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C-J DETONATION STUDIES IN HYDROGEN-CHLORINE, CARBON DISULFIDE-OXYGEN AND CARBON MONOXIDE-HYDROGEN-OXYGEN-NITROGEN MIXTURES

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C-J DETONATION STUDIES IN H_2-Cl_2, CS_2-O_2 AND CO-H_2-O_2-N_2 MIXTURES

by

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ABSTRACT

Detonation properties in steady, one-dimensional, equilibrium flows have been calculated for hydrogen-chlorine, carbon disulfide-oxygen and carbon monoxide-hydrogen-oxygen-nitrogen mixtures at an initial temperature of 25°C, initial pressures in the range from 30 to 760 torr and various initial mixture compositions. Experimental velocities in stoichiometric (H_2+Cl_2) and (CS_2+3O_2) mixtures, at atmospheric pressure initially, are about 2% larger than the calculated values and may reflect achievement of only partial equilibrium at the C-J plane.

TABLE OF CONTENTS

Page Nos.

LIST OF SYMBOLS

a_i = reactant mole number

A_i = chemical symbol for species i

b_i = product mole number

$B_i \equiv \log_e bi$

c_i = concentration of species i (mole/cm^3)

$c_2(fr)$ = frozen sound speed (cm/sec)

$C_i \equiv C_i(T_2, \mathcal{V}_2)$

$C_{p,i}$ = specific heat at constant pressure for species i (cal/mole -^{0}K)

D = detonation velocity (cm/sec)

H = enthalpy of reactive mixture (kcal/mole)

$(H^0-H^0{}_{298})_i \equiv \int_{298}^{T} C_{p,i}dT$ = difference between enthalpies in the standard states at temperatures T and 298^{0}K for species i (kcal/mole)

J = energy conversion factor = 4.187 x 10^{10}(ergs)

k_b = backward specific rate constant

k_f = forward specific rate constant

$K_c(T)$ = equilibrium constant in terms of concentrations

$K_p(T)$ = equilibrium constant in terms of partial pressures (in atm) = K_i

M = Mach number

n_i = mole number of species i

p = pressure (dyne/cm^2)

R^o = ideal gas constant = 8.3143 x 10^7erg/mole -^{o}K

T = temperature (^{o}K)

u = fluid particle velocity (cm/sec)

V = fluid velocity with respect to stationary detonation wave (c /sec)

$\mathcal{V}$ = volume (cm^3)

$\bar{W}$ = mean molecular weight of mixture (gm/mole)

W_i = molecular weight of species i (gm/mole)

X_i = mole fraction of species i

<u>Greek</u>

$\alpha_{s,i}$ = number of atoms of kind s in molecule of type i

$[\Delta F^o(T)]_i$ = standard free energy of formation of species i (kcal/mole)

$(\Delta H^{o}_{f})_i$ = standard heat of formation of species i (kcal/mole)

$\Delta\nu_i \equiv \nu_i'' - \nu_i'$

$\gamma_2(fr)$ = frozen specific heat ratio

ν_i' = stoichiometric coefficient for reactant species i

ν_i'' = stoichiometric coefficient for product species i

Subscripts

i = any species

= reactant

k = product

l = atom

s = atom

Index

1 = unburnt gas

2 = burnt gas

PREFACE

The research reported herein is a preliminary study of gaseous detonative combustion in novel chemical systems, namely in hydrogen-chlorine, carbon disulfide-oxygen and carbon monoxide-hydrogen-oxygen-nitrogen mixtures. The global objective of all gaseous detonation research is to further the understanding of the instability mechanism associated with the multi-headed structure observed universally in gaseous detonative combustion. The specific reasons whereby we have chosen to study the above mentioned reactive systems are twofold. In the first instance, the former two possess much simpler kinetic schemes than the oxyhydrocarbon systems conventionally studied in this research area. There are indications that the kinetic schemes may be linked to the instability mechanism and hence the simplified kinetics could help in isolating this linkage. Secondly, all of the above reactive systems produce potentially lasing media and it is of interest to investigate the feasibility of exploiting them in powerful, infrared, self-sustained chemical lasers.

As a first step, one must obtain reliable theoretical and experimental data on the global detonative behavior of the above mentioned gaseous systems. In this report, we present the theoretical aspect of the problem, i.e., the C-J calculations of detonation parameters in (H_2-Cl_2), (CS_2-O_2) and (CO-H_2-O_2-N_2) systems.

1. INTRODUCTION

Gaseous detonation waves have been extensively studied since the end of the 19th century. However, most of these theoretical and experimental investigations have been mainly devoted to hydrocarbon-oxygen systems for utilitarian purposes. Although the classical C-J model of a detonation wave which assumes [1, 2] the wave to possess a uniform and unidimensional structure predicts detonation velocities in good agreement with experimentally measured values, it has been demonstrated [3, 4] that planar detonation waves are inherently unstable, consisting of an intersecting transverse wave pattern composed of elemental triple point intersections. Sufficient experimental evidence exists [5, 6, 7] to infer that the onset of instability is in the form of periodic formation of randomly distributed reaction centers. From the striking qualitative resemblance of the onset of instability in gaseous detonations and in a reacting system involving autocatalytic or chain-branching steps in the reaction scheme [8, 9], we have postulated [10] that the instability mechanisms in gaseous detonations may also arise from such autocatalytic or chain-branching schemes. However, due to the complexity of the proposed chain-branching kinetic schemes in hydrocarbon-oxygen systems, we have suggested [10] to investigate systems with relatively simpler kinetic schemes such as the hydrogen-chlorine and/or the carbon disulfide-oxygen systems.

It is commonly admitted that, in both systems, chemical reactions proceed through a chain reaction mechanism. For the (H_2-Cl_2) system, the relevant kinetic steps are:

$$Cl_2 + M \rightarrow 2\underline{Cl} + M \qquad \text{initiation} \qquad (1.1.a)$$

$$\left.\begin{array}{ll} \underline{Cl} + H_2 \rightarrow HCl + \underline{H} & (1.1.b) \\ \underline{H} + Cl_2 \rightarrow HCl^* + \underline{Cl} & (1.1.c) \end{array}\right\} \text{propagation}$$

$$\left.\begin{array}{l} 2\underline{Cl} + M \rightarrow Cl_2 + M \\ 2\underline{H} + M \rightarrow H_2 + M \end{array}\right\} \text{termination} \qquad (1.1.d)$$

where underlined species denote chain carriers, HCl is a molecule in the electronic and vibrational ground state and HCl^*, a vibrationally excited molecule in the electronic ground state. Because it has been inferred from experiments [11, 12] that the energy liberated in reaction (1.1.c), namely 45.5 kcal/mole, is initially concentrated mainly in the HCl^* molecule (with vibrational quantum number $v = 6$), it has been postulated [13] that under flame conditions such energetic molecules could dissociate Cl_2 molecules through an energy chain-branching reaction, viz.,

$$HCl^* + Cl_2 \rightarrow 2\underline{Cl} + HCl \qquad (1.1.e)$$

this process being endothermic by 11.7 kcal/mole, only

Although no experimental evidence for the existence of reaction (1.1.e) has been found in (H_2-Cl_2) flames [14], the instability observed under detonative combustion [10] suggests the presence of the energy chain branching step in (H_2-Cl_2) detonations according to the autocatalytic instability mechanism.

On the other hand, two chain-branching steps are commonly considered in the (CS_2-O_2) kinetic scheme which is usually described by the following chain reaction mechanism [15, 16]

$$O_2 + M \rightarrow 2\underline{O} + M,$$

$$CS_2 + \underline{O} \rightarrow C\underline{S} + \underline{SO}, \quad \text{(branching)}$$

$$\underline{SO} + O_2 \rightarrow SO_2 + \underline{O},$$

$$\underline{CS} + \underline{O} \rightarrow CO^* + \underline{S},$$

$$\underline{CS} + O_2 \rightarrow COS + \underline{O},$$

$$\underline{S} + O_2 \rightarrow \underline{SO} + \underline{O}, \quad \text{(branching)}$$

$$2\underline{O} + M \rightarrow O_2 + M,$$

where CO^* denotes a vibrationally excited molecule in the electronic ground state. Although this chemical scheme is somewhat more complex than the (H_2-Cl_2) one, it is still much simpler than the oxyhydrocarbon one and the instability observed under detonative combustion in preliminary experiments can be easily linked to the chain-branching steps of the (CS_2-O_2) kinetic scheme.

In the context of the present report, C-J detonations in (H_2-Cl_2) systems have been investigated as early as the beginning of the 20th century [17-19]. Detonation velocities have been measured in stoichiometric [17-19] and fuel-rich mixtures [17] in the pressure range from 200 to 760 torr. Comparison with theoretical calculations in stoichiometric mixtures has shown a qualitative discrepancy, experimentally measured values of 1730 m/sec being pressure-independent from 760 to 200 torr [18, 19] whereas calculated values [20] decrease by approximately 2.5% from 1720 m/sec at 760 torr to 1680 m/sec at 200 torr. This discrepancy has been attributed [19, 20] to achievement of only partial equilibrium, the resulting Cl atom concentration being less than that corresponding to the equilibrium reaction $Cl_2 \rightleftarrows 2Cl$, therefore resulting in calculated detonation temperatures and velocities less than the true values. In preliminary investigations of spherical and cylindrical detonations in stoichiometric mixtures at subatmospheric pressures (30 - 120 torr), we have recently measured detonation velocities from 1470 m/sec at 30 torr to 1625 m/sec at 100 torr. At atmospheric pressure, with increasing fuel concentration, detonation velocities increase from 1729 m/sec for the stoichiometric mixture to 1855 m/sec in a ($3H_2$ + Cl_2) mixture [17]. Recently, soot film records in cylindrical and spherical detonations in stoichiometric (H_2-Cl_2) mixtures, at subatmospheric pressures, have given[10] a concrete evidence of the multi-headed structure in this system. Due to the lack of experimental and theoretical data at subatmospheric and atmospheric pressures and various initial compositions in (H_2-Cl_2) systems, we have started a detailed theoretical and experimental investigation of this system under detonative combustion conditions with the aim of ascertaining the relevant kinetic schemes and rate constants prevailing under non-equilibrium conditions in order to get some understanding of the instability mechanisms arising in most gaseous detonable systems and with the hope of achieving a more accurate description of the propagation of multi-headed detonation waves.

Detonation studies in (H_2-Cl_2) systems have also been motivated by their possible application to the development of powerful, infra-red, self-sustained, chemical lasers. At present, successful operation of pulsed and/or continuous wave mode (H_2-Cl_2) lasers have been reported[21, 22]. The feasibility of a detonation laser rests on the degree to which large population inversion in vibrationally excited reaction products formed in the reaction zone and/or in the hot combustion product region behind a detonation wave can be achieved. Because non-equilibrium prevails behind a detonation front and because of the fast hydrodynamic expansion accompanying a detonation wave, vibrational freezing should be readily achieved; in other words, collisional deactivation of excited species should be appreciably reduced by the resulting lowering of the translational temperature of the reacted mixture. Therefore, the non-linear coupling between chemical reactions and hydrodynamics in a transient flow field should guarantee the feasibility of population inversion under detonative combustion.

In addition to the (H_2-Cl_2) system, two other systems, namely, the carbon disulfide-oxygen and carbon monoxide-oxygen-hydrogen-nitrogen systems, appear to be possible candidates for detonative laser applications. The (CS_2-O_2) system has been successfully operated as a chemical laser, lasing resulting from vibrationally excited CO formed in chemical reactions initiated by an electrical discharge [23] and/or under deflagrative combustion [15]. Under detonative combustion, the (CS_2-O_2) system has been experimentally investigated since the beginning of the 20th century in relation with explosions in coal mines. Detonation velocities of 1800 m/sec have been measured [24, 25] in (CS_2 + $3O_2$) mixtures at atmospheric pressure. No experiments at subatmospheric pressures and other initial compositions have been reported and no theoretical data are available for comparison.

On the other hand, there have been extensive studies of detonation properties in (CO-O_2-H_2) systems.

The ($CO-O_2$) system supports a stable detonation wave in the presence of trace amounts of hydrogen [26, 27], whereas in a dry ($CO-O_2$) mixture, no self-developed detonation has ever been observed. The main products of the reaction between CO, O_2 and H_2 are CO_2 and H_2O. Therefore, the ($CO-O_2-H_2$) system should provide the essential species for CO_2 laser operation. CO_2 lasers have been extensively studied since the last decade, vibrationally excited CO_2 in the (00^01) level resulting from very efficient V-V exchange between $N_2(v = 1)$ and $CO_2(00^00)$ due to the near resonance between the $N_2(v = 1)$ and $CO_2(00^01)$ levels [28]. In addition, population inversion between the (00^01) and (10^00) CO_2 levels is enhanced by the presence of water vapour, one of the most efficient quenching molecules for the CO_2 lower laser level [28]. Addition of N_2 to a ($CO-O_2-H_2$) mixture should provide the main species, namely, CO_2, H_2O and N_2, for successful operation of a CO_2 detonation laser.

Therefore, the (H_2-Cl_2), (CS_2-O_2) and ($CO-O_2-H_2-N_2$) systems appear to be possible candidates for successful operation of detonation lasers. The first task in investigating the feasibility of such devices is to study theoretically and experimentally the behavior of these gaseous mixtures under detonative combustion. In this report, we present a theoretical investigation of the detonation properties of these systems. The classical C-J model has been used to calculate detonation parameters in (H_2-Cl_2), (CS_2-O_2) and (CO-O_2-H_2-N_2) mixtures under a wide variety of initial conditions. The method of computation is slightly different than that proposed by Eisen et al [29]. Instead of solving simultaneously the system of non-linear, algebraic equations (hydrodynamics + chemistry), we have devised a method by which for a given temperature of the burnt gases, the equilibrium composition at the C-J plane is obtained by iteration of the chemical equilibrium and atom balance equations, for an assumed volume of burnt gases. Then, iteration of the hydrodynamic equations yields a solution for all detonation parameters. The C-J solution is then obtained by finding the minimum detonation velocity compatible with the given initial conditions.

In the following, we shall first review the governing equations of the C-J model and describe the numerical method used to solve the corresponding system of non-linear, algebraic equations for any reacting gaseous mixture. Next, we shall present the relevant thermodynamic equilibrium and atom balance equations for each particular system, namely, (H_2-Cl_2), (CS_2-O_2) and (CO-O_2-H_2-N_2). Finally, the results will be discussed and compared with available experimental data.

2. Governing Equations

In the classical theory of detonation waves, the detonation process is considered as a one-dimensional one. The detonation front moves with uniform velocity D into a reactive gas mixture, initially at rest, $u_1 = 0$, at initial temperature and pressure, T_1 and p_1, respectively. The passage of the wave sets the gas behind it in motion at a velocity u_2 (Fig. 1a). In a reference system in which the wave is stationary, let V_1 and V_2 denote the gas velocities with respect to the stationary wave (Fig. 1.b), so that

$$V_1 = D \tag{2.1}$$

and

$$V_2 = D - u_2 \tag{2.2}$$

Across a detonation wave, the flux densities of mass, momentum and energy are continuous. In the stationary wave reference system, these conditions take the following forms:

- mass flux continuity:

$$\rho_1 V_1 = \rho_2 V_2 \tag{2.3}$$

where ρ denotes the gas density and subscripts 1 and 2, the unburnt and burnt gases, respectively.

- momentum flux continuity:

$$p_1 + \rho_1 V_1^2 = p_2 + \rho_2 V_2^2 \tag{2.4}$$

where p is the gas pressure.

- energy flux continuity:

$$H_1 + \sum_{i=1}^{j} n_i W_i \frac{V_1^2}{2} = H_2 + \sum_{i=1}^{k} n_i W_i \frac{V_2^2}{2} \qquad (2.5)$$

where n_i denotes the number of moles of specie i, $i = 1, 2, \ldots, j$ for reactants and $i = 1, 2, \ldots, k$ for reaction products. W_i is the molecular weight of species i and H, the enthalpy of the reactive mixture:

$$H = J \sum_{i=1}^{j \text{ or } k} \left[(\Delta H_f^0)_i + (H^0 - H_{298}^0)_i \right] \qquad (2.6)$$

where $(\Delta H_f^0)_i$ is the standard enthalpy of formation of species i, $(H^0 - H_{298}^0)_i = \int_{298}^{T} C_{p,i}\, dT$ is the difference between the enthalpies in the standard state at temperatures T and 298°K, respectively and J is the energy conversion factor.

Assuming a mixture of perfect gases, the equation of state is given by:

$$p = \rho \frac{R^0 T}{\bar{W}} = \sum_i n_i \frac{R^0 T}{v} \qquad (2.7)$$

where R^0 is the ideal gas constant, v is the gas volume and $\bar{W}$, the mean molecular weight of the mixture

$$\bar{W} = \sum_i X_i W_i \qquad (2.8)$$

where

$$X_i = n_i / \sum_i n_i \qquad (2.9)$$

is the mole fraction of species i.

The classical model of a detonation wave assumes the state of the burnt gas mixture to be the thermodynamic and chemical equilibrium state. The equilibrium composition at constant pressure and temperature, p_2 and T_2, respectively, is determined by writing that each chemical reaction taking place in the reaction zone behind the detonation front reaches equilibrium at section 2, the corresponding equations being:

i) the chemical equilibrium equations

ii) the conservation of mass (or atoms) equations.

For a given chemical reaction,

$$\sum_i \nu_i' A_i \underset{k_b}{\overset{k_f}{\rightleftharpoons}} \sum_i \nu_i'' A_i$$

the equilibrium constant K_c is defined as

$$K_c(T) \equiv \frac{k_f}{k_b} = \prod_i C_i^{\Delta\nu_i} \qquad (2.10)$$

where k_f and k_b denote the specific forward and backward reaction rates, respectively, $C_i \equiv n_i/v$ is the concentration of species i and $\Delta\nu_i \equiv \nu_i'' - \nu_i'$, where the ν's are the stoichiometric coefficients. Using Dalton's law for a mixture of ideal gases, viz.,

$$p_i = X_i p \qquad (2.11)$$

where p_i is the partial pressure of species i and the perfect gas law for species i,

$$p_i = n_i R^\circ T/v \qquad (2.12)$$

Eq. (2.10) can be rewritten in terms of partial pressures and/or number of moles, viz.,

$$K_c(T) = \prod_i p_i^{\Delta\nu_i} (R^\circ T)^{-\sum_i \Delta\nu_i}$$

$$= \prod_i n_i^{\Delta\nu_i} \cdot v^{-\sum_i \Delta\nu_i} \tag{2.13}$$

Defining the equilibrium constant K_p in terms of partial pressures, viz.,

$$K_p(T) = \prod_i p_i^{\Delta\nu_i} \tag{2.14}$$

Eq. (2.13) becomes

$$K_p(T) = \prod_i n_i^{\Delta\nu_i} \left(\frac{R^\circ T}{v}\right)^{\sum_i \Delta\nu_i} \tag{2.15}$$

The functions $K_p(T)$ are tabulated [30] or can be obtained from the well-known thermodynamic relation:

$$R^\circ T \log_e K_p(T) = -\sum_i \Delta\nu_i [\Delta F^\circ(T)]_i \tag{2.16}$$

where $[\Delta F^\circ(T)]_i$, the standard free energy of formation of species i is also tabulated in Ref. 30.

Finally, for a given gas mixture containing l different atoms, l atom balance equations can be written, viz.,

$$\sum_{i=1}^{k} \alpha_{s,i} n_i - \sum_{i=1}^{j} \alpha_{s,i} n_i = 0 ,$$

$$s = 1, 2, \cdots, l \tag{2.17}$$

where $\alpha_{s,i}$ is the number of atoms of kind s in molecule of type i.

3. METHOD OF SOLUTION

For given initial conditions, i.e., state 1, viz., p_1, T_1, v_1, X_i, $i = 1, 2, \ldots, j$ and $V_1 = D$, properties of state 2 are determined by solving the system of ($4+k$) non-linear, algebraic equations (Eqs. 2.3-2.5, 2.7, 2.15, 2.17) in ($4+k$) unknowns, namely, p_2, T_2, v_2, V_2 and the equilibrium composition (k species). However, since the detonation velocity V_1 (or D) is also unknown, the system can only be solved by assuming either the detonation velocity or any property of state 2. In the following, we shall assume a temperature T_2 and solve for the other unknowns. The Chapman-Jouguet state is the state 2 for which the detonation velocity is minimum.

For a given temperature T_2, the chemical equilibrium equations (Eq. 2.15) can always be expressed as functions of the volume v_2 and atom numbers only. Therefore, assuming a volume v_2, the atom balance equations can be solved by the Newton-Raphson method to yield the equilibrium composition. The pressure p_2 is then obtained from Eq. (2.7). Next, the hydrodynamic equations (Eqs. 2.3-2.5) are rewritten in the following forms. Combining Eqs. (2.3), (2.4) and (2.7) yields an expression for the detonation velocity, viz.,

$$V_1^2 = D^2 = \frac{R^\circ T_1}{\overline{W}_1} \cdot \frac{(1 - p_1/p_2)}{\frac{p_1}{p_2} \cdot \frac{\overline{W}_1}{\overline{W}_2} \cdot \frac{T_2}{T_1} - 1} \qquad (3.1)$$

$$= F_1(T_2, v_2)$$

A second expression for V_1^2 is obtained by combining Eqs. (2.3), (2.5)-(2.7), viz.,

$$V_1^2 = 2\left\{ \sum_{i=1}^{k} n_i\left[(\Delta H_f^\circ)_i + (H^\circ(T_2) - H^\circ_{298})_i\right] - \sum_{i=1}^{j} n_i\left[(\Delta H_f^\circ)_i + (H^\circ(T_1) - H^\circ_{298})_i\right] \right\}$$

$$\times\left\{ \sum_{i=1}^{j} n_i W_i - \sum_{i=1}^{k} n_i W_i \left(\frac{p_1}{p_2}\cdot\frac{\overline{W}_1}{\overline{W}_2}\cdot\frac{T_2}{T_1} \right)^2 \right\}^{-1}$$

$$= F_2(T_2, v_2) \qquad (3.2)$$

Equations (3.1) and (3.2) are then solved by iteration (false position method) to yield a solution for V_1 and v_2 when $|F^{(n)} - F^{(n-1)}|/|F^{(n-1)}| < 10^{-8}$, where $F = F_1(T_2, v_2) - F_2(T_2, v_2)$. Note that for each intermediate value of v_2, the equilibrium composition must be recomputed as described above. The advantage of this method over Eisen et al's method [29] is its simplicity, the rapidity of convergence to the solution, (usually, only four iterations by the false position method are necessary) and the absence of instability always present in the Newton-Raphson method when the number of equations increases with increasing complexity of the burnt gas mixture. Finally, the method of steepest descent is used to obtain the minimum detonation velocity D, i.e., the C-J state. The C-J state is considered to be reached when $|D^{(n)} - D^{(n-1)}|/D^{(n-1)} < 10^{-8}$

and the temperature step size $\Delta T_2 < 10^{-3}\,{}^{\circ}K$. Frozen specific heat ratios $\gamma_2(fr)$ and Mach numbers $M_2(fr)$ in the burnt gases have also been calculated using the following formulae:

$$\gamma_2(fr) = \frac{\sum_{i=1}^{k} n_i \cdot C_{p,i}}{\sum_{i=1}^{k} n_i\left[C_{p,i} - R^{\circ}\right]}$$

where $C_{p,i}$ is the molar specific heat at constant pressure of species i,

$$M_2(fr) = V_2/c_2(fr)$$

and

$$c_2(fr) = \left(\gamma_2(fr)\, R^{\circ} T_2/\bar{W}_2\right)^{\frac{1}{2}},$$

where $c_2(fr)$ is the frozen sound speed of the burnt gases. All thermodynamic data, namely, enthalpy differences, standard free energies of formation and molar specific heats at constant pressure tabulated in Ref. 30 were fitted by a least-squares fit program to polynomials of degree equal or greater than four, in the temperature range from 2000 to 5000°K. Calculations were performed in double precision on an IBM360/75 OS and the results shown in Tables I-XVIII are presented in computer outputs. In these tables, each specie name denotes the corresponding mole percent, the pressures are in atmospheres and the fluid velocities with respect to the stationary detonation wave are in km/sec.

4. RESULTS

In this section, we present the calculated properties of C-J detonation waves in (H_2-Cl_2), (CS_2-O_2) and (CO-O_2-H_2-N_2) systems. All calculations were performed with initial pressures ranging from 30 to 760 torr and an initial temperature of 298^0K. Initial mixture compositions were also varied.

4.1 The (H_2-Cl_2) System

The equilibrium composition at the C-J plane in (H_2-Cl_2) detonations consists of five species, namely, Cl_2, Cl, H_2, H and HCl. The relevant equations and detailed analysis of the (H_2-Cl_2) chemistry are given in Appendix I.

The detonation properties calculated by the method described in Section 3 are presented in Tables I to VII and plotted in Figs. 2 to 6 for Cl_2 initial mole percent ranging from 30 to 70 and initial pressures from 30 to 760 torr. At constant initial pressure, the detonation velocity (Fig. 2) first decreases quite linearly with increasing Cl_2 initial mole percent, up to 50%, then decreases sharply with Cl_2 increasing from 50 to ∿ 57.5%, then retains a negative slope with Cl_2 increasing up to 70%, the limit of the present calculation. At constant Cl_2 initial mole percent, decreasing the initial pressure causes a small decrease in the detonation velocity, the largest drop ($\simeq$ 6%) occurring for the stoichiometric mixture. Figure 3 shows the corresponding variations of the temperature ratio T_2/T_1 with initial pressure p_1 and Cl_2 initial mole percent. At any initial pressure (30 - 760 torr), the maximum temperature ratio does not occur for the stoichiometric mixture but is shifted towards lower Cl_2 concentration (approximately around 47.5%). The maximum also becomes quite flat at pressures below 100 torr. On the other hand, the pressure ratio $\bar{p}_2/p_1$ and the detonation Mach number M_1, shown in Figs. 4 and 5, peak at 50% Cl_2 initial mole fraction for all initial pressures as expected from stoichiometry, while retaining the same qualitative shape as the temperature ratio. The HCl mole percent variations shown in Fig. 6 exhibit the same qualitative behavior as the other thermodynamic parameters but the maximum HCl mole percent shifts from 50% initial Cl_2 at atmospheric pressure, as expected from stoiometry, to ∿ 55% initial Cl_2 at 30 torr. The present results are in good agreement with Zel'dovich's calculated detonation parameters [20] in stoichiometric mixtures at 760 and 200 torr, initial pressure. Therefore, the qualitative discrepancy between calculated [20] and experimentally measured [18, 19] detonation velocities, already discussed in Section 1, is also reflected by the present calculation. Similarly, comparison of the present calculation with Dixon's measurements [17] at atmospheric pressure and varying initial composition shows a poor agreement (Fig. 2), calculated detonation velocities being higher at low Cl_2 mole percent and lower for the stoichiometric mixture. Experiments at subatmospheric pressures are in progress and the results will be compared to the theoretical values in a near future.

