{a,D}$ °K	$T_{a,N.S.}$ °K	$p_{a,D}$ atm	$p_{a,N.S.}$ atm	p_{imp} atm	U_a m/sec	U_D m/sec	$\frac{\rho_{a,D}}{\rho_b}$	$M_D = \frac{U_D}{a_b}$
10	313.16	1632	1077	42.07	74.33	63.00	751	1277	1.699	3.59
20	313.16	2563	1501	65.89	114.8	108.6	889	1586	1.784	4.45
29.6	313.16	2982	1673	76.01	131.3	128.5	936	1698	1.813	4.76
40	313.16	3008	1688	75.82	132.7	127.1	953	1709	1.794	4.79
50	313.16	2728	1579	68.30	122.3	110.9	939	1644	1.751	4.59

TABLE 4. PROPERTIES OF A CARBON MONOXIDE - AIR DETONATION WAVE, p_b = 25 atm

Molar per cent fuel in mixture	T_b ^oK	$T_{a,D}$ ^oK	$T_{a,N.S.}$ ^oK	$p_{a,D}$ atm	$p_{a,N.S.}$ atm	p_{imp} atm	U_a m/sec	U_D m/sec	$\frac{\rho_{a,D}}{\rho_b}$	$M_D = \frac{U_D}{a_b}$
10	313.16	1632	1077	210.4	371.7	315.0	751	1277	1.699	3.59
20	313.16	2583	1510	329.9	578.6	541.1	897	1592	1.775	4.47
29.6	313.16	3090	1717	389.5	677.3	658.4	955	1724	1.806	4.83
40	313.16	3066	1714	381.4	675.9	633.6	971	1725	1.777	4.83
50	313.16	2732	1581	341.4	612.5	553.4	941	1645	1.749	4.60

TABLE 5. PROPERTIES OF A CARBON MONOXIDE - AIR DETONATION WAVE, p_b = 100 atm

Molar per cent fuel in mixture	T_b ^oK	$T_{a,D}$ ^oK	$T_{a,N.S.}$ ^oK	$p_{a,D}$ atm	$p_{a,N.S.}$ atm	p_{imp} atm	U_a m/sec	U_D m/sec	$\frac{\rho_{a,D}}{\rho_b}$	$M_D = \frac{U_D}{a_b}$
10	313.16	1632	1077	841.4	1487	1260	751	1277	1.699	3.59
20	313.16	2589	1514	1312	2322	2136	905	1595	1.762	4.48
29.6	313.16	3173	1750	1583	2773	2666	971	1744	1.797	4.89
40	313.16	3093	1725	1534	2725	2545	976	1732	1.774	4.85
50	313.16	2733	1582	1365	2451	2209	942	1646	1.747	4.60

TABLE 6

EQUILIBRIUM CONSTANTS

T $^\circ K$	K_{CO_2} Atm.	K_{O_2} Atm.	K_{NO} Atm.
1500	4.843×10^{-6}	4.628×10^{-6}	3.087×10^{-3}
2000	1.310×10^{-3}	7.374×10^{-4}	1.920×10^{-2}
2500	3.627×10^{-2}	1.564×10^{-2}	5.744×10^{-2}
3000	3.242×10^{-1}	1.205×10^{-1}	1.190×10^{-1}
3500	1.517	5.198×10^{-1}	1.997×10^{-1}
4000	4.759	1.559	2.941×10^{-1}
4500	11.43	3.664	3.957×10^{-1}
5000	22.77	7.271	4.998×10^{-1}

ΔE_o = 66,767 cal/mole CO_2

ΔE_o = 58,532 cal/mole O_2

ΔE_o = 21,600 cal/mole NO

TABLE 7

HEATS OF FORMATION $\left(\frac{\Delta H_f}{\mathcal{R} T}\right)_i^T$

T °K	CO_2	CO	O_2	O	N_2	NO
298.16	-158.7954	-44.6155	0	99.8153	0	36.6859
300	-157.7929	-44.3197	0.02266	99.2197	0.02216	36.4839
400	-117.1620	-32.3613	0.91113	75.0662	0.89401	28.2603
500	- 92.69516	-25.1785	1.46526	60.5665	1.42236	23.3355
600	- 76.32368	-20.3781	1.85448	50.8971	1.78348	20.0650
700	- 64.58725	-16.9379	2.14861	43.9881	2.05086	17.7426
1000	- 43.32795	-10.6938	2.73212	31.5483	2.58177	13.6129
1500	- 26.61104	- 5.75287	3.25747	21.8691	3.08103	10.4794
2000	- 18.16171	- 3.23862	3.56067	17.0279	3.37749	8.95096
2500	- 13.05162	- 1.71094	3.76959	14.1237	3.57631	8.05059
3000	- 9.62325	- 0.683082	3.93051	12.1885	3.71994	7.45841
3500	- 7.16045	- 0.056999	4.06172	10.8084	3.82800	7.04096
4000	- 5.30190	0.615081	4.17082	9.77631	3.91357	6.73253
4500	- 3.84864	1.05183	4.26418	8.97617	3.98225	6.49661
5000	- 2.68039	1.40334	4.34421	8.33927	4.03972	6.31331