4.2 The (CS_2-O_2) System

Whereas the (H_2-Cl_2) system has only one stoichiometric composition, the equimolar one, the (CS_2-O_2) system possesses at least three stoichiometries, namely:

$$CS_2 + 3O_2 \rightarrow CO_2 + 2SO_2, \tag{4.2.1}$$

$$CS_2 + 2O_2 \rightarrow CO_2 + 2SO, \tag{4.2.2}$$

and

$$CS_2 + O_2 \rightarrow 2CO + 2S_2 \tag{4.2.3}$$

Therefore, under detonative combustion, CO, CO_2, SO, SO_2 and S_2 are likely to be found in the burnt gas at the C-J flame. In addition, kinetic studies in shocked-heated (CS_2-O_2) mixtures, highly diluted in A, also include among the product, carbonyl sulfide, COS [16, 31]. Hence, the equilibrium composition at the C-J plane should consist of 11 species, namely, CS_2, CS, CO, CO_2, COS, O_2, O, SO_2, SO, S_2 and S. We have also included in the calculation C_2 and C to account for CO and CS dissociations. The detailed analysis of the equilibrium composition at the C-J plane in (CS_2-O_2) mixtures is given in Appendix II. The results are presented in Tables VIII to XIII and Figs. 7 to 19, for initial pressures ranging from 30 to 760 torr and CS_2 initial mole percent from 25 to 80%. Below 25% initial CS_2 and above 80% initial CS_2, no solution could be obtained. The absence of theoretical solutions beyond these initial compositions may correspond to the detonability limits of the (CS_2-O_2) mixture, although the model does not account for these limits. At constant initial pressure, detonation velocities decrease with increasing CS_2 initial mole percent and seem to be maximum at 25% initial CS_2 (Figs. 7, 11). At constant initial composition, decreasing the initial pressure from 760 to 30 torr decreases the detonation velocity comparison with an experimentally measured value in ($CS_2 + 3O_2$) mixture at 1 atm. initial pressure [25] shows some disagreement, the calculated value being ∿ 1.4% less than the measured one. Such a discrepancy may result from achievement of partial equilibrium at the C-J plane. Due to the various possible stoichiometries of the (CS_2-O_2) system, it is difficult to define a priori the stoichiometry for which all thermodynamic parameters will be maximum. From Figs. 8 and 12, it is seen that the temperature ratio T_2/T_1 is maximum at ∿ 30% initial CS_2 for all initial pressures considered in the present calculation whereas the pressure ratio P_2/p_1 (Figs. 9, 13) and detonation Mach number M_1 (Figs. 10, 14) are both maximum at ∿ 35% initial CS_2, for the same range of initial pressures. Therefore, the stoichiometry described by Eqs. (4.2.2) corresponding to a ($CS_2 + 2O_2$) mixture seems to prevail under detonative combustion. In addition, all detonation parameters (Figs. 11-14) show a very sharp decrease at 60% initial CS_2. This behavior may reflect a shift in shoichiometry from (CS_2 + $2O_2$) to ($2CS_2$ + O_2) and is supported by the corresponding variations in product mole percents as shown in Figs. 15 - 19. As expected from stoichiometry (Eq. 4.2.1), CO_2 is maximum, although much smaller than the CO mole percent, for (CS_2) initial = 25% at all initial pressures considered Fig. 15). Similarly, SO_2 is also maximum for the same initial composition (Fig. 16). Increasing the fuel mole percent shifts the stoichiometry to the reaction described by Eqs. (4.2.2), hence resulting in SO reaching a maximum at ∿ 35% (Fig. 17). Further increase in fuel concentration shifts again the stoichiometry to the reaction described by Eq. (4.2.3), resulting in CO and S_2 reaching a maximum at ∿ 70% initial CS_2 (Figs. 18, 19). Moreover, in this case, equal mole percents of CO and S_2 are approximately formed, in good agreement with the corresponding stoichiometry. Whereas all detonation parameters decrease with decreasing initial pressures, the CO mole percent increase with increasing initial pressure (Fig. 18), S_2 and SO mole percents first decrease, then increase after reaching their maximum (Figs. 17 and 19) and CO_2 and SO_2 mole percents exhibit the same qualitative behavior as the detonation parameters (Fig. 15, 16). The lack of experimental data makes it difficult to draw any conclusion on the behavior of the (CS_2-O_2) system under detonative combustion. Experiments are in progress and will be compared with theoretical data in a near future.

4.3 The $(CO-H_2-O_2-N_2)$ System

For an (H_2-O_2) system, the relevant stoichiometry is:

$$H_2 + .5O_2 \rightarrow H_2O \qquad (4.3.1)$$

Accounting for dissociation and recombination under detonative combustion, the equilibrium composition should consist of six species, namely, H_2, O_2, H, O, OH and H_2O. Addition of carbon monoxide to the (H_2-O_2) system while maintaining the stoichiometry, i.e., fuel/oxidizer = 2, viz.,

$$[yH_2 + (1-y)CO] + .5O_2 \rightarrow yH_2O + (1-y)CO_2 \qquad (4.3.2)$$

yields CO_2 as reaction product. Again, accounting for dissociation and recombination, the relevant equilibrium composition for the $(CO-O_2-H_2)$ system should consist of ten species, namely, H_2, O_2, CO, CO_2, H, O, OH, H_2O, C_2 and C. Finally, with nitrogen distribution, N_2, N, NO, NO_2, N_2O, HN and HNO should also be included in the equilibrium composition at the C-J plane. Therefore, we shall consider seventeen species to be present at the C-J plane in detonations in $(CO-O_2-H_2-N_2)$ system. The detailed analysis of the chemistry of this system is presented in Appendix III.

Because experimental data are available for the undiluted system only, we have first calculated detonation parameters in the stoichiometric mixture given by Eq. (4.3.2) at atmospheric pressure, initially. The results of these calculations with varying initial CO mole percent are shown in Table XIV and Figs. 20 - 24. Complete agreement with Lu et al's [26] calculated detonation velocities is shown in Fig. 20 whereas experimental data [26, 27] are about 2% lower than the theoretical ones. As shown in Figs. 21 - 23, temperature and pressure ratios and detonation Mach number all exhibit a minimum at a high CO content. However, the minimum temperature ratio occurs at ∿ 85% initial $CO/(CO + H_2)$ whereas the pressure ratio and detonation Mach number have a minimum at ∿ 80% initial $CO/(CO + H_2)$. CO and CO_2 product mole percents (Fig. 24) are seen to increase with increasing $CO/(CO + H_2)$ initial mole percent, the CO mole percent being larger than the CO_2 mole percent at low initial $CO/(CO + H_2)$ content whereas the reverse is true at high initial $CO/(CO + H_2)$ content, both product percentages being equal for ∿ 80% $CO/(CO + H_2)$ initial.

With nitrogen dilution, no experimental data are yet available for comparison with the theoretical results presented in Tables 15 - 18 and Figs. 25 - 29. In these calculations, we maintain the stoichiometry as given by Eqs. (4.3.2), the initial H_2 mole percent being fixed at 1% and the initial N_2 mole percent varying from 10 to 40%. At constant initial pressure, with increasing N_2 dilution, all detonation properties decrease monotonically. Similarly, at constant N_2 dilution, decreasing the initial pressure also decreases all detonation properties. The corresponding variations of the CO_2 and CO product mole percents are shown in Fig. 29. The CO_2 mole percent exhibits the same qualitative behavior as the thermodynamic properties when the initial pressure and/or the N_2 dilution are varied whereas the CO mole percent increases with decreasing initial pressure at constant N_2 dilution being slightly larger (a few percent) than the CO_2 mole percent at low dilution and initial pressure and smaller (∿ 15%) than the CO_2 mole percent at larger N_2 dilution for any initial pressure in the range (760 - 30 torr). The calculation was not carried beyond 40% N_2 dilution because one may expect quenching of the detonation in highly diluted mixture. These results will be compared with experimental data in a near future.

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Appendix I

The overall reaction for the equilibrium composition at the C-J plane in $(H_2\text{-}Cl_2)$ mixtures can be written as:

$$a_1 Cl_2 + a_2 H_2 \rightarrow b_1 Cl_2 + b_2 H_2 + b_3 Cl + b_4 H + b_5 HCl \quad (I.1)$$

where the a's and b's denote reactant and product mole numbers, respectively. The corresponding atom balance equations are:

$$[Cl] \quad 2a_1 = 2b_1 + b_3 + b_5 \quad (I.2)$$

$$[H] \quad 2a_2 = 2b_2 + b_4 + b_5 \quad (I.3)$$

For a given temperature T_2 and a given volume v_2 of the burnt mixture, the equilibrium composition is determined by solving simultaneously the atom balance and equilibrium equations. Therefore, three equilibrium equations are needed corresponding to the following chemical reactions, viz.,

$$\frac{1}{2} H_2 \overset{K_1}{\rightleftharpoons} H \quad (I.4)$$

$$\frac{1}{2} Cl_2 \overset{K_2}{\rightleftharpoons} Cl \quad (I.5)$$

$$\frac{1}{2} H_2 + \frac{1}{2} Cl_2 \overset{K_3}{\rightleftharpoons} HCl \quad (I.6)$$

where the K's are the corresponding equilibrium constants, namely,

$$K_1 = p_H / p_{H_2}^{\frac{1}{2}} = (b_4 / b_2^{1/2})\chi \tag{I.7}$$

$$K_2 = p_{Cl} / p_{Cl_2}^{1/2} = (b_3 / b_1^{\frac{1}{2}})\chi \tag{I.8}$$

$$K_3 = p_{HCl} / (p_{Cl_2} p_{H_2})^{1/2} = b_5 / (b_1 b_2)^{1/2} \tag{I.9}$$

where

$$\chi = (R^\circ T_2 / v_2)^{1/2} \tag{I.10}$$

Defining

$$B_i = \log_e b_i \quad , \; i = 1, 2, \cdot\cdot, 5$$

it can be seen that Eqs. (I.2, I.3, I.7-I.9) can be expressed in terms of B_3 and B_4 for given T_2 and v_2. Solving Eqs. (I.7-I.9) yields:

$$b_1 = b_3^2 / C_1 \tag{I.11}$$

$$b_2 = b_4^2 / C_2 \tag{I.12}$$

$$b_5 = b_3 b_4 / C_3 \tag{I.13}$$

where the C's are functions of T_2 and v_2, only, viz.,

$$C_1 = k_2^2(T_2)/\chi^2 \tag{I.14.a}$$

$$C_2 = k_1^2(T_2)/\chi^2 \tag{I.14.b}$$

$$C_3 = k_1(T_2)k_2(T_2)/(k_3(T_2)\chi^2) \tag{I.14.c}$$

Using Eqs. (I.11-I.14) into Eqs. (I.2, I.3) yields a system of two non-linear, algebraic equations in b_3, b_4, T_2 and v_2, viz.,

$$F(x, y, T_2, v_2) \equiv \left[\frac{2x^2}{C_1} + x + \frac{xy}{C_3}\right] - 2a_1 = 0$$

$$G(x, y, T_2, v_2) \equiv \left[\frac{2y^2}{C_2} + y + \frac{xy}{C_3}\right] - 2a_2 = 0$$

where $x \equiv b_3$ and $y \equiv b_4$. For given values of T_2 and v_2, this system can readily be solved for x and y by the Newton-Raphson method and the remaining unknowns, namely, b_1, b_2 and b_5 are then given by Eqs. (I.11-I.13).

Appendix II

The overall reaction for the equilibrium composition at the C-J plane in (CS_2-O_2) mixtures is:

$$a_1 CS_2 + a_2 O_2 \rightarrow b_1 CS_2 + b_2 CS + b_3 CO + b_4 COS + b_5 C_2 + b_6 C + b_7 O_2 + b_8 O + b_9 SO_2 + b_{10} SO + b_{11} S_2 + b_{12} S + b_{13} CO_2 \qquad (II.1)$$

The corresponding atom balance equations are written as:

$$[C]: a_1 = b_1 + b_2 + b_3 + b_4 + 2b_5 + b_6 + b_{13} \qquad (II.2)$$

$$[S]: 2a_1 = 2b_1 + b_2 + b_4 + b_9 + b_{10} + 2b_{11} + b_{12} \qquad (II.3)$$

$$[O]: 2a_2 = b_3 + b_4 + 2b_7 + b_8 + 2b_9 + b_{10} + 2b_{13} \qquad (II.4)$$

Since thirteen species are assumed to be present at the C-J plane and three atom balance equations can be written for the (CS_2-O_2) system, ten equilibrium equations are needed to obtain the equilibrium composition for given T_2 and v_2. These equations correspond to the following chemical reactions, viz.,

$$\frac{1}{2}O_2 \overset{k_1}{\rightleftharpoons} O \qquad \text{(II.5.a)}$$

$$SO_2 \overset{k_2}{\rightleftharpoons} SO + \frac{1}{2}O_2 \qquad \text{(II.5.b)}$$

$$CS_2 \overset{k_3}{\rightleftharpoons} CS + \frac{1}{2}S_2 \qquad \text{(II.5.c)}$$

$$SO \overset{k_4}{\rightleftharpoons} \frac{1}{2}S_2 + \frac{1}{2}O_2 \qquad \text{(II.5.d)}$$

$$\frac{1}{2}S_2 \overset{k_5}{\rightleftharpoons} S \qquad \text{(II.5.e)}$$

$$CS \overset{k_6}{\rightleftharpoons} \frac{1}{2}C_2 + \frac{1}{2}S_2 \qquad \text{(II.5.f)}$$

$$\frac{1}{2}C_2 \overset{k_7}{\rightleftharpoons} C \qquad \text{(II.5.g)}$$

$$COS \overset{k_8}{\rightleftharpoons} CS + \frac{1}{2}O_2 \qquad \text{(II.5.h)}$$

$$CO \overset{k_9}{\rightleftharpoons} \frac{1}{2}C_2 + \frac{1}{2}O_2 \qquad \text{(II.5.i)}$$

$$CO_2 \overset{k_{10}}{\rightleftharpoons} CO + \frac{1}{2}O_2 \qquad \text{(II.5.j)}$$

and the corresponding equilibrium equations in terms of equilibrium constants are:

$$K_1 = \frac{p_O}{p_{O_2}^{1/2}} = \frac{b_8}{b_7^{1/2}}\chi \qquad \text{(II.6)}$$

$$K_2 = \frac{p_{SO}\,p_{O_2}^{1/2}}{p_{SO_2}} = \frac{b_7^{1/2}\,b_{10}}{b_9}\chi \qquad \text{(II.7)}$$

$$K_3 = \frac{p_{CS}\,p_{S_2}^{1/2}}{p_{CS_2}} = \frac{b_2\,b_{11}^{1/2}}{b_1}\chi \qquad \text{(II.8)}$$

$$K_4 = \frac{(p_{S_2}\,p_{O_2})^{1/2}}{p_{SO}} = \frac{(b_7\,b_{11})^{1/2}}{b_{10}} \qquad \text{(II.9)}$$

$$K_5 = \frac{p_S}{p_{S_2}^{1/2}} = \frac{b_{12}}{b_{11}^{1/2}}\chi \qquad \text{(II.10)}$$

$$K_6 = \frac{(p_{C_2}\,p_{S_2})^{1/2}}{p_{CS}} = \frac{(b_5\,b_{11})^{1/2}}{b_2} \qquad \text{(II.11)}$$

$$K_7 = \frac{p_C}{p_{C_2}^{1/2}} = \frac{b_6}{b_5^{1/2}}\chi \qquad \text{(II.12)}$$

$$K_8 = \frac{p_{CS}\, p_{O_2}^{1/2}}{p_{COS}} = \frac{b_2\, b_7^{1/2}}{b_4}\, \chi \qquad \text{(II.13)}$$

$$K_9 = \frac{(p_{C_2}\, p_{O_2})^{1/2}}{p_{CO}} = \frac{(b_5 b_7)^{1/2}}{b_3} \qquad \text{(II.14)}$$

$$K_{10} = \frac{p_{CO}\, p_{O_2}^{1/2}}{p_{CO_2}} = \frac{b_3\, b_7^{1/2}}{b_{13}}\, \chi \qquad \text{(II.15)}$$

where

$$\chi = (R^\circ T_2 / v_2)^{1/2} \qquad \text{(II.16)}$$

Defining:

$$B_i = \log_e b_i \ , \quad i = 1, 2, \cdots, 13 \ .$$

it can be seen that all the b's in Eqs. (II.6-II.16) can be expressed as functions of T_2 , v_2 and b_6 , b_8 , b_{12} , the C , O and S atom numbers, respectively, viz.,

$$b_1 = b_6\, b_{12}^2 / C_1$$

$$b_2 = b_6\, b_{12} / C_2$$

$$b_3 = b_6\, b_8 / C_3$$

$$b_4 = b_6 b_8 b_{12}/C_4$$

$$b_5 = b_6^2/C_5$$

$$b_7 = b_8^2/C_6$$

$$b_9 = b_8^2 b_{12}/C_7 \qquad \text{(II.17)}$$

$$b_{10} = b_8 b_{12}/C_8$$

$$b_{11} = b_{12}^2/C_9$$

$$b_{13} = b_6 b_8^2/C_{10}$$

where the C's are functions of T_2 and v_2, only, viz.,

$$C_1 = K_3 K_5^2 K_6 K_7/\chi^2$$

$$C_2 = K_5 K_6 K_7/\chi^2$$

$$C_3 = K_1 K_7 K_9/\chi^2$$

$$\begin{aligned}
C_4 &= K_1 K_5 K_6 K_7 K_8 / \chi^4 \\
C_5 &= K_7^2 / \chi^2 \\
C_6 &= K_1^2 / \chi^2 \\
C_7 &= K_1^2 K_2 K_4 K_5 / \chi^4 \\
C_8 &= K_1 K_4 K_5 / \chi^2 \\
C_9 &= K_5^2 / \chi^2 \\
C_{10} &= K_1^2 K_7 K_9 K_{10} / \chi^4
\end{aligned} \tag{II.18}$$

Using Eqs. (II.17) into Eqs. (II.2-II.4) yields a system of three, non-linear, algebraic equations in five unknowns b_6, b_8, b_{12}, T_2 and v_2, namely,

$$F(x,y,z,T_2,v_2) = \frac{xy^2}{C_1} + \frac{xy}{C_2} + \frac{xz}{C_3} + \frac{xyz}{C_4}$$

$$+ \frac{2x^2}{C_5} + x + \frac{xz^2}{C_{10}} - a_1 = 0$$

$$G(x,y,z,T_2,v_2) = \frac{2xy^2}{C_1} + \frac{xy}{C_2} + \frac{xyz}{C_4} + \frac{yz^2}{C_7}$$

$$+ \frac{yz}{C_8} + \frac{2y^2}{C_9} + y - 2a_1 = 0$$

$$H(x,y,z,T_2,v_2) = \frac{xz}{C_3} + \frac{xyz}{C_4} + \frac{2z^3}{C_6} + z$$

$$+ \frac{2yz^2}{C_7} + \frac{yz}{C_8} + \frac{2xz^2}{C_{10}} - 2a_2 = 0$$

where $x \equiv b_6$, $y \equiv b_{12}$ and $z \equiv b_8$. These equations are readily solved for given v_2 and T_2 by the Newton-Raphson method, then Eqs. (II.17) give the remaining unknown b's.

Appendix III

A. The $(CO-H_2-O_2)$ System

The overall reaction for the equilibrium composition at the C-J plane is written as:

$$a_1 CO + a_2 O_2 + a_3 H_2 \rightarrow b_1 CO_2 + b_2 CO + b_3 O_2 + b_4 O + b_5 H_2O + b_6 OH + b_7 H_2 + b_8 H + b_9 C_2 + b_{10} C \quad \text{(III.A.1)}$$

The corresponding atom balance equations are:

$$[C]: \quad a_1 = b_1 + b_2 + 2b_9 + b_{10} \quad \text{(III.A.2)}$$

$$[O]: \quad a_1 + 2a_2 = 2b_1 + b_2 + 2b_3 + b_4 + b_5 + b_6 \quad \text{(III.A.3)}$$

$$[H]: \quad 2a_3 = 2b_5 + b_6 + 2b_7 + b_8 \quad \text{(III.A.4)}$$

For given temperature and volume of the burnt gas mixture, the equilibrium composition (10 species) is completely determined by solving simultaneously the atom balance and equilibrium equations. Therefore, seven equilibrium equations are needed, representing the following reactions:

$$CO_2 \overset{K_1}{\rightleftharpoons} CO + \frac{1}{2}O_2 \tag{III.A.5}$$

$$CO \overset{K_2}{\rightleftharpoons} \frac{1}{2}C_2 + \frac{1}{2}O_2 \tag{III.A.6}$$

$$\frac{1}{2}O_2 \overset{K_3}{\rightleftharpoons} O \tag{III.A.7}$$

$$\frac{1}{2}C_2 \overset{K_4}{\rightleftharpoons} C \tag{III.A.8}$$

$$\frac{1}{2}H_2 \overset{K_5}{\rightleftharpoons} H \tag{III.A.9}$$

$$H_2O \overset{K_6}{\rightleftharpoons} H_2 + \frac{1}{2}O_2 \tag{III.A.10}$$

$$OH \overset{K_7}{\rightleftharpoons} \frac{1}{2}O_2 + \frac{1}{2}H_2 \tag{III.A.11}$$

where the K's are the corresponding equilibrium constants, viz.,

$$K_1 = \frac{p_{CO}\,p_{O_2}^{1/2}}{p_{CO_2}} = \frac{b_2 b_3^{1/2}}{b_1}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \tag{III.A.12}$$

$$K_2 = \frac{p_{C_2}^{1/2}\,p_{O_2}^{1/2}}{p_{CO}} = \frac{(b_3 b_9)^{1/2}}{b_2} \tag{III.A.13}$$

$$K_3 = \frac{p_O}{p_{O_2}^{1/2}} = \frac{b_4}{b_3^{1/2}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \tag{III.A.14}$$

$$K_4 = \frac{p_C}{p_{C_2}^{1/2}} = \frac{b_{10}}{b_9^{1/2}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \tag{III.A.15}$$

$$K_5 = \frac{p_H}{p_{H_2}^{1/2}} = \frac{b_8}{b_7^{1/2}}\left(\frac{R^0 T_2}{v_2}\right)^{1/2} \qquad \text{(III.A.16)}$$

$$K_6 = \frac{p_{OH} \cdot p_{H_2}^{1/2}}{p_{H_2O}} = \frac{b_6 b_7^{1/2}}{b_5}\left(\frac{R^0 T_2}{v_2}\right)^{1/2} \qquad \text{(III.A.17)}$$

and

$$K_7 = \frac{(p_{O_2} p_{H_2})^{1/2}}{p_{OH}} = \frac{(b_3 b_7)^{1/2}}{b_6} \qquad \text{(III.A.18)}$$

Defining: $B_i \equiv \log_e b_i$ and $\chi \equiv (R^0 T_2 / v_2)^{1/2}$, inspection of Eqs. (III.A.2 - III.A.4, III.A.12 - III.A.18) shows that for given T_2 and v_2, all the b's are functions of the atom numbers only, namely, b_4, b_8 and b_{10}, respectively. Solving Eqs. (III.A.13 - III.A.18) in terms of b_4, b_8 and b_{10} yields the equilibrium composition, viz.,

$$b_1 = b_4^2 b_{10} / C_1 \qquad \text{(III.A.19)}$$

$$b_2 = b_4 b_{10} / C_2 \qquad \text{(III.A.20)}$$

$$b_3 = b_4^2 / C_3 \qquad \text{(III.A.21)}$$

$$b_5 = b_4 b_8^2 / C_4 \qquad \text{(III.A.22)}$$

$$b_6 = b_4 b_8 / C_5 \qquad \text{(III.A.23)}$$

$$b_7 = b_8^2 / C_6 \qquad \text{(III.A.24)}$$

$$b_9 = b_{10}^2 / C_7 \qquad \text{(III.A.25)}$$

where the C's are functions of T_2 and v_2 only, and are given by the following relations:

$$C_1 = k_1 k_2 k_3^2 k_4 / \chi^4 \tag{III.A.26}$$

$$C_2 = k_2 k_3 k_4 / \chi^2 \tag{III.A.27}$$

$$C_3 = k_3^2 / \chi^2 \tag{III.A.28}$$

$$C_4 = k_3 k_5^2 k_6 k_7 / \chi^4 \tag{III.A.29}$$

$$C_5 = k_3 k_5 k_7 / \chi^2 \tag{III.A.30}$$

$$C_6 = k_5^2 / \chi^2 \tag{III.A.31}$$

$$C_7 = k_4^2 / \chi^2 \tag{III.A.32}$$

Using Eqs. (III.A. 19 - III.A.25), Eqs. (III.A.2 - III.A.4) become:

$$F(x,y,z,T_2,v_2) \equiv \frac{x^2 z}{C_1} + \frac{xz}{C_2} + \frac{2z^2}{C_7} + z - a_1 = 0$$

$$\begin{aligned} G(x,y,z,T_2,v_2) \equiv {} & \frac{2x^2 z}{C_1} + \frac{xz}{C_2} + \frac{2x^2}{C_3} \\ & + x + \frac{xy^2}{C_4} + \frac{xy}{C_5} \\ & - (a_1 + 2a_2) = 0 \end{aligned}$$

$$H(x,y,z,T_2,v_2) \equiv \frac{2xy^2}{C_4} + \frac{xy}{C_5} + \frac{2y^2}{C_6} + y - 2a_3 = 0$$

where $x \equiv b_4$, $y \equiv b_8$ and $z \equiv b_{10}$, respectively. This system of three, non-linear, algebraic equations may be solved by the Newton-Raphson method for a given temperature T_2 and a given volume v_2 and the corresponding equilibrium composition is completely determined by using Eqs. (III.A.19 - III.A.25).

B. The $(CO\text{-}H_2\text{-}O_2\text{-}N_2)$ System

The overall reaction for the equilibrium composition at the C-J plane is given by:

$$\begin{aligned} a_1 CO + a_2 O_2 + a_3 N_2 + a_4 H_2 \longrightarrow \\ b_1 CO_2 + b_2 CO + b_3 O_2 + b_4 O \\ + b_5 N_2 + b_6 N + b_7 NO + b_8 N_2O \\ + b_9 NO_2 + b_{10} H_2O + b_{11} OH + b_{12} H_2 \\ + b_{13} H + b_{14} C_2 + b_{15} C + b_{16} NH + b_{17} HNO \end{aligned} \qquad \text{(III.B.1)}$$

The corresponding atom balance equations are:

$$[C]:\ a_1 = b_1 + b_2 + 2b_{14} + b_{15} \qquad \text{(III.B.2)}$$

$$\begin{aligned} [O]:\ a_1 + 2a_2 = 2b_1 + b_2 + 2b_3 + b_4 + b_7 \\ + b_8 + 2b_9 + b_{10} + b_{11} + b_{17} \end{aligned} \qquad \text{(III.B.3)}$$

$$[N]:\ 2a_3 = 2b_5 + b_6 + b_7 + 2b_8 + b_9 + b_{16} + b_{17} \tag{III.B.4}$$

$$[H]:\ 2a_4 = 2b_{10} + b_{11} + 2b_{12} + b_{13} + b_{16} + b_{17} \tag{III.B.5}$$

The equilibrium composition consisting of 17 species is obtained by solving simultaneously the atom balance and equilibrium equations for a given temperature T_2 and a given volume $\mathcal{V}_2$ of the burnt mixture. Therefore, 13 equilibrium equations are needed, corresponding to the following reactions:

$$CO_2 \overset{K_1}{\rightleftharpoons} CO + \tfrac{1}{2}O_2 \tag{III.B.6}$$

$$CO \overset{K_2}{\rightleftharpoons} \tfrac{1}{2}C_2 + \tfrac{1}{2}O_2 \tag{III.B.7}$$

$$\tfrac{1}{2}O_2 \overset{K_3}{\rightleftharpoons} O \tag{III.B.8}$$

$$\tfrac{1}{2}C_2 \overset{K_4}{\rightleftharpoons} C \tag{III.B.9}$$

$$\tfrac{1}{2}N_2 \overset{K_5}{\rightleftharpoons} N \tag{III.B.10}$$

$$NO \overset{K_6}{\rightleftharpoons} \tfrac{1}{2}N_2 + \tfrac{1}{2}O_2 \tag{III.B.11}$$

$$NO_2 \overset{K_7}{\rightleftharpoons} \tfrac{1}{2}O_2 + NO \tag{III.B.12}$$

$$N_2O \overset{K_8}{\rightleftharpoons} \tfrac{1}{2}N_2 + NO \qquad \text{(III.B.13)}$$

$$\tfrac{1}{2}H_2 \overset{K_9}{\rightleftharpoons} H \qquad \text{(III.B.14)}$$

$$H_2O \overset{K_{10}}{\rightleftharpoons} OH + \tfrac{1}{2}H_2 \qquad \text{(III.B.15)}$$

$$OH \overset{K_{11}}{\rightleftharpoons} \tfrac{1}{2}O_2 + \tfrac{1}{2}H_2 \qquad \text{(III.B.16)}$$

$$NH \overset{K_{12}}{\rightleftharpoons} \tfrac{1}{2}N_2 + \tfrac{1}{2}H_2 \qquad \text{(III.B.17)}$$

$$HNO \overset{K_{13}}{\rightleftharpoons} \tfrac{1}{2}H_2 + NO \qquad \text{(III.B.18)}$$

where the K's are the corresponding equilibrium constants, viz.,

$$K_1 = \frac{p_{CO}\,p_{O_2}^{1/2}}{p_{CO_2}} = \frac{b_2 b_3^{1/2}}{b_1}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.19)}$$

$$K_2 = \frac{(p_{C_2}\,p_{O_2})^{1/2}}{p_{CO}} = \frac{(b_3 b_4)^{1/2}}{b_2} \qquad \text{(III.B.20)}$$

$$K_3 = \frac{p_O}{p_{O_2}^{1/2}} = \frac{b_4}{b_3^{1/2}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.21)}$$

$$K_4 = \frac{p_C}{p_{C_2}^{1/2}} = \frac{b_{15}}{b_{14}^{1/2}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.22)}$$

$$K_5 = \frac{p_N}{p_{N_2}^{1/2}} = \frac{b_6}{b_5^{1/2}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.23)}$$

$$K_6 = \frac{(p_{N_2} p_{O_2})^{1/2}}{p_{NO}} = \frac{(b_3 b_5)^{1/2}}{b_7} \qquad \text{(III.B.24)}$$

$$K_7 = \frac{p_{NO} p_{O_2}^{1/2}}{p_{NO_2}} = \frac{b_7 b_3^{1/2}}{b_9}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.25)}$$

$$K_8 = \frac{p_{NO} p_{N_2}^{1/2}}{p_{N_2O}} = \frac{b_7 b_5^{1/2}}{b_8}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.26)}$$

$$K_9 = \frac{p_H}{p_{H_2}^{1/2}} = \frac{b_{13}}{b_{12}^{1/2}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.27)}$$

$$K_{10} = \frac{p_{H_2}^{1/2} p_{OH}}{p_{H_2O}} = \frac{b_{12}^{1/2} b_{11}}{b_{10}}\left(\frac{R^\circ T_2}{v_2}\right)^{1/2} \qquad \text{(III.B.28)}$$

$$K_{11} = \frac{(p_{H_2} p_{O_2})^{1/2}}{p_{OH}} = \frac{(b_3 b_{12})^{1/2}}{b_{11}} \qquad \text{(III.B.29)}$$

$$K_{12} = \frac{(p_{N_2} p_{H_2})^{1/2}}{p_{NH}} = \frac{(b_5 b_{12})^{1/2}}{b_{16}} \qquad \text{(III.B.30)}$$

$$K_{13} = \frac{p_{H_2}^{1/2} p_{NO}}{p_{HNO}} = \frac{b_7 b_{12}^{1/2}}{b_{17}} \left(\frac{R^\circ T_2}{V_2}\right)^{1/2} \qquad \text{(III.B.31)}$$

Defining $B_i \equiv \log_e b_i$ and $\chi \equiv (R^\circ T_2/V_2)^{1/2}$, inspection of Eqs. (III.B.2 - III.B.31) shows that b_4, b_6, b_{13} and b_{15} (the O, N, H and C atom numbers, respectively) can be chosen as independent variables. Solving Eqs. (III.B.19 - III.B.31) in terms of these variables yields:

$$b_1 = b_4^2 b_{15} / C_1 \qquad \text{(III.B.32)}$$

$$b_2 = b_4 b_{15} / C_2 \qquad \text{(III.B.33)}$$

$$b_3 = b_4^2 / C_3 \qquad \text{(III.B.34)}$$

$$b_5 = b_6^2 / C_4 \qquad \text{(III.B.35)}$$

$$b_7 = b_4 b_6 / C_5 \qquad \text{(III.B.36)}$$

$$b_8 = b_4 b_6^2 / C_6 \qquad \text{(III.B.37)}$$

$$b_9 = b_4^2 b_6 / C_7 \qquad \text{(III.B.38)}$$

$$b_{10} = b_4 b_{13}^2 / C_8 \qquad \text{(III.B.39)}$$

$$b_{11} = b_4 b_{13} / C_9 \qquad \text{(III.B.40)}$$

$$b_{12} = b_{13}^2 / C_{10} \tag{III.B.41}$$

$$b_{14} = b_{15}^2 / C_{11} \tag{III.B.42}$$

$$b_{16} = b_6 b_{13} / C_{12} \tag{III.B.43}$$

$$b_{17} = b_4 b_6 b_{13} / C_{13} \tag{III.B.44}$$

where the C's are functions of v_2 and T_2 only and are given by:

$$\begin{aligned}
C_1 &= K_1 K_2 K_3^2 K_4 / \chi^4 \\
C_2 &= K_2 K_3 K_4 / \chi^2 \\
C_3 &= (K_3 / \chi)^2 \\
C_4 &= (K_5 / \chi)^2 \\
C_5 &= K_3 K_5 K_6 / \chi^2 \\
C_6 &= K_3 K_5^2 K_6 K_8 / \chi^4 \\
C_7 &= K_3^2 K_5 K_6 K_7 / \chi^4 \\
C_8 &= K_3 K_9^2 K_{10} K_{11} / \chi^4 \\
C_9 &= K_3 K_9 K_{11} / \chi^2 \\
C_{10} &= (K_9 / \chi)^2 \\
C_{11} &= (K_4 / \chi)^2 \\
C_{12} &= K_5 K_9 K_{12} / \chi^2 \\
C_{13} &= K_3 K_5 K_6 K_9 K_{13} / \chi^4
\end{aligned} \tag{III.B.45}$$

Substitition of Eqs. (III.B.32 - III.B.44) into Eqs. (III.B.2 - III.B.5) yields a system of four, non-linear, algebraic equations, viz.,

$$F(w,x,y,z,T_2,U_2) \equiv \frac{w^2z}{C_1} + \frac{wz}{C_2} + \frac{2z^2}{C_{11}} + z - a_1 \quad = 0$$

$$G(w,x,y,z,T_2,U_2) \equiv \frac{2w^2z}{C_1} + \frac{wz}{C_2} + \frac{2w^2}{C_3}$$

$$+ w + \frac{wx}{C_5} + \frac{wx^2}{C_6} + \frac{2w^2x}{C_7}$$

$$+ \frac{wy^2}{C_8} + \frac{wy}{C_9} + \frac{wxy}{C_{13}}$$

$$- (a_1 + 2a_2) = 0$$

$$H(w,x,y,z,T_2,U_2) = \frac{2x^2}{C_4} + x + \frac{wx}{C_5} + \frac{2w^2x}{C_6}$$

$$+ \frac{w^2x}{C_7} + \frac{xy}{C_{12}} + \frac{wxy}{C_{13}}$$

$$- 2a_3 \quad = 0$$

$$I(w,x,y,z,T_2,v_2) = \frac{2wy^2}{C_8} + \frac{wy}{C_9} + \frac{2y^2}{C_{10}}$$

$$+ y + \frac{xy}{C_{12}} + \frac{wxy}{C_{13}} - 2a_4 = 0$$

where $w \equiv b_4$, $x \equiv b_6$, $y \equiv b_{13}$ and $z \equiv b_{15}$, respectively. Solving this system by the Newton-Raphson method for given T_2 and v_2 yields the equilibrium atom numbers and the mole numbers are then obtained from Eqs. (III.B.32 - III.B.44).

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Table I

$(Cl_2)_1{}^c$ = .300D 02 γ_1 = .138D 01

$P_1{}^a$	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.917D 01	.904D 01	.890D 01	.880D 01
P_2/P_1	.164D 02	.162D 02	.161D 02	.160D 02
ρ_1/ρ_2	.566D 00	.564D 00	.562D 00	.561D 00
$V_1{}^b$	.197D 01	.195D 01	.194D 01	.193D 01
$V_2{}^b$	.111D 01	.110D 01	.109D 01	.108D 01
M_1	.507D 01	.504D 01	.500D 01	.497D 01
M_2(fr)	.972D 00	.967D 00	.962D 00	.958D 00
γ_2(fr)	.130D 01	.130D 01	.130D 01	.130D 01
$Cl_2{}^c$	.528D-02	.565D-02	.402D-02	.361D-02
$H_2{}^c$	.396D 02	.395D 02	.394D 02	.394D 02
Cl^c	.104D 01	.128D 01	.155D 01	.173D 01
H^c	.993D 00	.122D 01	.148D 01	.166D 01
HCl^c	.583D 02	.580D 02	.575D 02	.572D 02

[a] pressures are in atmospheres; [b] velocities are in km/sec; [c] mole fraction percentage.

Table I (continued)

p_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.876D 01	.871D 01	.864D 01	.854D 01	.847D 01
p_2/p_1	.159D 02	.158D 02	.158D 02	.156D 02	.156D 02
ρ_1/ρ_2	.560D 00	.560D 00	.559D 00	.558D 00	.557D 00
V_1	.192D 01	.192D 01	.191D 01	.190D 01	.189D 01
V_2	.108D 01	.107D 01	.107D 01	.106D 01	.106D 01
M_1	.496D 01	.495D 01	.493D 01	.491D 01	.489D 01
M_2(fr)	.957D 00	.955D 00	.953D 00	.950D 00	.948D 00
γ_2(fr)	.130D 01	.131D 01	.131D 01	.131D 01	.131D 01
Cl_2	.345D-02	.326D-02	.302D-02	.271D-02	.250D-02
H_2	.393D 02	.393D 02	.393D 02	.392D 02	.391D 02
Cl	.181D 01	.190D 01	.203D 01	.220D 01	.233D 01
H	.173D 01	.182D 01	.194D 01	.210D 01	.223D 01
HCl	.571D 02	.570D 02	.568D 02	.565D 02	.563D 02

Table II

$(Cl_2)_1$ = .400D 02 γ_1 = .137D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.103D 02	.100D 02	.975D 01	.958D 01
P_2/P_1	.191D 02	.187D 02	.184D 02	.181D 02
ρ_1/ρ_2	.557D 00	.555D 00	.554D 00	.553D 00
V_1	.185D 01	.183D 01	.181D 01	.179D 01
V_2	.103D 01	.101D 01	.100D 01	.990D 00
M_1	.545D 01	.540D 01	.533D 01	.529D 01
M_2(fr)	.95[illegible] 00	.948D 00	.943D 00	.940D 00
γ_2(fr)	.131D 01	.131D 01	.132D 01	.132D 01
Cl_2	.380D-01	.306D-01	.243D-01	.207D-01
H_2	.208D 02	.208D 02	.209D 02	.209D 02
Cl	.470D 01	.530D 01	.590D 01	.629D 01
H	.194D 01	.221D 01	.249D 01	.267D 01
HCl	.726D 02	.716D 02	.707D 02	.701D 02

Table II (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.951D 01	.943D 01	.933D 01	.918D 01	.908D 01
P_2/P_1	.181D 02	.179D 02	.178D 02	.176D 02	.174D 02
ρ_1/ρ_2	.552D 00	.552D 00	.551D 00	.551D 00	.550D 00
V_1	.179D 01	.178D 01	.177D 01	.176D 01	.175D 01
V_2	.986D 00	.982D 00	.976D 00	.968D 00	.962D 00
M_1	.528D 01	.526D 01	.523D 01	.519D 01	.517D 01
M_2(fr)	.939D 00	.937D 00	.936D 00	.933D 00	.932D 00
γ_2(fr)	.132D 01	.132D 01	.132D 01	.133D 01	.133D 01
Cl_2	.195D-01	.180D-01	.162D-01	.140D-01	.126D-01
H_2	.210D 02	.210D 02	.210D 02	.210D 02	.211D 02
Cl	.644D 01	.663D 01	.686D 01	.719D 01	.742D 01
H	.274D 01	.283D 01	.294D 01	.309D 01	.320D 01
HCl	.698D 02	.696D 02	.692D 02	.687D 02	.683D 02

Table III

$(Cl_2)_1$ = .450D 02

γ_1 = .136D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.105D 02	.102D 02	.994D 01	.976D 01
P_2/P_1	.200D 02	.196D 02	.191D 02	.189D 02
ρ_1/ρ_2	.554D 00	.553D 00	.552D 00	.551D 00
V_1	.179D 01	.176D 01	.174D 01	.173D 01
V_2	.989D 00	.975D 00	.961D 00	.951D 00
M_1	.558D 01	.551D 01	.545D 01	.540D 01
M_2(fr)	.944D 00	.939D 00	.935D 00	.932D 00
γ_2(fr)	.132D 01	.133D 01	.133D 01	.134D 01
Cl_2	.865D-01	.672D-01	.517D-01	.433D-01
H_2	.126D 02	.128D 02	.130D 02	.131D 02
Cl	.787D 01	.863D 01	.935D 01	.982D 01
H	.186D 01	.209D 01	.231D 01	.246D 01
HCl	.776D 02	.764D 02	.753D 02	.746D 02

Table III (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.968D 01	.959D 01	.948D 01	.932D 01	.921D 01
P_2/P_1	.188D 02	.186D 02	.185D 02	.182D 02	.180D 02
ρ_1/ρ_2	.551D 00	.550D 00	.550D 00	.549D 00	.549D 00
V_1	.172D 01	.171D 01	.171D 01	.169D 01	.168D 01
V_2	.948D 00	.943D 00	.937D 00	.929D 00	.924D 00
M_1	.538D 01	.536D 01	.533D 01	.529D 01	.526D 01
M_2	.931D 00	.929D 00	.928D 00	.925D 00	.924D 00
γ_2(fr)	.134D 01	.134D 01	.134D 01	.134D 01	.135D 01
Cl_2	.404D-01	.370D-01	.330D-01	.280D-01	.250D-01
H_2	.132D 02	.132D 02	.133D 02	.134D 02	.134D 02
Cl	.100D 02	.102D 02	.105D 02	.109D 02	.111D 02
H	.252D 01	.259D 01	.268D 01	.281D 01	.290D 01
HCl	.743D 02	.739D 02	.735D 02	.729D 02	.725D 02

Table IV

$(Cl_2)_1$ = .500D 02 γ_1 = .136D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.105D 02	.102D 02	.994D 01	.975D 01
P_2/P_1	.204D 02	.200D 02	.195D 02	.193D 02
ρ_1/ρ_2	.554D 00	.552D 00	.551D 00	.550D 00
V_1	.172D 01	.170D 01	.167D 01	.166D 01
V_2	.951D 00	.937D 00	.929D 00	.914D 00
M_1	.565D 01	.558D 01	.551D 01	.546D 01
M_2(fr)	.936D 00	.931D 00	.927D 00	.924D 00
γ_2(fr)	.135D 01	.135D 01	.136D 01	.136D 01
Cl_2	.210D 00	.156D 00	.116D 00	.950D-01
H_2	.568D 01	.597D 01	.624D 01	.641D 00
Cl	.122D 02	.130D 02	.138D 02	.143D 02
H	.125D 01	.141D 01	.158D 01	.169D 01
HCl	.807D 02	.794D 02	.782D 02	.775D 02

Table IV (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.967D 01	.958D 01	.946D 01	.930D 01	.919D 01
P_2/P_1	.191D 02	.190D 02	.188D 02	.186D 02	.184D 02
ρ_1/ρ_2	.550D 00	.550D 00	.549D 00	.549D 00	.548D 00
V_1	.165D 01	.165D 01	.164D 01	.163D 01	.162D 01
V_2	.910D 00	.906D 00	.900D 00	.892D 00	.887D 00
M_1	.544D 01	.542D 01	.539D 01	.535D 01	.532D 01
M_2(fr)	.923D 00	.921D 00	.920D 00	.917D 00	.916D 00
γ_2(fr)	.136D 01	.136D 01	.136D 01	.137D 01	.137D 01
Cl_2	.877D-01	.796D-01	.702D-01	.587D-01	.517D-01
H_2	.648D 01	.656D 01	.666D 01	.680D 01	.690D 01
Cl	.145D 02	.147D 02	.150D 02	.154D 02	.157D 02
H_2	.173D 01	.179D 01	.185D 01	.195D 01	.202D 01
HCl	.772D 02	.768D 02	.764D 02	.758D 02	.753D 02

Table V

$(Cl_2)_1$ = .550D 02 γ_1 = .136D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.984D 01	.962D 01	.940D 01	.925D 01
P_2/P_1	.193D 02	.190D 02	.187D 02	.185D 02
ρ_1/ρ_2	.563D 00	.561D 00	.559D 00	.557D 00
V_1	.161D 01	.159D 01	.158D 01	.157D 01
V_2	.906D 00	.894D 00	.882D 00	.874D 00
M_1	.555D 01	.550D 01	.544D 01	.540D 01
M_2(fr)	.940D 00	.934D 00	.929D 00	.925D 00
γ_2(fr)	.138D 01	.138D 01	.139D 01	.139D 01
Cl_2	.883D 00	.605D 00	.413D 00	.321D 00
H_2	.788D 00	.943D 00	.112D 01	.125D 01
Cl	.182D 02	.191D 02	.198D 02	.203D 02
H	.257D 00	.323D 00	.401D 00	459D 00
HCl	.799D 02	.791D 02	.783D 02	.777D 02

Table V (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.920D 01	.913D 01	.903D 01	.891D 01	.881D 01
P_2/P_1	.184D 02	.183D 02	.182D 02	.180D 02	.179D 02
ρ_1/ρ_2	.557D 00	.556D 00	.555D 00	.554D 00	.554D 00
V_1	.156D 01	.156D 01	.155D 01	.154D 01	.153D 01
V_2	.870D 00	.866D 00	.861D 00	.854D 00	.849D 00
M_1	.539D 01	.537D 01	.534D 01	.531D 01	.528D 01
M_2(fr)	.923D 00	.922D 00	.919D 00	.916D 00	.914D 00
γ_2(fr)	.139D 01	.140D 01	.140D 01	.140D 01	.140D 01
Cl_2	.290D 00	.257D 00	.220D 00	.177D 00	.152D 00
H_2	.131D 01	.137D 01	.146D 01	.158D 01	.167D 01
Cl	.204D 02	.206D 02	.209D 02	.212D 02	.215D 02
H_2	.484D 00	.514D 00	.554D 00	.613D 00	.655D 00
HCl	.775D 02	.772D 02	.769D 02	.764D 02	.760D 02

Table VI

$(Cl_2)_1$ = .600D 02 γ_1 = .135D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.825D 01	.796D 01	.769D 01	.751D 01
P_2/P_1	.163D 02	.158D 02	.154D 02	.151D 02
ρ_1/ρ_2	.566D 00	.566D 00	.566D 00	.566D 00
V_1	.142D 01	.140D 01	.138D 01	.136D 01
V_2	.804D 00	.792D 00	.780D 00	.772D 00
M_1	.510D 01	.503D 01	.496D 01	.491D 01
M_2(fr)	.939D 00	.935D 00	.931D 00	.928D 00
γ_2(fr)	.139D 01	.140D 01	.141D 01	.141D 01
Cl_2	.742D 01	.553D 01	.570D 01	.518D 01
H_2	.167D-01	.133D-01	.106D-01	.911D-02
Cl	.210D 02	.225D 02	.239D 02	.247D 02
H	.669D-02	.570D-02	.482D-02	.429D-02
HCl	.716D 02	.710D 02	.704D 02	.701D 02

Table VI (continued)

P_1	.132D 00	.1050D 00	.789D-01	.525D-01	.395D-01
T_2/T_1	.744D 01	.736D 01	.726D 01	.712D 01	.702D 01
P_2/P_1	.150D 02	.149D 02	.147D 02	.145D 02	.143D 02
ρ_1/ρ_2	.566D 00	.566D 00	.566D 00	.565D 00	.567D 00
V_1	.136D 01	.135D 01	.134D 01	.133D 01	.133D 01
V_2	.769D 00	.766D 00	.761D 00	.755D 00	.751D 00
M_1	.489D 01	.487D 01	.484D 01	.480D 01	.477D 01
M_2(fr)	.927D 00	.926D 00	.925D 00	.924D 00	.923D 00
γ_2(fr)	.142D 01	.142D 01	.142D 01	.142D 01	.143D 01
Cl_2	.500D 01	.475D 01	.446D 01	.407D 01	.380D 01
H_2	.859D-02	.800D-02	.731D-02	.645D-02	.592D-02
Cl	.250D 02	.254D 02	.259D 02	.266D 02	.270D 02
H_2	.410D-02	.387D-02	.360D-02	.326D-02	.303D-02
HCl	.700D 02	.698D 02	.696D 02	.694D 02	.692D 02

Table VII

$(Cl_2)_1$ = .700D 02 γ_1 = .134D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.688D 01	.665D 01	.643D 01	.628D 01
P_2/P_1	.131D 02	.128D 02	.125D 02	.122D 02
ρ_1/ρ_2	.564D 00	.563D 00	.562D 00	.561D 00
V_1	.117D 01	.115D 01	.113D 01	.112D 01
V_2	.659D 00	.648D 00	.637D 00	.630D 00
M_1	.454D 01	.447D 01	.441D 01	.436D 01
M_2(fr)	.942D 00	.937D 00	.932D 00	.929D 00
γ_2(fr)	.134D 01	.135D 01	.136D 01	.136D 01
Cl_2	.304D 02	.296D 02	.287D 02	.282D 01
H_2	.384D-03	.266D-03	.181D-03	.139D-03
Cl	.136D 02	.149D 02	.161D 02	.169D 02
H	.123D-03	.926D-04	.680D-04	.546D-04
HCl	.559D 02	.555D 02	.552D 02	.549D 02

Table VII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.623D 01	.616D 01	.607D 01	.595D 01	.587D 01
P_2/P_1	.122D 02	.121D 02	.119D 02	.117D 02	.116D 02
ρ_1/ρ_2	.561D 00	.560D 00	.560D 00	.560D 00	.559D 00
V_1	.112D 01	.111D 01	.111D 01	.110D 01	.109D 01
V_2	.627D 00	.624D 00	.619D 00	.613D 00	.609D 00
M_1	.434D 01	.432D 01	.430D 01	.426D 01	.423D 01
M_2(fr)	.927D 00	.926D 00	.924D 00	.921D 00	.920D 00
γ_2(fr)	.136D 01	.136D 01	.137D 01	.137D 01	.137D 01
Cl_2	.280D 02	.277D 02	.274D 02	.269D 02	.266D 02
H_2	.125D-03	.110D-03	.927D-04	.725D-04	.608D-04
Cl	.172D 02	.176D 02	.180D 02	.186D 02	.191D 02
H	.499D-04	.446D-04	.385D-04	.311D-04	.266D-04
HCl	.548D 02	.547D 02	.546D 02	.544D 02	.543D 02

Table VIII

$(CS_2)_1$ = .250D 02 γ_1 = .133D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.136D 02	.131D 02	.126D 02	.123D 02
P_2/P_1	.262D 02	.255D 02	.248D 02	.244D 02
ρ_1/ρ_2	.540D 00	.540D 00	.539D 00	.539D 00
V_1	.178D 01	.175D 01	.173D 01	.171D 01
V_2	.959D 00	.945D 00	.931D 00	.921D 00
M_1	.641D 01	.632D 01	.623D 01	.618D 01
M_2(fr)	.984D 00	.975D 00	.967D 00	.962D 00
γ_2(fr)	.117D 01	.119D 01	.120D 01	.121D 01

Table VIII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.122D 02	.121D 02	.119D 02	.117D 02	.115D 02
P_2/P_1	.243D 02	.241D 02	.238D 02	.234D 02	.232D 02
ρ_1/ρ_2	.539D 00	.538D 00	.538D 00	.538D 00	.538D 00
V_1	.170D 01	.170D 01	.169D 01	.167D 01	.166D 01
V_2	.918D 00	.913D 00	.908D 00	.900D 00	.894D 00
M_1	.615D 01	.613D 01	.609D 01	.604D 01	.601D 01
M_2(fr)	.961D 00	.959D 00	.956D 00	.953D 00	.951D 00
γ_2(fr)	.121D 01	.122D 01	.122D 01	.123D 01	.123D 01

Table VIII (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CS_2	.205D-05	.113D-05	.618D-06	.413D-06
CS	.940D-04	.614D-04	.397D-04	.296D-04
CO	.174D 02	.176D 02	.177D 02	.178D 02
CO_2	.661D 01	.620D 01	.584D 01	.563D 01
COS	.824D-02	.591D-02	.423D-02	.338D-02
C_2	.565D-11	.181D-11	.563D-12	.257D-12
C	.106D-05	.615D-06	.350D-06	.238D-06
O_2	.158D 02	.156D 02	.153D 02	.151D 02
O	.124D 02	.133D 02	.142D 02	.148D 02
SO_2	.242D 02	.237D 02	.232D 02	.229D 02
SO	.208D 02	.208D 02	.208D 02	.208D 02
S_2	.209D 00	.184D 00	.162D 00	.149D 00
S	.251D 01	.265D 01	.279D 01	.287D 01

Table VIII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
CS_2	.352D-06	.289D-06	.224D-06	.156D-06	.121D-06
CS	.263D-04	.227D-04	.188D-04	.144D-04	.119D-04
CO	.178D 02	.179D 02	.179D 02	.180D 02	.180D 02
CO_2	.555D 01	.546D 01	.534D 01	.518D 01	.508D 01
COS	.310D-02	.278D-02	.242D-02	.199D-02	.173D-02
C_2	.188D-12	.127D-12	.773D-13	.380D-13	.229D-13
C	.204D-06	.169D-06	.132D-06	.939D-07	.722D-07
O_2	.150D 02	.149D 02	.148D 02	.146D 02	.145D 02
O	.150D 02	.152D 02	.156D 02	.160D 02	.164D 02
SO_2	.228D 02	.227D 02	.225D 02	.223D 02	.222D 02
SO	.208D 02	.208D 02	.207D 02	.207D 02	.207D 02
S_2	.144D 00	.138D 00	.130D 00	.121D 00	.114D 00
S	.290D 01	.294D 01	.299D 01	.305D 01	.310D 01

Table IX

$(CS_2)_1$ = .300D 02

γ_1 = .132D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.137D 02	.132D 02	.127D 02	.124D 02
P_2/P_1	.273D 02	.266D 02	.[illegible]0D 02	.255D 02
ρ_1/ρ_2	.540D 00	.540D 00	.539D 00	.539D 00
V_1	.177D 01	.175D 01	.172D 01	.171D 01
V_2	.957D 00	.943D 00	.929D 00	.919D 00
M_1	.659D 01	.649D 01	.640D 01	.634D 01
M_2(fr)	.982D 00	.973D 00	.965D 00	.960D 00
γ_2(fr)	.117D 01	.119D 01	.121D 01	.122D 01

Table IX (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.123D 02	.122D 02	.120D 02	.118D 02	.116D 02
P_2/P_1	.253D 02	.251D 02	.249D 02	.245D 02	.242D 02
ρ_1/ρ_2	.539D 00	.538D 00	.538D 00	.538D 00	.538D 00
V_1	.170D 01	.169D 01	.168D 01	.167D 01	.166D 01
V_2	.916D 00	.911D 00	.905D 00	.897D 00	.892D 00
M_1	.632D 01	.629D 01	.625D 01	.620D 01	.617D 01
M_2(fr)	.959D 00	.957D 00	.954D 00	.951D 00	.949D 00
γ_2(fr)	.122D 01	.122D 01	.123D 01	.123D 01	.124D 01

Table IX (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CS_2	.137D-04	.743D-05	.401D-05	.266D-05
CS	.345D-03	.224D-03	.144D-03	.107D-03
CO	.221D 02	.222D 02	.223D 02	.224D 02
CO_2	.571D 01	.533D 01	.500D 01	.480D 01
COS	.198D-01	.141D-01	.997D-02	.794D-02
C_2	.237D-10	.756D-11	.236D-11	.108D-11
C	.230D-05	.134D-05	.765D-06	.523D-06
O_2	.807D 01	.799D 01	.789D 01	.781D 01
O	.930D 01	.100D 02	.108D 02	.112D 02
SO_2	.216D 02	.210D 02	.206D 02	.203D 02
SO	.276D 02	.275D 02	.275D 02	.274D 02
S_2	.742D 00	.650D 00	.568D 00	.519D 00
S	.492D 01	.518D 01	.543D 01	.560D 01

Table IX (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
CS_2	.226D-05	.185D-05	.143D-05	.994D-06	.767D-06
CS	.948D-04	.819D-04	.678D-04	.518D-04	.427D-04
CO	.224D 02	.224D 02	.224D 02	.225D 02	.225D 02
CO_2	.473D 01	.464D 01	.453D 01	.439D 01	.429D 01
COS	.726D-02	.650D-02	.564D-02	.462D-02	.401D-02
C_2	.786D-12	.534D-12	.324D-12	.159D-12	.960D-13
C	.449D-06	.371D-06	.291D-06	.205D-06	.159D-06
O_2	.778D 01	.774D 01	.769D 01	.761D 01	.755D 01
O	.114D 02	.116D 02	.119D 02	.123D 02	.125D 02
SO_2	.202D 02	.200D 02	.199D 02	.197D 02	.195D 02
SO	.274D 02	.274D 02	.273D 02	.272D 02	.272D 02
S_2	.501D 00	.479D 00	.452D 00	.417D 00	.394D 00
S	.566D 01	.573D 01	.583D 01	.595D 01	.604D 01

Table X

$(CS_2)_1$ = .350D 02 γ_1 = .131D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.135D 02	.130D 02	.126D 02	.123D 02
P_2/P_1	.278D 02	.272D 02	.265D 02	.261D 02
ρ_1/ρ_2	.542D 00	.541D 00	.540D 00	.540D 00
V_1	.175D 01	.173D 01	.170D 01	.169D 01
V_2	.948D 00	.934D 00	.920D 00	.911D 00
M_1	.668D 01	.660D 01	.651D 01	.645D 01
M_2(fr)	.979D 00	.970D 00	.962D 00	.958D 00
γ_2(fr)	.119D 01	.121D 01	.122D 01	.123D 01