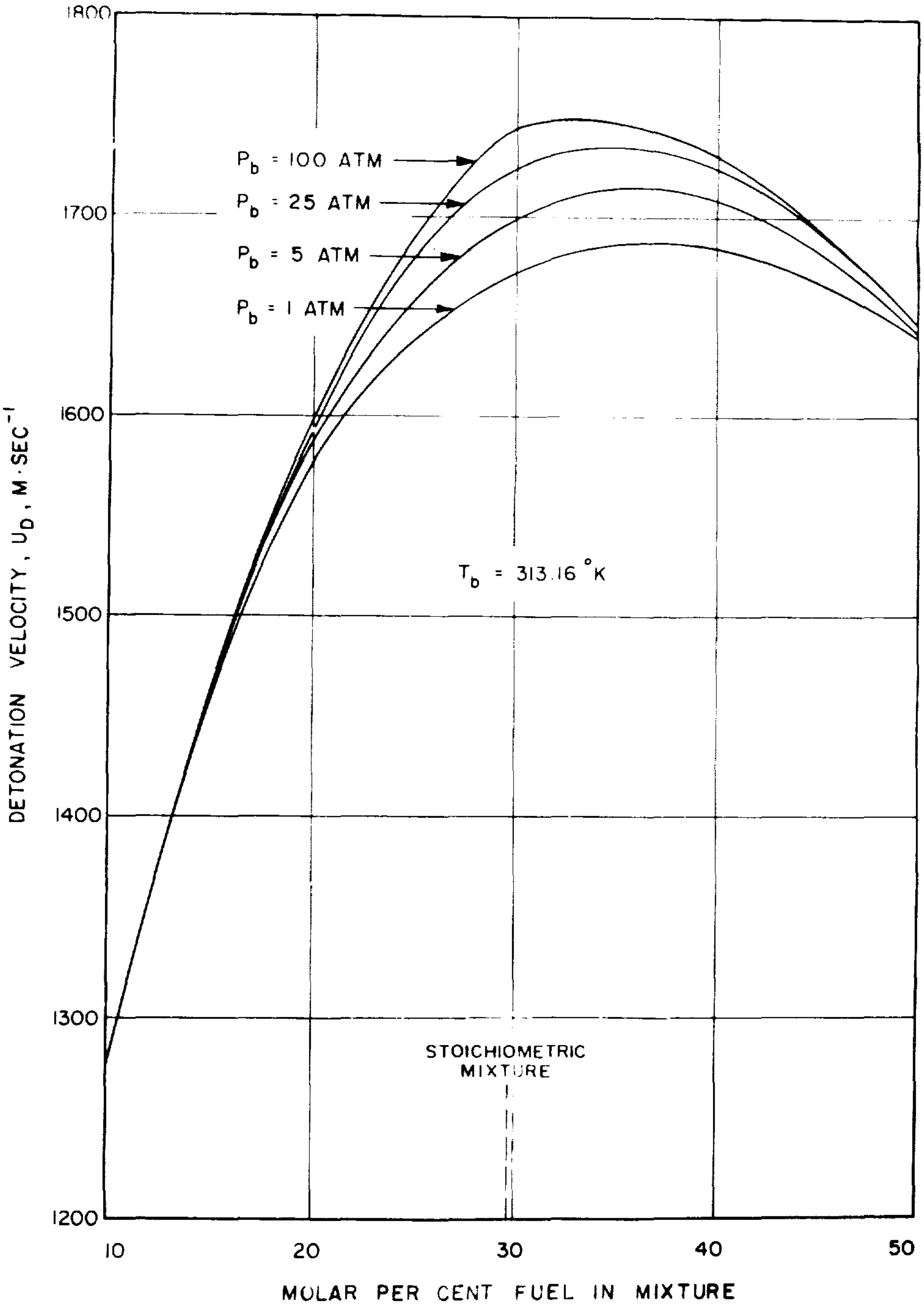

FIG. 1 CALCULATED DETONATION VELOCITIES OF CARBON MONOXIDE - AIR MIXTURES

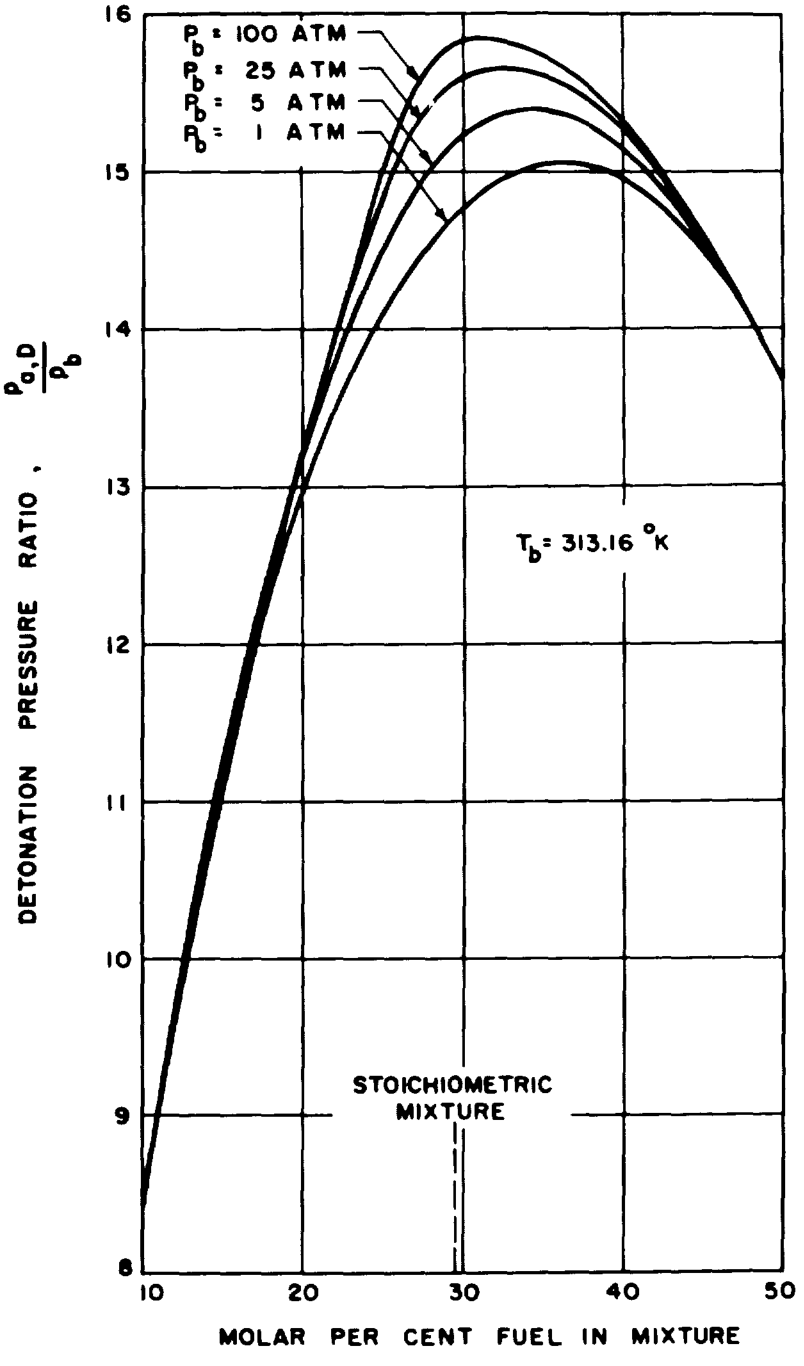