Table X (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	395D-01
T_2/T_1	.122D 02	.121D 02	.119D 02	.117D 02	.115D 02
P_2/P_1	.259D 02	.257D 02	.254D 02	.251D 02	.248D 02
ρ_1/ρ_2	.540D 00	.539D 00	.539D 00	.539D 00	.538D 00
V_1	.168D 01	.167D 01	.166D 01	.165D 01	.164D 01
V_2	.907D 00	.903D 00	.897D 00	.890D 00	.884D 00
M_1	.642D 01	.640D 01	.636D 01	.631D 01	.627D 01
M_2(fr)	.957D 00	.955D 00	.952D 00	.949D 00	.947D 00
γ_2(fr)	.123D 01	.124D 01	.124D 01	.124D 01	.125D 01

Table X (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CS_2	.774D-04	.417D-04	.224D-04	.148D-04
CS	.990D-03	.643D-03	.414D-03	.308D-03
CO	.264D 02	.264D 02	.265D 02	.265D 02
CO_2	.490D 01	.455D 01	.425D 01	.407D 01
COS	.436D-01	.307D-01	.217D-01	.172D-01
C_2	.529D-10	.172D-10	.547D-11	.252D-11
C	.298D-05	.177D-05	.103D-05	.713D-06
O_2	.325D 01	.326D 01	.325D 01	.324D 01
O	.523D 01	.573D 01	.622D 01	.654D 01
SO_2	.182D 02	.178D 02	.173D 02	.171D 02
SO	.318D 02	.319D 02	.319D 02	.319D 02
S_2	.232D 01	.203D 01	.177D 01	.162D 01
S	.783D 01	.831D 01	.876D 01	.905D 01

Table X (continued)

P_1	.132D 00	.105D 00	.789D-01	.726D-01	.395D-01
CS_2	.126D-04	.103D-04	.792D-05	.548D-05	.422D-05
CS	.273D-03	.236D-03	.196D-03	.150D-03	.123D-03
CO	.265D 02	.265D 02	.265D 02	.266D 02	.266D 02
CO_2	.400D 01	.393D 01	.383D 01	.370D 01	.361D 01
COS	.157D-01	.141D-01	.122D-01	.995D-02	.862D-02
C_2	.185D-11	.126D-11	.772D-12	.383D-12	.232D-12
C	.614D-06	.511D-06	.403D 06	.285D-06	.224D-06
O_2	.324D 01	.323D 01	.322D 01	.321D 01	.319D 01
O	.667D 01	.682D 01	.701D 01	.729D 01	.748D 01
SO_2	.170D 02	.169D 02	.167D 02	.165D 02	.164D 02
SO	.318D 02	.318D 02	.318D 02	.317D 02	.317D 02
S_2	.156D 01	.149D 01	.140D 01	.129D 01	.122D 01
S	.916D 01	.930D 01	.947D 01	.970D 01	.985D 01

Table XI

$(CS_2)_1$ = .400D 02 γ_1 = .130D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.129D 02	.125D 02	.121D 02	.118D 02
P_2/P_1	.274D 02	.268D 02	.262D 02	.258D 02
ρ_1/ρ_2	.545D 00	.545D 00	.544D 00	.543D 00
V_1	.170D 01	.168D 01	.166D 01	.164D 01
V_2	.928D 00	.915D 00	.902D 00	.894D 00
M_1	.668D 01	.659D 01	.651D 01	.645D 01
M_2(fr)	.976D 00	.968D 00	.962D 00	.958D 00
γ_2(fr)	.121D 01	.123D 01	.124D 01	.125D 01

Table XI (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.117D 02	.116D 02	.115D 02	.113D 02	.111D 02
P_2/P_1	.256D 02	.254D 02	.252D 02	.248D 02	.246D 02
ρ_1/ρ_2	.543D 00	.543D 00	.542D 00	.542D 00	.542D 00
V_1	.164D 01	.163D 01	.162D 01	.161D 01	.160D 01
V_2	.890D 00	.886D 00	.881D 00	.874D 00	.868D 00
M_1	.643D 01	.640D 01	.637D 01	.632D 01	.629D 01
M_2(fr)	.957D 00	.955D 00	.953D 00	.951D 00	.949D 00
γ_2(fr)	.125D 01	.125D 01	.125D 01	.126D 01	.126D 01

Table XI (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CS_2	.389D-03	.217D-03	.121D-03	.814D-03
CS	.219D-02	.146D-02	.957D-03	.721D-03
CO	.302D 02	.302D 02	.303D 02	.303D 02
CO_2	.432D 01	.398D 01	.370D 01	.353D 01
COS	.913D-01	.654D-01	.468D-01	.375D-01
C_2	.550D-10	.183D-10	.594D-11	.278D-11
C	.203D-05	.122D-05	.722D-06	.504D-06
O_2	.942D 00	.939D 00	.931D 00	.925D 00
O	.200D 01	.219D 01	.238D 01	.250D 01
SO_2	.148D 02	.144D 02	.140D 02	.138D 02
SO	.314D 02	.318D 02	.321D 02	.322D 02
S_2	.654D 01	.588D 01	.527D 01	.489D 01
S	.979D 01	.106D 02	.113D 02	.118D 02

Table XI (continued)

P_1	.132D 00	.105D 00	.789D-01	.726D-01	.395D-01
CS_2	.690D-04	.574D-04	.447D-04	.315D-04	.245D-04
CS	.643D-03	.560D-03	.467D-03	.360D-03	.300D-03
CO	.303D 02	.303D 02	.303D 02	.303D 02	.303D 02
CO_2	.346D 01	.339D 01	.330D 01	.317D 01	.309D 01
COS	.343D-01	.308D-01	.268D-01	.220D-01	.191D-01
C_2	.205D-11	.141D-11	.869D-12	.436D-12	.267D-12
C	.436D-06	.364D-06	.288D-06	.207D-06	.163D-06
O_2	.923D 00	.919D 00	.914D 00	.908D 00	.903D 00
O	.255D 01	.261D 01	.268D 01	.279D 01	.286D 01
SO_2	.137D 02	.136D 02	.135D 02	.133D 02	.132D 02
SO	.323D 02	.323D 02	.324D 02	.325D 02	.325D 02
S_2	.474D 01	.457D 01	.435D 01	.405D 01	.385D 01
S	.120D 02	.123D 02	.126D 02	.130D 02	.133D 02

Table XII

P_1 = .100D 01

$(CS_2)_1$	.500D 02	.600D 02	.700D 02	.800D 02
T_2/T_1	.114D 02	.989D 01	.748D 01	.533D 01
P_2/P_1	.253D 02	.228D 02	.170D 02	.110D 02
ρ_1/ρ_2	.549D 00	.554D 00	.569D 00	.569D 00
V_1	.157D 01	.144D 01	121D 01	.192D 01
V_2	.864D 00	.797D 00	.688D 00	.525D 00
M_1	.648D 01	.620D 01	.543D 01	.431D 01
M_2(fr)	.968D 00	.967D 00	.991D 00	.991D 00
γ_1	.129D 01	.127D 01	.126D 01	.124D 01
γ_2(fr)	.125D 01	.127D 01	.127D 01	.122D 01

Table XII (continued)

$(CS_2)_1$	.500D 02	.600D 02	.700D 02	800D 02
CS_2	.375D-02	.212D-01	.773D 01	.343D 02
CS	.453D-02	.581D-02	.104D 00	.370D-02
CO	.367D 02	.428D 02	.447D 02	.292D 02
CO_2	.401D 01	.355D 01	.765D-01	.141D 00
COS	.270D 00	.599D 00	.165D 01	.464D 01
C_2	.143D-10	.179D-11	.395D-11	.232D-17
C	.305D-06	.222D-07	.716D-09	.945D-15
O_2	.637D-01	.219D-02	.921D-09	.604D-13
O	.187D 00	.915D-02	.239D-06	.932D-11
SO_2	838D 01	.262D 01	.119D-03	.13[illegible]D-04
SO	.199D 02	.688D 01	.108D-01	.286D-03
S_2	.229D 02	.402D 02	.455D 02	.317D 02
S	.767D 01	.330D 01	.235D 00	.222D-02

Table XIII

P_1 = .132D 00

$(CS_2)_1$	.500D 02	.600D 02	.700D 02	.800D 02
T_2/T_1	.104D 02	.924D 01	.732D 01	.514D 01
P_2/P_1	.238D 02	.218D 02	.168D 02	.107D 02
ρ_1/ρ_2	.547D 00	.550D 00	.567D 00	.572D 00
V_1	.152D 01	.140D 01	.120D 01	.911D 00
V_2	.829D 00	.770D 00	.679D 00	.521D 00
M_1	.625D 01	.603D 01	.538D 01	.426D 01
M_2(fr)	.955D 00	.956D 00	.985D 00	.973D 00
γ_1	.129D 01	.127D 01	.126D 01	.124D 01
γ_2(fr)	.127D 01	.128D 01	.127D 01	.123D 01

Table XIII (continued)

$(CS_2)_1$	.500D 02	.600D 02	.700D 02	.800D 02
CS_2	.895D-03	.543D-02	.750D 01	.338D 02
CS	.151D-02	.217D-02	.209D 00	.509D-02
CO	.369D 02	.433D 02	.454D 02	.314D 02
CO_2	.314D 01	.272D 01	.131D-01	.353D-01
COS	.116D 00	.264D 00	.672D 00	.230D 01
C_2	.518D-12	.893D-13	.100D-10	.152D-17
C	.610D-07	.581D-08	.218D-08	.920D-15
O_2	.528D-01	.205D-02	.101D-09	.537D-14
O	.208D 00	.119D-01	.160D-06	.381D-11
SO_2	.776D 01	.244D 01	.737D-05	.123D-05
SO	.212D 02	.782D 01	.389D-02	.103D-03
S_2	.206D 02	.386D 02	.457D 02	.325D 02
S	.101D 02	.484D 01	.500D-01	.353D-01

Table XIV

P_1 = .100D 01 O_2 = .333D 02

$CO/(CO+H_2)$	.985D 02	.850D 02	.700D 02
T_2/T_1	.118D 02	.117D 02	.118D 02
P_2/P_1	.184D 02	.183D 02	.183D 02
ρ_1/ρ_2	.543D 00	.543D 00	.543D 00
V_1	.180D 01	.187D 01	.197D 01
V_2	.980D 00	.102D 01	.107D 01
M_1	.523D 01	.521D 01	.521D 01
M_2(fr)	.100D 01	.996D 00	.992D 00
γ_1	.140D 01	.140D 01	.140D 01
γ_2(fr)	.112D 01	.113D 01	.114D 01

Table XIV (continued)

$CO/(CO+H_2)$	.550D 02	.400D 02	.250D 02
T_2/T_1	.119D 02	.120D 02	.121D 02
P_2/P_1	.184D 02	.185D 02	.186D 02
ρ_1/ρ_2	.543D 00	.544D 00	.544D 00
V_1	.209D 01	.224D 01	.242D 01
V_2	.114D 01	.122D 01	.131D 01
M_1	.522D 01	.523D 01	.525D 01
M_2(fr)	.987D 00	.981D 00	.975D 00
γ_1	.140D 01	.140D 01	.140D 01
γ_2(fr)	.116D 01	.117D 01	.119D 01

Table XIV (continued)

CO/(CO+H_2)	.985D 02	.850D 02	.700D 02
CO_2	.400D 02	.339D 02	.265D 02
CO	.373D 02	.330D 02	.288D 02
O_2	.160D 02	.138D 02	.121D 02
O	.472D 01	.426D 01	.413D 01
H_2O	.381D 00	.765D 01	.166D 02
OH	.120D 01	.510D 01	.746D 01
H_2	.444D-01	.932D 00	.226D 01
H	.297D 00	.133D 01	.214D 01
C_2	.210D-12	.167D-12	.171D 12
C	.623D-07	.537D-07	.569D-07

Table XIV (continued)

$CO/(CO+H_2)$	.550D 02	.400D 02	.250D 02
CO_2	.194D 02	.129D 02	.718D 01
CO	.242D 02	.190D 02	.128D 02
O_2	.104D 02	.883D 01	.727D 01
O	.410D 01	.408D 01	.405D 01
H_2O	.256D 02	.341D 02	.420D 02
OH	.928D 01	.108D 02	.121D 02
H_2	.397D 01	.623D 01	.924D 01
H	.300D 01	.404D 01	.533D 01
C_2	.185D-12	.189D-12	.154D-12
C	.637D-07	.709D-07	.712D-07

Table XV

$(N_2)_1$ = .100D 02 γ_1 = .140D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.115D 02	.112D 02	.108D 02	.106D 02
P_2/P_1	.180D 02	.176D 02	.173D 02	.170D 02
ρ_1/ρ_2	.543D 00	.543D 00	.542D 00	.542D 00
V_1	.179D 01	.176D 01	.174D 01	.173D 01
V_2	.970D 00	.958D 00	.946D 00	.938D 00
M_1	.516D 01	.510D 01	.504D 01	.500D 01
M_2(fr)	.994D 00	.987D 00	.980D 00	.975D 00
γ_2(fr)	.114D 01	.115D 01	.116D 01	.117D 01

Table XV (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.105D 02	.104D 02	.103D 02	.102D 02	.100D 02
P_2/P_1	.169D 02	.168D 02	.166D 02	.164D 02	.163D 02
ρ_1/ρ_2	.542D 00	.542D 00	.542D 00	.542D 00	.542D 00
V_1	.172D 01	.172D 01	.171D 01	.170D 01	.169D 01
V_2	.935D 00	.931D 00	.926D 00	.920D 00	.915D 00
M_1	.499D 01	.497D 01	.494D 01	.491D 01	.488D 01
M_2(fr)	.974D 00	.972D 00	.969D 00	.966D 00	.964D 00
γ_2(fr)	.117D 01	.118D 01	.118D 01	.119D 01	.119D 01

Table XV (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CO_2	.379D 02	.365D 02	.353D 02	.346D 02
CO	.314D 02	.322D 02	.329D 02	.333D 02
O_2	.127D 02	.130D 02	.133D 02	.135D 02
O	.336D 01	.372D 01	.408D 01	.432D 01
N_2	.106D 02	.106D 02	.106D 02	.106D 02
N	.116D-02	.998D-03	.850D-03	.760D-03
NO	.221D 01	.204D 01	.187D 01	.177D 01
N_2O	.179D-03	.115D-03	.734D-04	.544D-04
NO_2	.282D-02	.196D-02	.135D-02	.105D-02
H_2O	.458D 00	.436D 00	.415D 00	.402D 00
OH	.108D 01	.107D 01	.106D 01	.104D 01
H_2	.481D-01	.495D-01	.508D-01	.516D-01
H	.254D 00	.289D 00	.327D 00	.353D 00
C_2	.707D-13	.236D-13	.765D-14	.358D-14
C	.277D-07	.166D-07	.978D-08	.681D-08
N^+	.533D-04	.379D-04	.267D-04	.211D-04
HNO	.987D-04	.541D-04	.414D-04	.309D-04

Table XV (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
CO_2	.343D 02	.340D 02	.336D 02	.330D 02	.326D 02
CO	.335D 02	.337D 02	.340D 02	.343D 02	.345D 02
O_2	.135D 02	.136D 02	.137D 02	.138D 02	.139D 02
O	.441D 01	.453D 01	.468D 01	.490D 01	.505D 01
N_2	.106D 02	.106D 02	.106D 02	.106D 02	.106D 02
N	.726D-03	.686D-03	.637D-03	.572D-03	.529D-03
NO	.172D 01	.167D 01	.161D 01	.153D 01	.147D 01
N_2O	.483D-04	.418D-04	.346D-04	.265D-04	.219D-04
NO_2	.954D-03	.845D-03	.722D-03	.578D-03	.493D-03
H_2O	.397D 00	.390D 00	.383D 00	.372D 00	.365D 00
OH	.104D 01	.103D 01	.102D 01	.101D 01	.997D 00
H_2	.519D-01	.522D-01	.527D-01	.532D-01	.536D-01
H	.364D 00	.378D 00	.396D 00	.422D 00	.441D 00
C_2	.265D-14	.182D-14	.112D-14	.563D-15	.344D-15
C	.589D-08	.492D-08	.389D-08	.279D-08	.219D-08
NH	.192D-04	.171D-04	.147D-04	.118D-04	.101D-04
HNO	.275D-04	.238D-04	.198D-04	.150D-04	.126D-04

Table XVI

$(N_2)_1$ = .200D 02

γ_1 = .140D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.112D 02	.109D 02	.106D 02	.104D 02
P_2/P_1	.176D 02	.173D 02	.169D 02	.167D 02
ρ_1/ρ_2	.544D 00	.543D 00	.543D 00	.543D 00
V_1	.177D 01	.175D 01	.173D 01	.172D 01
V_2	.962D 00	.951D 00	.940D 00	.932D 00
M_1	.511D 01	.505D 01	.499D 01	.495D 01
M_2(fr)	.988D 00	.981D 00	.975D 00	.971D 00
γ_2(fr)	.115D 01	.116D 01	.118D 01	.118D 01

Table XVI (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.103D 02	.102D 02	.101D 02	.995D 01	.984D 01
P_2/P_1	.166D 02	.165D 02	.164D 02	.162D 02	.160D 02
ρ_1/ρ_2	.543D 00	.542D 00	.542D 00	.542D 00	.542D 00
V_1	.171D 01	.171D 01	.170D 01	.169D 01	.168D 01
V_2	.929D 00	.926D 00	.921D 00	.915D 00	.910D 00
M_1	.494D 01	.492D 01	.490D 01	.487D 01	.484D 01
M_2(fr)	.970D 00	.968D 00	.966D 00	.963D 00	.961D 00
γ_2(fr)	.119D 01	.119D 01	.119D 01	.120D 01	.120D 01

Table XVI (continued)

P_1	.100D 01	.500D 00	.250D 00	.153D 00
CO_2	.354D 02	.342D 02	.331D 02	.324D 02
CO	.257D 02	.265D 02	.272D 02	.276D 02
O_2	.102D 02	.105D 02	.108D 02	.110D 02
O	.238D 01	.267D 01	.297D 01	.317D 01
N_2	.220D 02	.220D 02	.219D 02	.219D 02
N	.107D-02	.934D-03	.808D-03	.730D-03
NO	.262D 01	.243D 01	.224D 01	.212D 01
N_2O	.300D-03	.194D-03	.124D-03	.927D-04
NO_2	.312D-02	.218D-02	.152D-02	.119D-02
H_2O	.535D 00	.510D 00	.486D 00	.471D 00
OH	.954D 00	.953D 00	.947D 00	.941D 00
H_2	.500D-01	.517D-01	.534D-01	.544D-01
H	.210D 00	.242D 00	.277D 00	.301D 00
C_2	.215D-13	.746D-14	.252D-14	.121D-14
C	.116D-07	.718D-08	.435D-08	.309D-08
NH	.568D-04	.410D-04	.293D-04	.233D-04
HNO	.117D-03	.767D-04	.500D-04	.376D-04

Table XVI (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
CO_2	.321D 02	.318D 02	.314D 02	.309D 02	.305D 02
CO	.278D 02	.280D 02	.283D 02	.286D 02	.288D 02
O_2	.111D 02	.112D 02	.113D 02	.114D 02	.115D 02
O	.325D 01	.335D 01	.348D 01	.366D 01	.379D 01
N_2	.219D 02	.218D 02	.218D 02	.218D 02	.218D 02
N	.700D-03	.665D-03	.621D-03	.562D-03	.523D-03
NO	.208D 01	.202D 01	.195D 01	.185D 01	.178D 01
N_2O	.824D-04	.713D-04	.592D-04	.455D-04	.377D-04
NO_2	.108D-02	.960D-03	.823D-03	.662D-03	.566D-03
H_2O	.465D 00	.458D 00	.450D 00	.437D 00	.429D 00
OH	.938D 00	.934D 00	.929D 00	.920D 00	.913D 00
H_2	.548D-01	.553D-01	.559D-03	.566D-03	.572D-03
H	.311D 00	.324D 00	.341D 00	.365D 00	.383D 00
C_2	.904D-15	.630D-15	.394D-15	.218D-15	.125D-15
C	.269D-08	.227D-08	.182D-08	.132D-08	.105D-08
NH	.213D-04	.190D-04	.164D-04	.133D-04	.115D-04
HNO	.335D-04	.291D-04	.243D-04	.187D-04	.156D-04

Table XVII

$(N_2)_1$ = .300D 02

γ_1 = .140D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.108D 02	.106D 02	.101D 02	.101D 02
P_2/P_1	.172D 02	.169D 02	.165D 02	.163D 02
ρ_1/ρ_2	.544D 00	.544D 00	.544D 00	.543D 00
V_1	.175D 01	.173D 01	.172D 01	.170D 01
V_2	.954D 00	.943D 00	.933D 00	.925D 00
M_1	.504D 01	.499D 01	.494D 01	.490D 01
M_2(fr)	.982D 00	.976D 00	.971D 00	.967D 00
γ_2(fr)	.117D 01	.118D 01	.119D 01	.119D 01

Table XVII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.101D 02	.997D 01	.987D 01	.972D 01	.962D 01
P_2/P_1	.162D 02	.161D 02	.160D 02	.158D 02	.157D 02
ρ_1/ρ_2	.543D 00	.543D 00	.543D 00	.543D 00	.543D 00
V_1	.170D 01	.169D 01	.168D 01	.167D 01	.167D 01
V_2	.923D 00	.919D 00	.915D 00	.909D 00	.904D 00
M_1	.489D 01	.487D 01	.485D 01	.482D 01	.480D 01
M_2(fr)	.966D 00	.965D 00	.963D 00	.960D 00	.959D 00
γ_2(fr)	.120D 01	.120D 01	.120D 01	.121D 01	.121D 01

Table XVII (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CO_2	.328D 02	.317D 02	.307D 02	.301D 02
CO	.201D 02	.209D 02	.216D 02	.220D 02
O_2	.785D 01	.821D 01	.854D 01	.875D 01
O	.159D 01	.181D 01	.204D 01	.219D 01
N_2	.335D 02	.333D 02	.332D 02	.332D 02
N	.770D-03	.688D-03	.607D-03	.555D-03
NO	.256D 01	.240D 01	.223D 01	.212D 03
N_2O	.355D-03	.232D-03	.150D-03	.112D-03
NO_2	.282D-02	.200D-02	.141D-02	.111D-02
H_2O	.622D 00	.595D 00	.569D 00	.553D 00
OH	.807D 00	.816D 00	.820D 00	.820D 00
H_2	.502D-01	.525D-01	.546D-01	.560D-01
H	.164D 00	.192D 00	.222D 00	.244D 00
C_2	.508D-14	.186D-14	.659D-15	.327D-15
C	.404D-08	.260D-08	.164D-08	.119D-08
NH	.478D-04	.351D-04	.256D-04	.206D-04
HNO	.112D-03	.748D-04	.494D-04	.374D-04

Table XVII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
CO_2	.298D 02	.295D 02	.292D 02	.287D 02	.283D 02
CO	.222D 02	.224D 02	.227D 02	.230D 02	.232D 02
O_2	.882D 01	.891D 01	.903D 01	.918D 01	.928D 01
O	.226D 01	.234D 01	.244D 01	.259D 01	.270D 01
N_2	.331D 02	.331D 02	.331D 02	.330D 02	.330D 02
N	.534D-03	.510D-03	.480D-03	.439D-03	.411D-03
NO	.208D 01	.203D 01	.196D 01	.187D 01	.181D 01
N_2O	.100D-03	.869D-04	.724D-04	.559D-04	.464D-04
NO_2	.101D-02	.901D-03	.775D-03	.626D-03	.538D-03
H_2O	.547D 00	.539D 00	.529D 00	.515D 00	.506D 00
OH	.819D 00	.818D 00	.816D 00	.812D 00	.809D 00
H_2	.565D-01	.571D-01	.579D-01	.590D-01	.597D-01
H	.253D 00	.265D 00	.280D 00	.302D 00	.318D 00
C_2	.246D-15	.174D-15	.111D-15	.582D-16	.367D-16
C	.104D-08	.890D-09	.722D-09	.535D-09	.431D-09
NH	.189D-04	.170D-04	.147D-04	.121D-04	.105D-04
HNO	.335D-04	.292D-04	.245D-04	.190D-04	.159D-04

Table XVIII

$(N_2)_1$ = .400D 02 γ_1 = .140D 01

P_1	.100D 01	.500D 00	.250D 00	.158D 00
T_2/T_1	.104D 02	.102D 02	.996D 01	.981D 01
P_2/P_1	.167D 02	.164D 02	.161D 02	.159D 02
ρ_1/ρ_2	.546D 00	.545D 00	.545D 00	.545D 00
V_1	.173D 01	.171D 01	.170D 01	.168D 01
V_2	.944D 00	.934D 00	.924D 00	.917D 00
M_1	.497D 01	.492D 01	.487D 01	.484D 01
M_2(fr)	.976D 00	.971D 00	.967D 00	.964D 00
γ_2(fr)	.119D 01	.119D 01	.120D 01	.121D 01

Table XVIII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
T_2/T_1	.975D 01	.967D 01	.958D 01	.945D 01	.935D 01
P_2/P_1	.158D 02	.157D 02	.156D 02	.154D 02	.153D 02
ρ_1/ρ_2	.545D 00	.544D 00	.544D 00	.544D 00	.544D 00
V_1	.168D 01	.167D 01	.167D 01	.166D 01	.165D 01
V_2	.915D 00	.911D 00	.907D 00	.901D 00	.897D 00
M_1	.482D 01	.481D 01	.479D 01	.476D 01	.474D 01
M_2(fr)	.963D 00	.962D 00	.960D 00	.958D 00	.956D 00
γ_2(fr)	.121D 01	.121D 01	.121D 01	.122D 01	.122D 01

Table XVIII (continued)

P_1	.100D 01	.500D 00	.250D 00	.158D 00
CO_2	.300D 02	.290D 02	.281D 02	.276D 02
CO	.148D 02	.155D 02	.162D 02	.166D 02
O_2	.572D 01	.606D 01	.637D 01	.657D 01
O	.950D 00	.110D 01	.127D 01	.138D 01
N_2	.448D 02	.446D 02	.445D 02	.444D 02
N	.452D-03	.415D-03	.375D-03	.348D-03
NO	.222D 01	.210D 01	.198D 01	.189D 01
N_2O	.349D-03	.230D-03	.151D-03	.114D-03
NO_2	.223D-02	.161D-02	.115D-02	.914D-03
H_2O	.721D 00	.693D 00	.667D 00	.649D 00
OH	.641D 00	.657D 00	.669D 00	.675D 00
H_2	.481D-01	.509D-01	.536D-01	.554D-01
H	.117D 00	.140D 00	.165D 00	.183D 00
C_2	.813D-15	.318D-15	.120D-15	.619D-16
C	.106D-08	.717D-09	.473D-09	.354D-09
NH	.333D-04	.251D-04	.187D-04	.153D-04
HNO	.930D-04	.631D-04	.424D-04	.325D-04

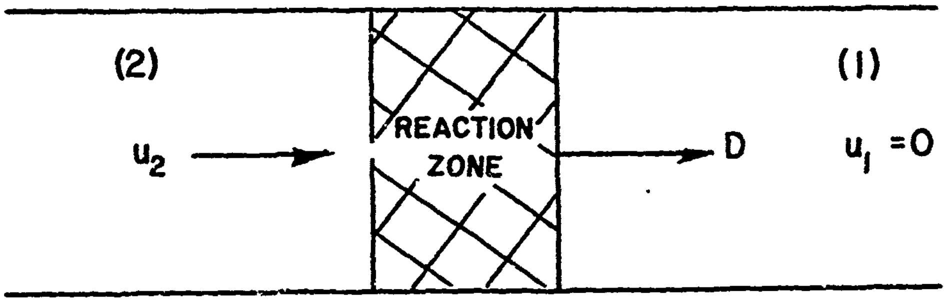
Table XVIII (continued)

P_1	.132D 00	.105D 00	.789D-01	.526D-01	.395D-01
CO_2	.274D 02	.271D 02	.268D 02	.263D 02	.260D 02
CO	.168D 02	.170D 02	.172D 02	.176D 02	.178D 02
O_2	.665D 01	.674D 01	.685D 01	.701D 01	.711D 01
O	.143D 01	.149D 01	.156D 01	.168D 01	.176D 01
N_2	.443D 02	.443D 02	.442D 02	.442D 02	.441D 02
N	.337D-03	.325D-03	.308D-03	.285D-03	.270D-03
NO	.186D 01	.182D 01	.177D 01	.169D 01	.164D 01
N_2O	.102D-03	.887D-04	.742D-04	.576D-04	.481D-04
NO_2	.834D-03	.746D-03	.645D-03	.525D-03	.453D-03
H_2O	.642D 00	.634D 00	.624D 00	.609D 00	.599D 00
OH	.676D 00	.678D 00	.680D 00	.682D 00	.682D 00
H_2	.560D-01	.569D-01	.579D-01	.593D-01	.603D-01
H	.190D 00	.200D 00	.213D 00	.232D 00	.246D 00
C_2	.474D-16	.341D-16	.222D-16	.121D-16	.777D-17
C	.315D-09	.272D-09	.224D-09	.170D-09	.139D-09
NH	.141D-04	.127D-04	.112D-04	.926D-05	.809D-05
HNO	.292D-04	.256D-04	.216D-04	.169D-04	.142D-04

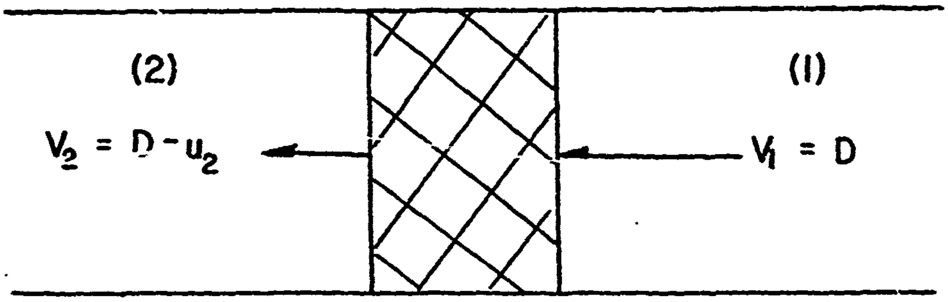
FIGURE CAPTIONS

FIGURE 1	Detonation Wave in a) Laboratory System b) Stationary Wave System
FIGURE 2	Detonation velocity in (H_2-Cl_2) mixture at 298°K.
FIGURE 3	Theoretical temperature ratio in detonated (H_2-Cl_2) mixture at 298°K.
FIGURE 4	Theoretical pressure ratio in detonated (H_2-Cl_2) mixture at 298°K.
FIGURE 5	Theoretical Mach number in detonated (H_2-Cl_2) mixture at 298°K.
FIGURE 6	Theoretical HCl mole percent in detonated (H_2-Cl_2) mixture at 298°K.
FIGURE 7	Detonation velocity in detonated (CS_2-O_2) mixture at 298°K.
FIGURE 8	Theoretical temperature ratio in detonated (CS_2-O_2) mixture at 298°K.