FIG. 2 PRESSURE RATIOS ACROSS CARBON MONOXIDE - AIR DETONATION WAVES

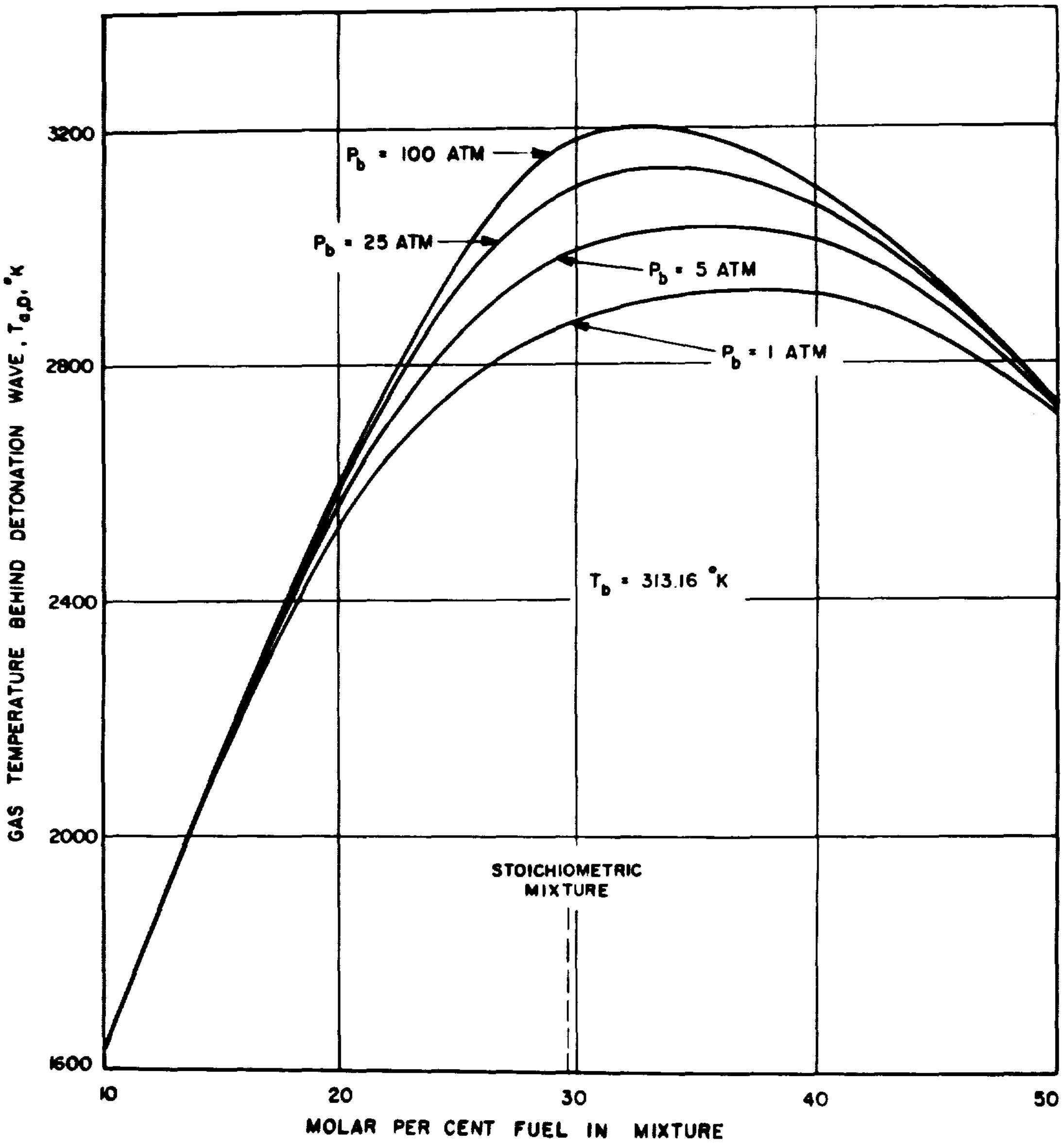

FIG. 3 GAS TEMPERATURES BEHIND CARBON MONOXIDE - AIR DETONATION WAVES

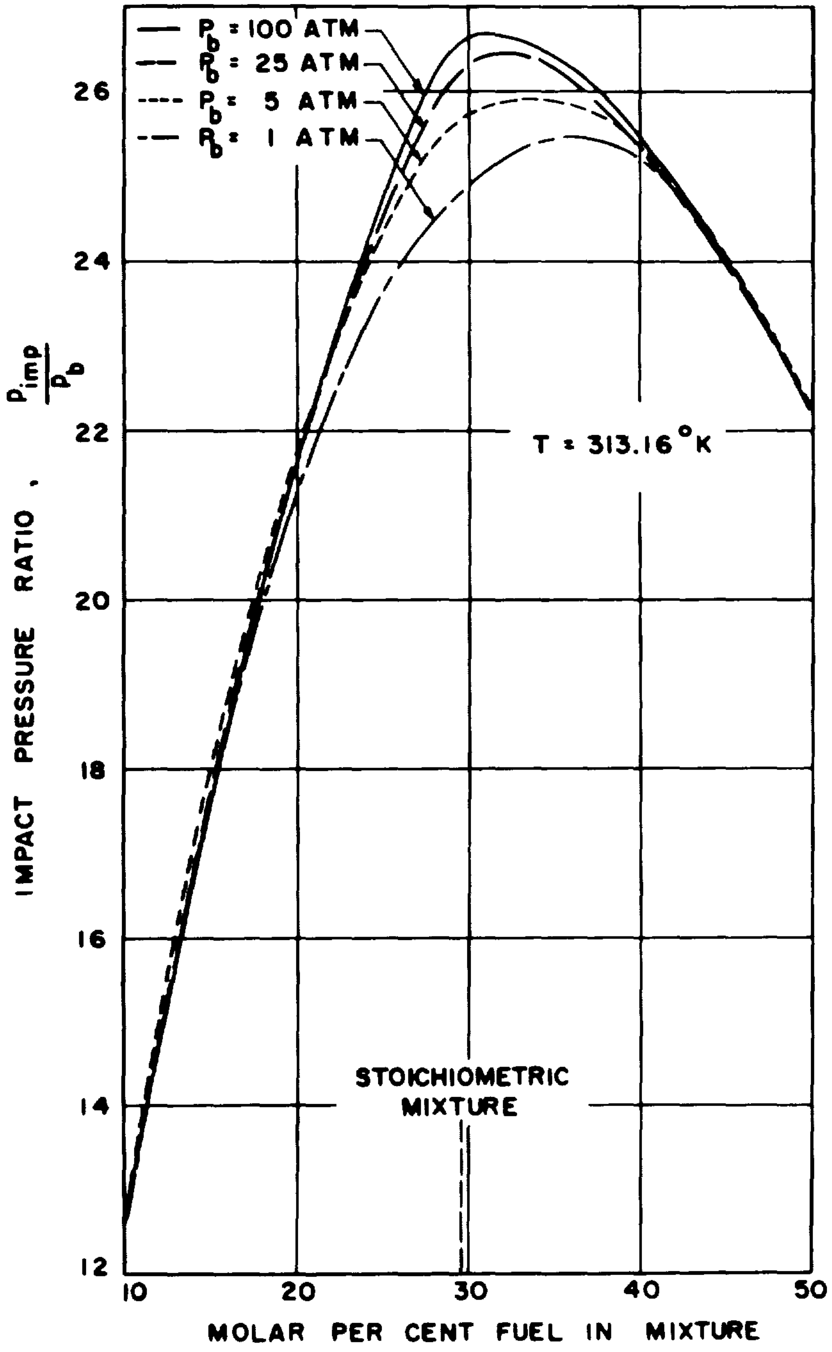

FIG. 4 IMPACT PRESSURE RATIOS OF CARBON MONOXIDE - AIR DETONATION WAVES