FIGURE 18	Theoretical CO mole percent in detonated (CS_2-O_2) mixture at 298°K.
FIGURE 19	Theoretical S_2 mole percent in detonated (CS_2-O_2) mixture at 298°K.
FIGURE 20	Detonation velocity in $2(H_2 + CO) + O_2$ mixture at one atmosphere and 298°K.
FIGURE 21	Theoretical detonation temperature ratio in $2(H_2 + CO) + O_2$ mixture at one atmosphere and 298°K.
FIGURE 22	Theoretical detonation pressure ratio in $2(H_2 + CO) + O_2$ mixture at one atmosphere and 298°K.
FIGURE 23	Theoretical detonation Mach number in $2(H_2 + CO) + O_2$ mixture at one atmosphere and 298°K.
FIGURE 24	Theoretical CO_2 and CO mole percents in detonated $2(H_2 + CO) + O_2$ mixture at one atmosphere and 298°K.
FIGURE 25	Theoretical detonation velocity in (CO-H_2-O_2-N_2) mixture at 298°K.



a. LABORATORY SYSTEM



b. STATIONARY WAVE SYSTEM

FIG. 1

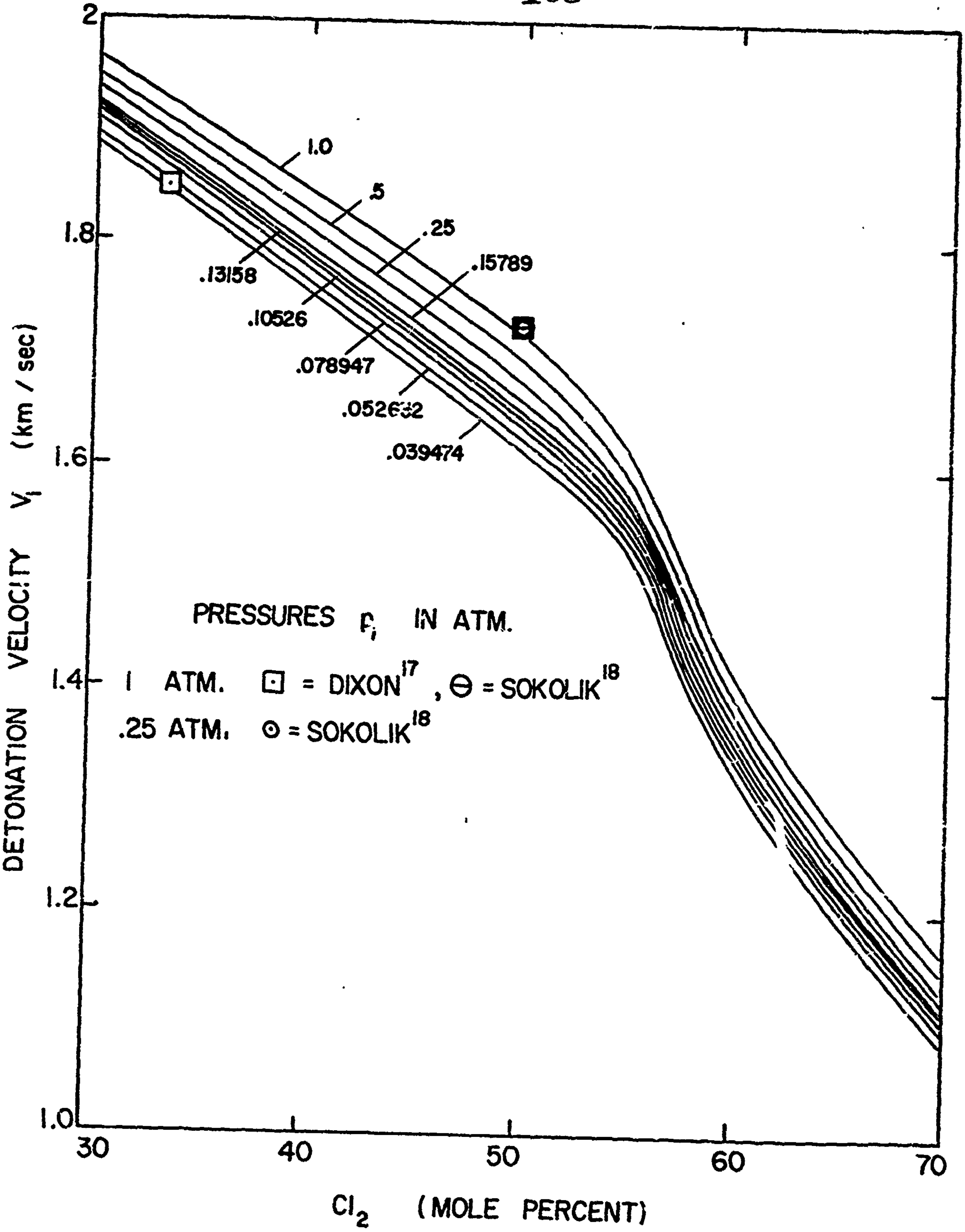

2
1.8
1.6
1.4
1.2
1.0
30
40
50
60
70
DETONATION VELOCITY V_i (km / sec)
Cl_2 (MOLE PERCENT)
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
PRESSURES p_i IN ATM.
1 ATM. ⊡ = DIXON[17], ⊖ = SOKOLIK[18]
.25 ATM. ⊙ = SOKOLIK[18]

FIG. 2

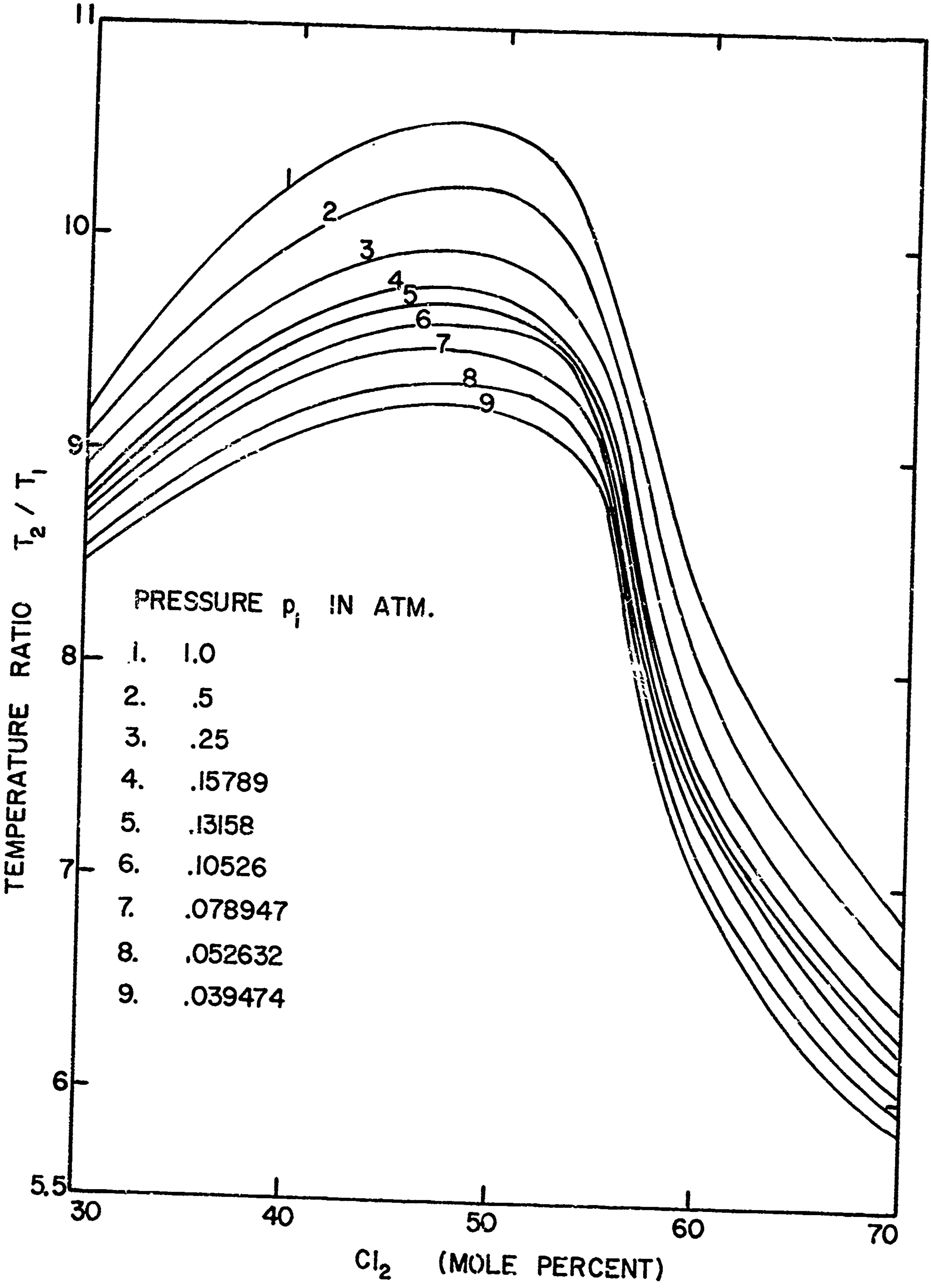

11
10
9
8
7
6
5.5
TEMPERATURE RATIO T_2 / T_1
1
2
3
4
5
6
7
8
9
PRESSURE p_i IN ATM.
1. 1.0
2. .5
3. .25
4. .15789
5. .13158
6. .10526
7. .078947
8. .052632
9. .039474
30
40
50
60
70
Cl_2 (MOLE PERCENT)

FIG. 3

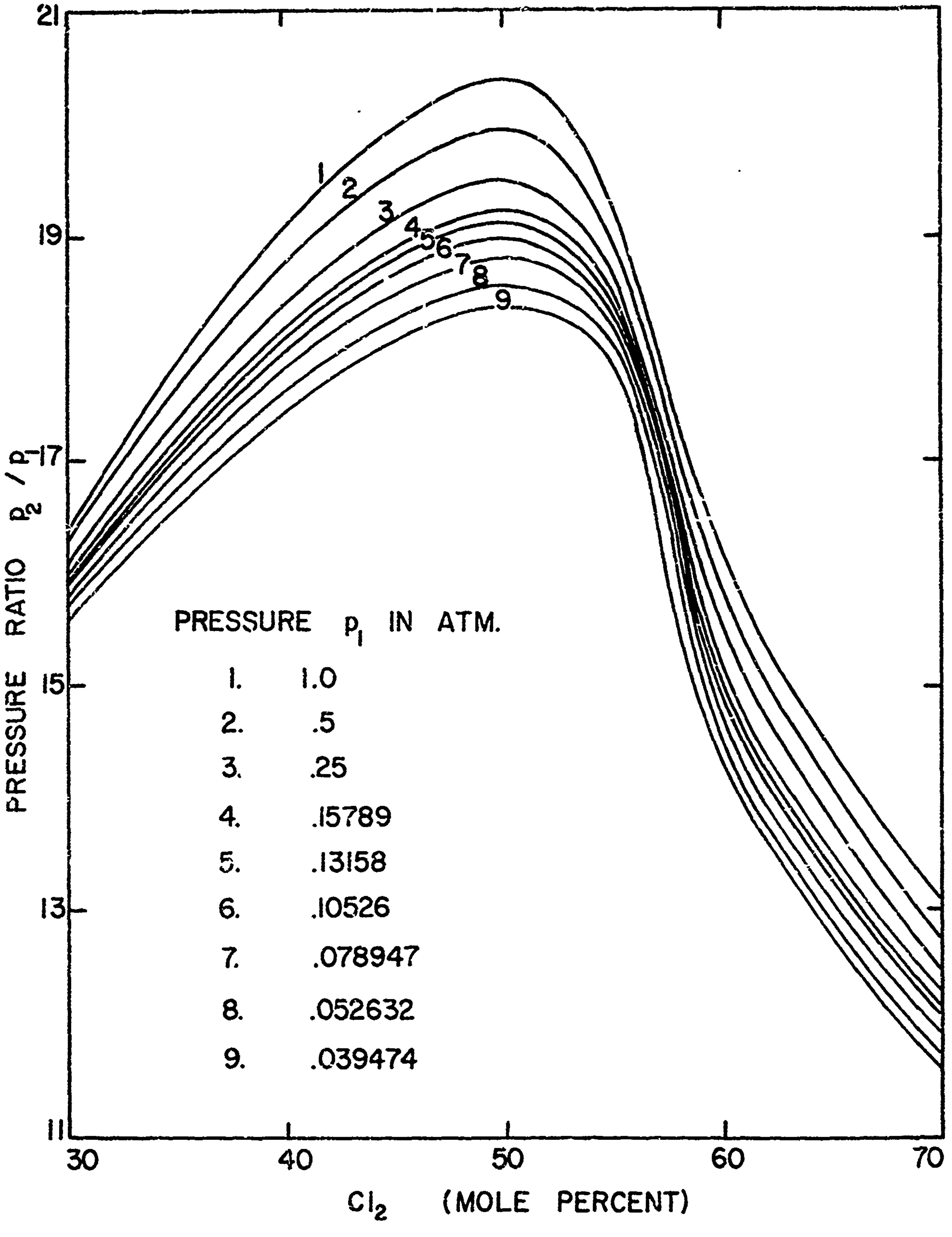

21
19
17
15
13
11
PRESSURE RATIO p_2/p_1
30
40
50
60
70
Cl_2 (MOLE PERCENT)
1
2
3
4
5
6
7
8
9
PRESSURE p_1 IN ATM.
1. 1.0
2. .5
3. .25
4. .15789
5. .13158
6. .10526
7. .078947
8. .052632
9. .039474

FIG. 4

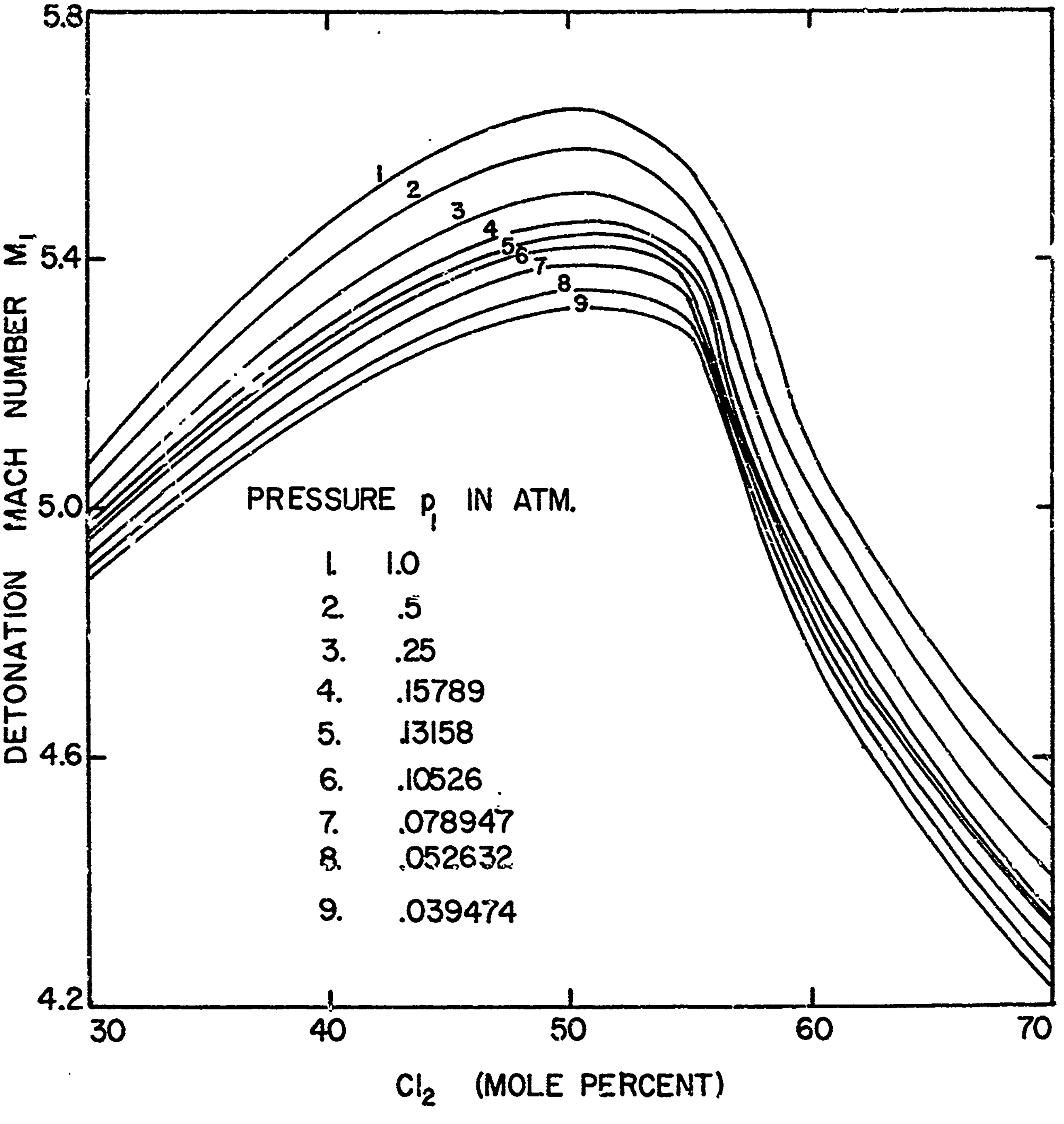

5.8
5.4
5.0
4.6
4.2
DETONATION MACH NUMBER M_1
30
40
50
60
70
Cl_2 (MOLE PERCENT)
1
2
3
4
5
6
7
8
9
PRESSURE p_1 IN ATM.
1. 1.0
2. .5
3. .25
4. .15789
5. .13158
6. .10526
7. .078947
8. .052632
9. .039474

FIG.5

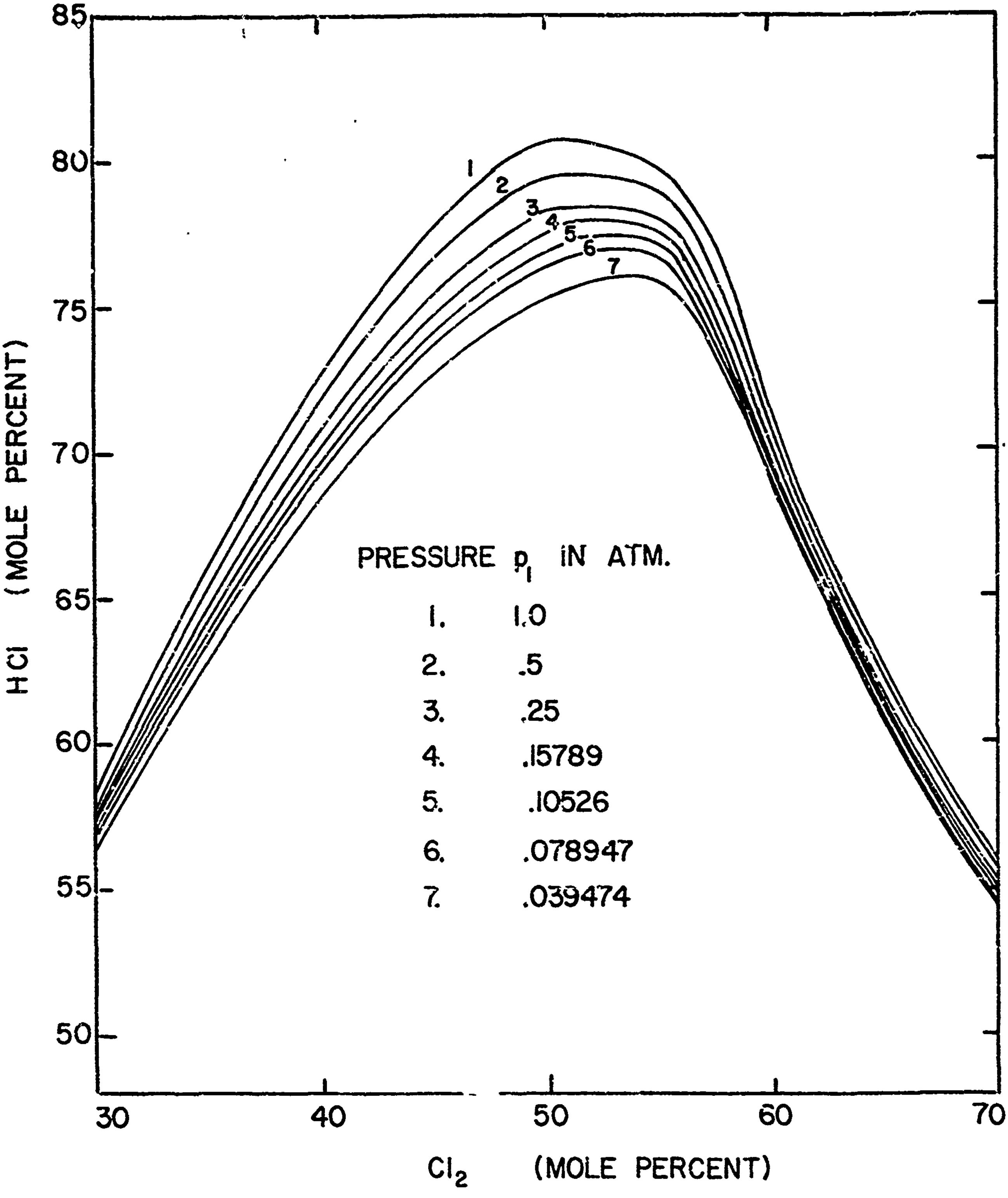

85
80
75
70
65
60
55
50
HCl (MOLE PERCENT)
30
40
50
60
70
Cl_2 (MOLE PERCENT)
1
2
3
4
5
6
7
PRESSURE p_1 IN ATM.
1. 1.0
2. .5
3. .25
4. .15789
5. .10526
6. .078947
7. .039474

FIG. 6

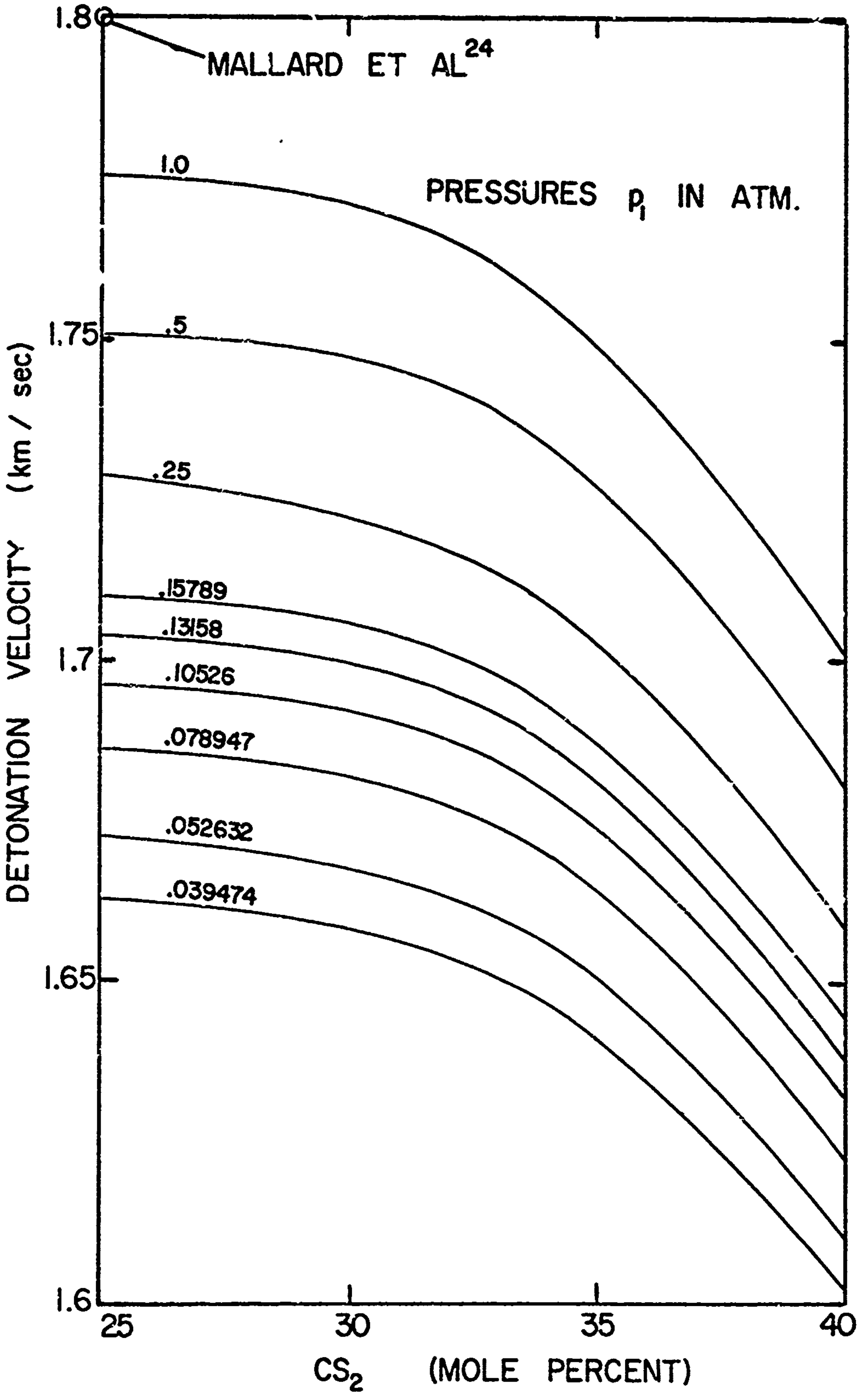

1.80
MALLARD ET AL[24]
PRESSURES p_1 IN ATM.
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
1.75
1.7
1.65
1.6
DETONATION VELOCITY (km / sec)
25
30
35
40
CS_2 (MOLE PERCENT)