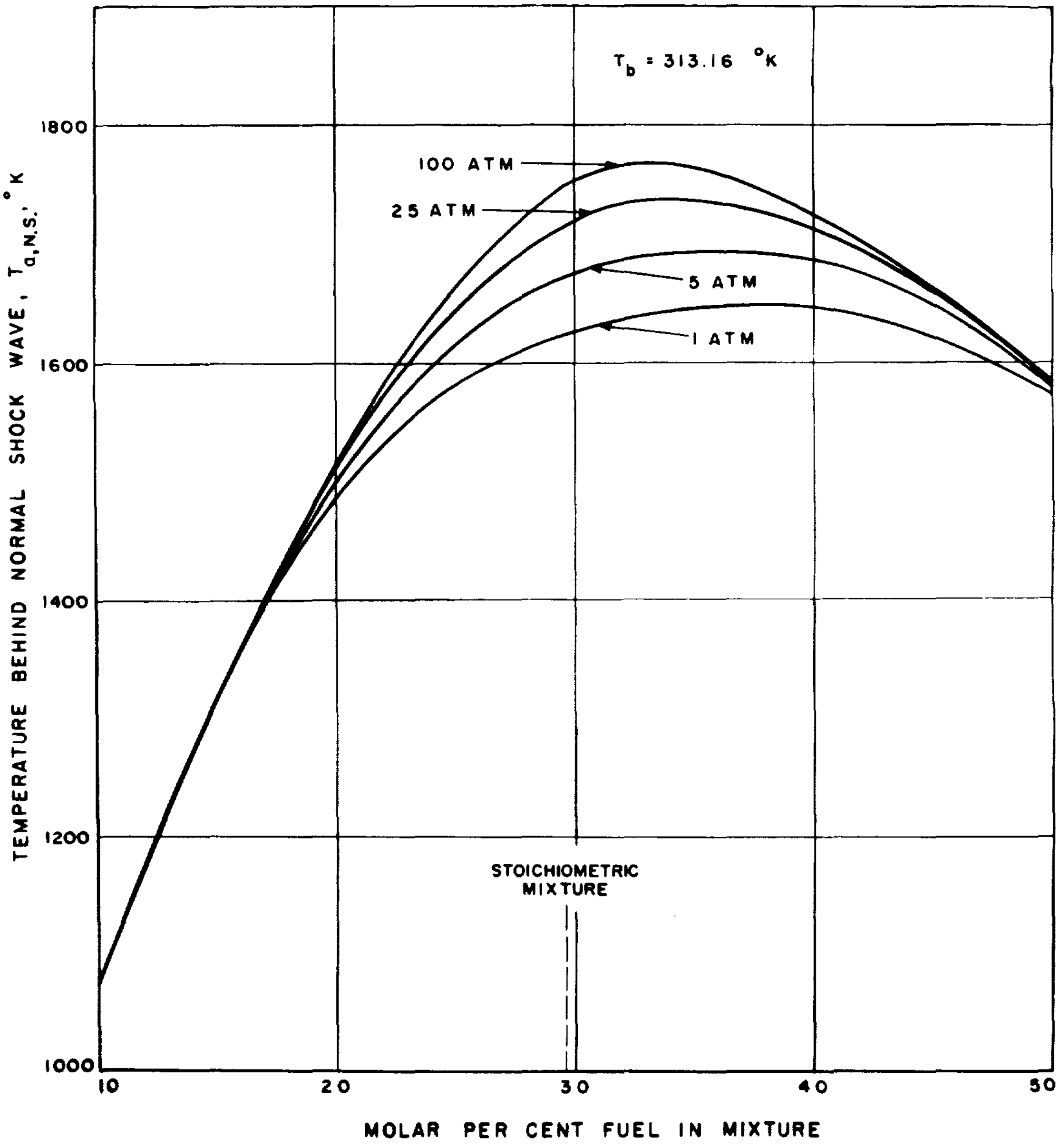

FIG. 5 GAS TEMPERATURES BEHIND NORMAL SHOCK WAVES OF CARBON MONOXIDE - AIR DETONATION WAVES

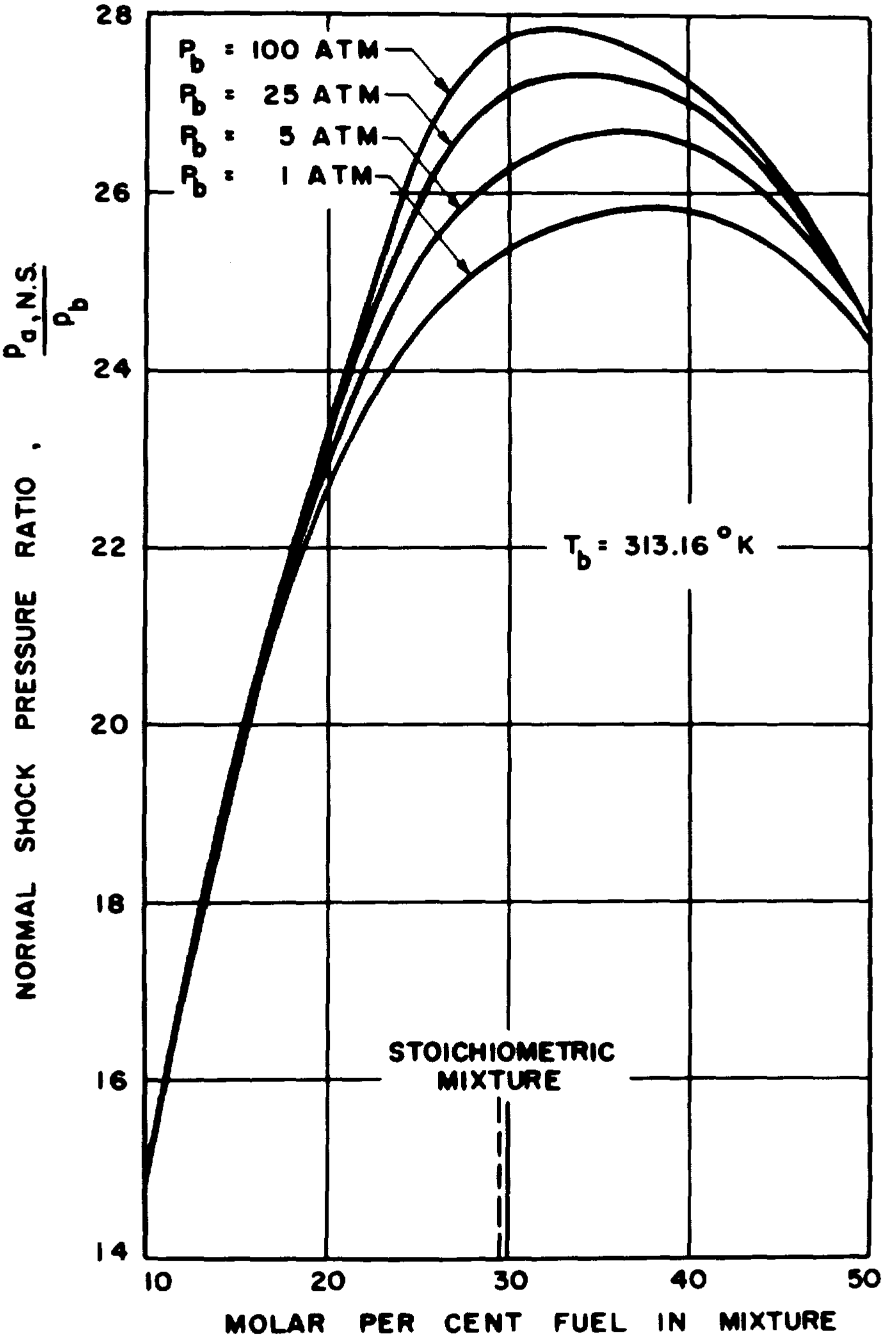

FIG. 6 PRESSURE RATIOS ACROSS SHOCK WAVES OF CARBON MONOXIDE - AIR DETONATION WAVES

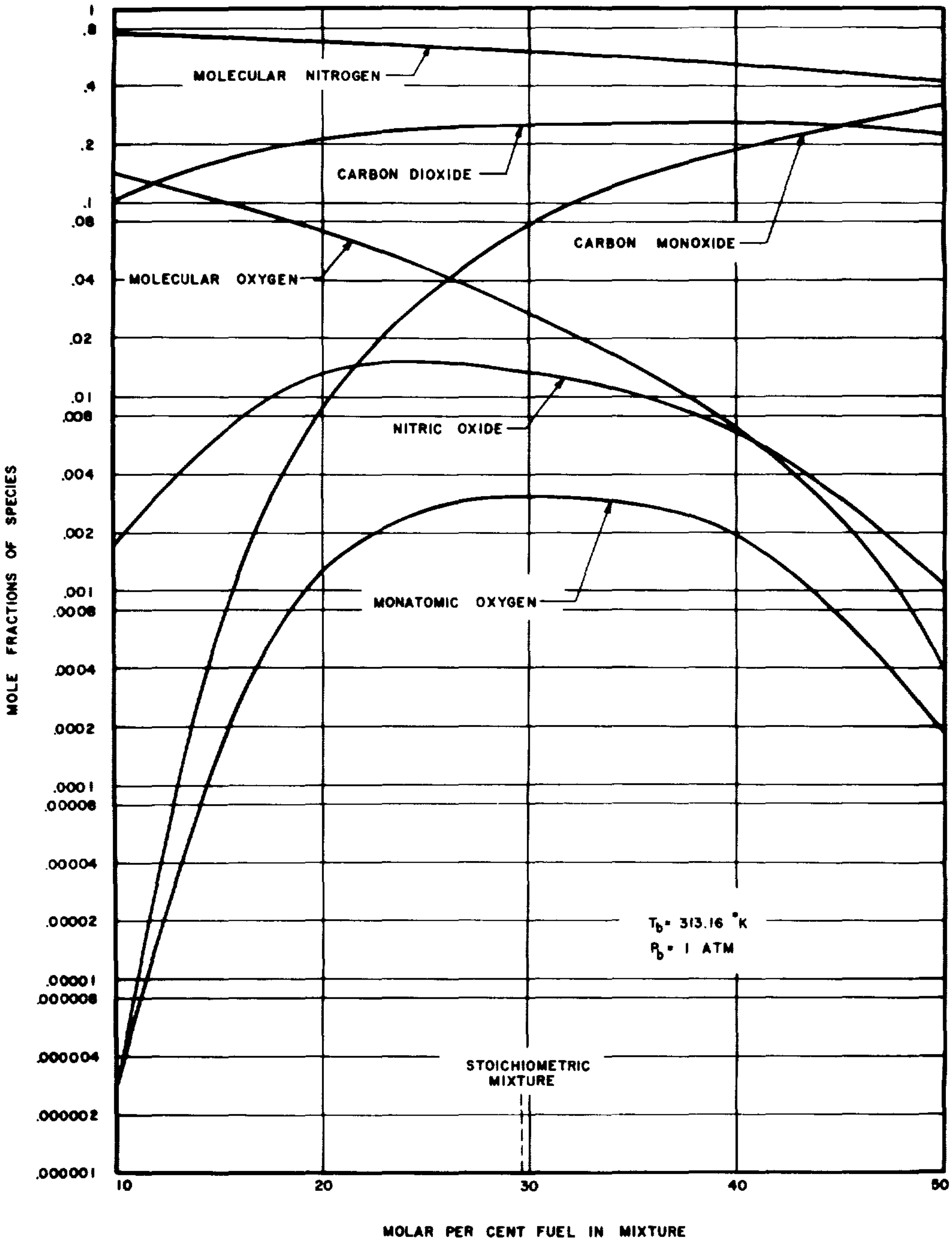