FIG. 7

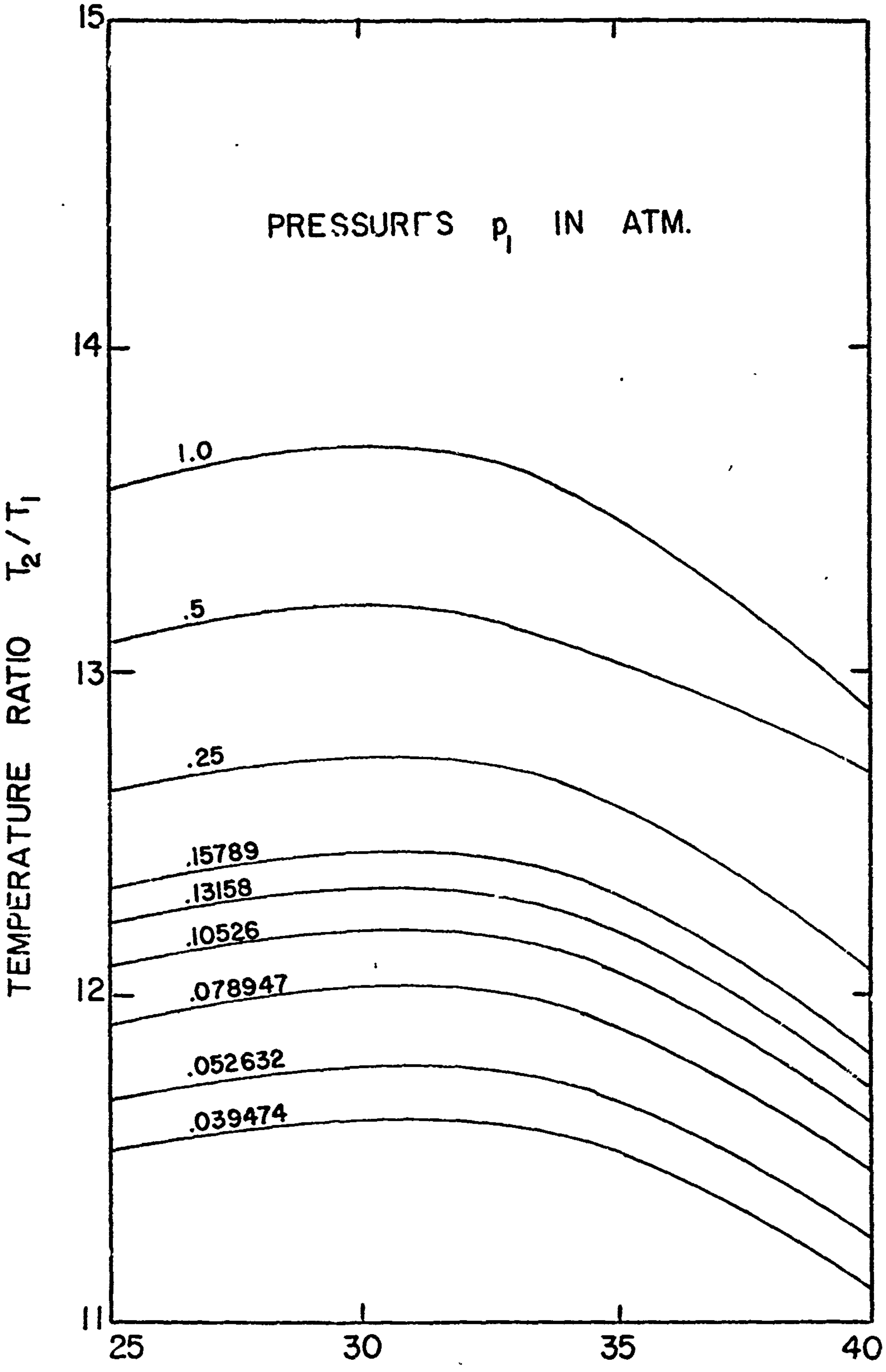

PRESSURES p_1 IN ATM.
15
14
13
12
11
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
TEMPERATURE RATIO T_2/T_1
25
30
35
40
CS_2 (MOLE PERCENT)

FIG. 8

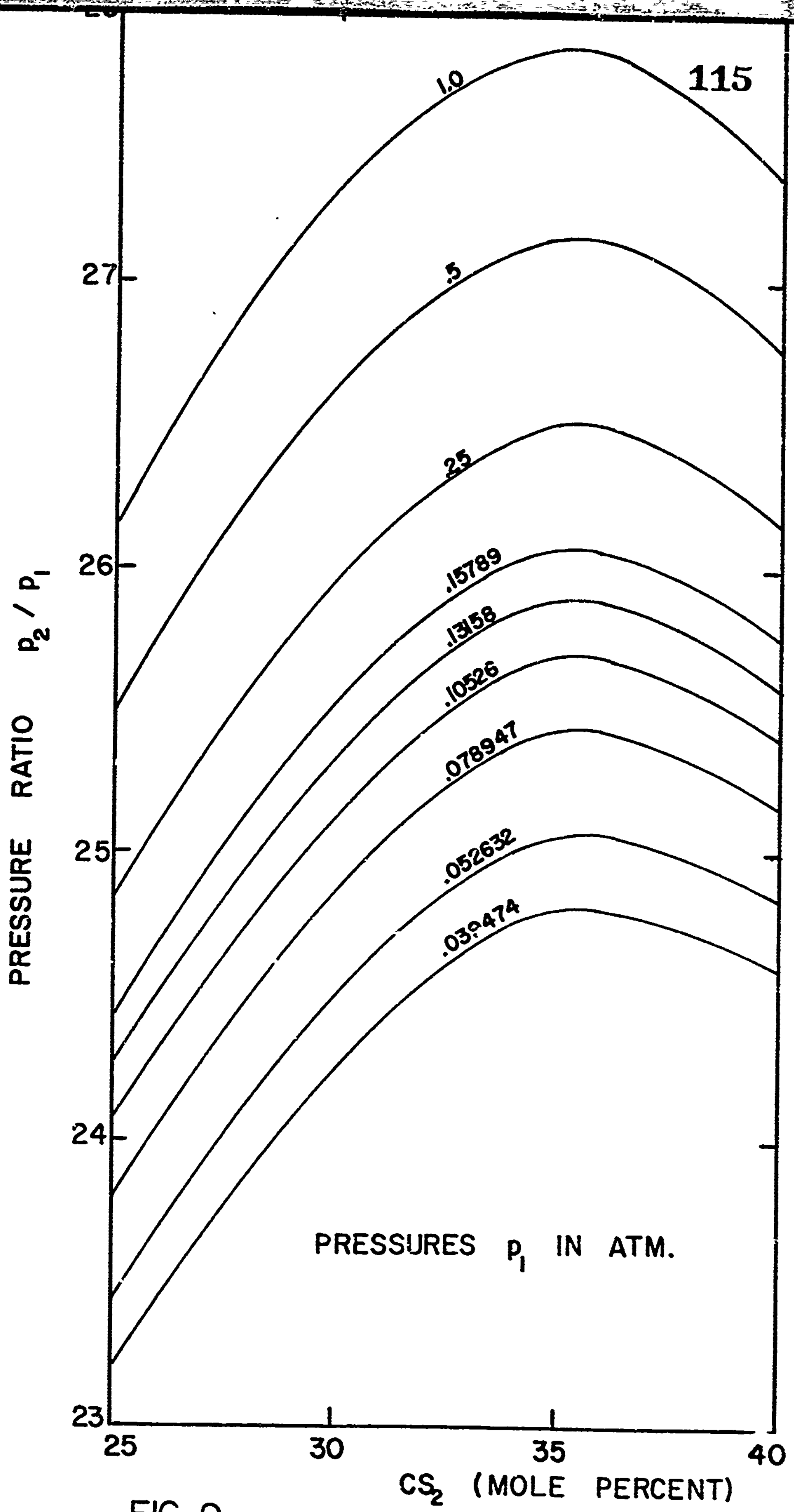

1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
PRESSURES p_1 IN ATM.
PRESSURE RATIO p_2 / p_1
27
26
25
24
23
25
30
35
40
CS_2 (MOLE PERCENT)

FIG. 9

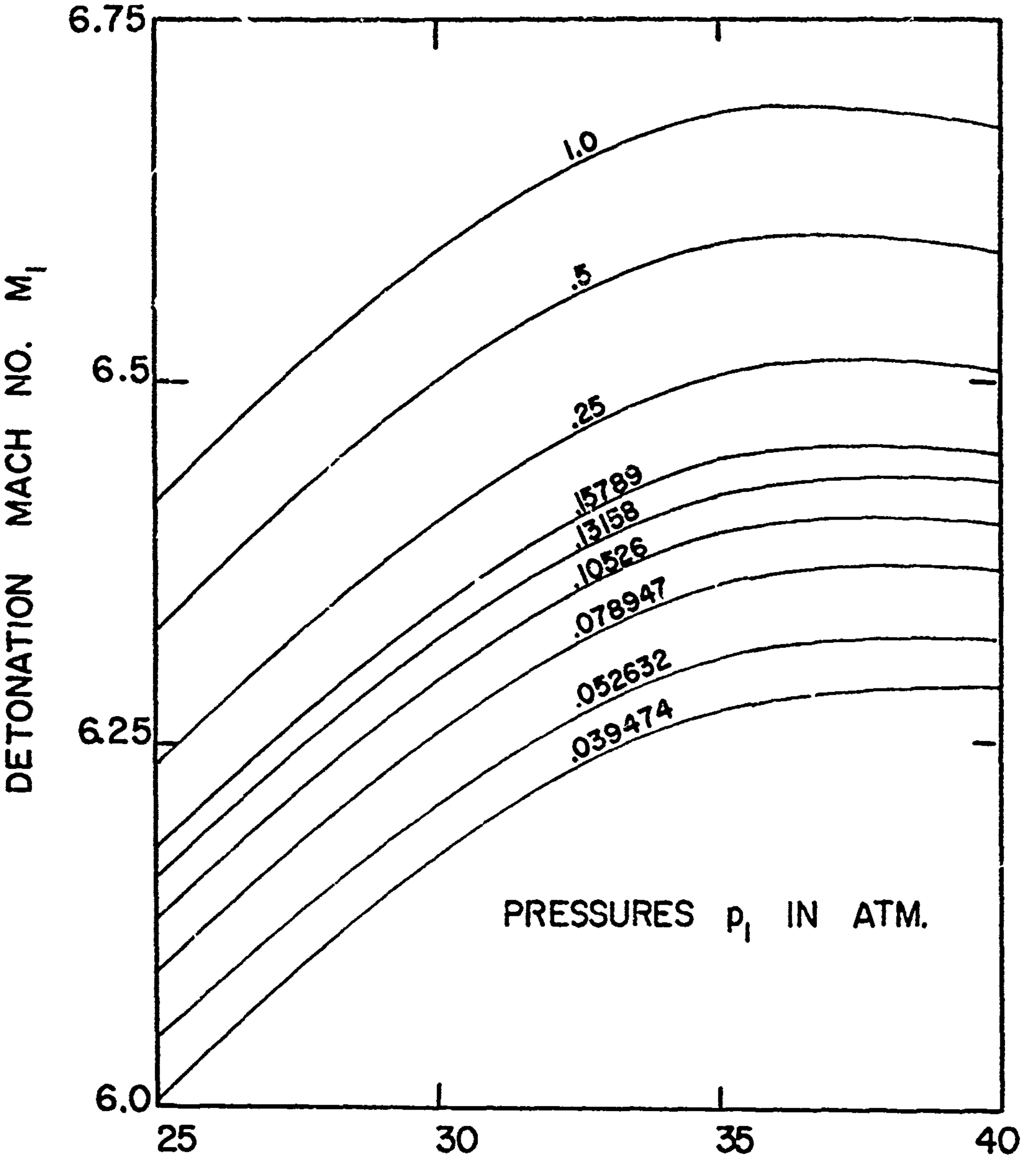

DETONATION MACH NO. M_1
6.75
6.5
6.25
6.0
25
30
35
40
CS$_2$ (MOLE PERCENT)
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
PRESSURES p_1 IN ATM.

FIG. 10

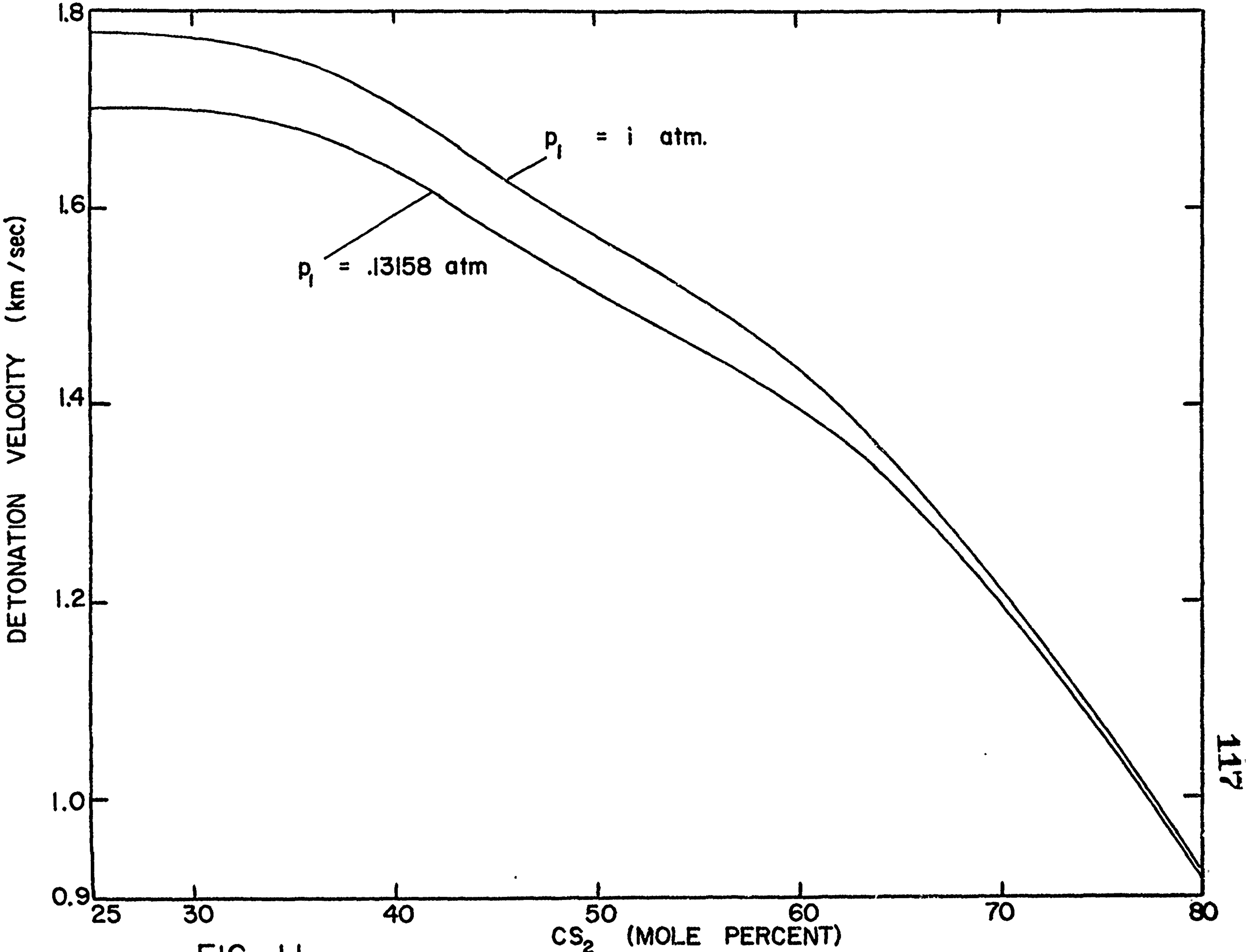

DETONATION VELOCITY (km / sec)
1.8
1.6
1.4
1.2
1.0
0.9
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)
p_1 = 1 atm.
p_1 = .13158 atm

FIG. 11

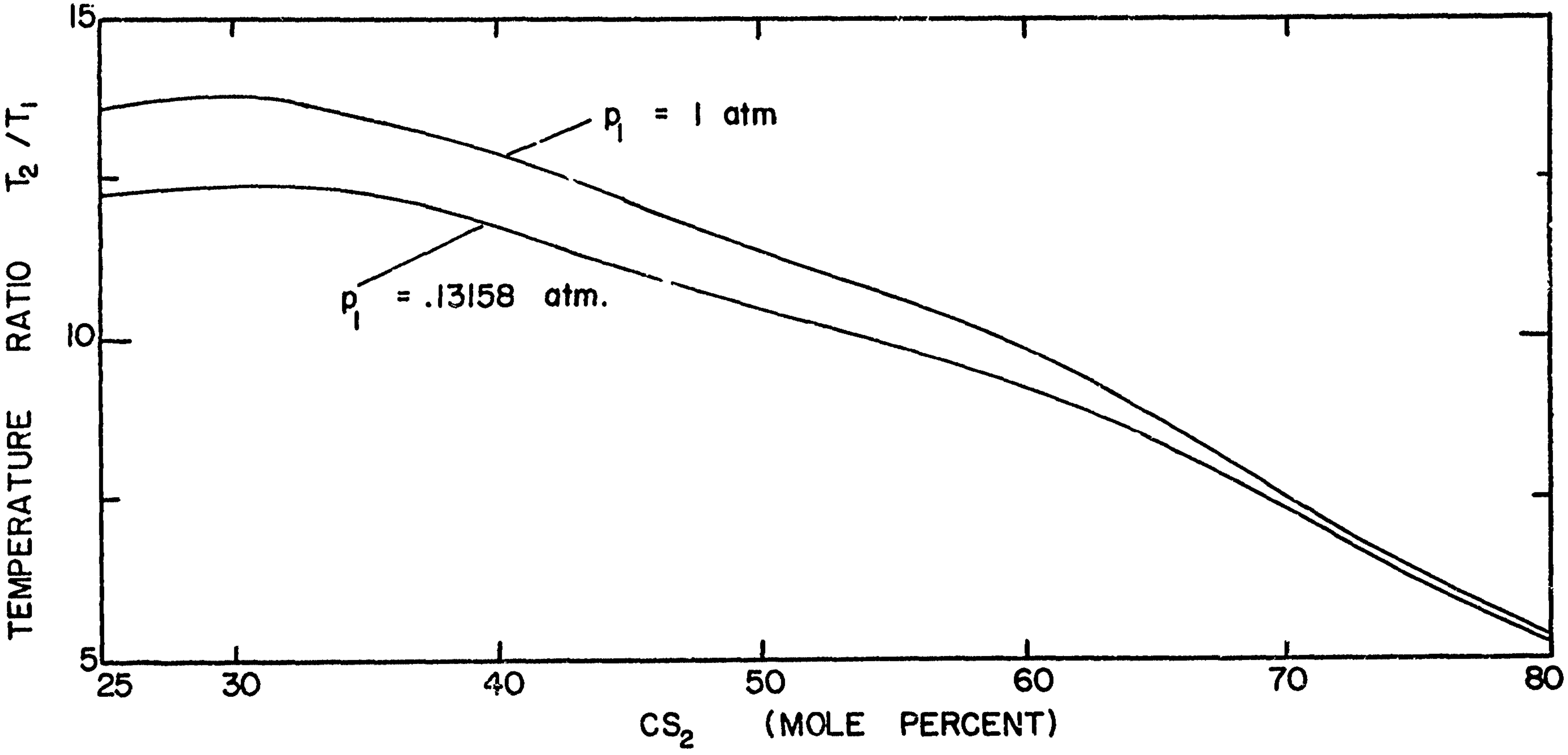

15
10
5
TEMPERATURE RATIO T_2/T_1
p_1 = 1 atm
p_1 = .13158 atm.
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)

FIG. 12

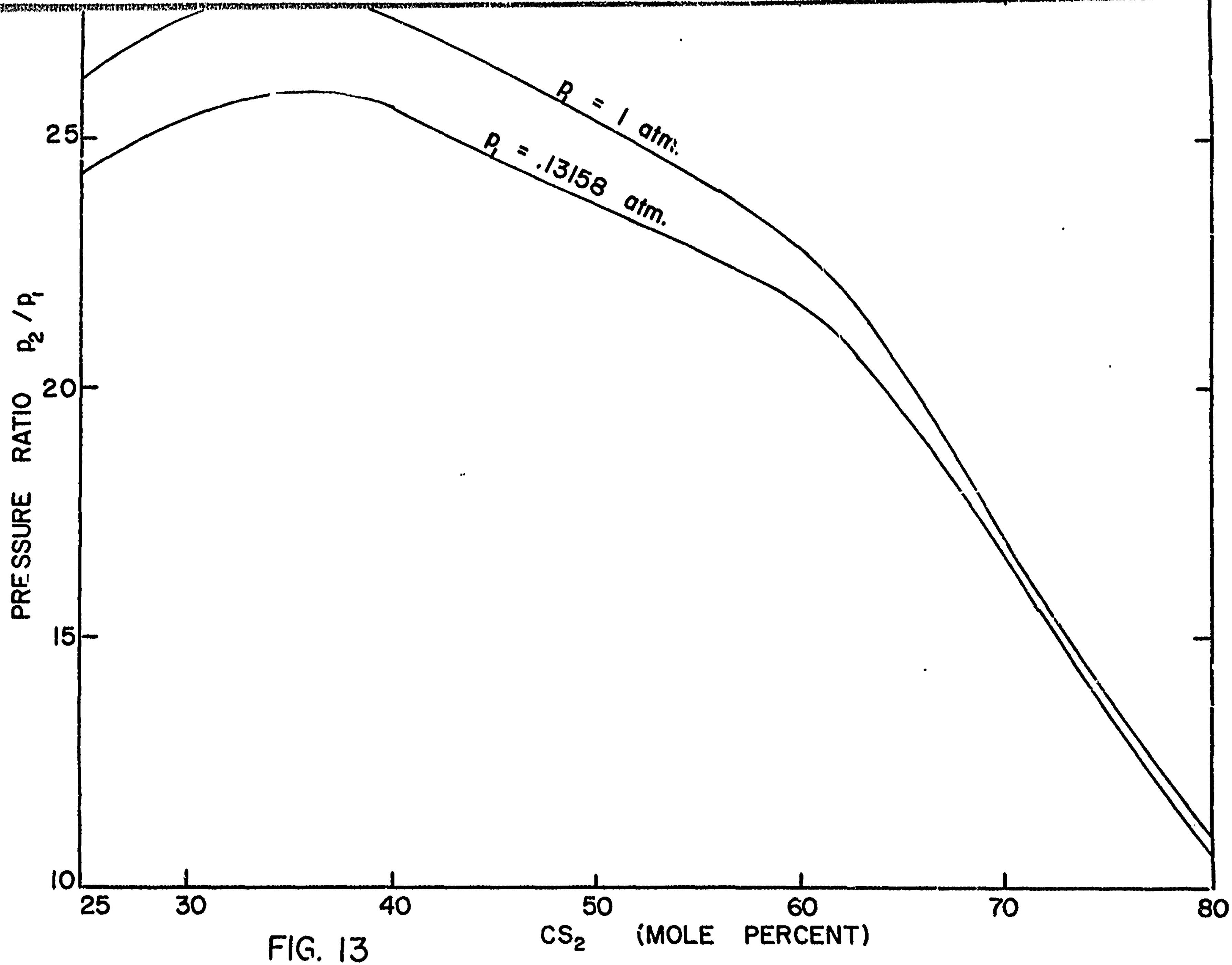

P_1 = 1 atm.
P_1 = .13158 atm.
PRESSURE RATIO P_2/P_1
10
15
20
25
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)

FIG. 13

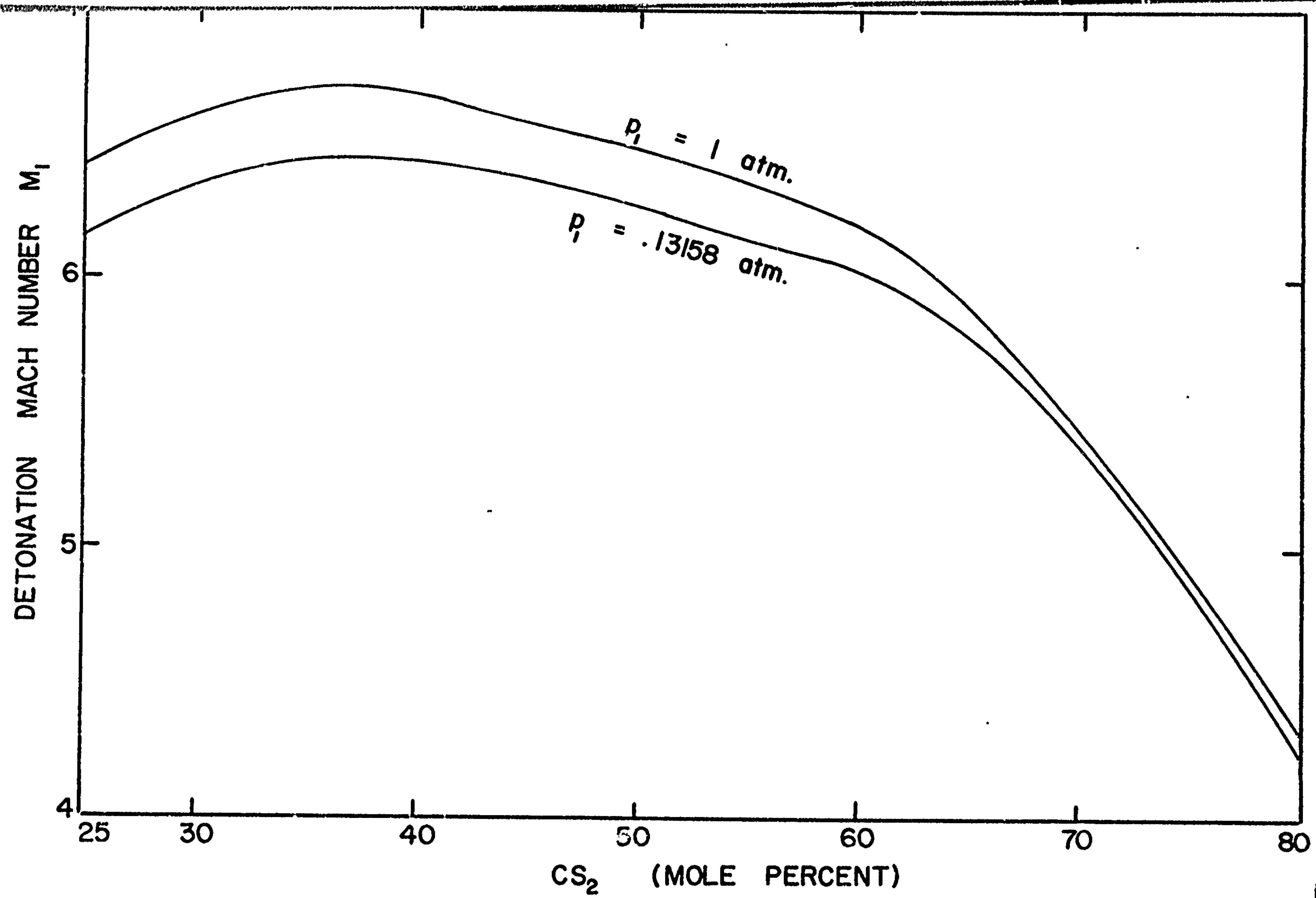

DETONATION MACH NUMBER M_1
6
5
4
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)
p_1 = 1 atm.
p_1 = .13158 atm.