FIG. 7 MOLE FRACTIONS OF SPECIES; INITIAL PRESSURE = 1 ATMOSPHERE

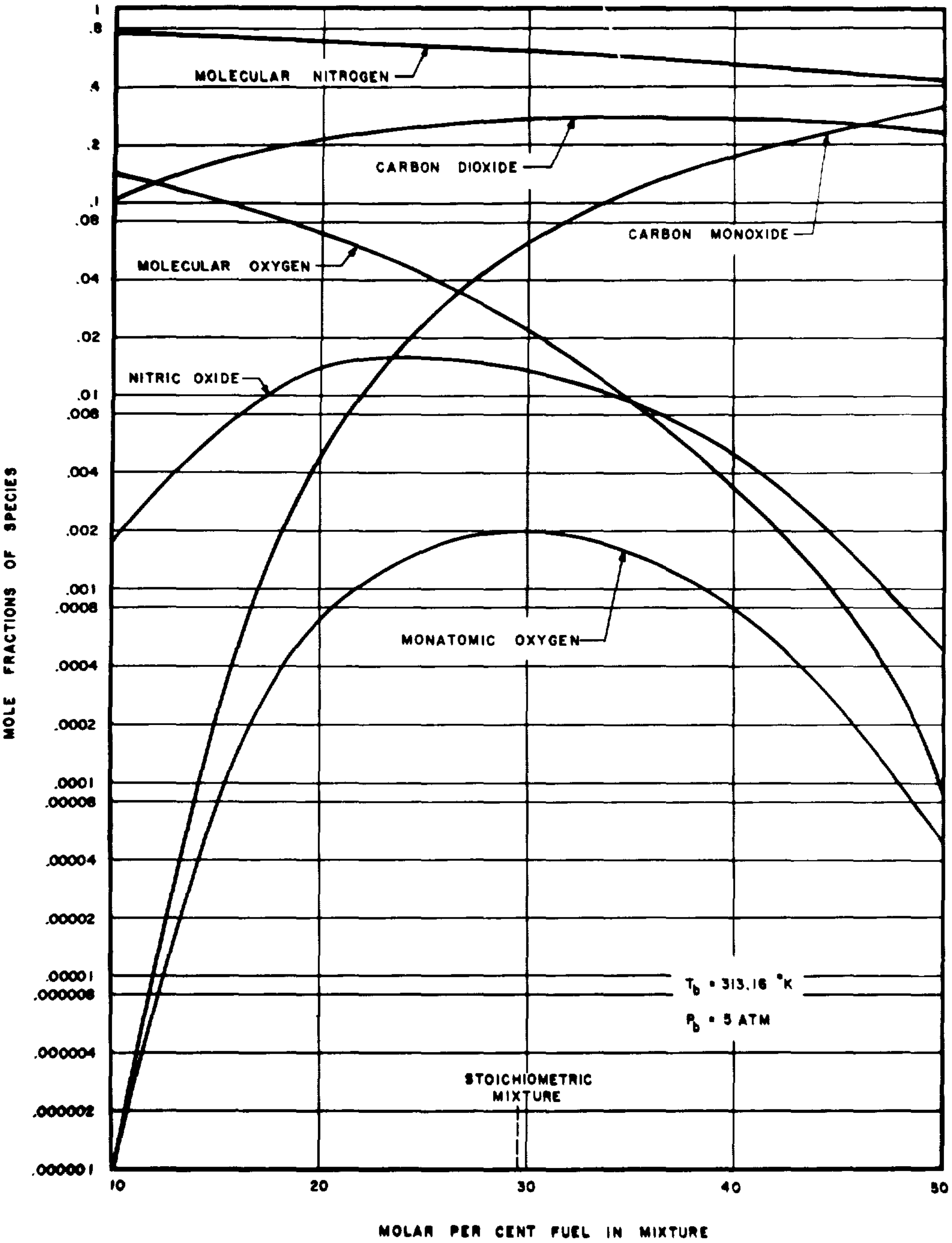

FIG. 8 MOLE FRACTIONS OF