FIG. 14

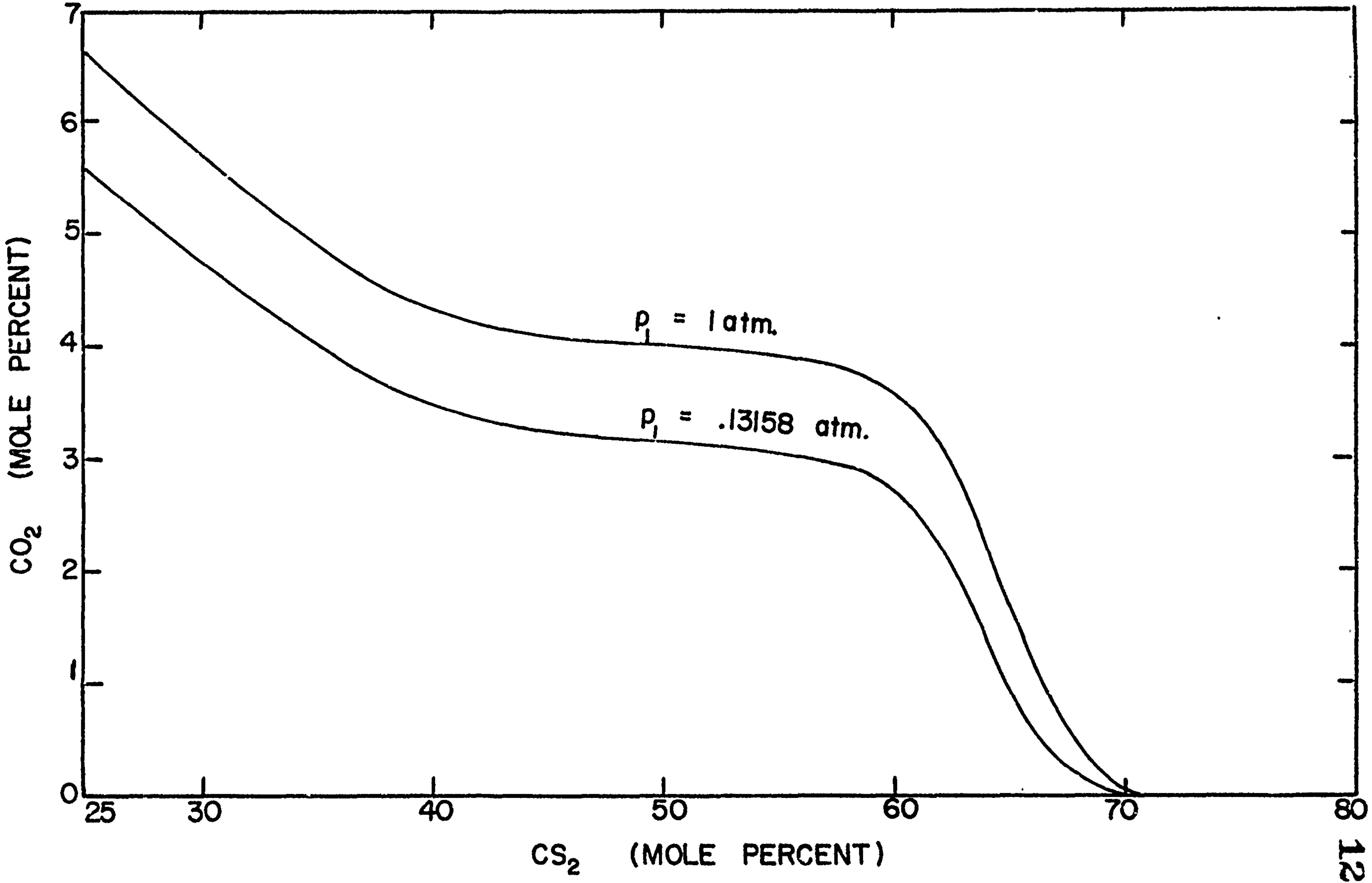

CO_2 (MOLE PERCENT)
7
6
5
4
3
2
1
0
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)
p_1 = 1 atm.
p_1 = .13158 atm.

FIG. 15

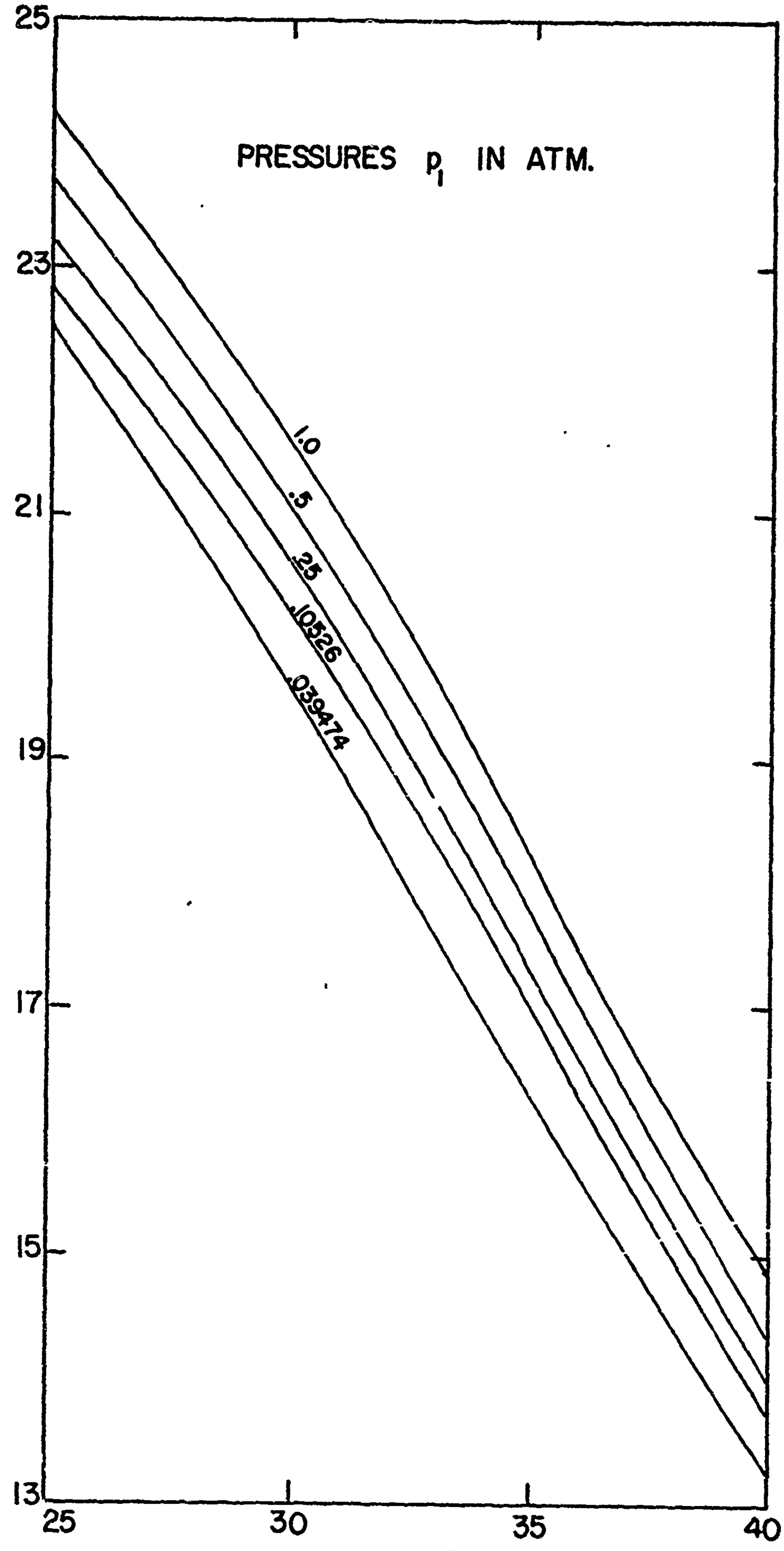

PRESSURES p_1 IN ATM.
1.0
.5
.25
.10526
.039474
25
23
21
19
17
15
13
25
30
35
40
SO_2 (MOLE PERCENT)
CS_2 (MOLE PERCENT)

FIG. 16

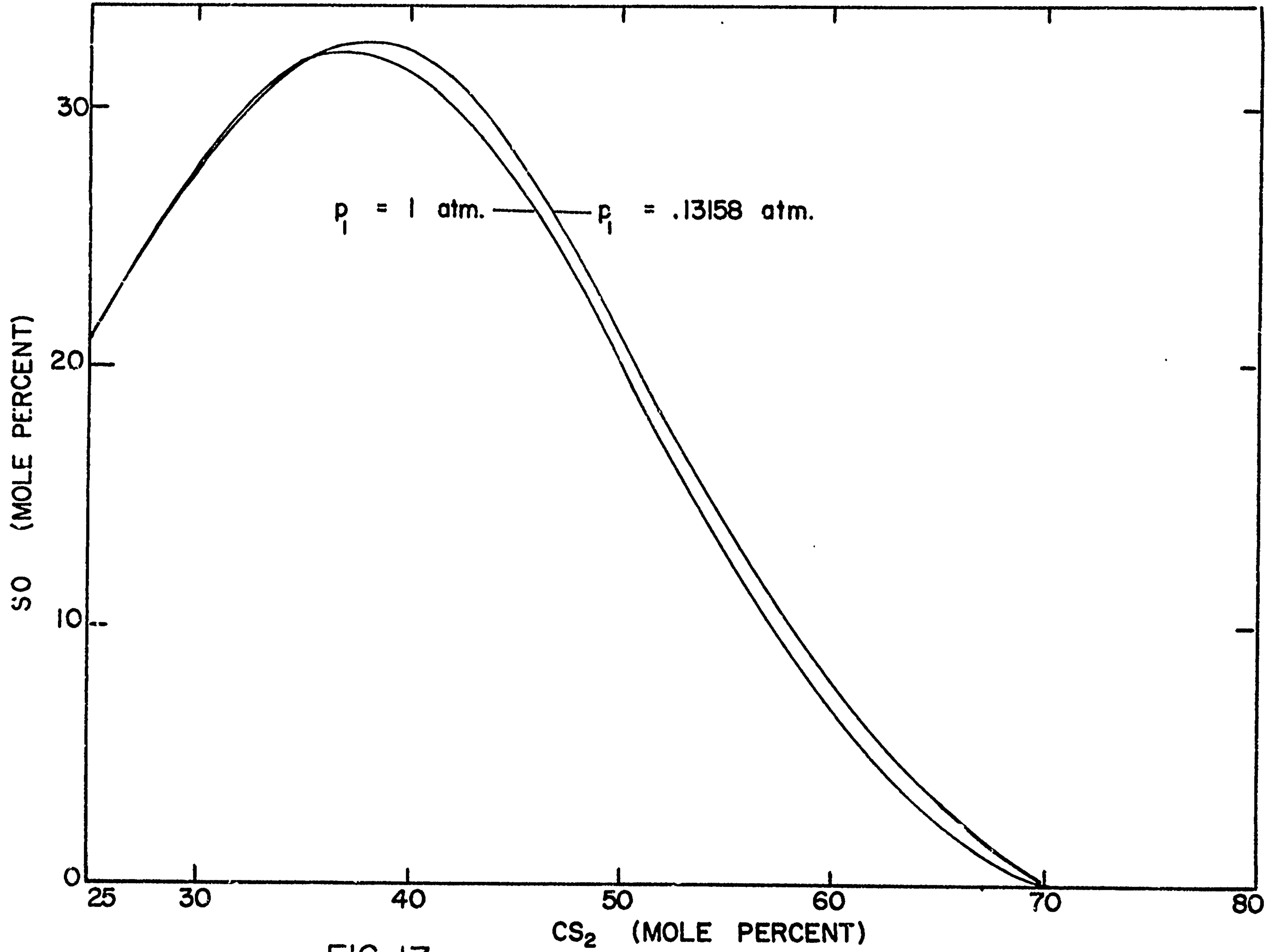

30
20
10
0
SO (MOLE PERCENT)
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)
p_1 = 1 atm.
p_1 = .13158 atm.

FIG. 17

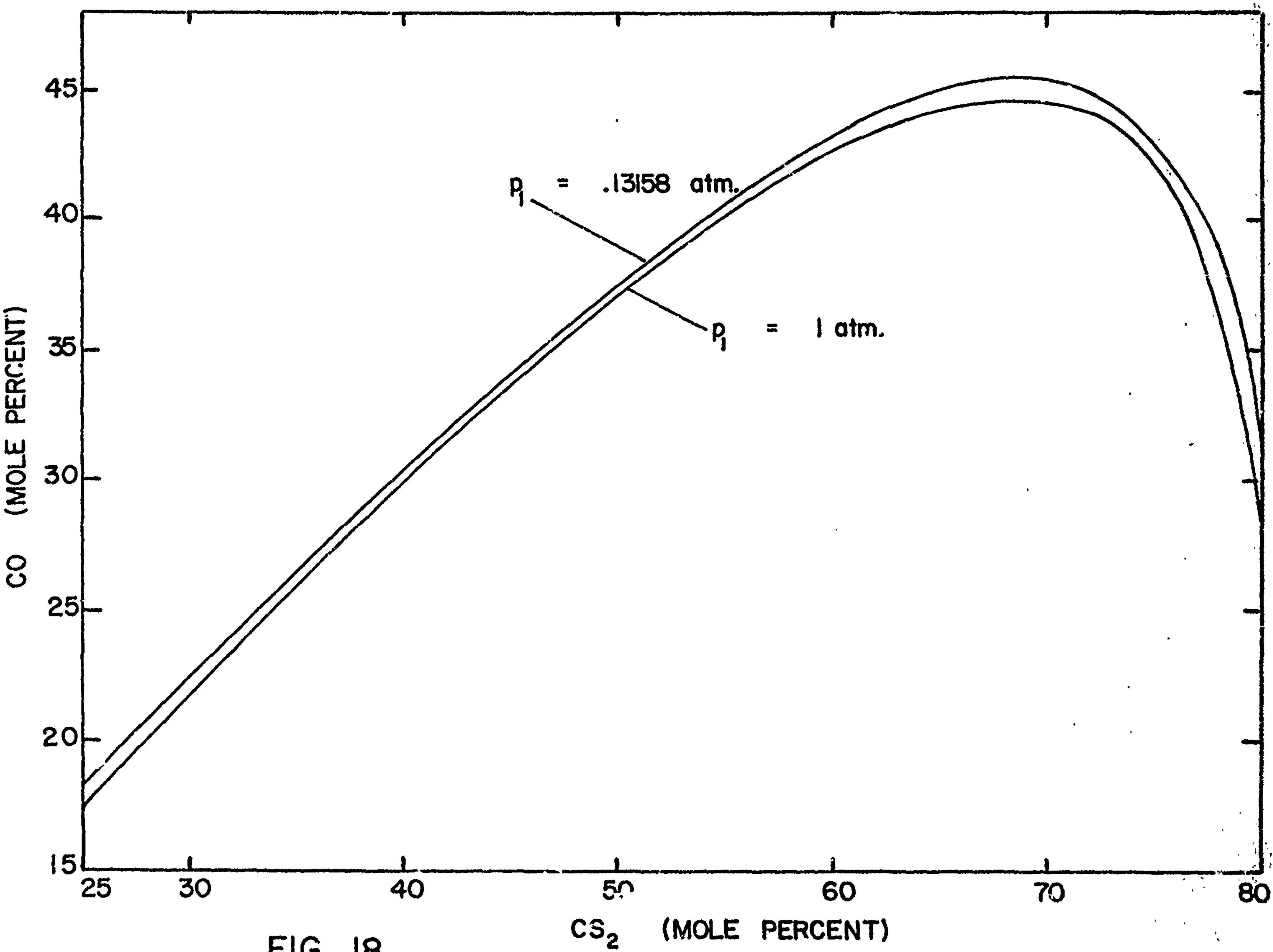

CO (MOLE PERCENT)
45
40
35
30
25
20
15
25
30
40
50
60
70
80
CS_2 (MOLE PERCENT)
P_1 = .13158 atm.
P_1 = 1 atm.

FIG. 18

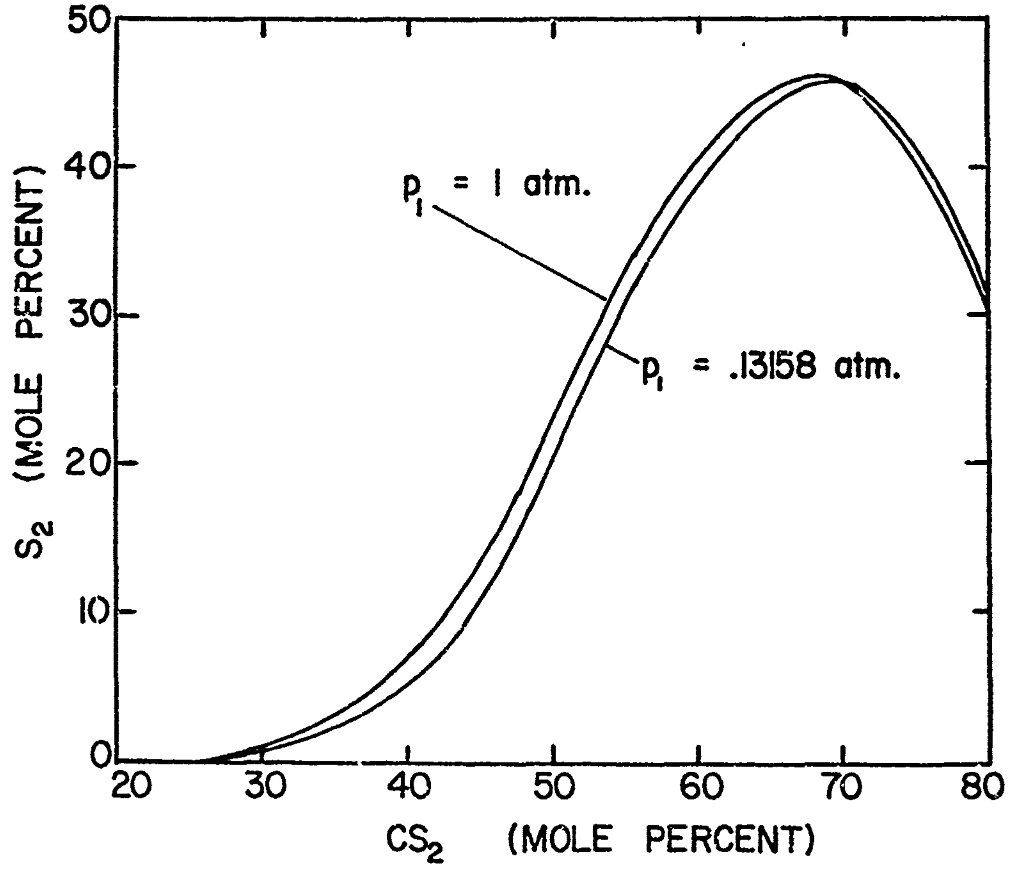

p_1 = 1 atm.
p_1 = .13158 atm.
S_2 (MOLE PERCENT)
CS_2 (MOLE PERCENT)
0
10
20
30
40
50
20
30
40
50
60
70
80

FIG. 19

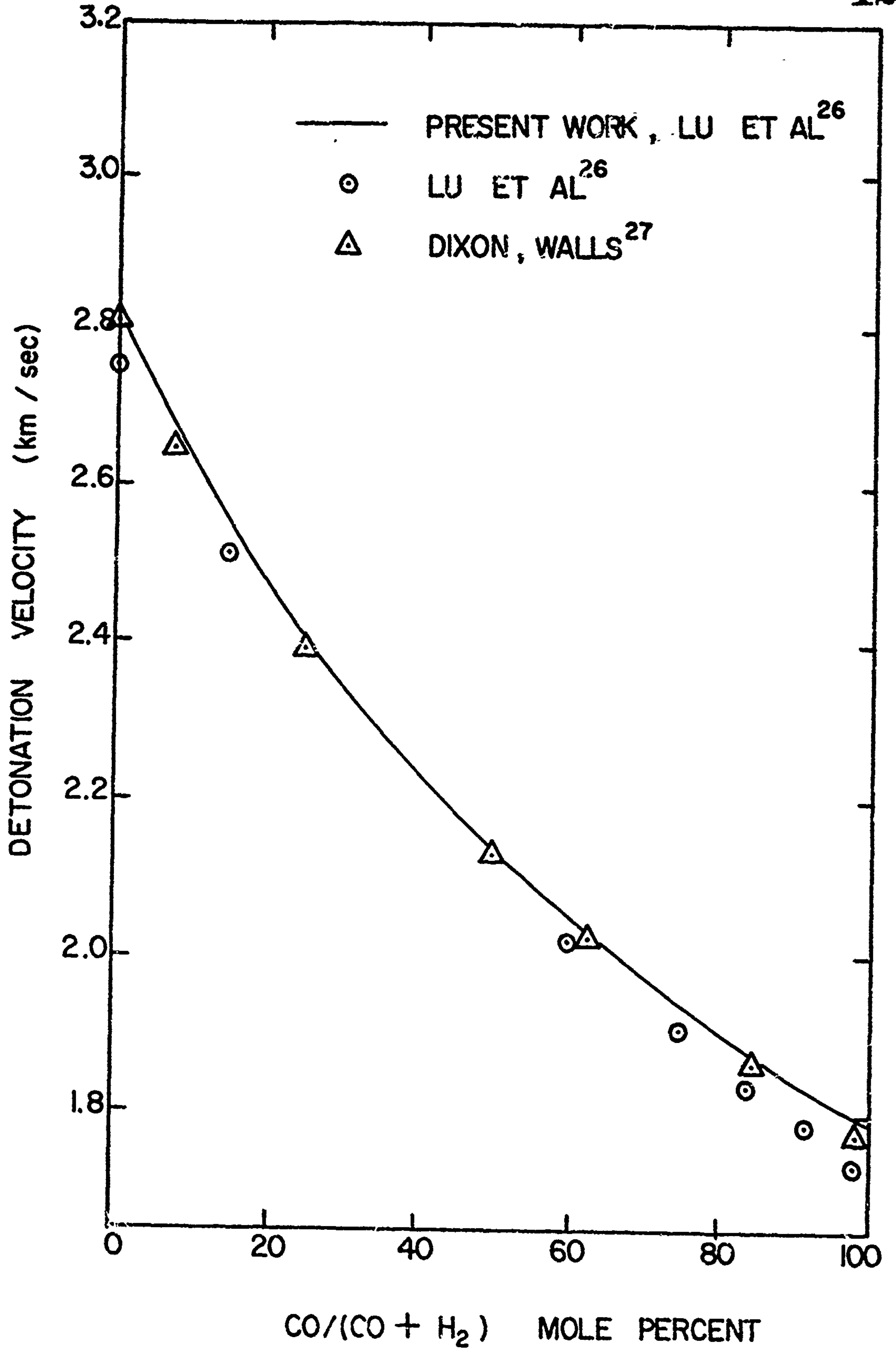

PRESENT WORK, LU ET AL^{26}
LU ET AL^{26}
DIXON, WALLS^{27}
DETONATION VELOCITY (km / sec)
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
0
20
40
60
80
100
CO/(CO + H_2) MOLE PERCENT

FIG. 20

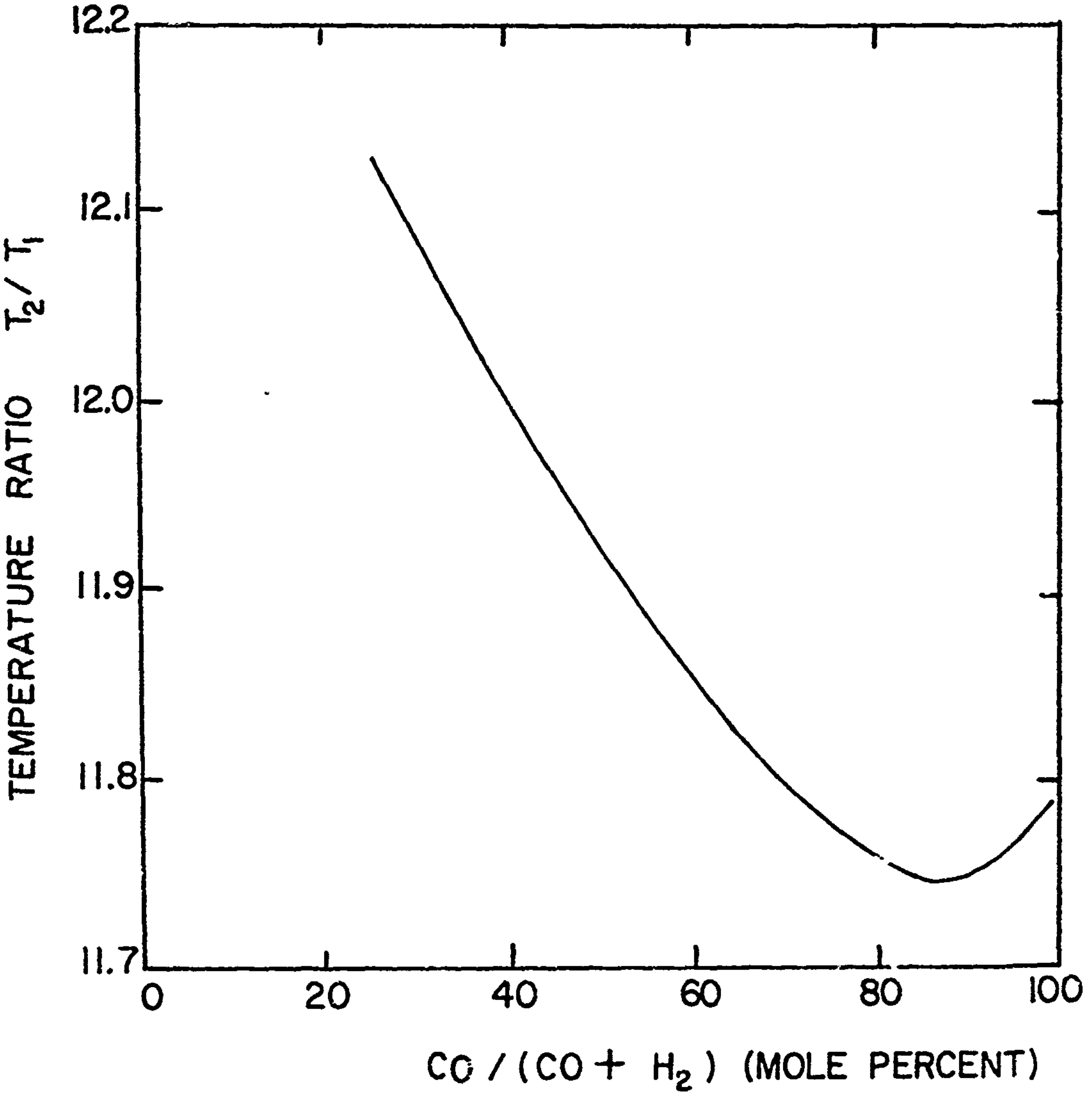

12.2
12.1
12.0
11.9
11.8
11.7
TEMPERATURE RATIO T_2/T_1
0
20
40
60
80
100
CO / (CO + H_2) (MOLE PERCENT)