SPECIES; INITIAL PRESSURE = 5 ATMOSPHERES

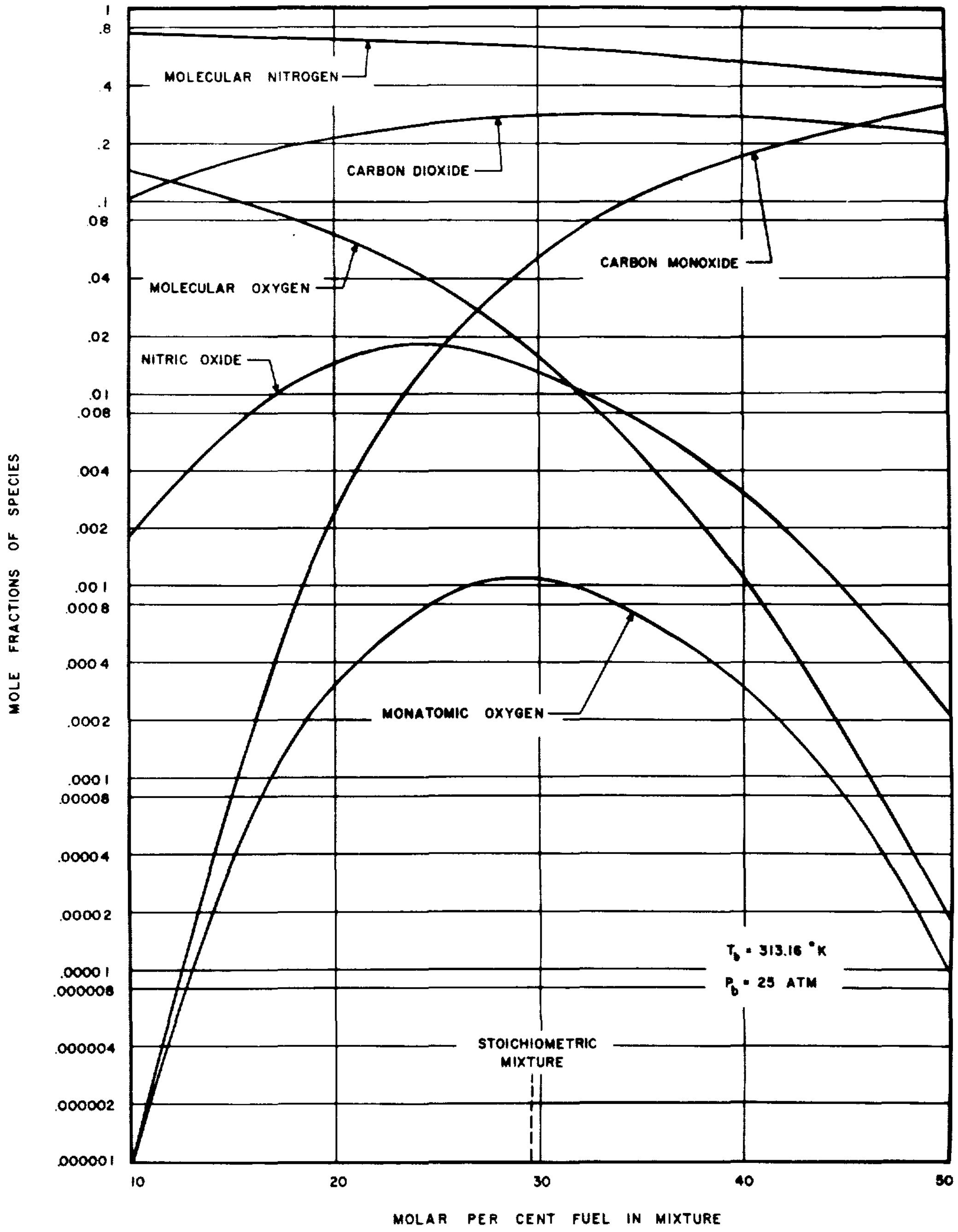

FIG. 9 MOLE FRACTIONS OF SPECIES; INITIAL PRESSURE = 25 ATMOSPHERES