FIG. 21

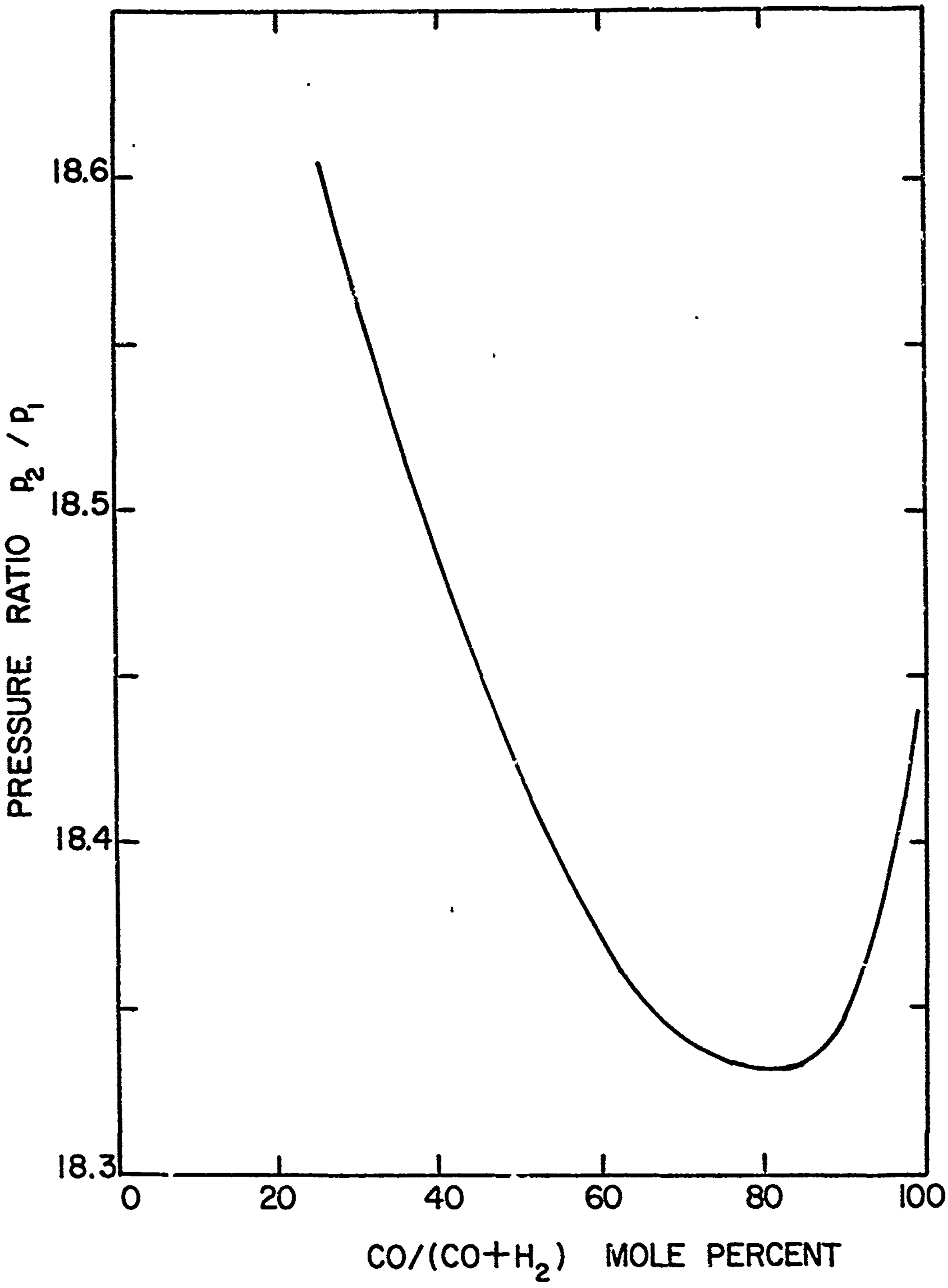

PRESSURE RATIO P_2 / P_1
18.6
18.5
18.4
18.3
0
20
40
60
80
100
$CO/(CO+H_2)$ MOLE PERCENT

FIG. 22

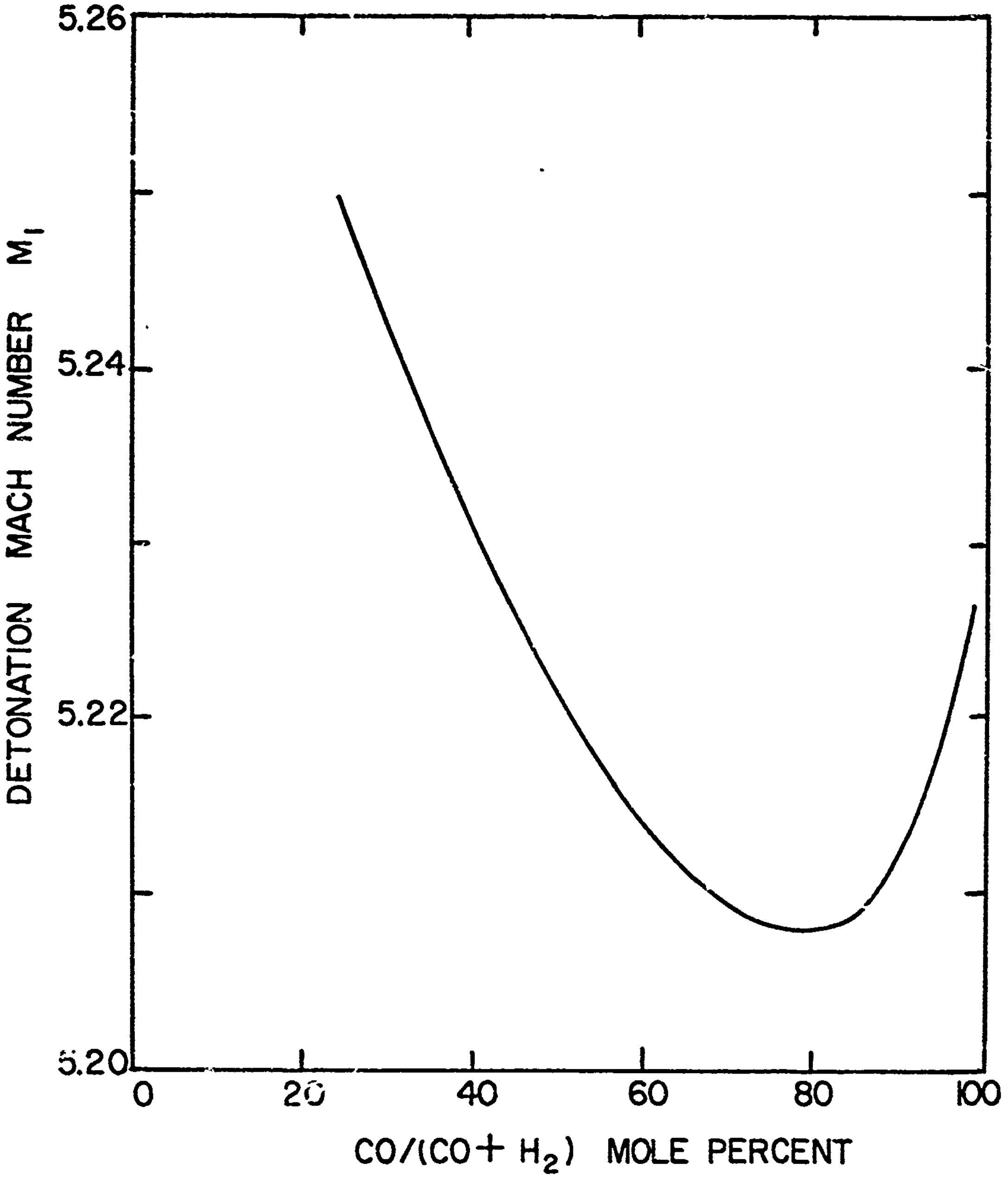

DETONATION MACH NUMBER M_1
5.26
5.24
5.22
5.20
0
20
40
60
80
100
CO/(CO+ H_2) MOLE PERCENT

FIG. 23

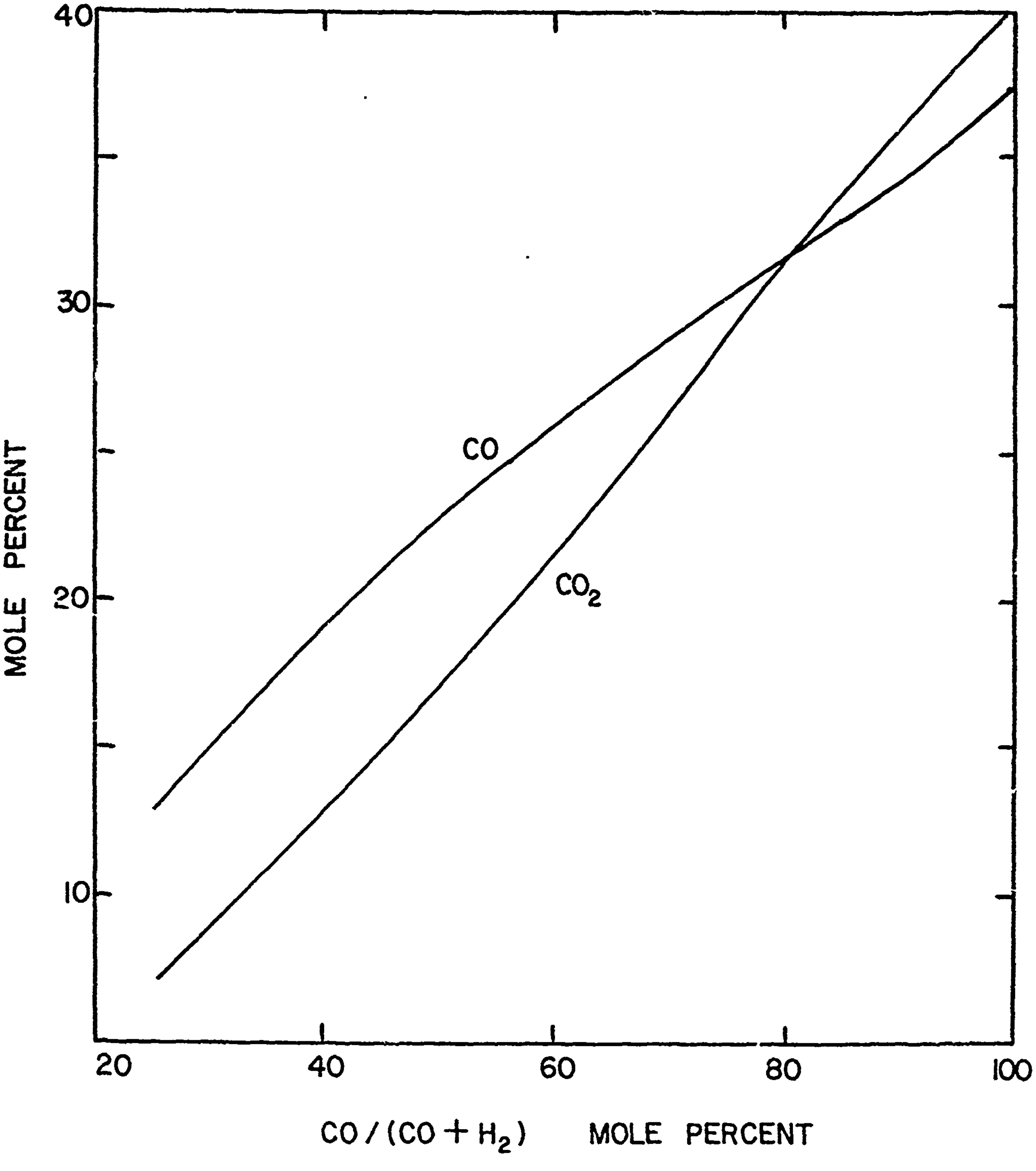

40
30
20
10
MOLE PERCENT
CO
CO_2
20
40
60
80
100
$CO/(CO+H_2)$ MOLE PERCENT

FIG. 24

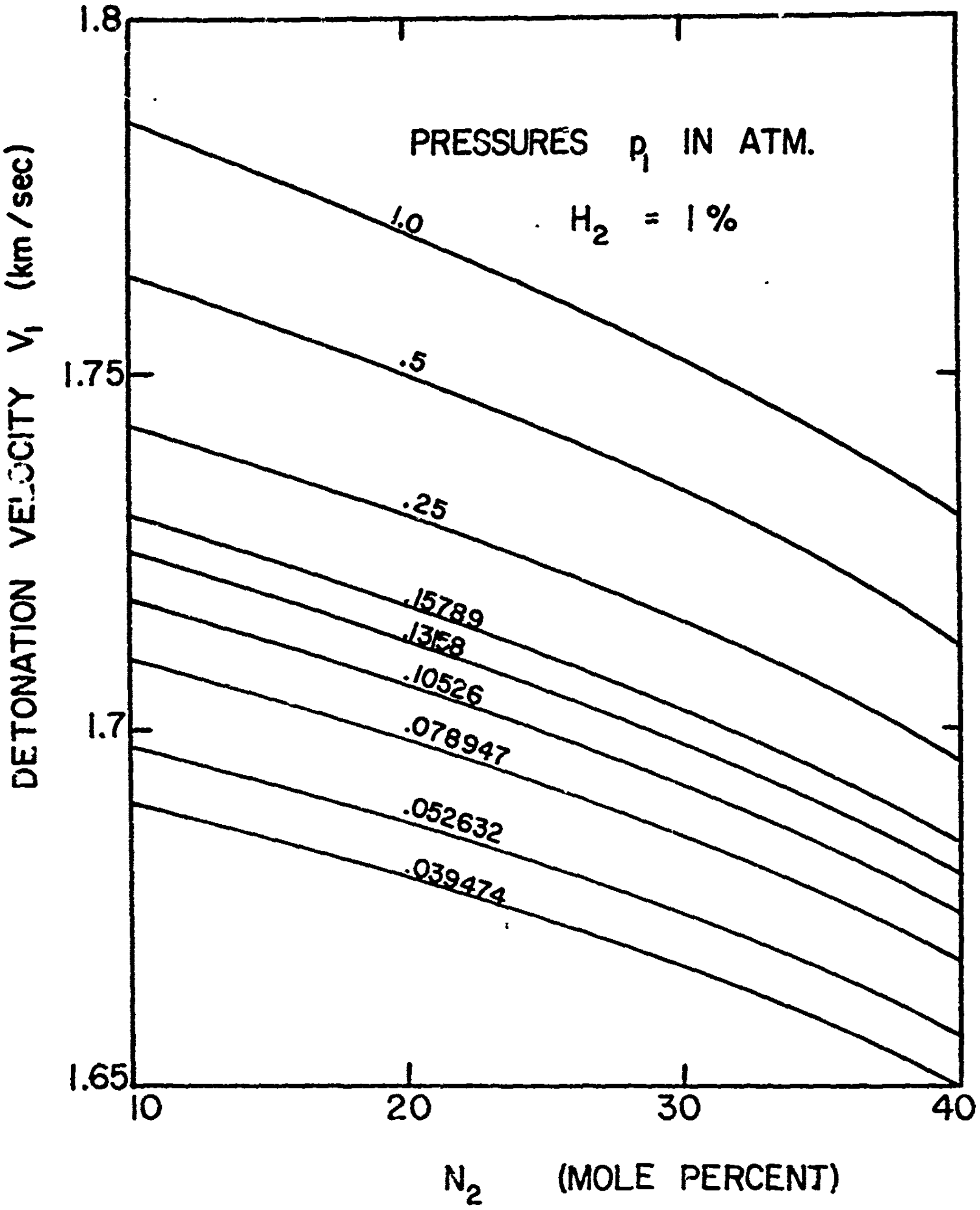

PRESSURES p_1 IN ATM.
H_2 = 1%
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
DETONATION VELOCITY V_1 (km/sec)
1.8
1.75
1.7
1.65
10
20
30
40
N_2 (MOLE PERCENT)

FIG. 25

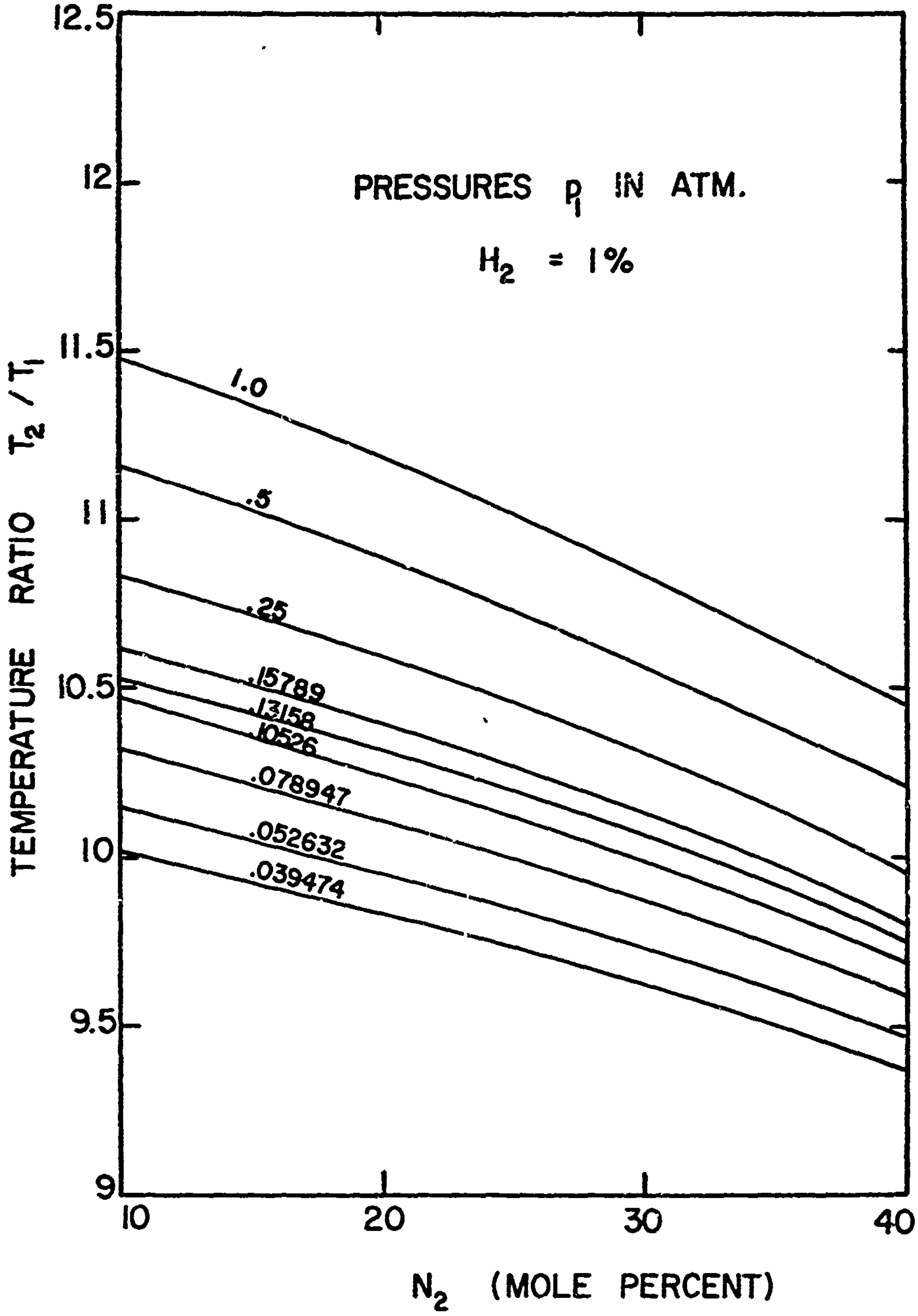

PRESSURES p_1 IN ATM.
H_2 = 1%
TEMPERATURE RATIO T_2 / T_1
12.5
12
11.5
11
10.5
10
9.5
9
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
10
20
30
40
N_2 (MOLE PERCENT)

FIG. 26

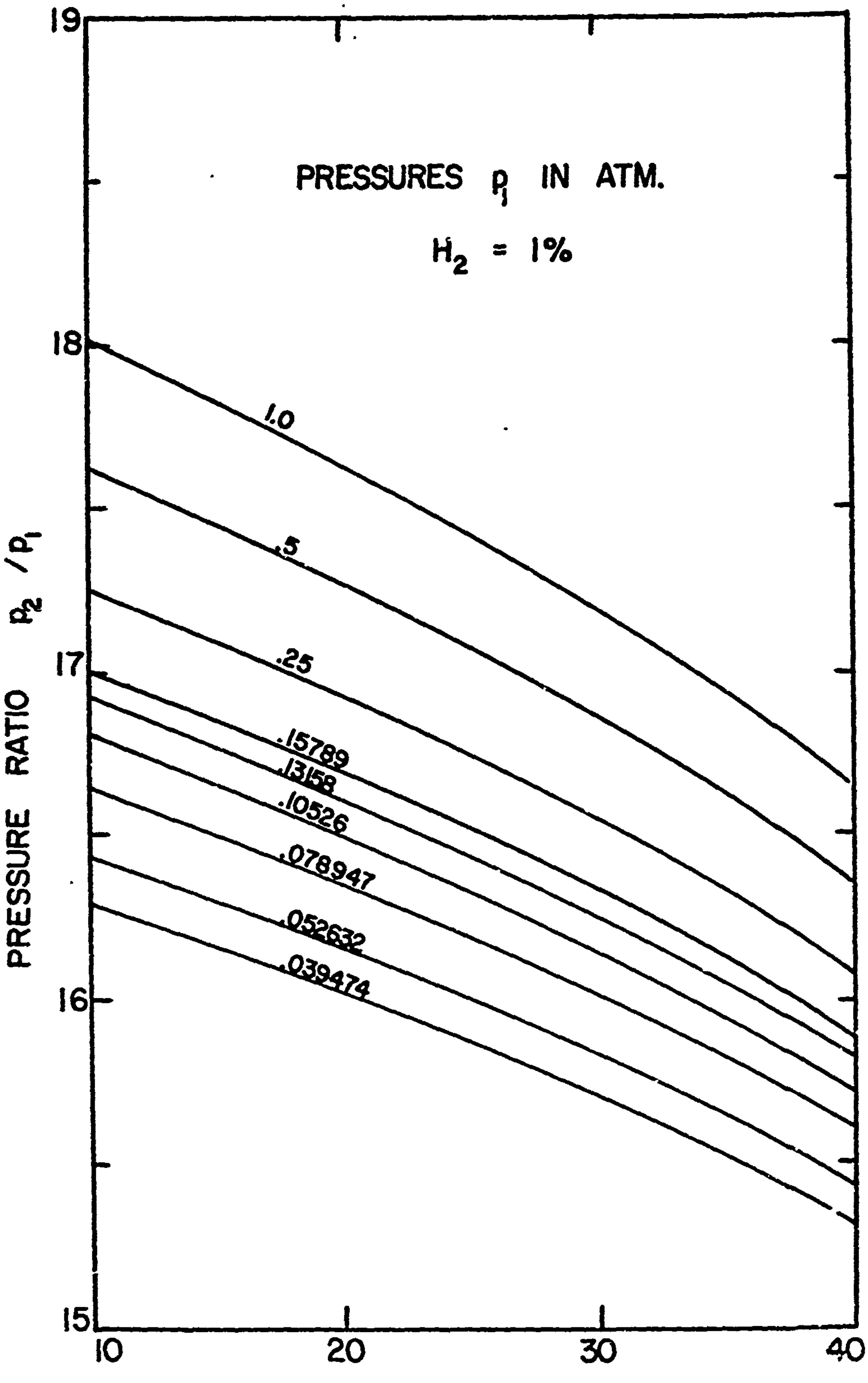

PRESSURES p_1 IN ATM.
H_2 = 1%
19
18
17
16
15
PRESSURE RATIO p_2/p_1
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
10
20
30
40
N_2 (MOLE PERCENT)

FIG. 27

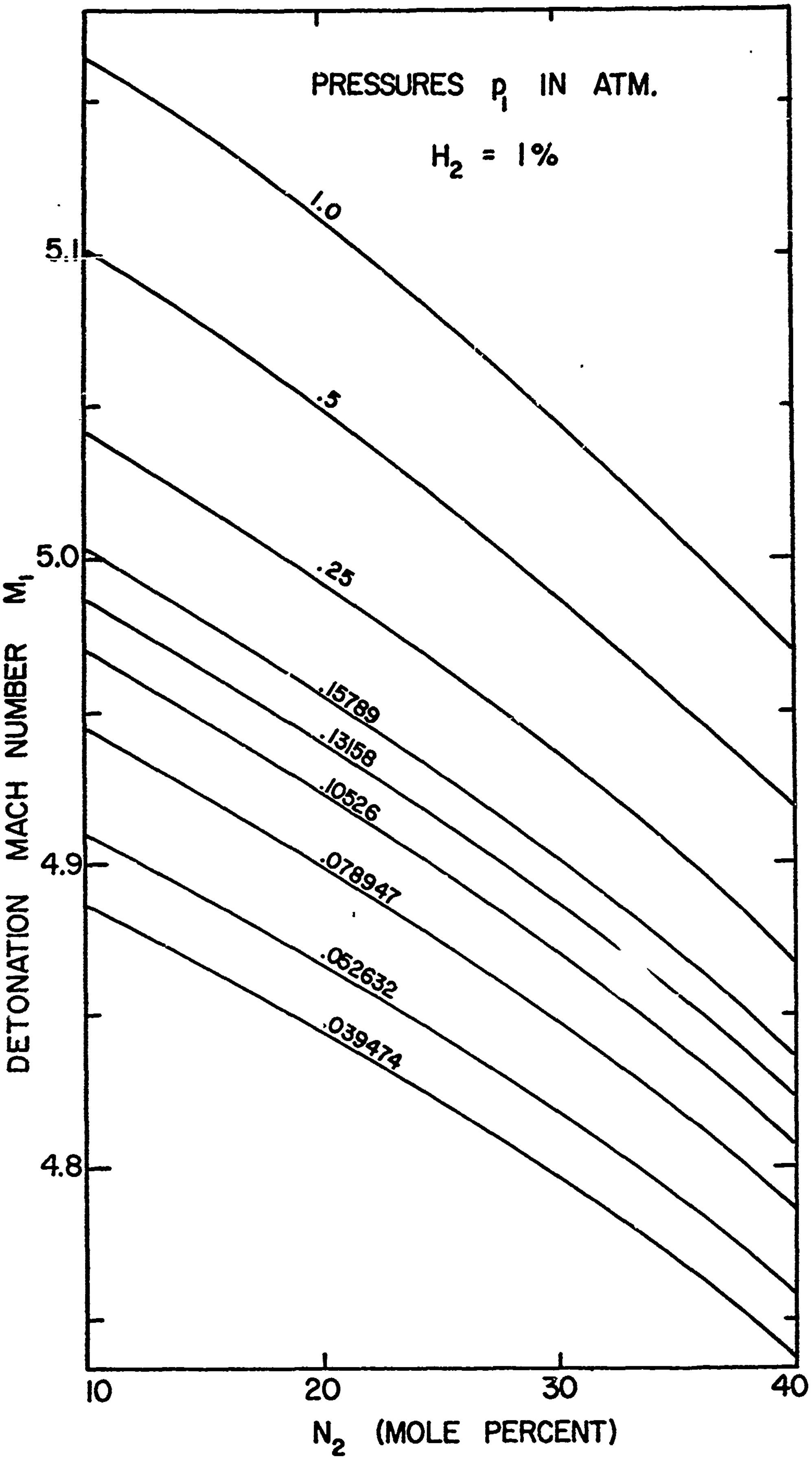

PRESSURES p_1 IN ATM.
H_2 = 1%
1.0
.5
.25
.15789
.13158
.10526
.078947
.052632
.039474
DETONATION MACH NUMBER M_1
5.1
5.0
4.9
4.8
10
20
30
40
N_2 (MOLE PERCENT)

FIG. 28

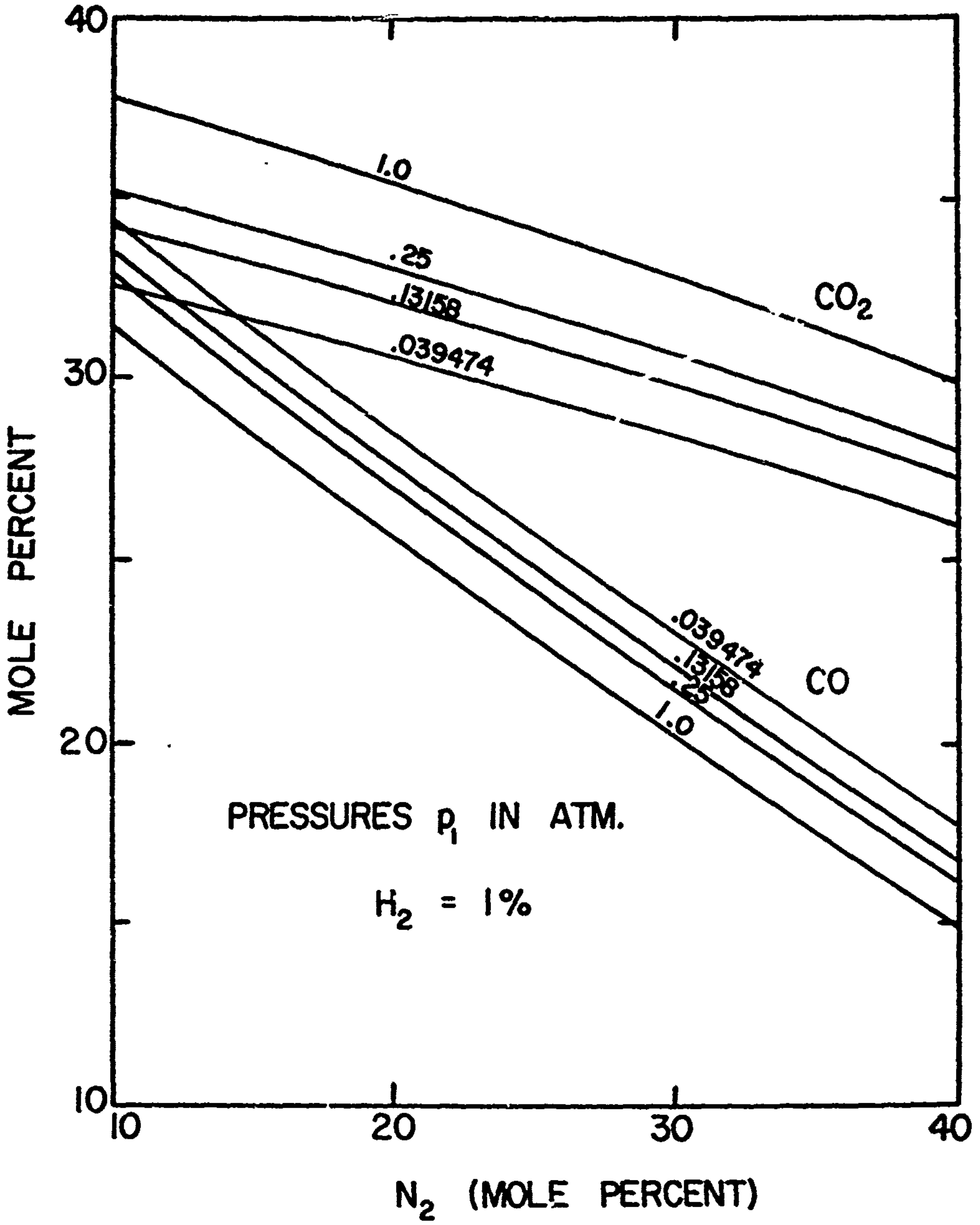

MOLE PERCENT
N$_2$ (MOLE PERCENT)
40
30
20
10
10
20
30
40
1.0
.25
.13158
.039474
CO$_2$
.039474
.13158
.25
1.0
CO
PRESSURES p_1 IN ATM.
H_2 = 1%

FIG. 29