not change with respect to expansion ratios except when compared over very large expansion ratios as is shown in Ref. 6; nor do they change markedly when compared on a frozen equilibrium basis. However, as some of the propellant systems considered here have phase changes of combustion products predicted during the expansion, it is well to compare

Table 5 Densities and heats of formation of propellant components

Reactants	ρ, gm/cm^3	ΔH_{f298}, kcal/mole
H_2O_2	1.47	−44.84
O_2	1.14	−3.08
N_2O_4	1.49	−6.8
F_2	1.5	−3.02
ClF_3	1.83	−44.53
$-CH_2-$	0.807	−6.03
H_2	0.07	−2.13
N_2H_4	1.01	+12.05
Be	1.85	0
Li	0.53	0
Al	2.70	0
B	2.54	0

Table 6 Enthalpies of formation of combustion products

Species	ΔH_{f298}	Species	ΔH_{f298}
$BeO(l)$	−129.06	$Li_2O(l)$	−132.32
$BeO(s)$	−143.10	$LiOH(v)$	−57.70
$Al_2O_3(l)$	−313.35	$BeF_2(l)$	−182.80
$Al_2O_3(s)$	−400.40	$BeF_2(l)$	−238.63
$AlF_3(v)$	−273.50	$BF_3(v)$	−270.00
$LiF(v)$	−79.30	$B_2O_3(l)$	−300.34
$LiF(l)$	−140.72	$B_2O_3(s)$	−305.34
$Li_2O(v)$	−34.10	$HBO_2(v)$	−135.32

a few systems at other conditions to check the validity of the 1000/14.7 psia shifting equilibrium ideal expansion comparison. Fig. 14 presents I_s (vacuum) vs. area ratio for several of the high I_s systems. It is seen that there is only a small change in relative I_s values over a relatively wide range in nozzle expansion area ratios. Frozen equilibrium I_s values for the same propellants are given in Tables 2 and 3. Although the differences between shifting and frozen equilibrium values shown there do vary from 5 to 32 sec, there is no difference in the relative I_s values of those propellants.

In conclusion, it must be pointed out that the uncertainties in heats of formation of both reactants and products plus uncertainties in heat capacities, heats of fusion, and heats of vaporization of combustion products are such that there may be uncertainties of ±15 sec in some of the I_s values presented here. Tables 5 and 6 list some of the data used in the calculations. The combustion product data used were taken as much as possible from the recently published JANAF tables (7)

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Calculation of Detonation Properties and Effect of Independent Parameters on Gaseous Detonations

FRANK J. ZELEZNIK
SANFORD GORDON

NASA Lewis Research Center
Cleveland, Ohio

A general iterative method for obtaining detonation parameters for any chemical reactants is presented. A systematic procedure is described for obtaining good initial estimates of the detonation temperature and pressure for any gaseous reactants. Equations are also presented for obtaining partial derivatives of the detonation parameters. These derivatives permit detonation parameters calculated for one set of initial conditions to be extrapolated with good accuracy for moderate changes in initial conditions. Detailed results are tabulated for stoichiometric hydrogen-oxygen for a wide range of initial temperatures and pressures. A comparison is made with results obtained by using an equilibrium gamma and an equilibrium specific heat ratio for calculating sonic velocity.

$\mathbb{M}$ANY articles describe methods for the thermodynamic-hydrodynamic calculation of Chapman-Jouguet detonations (e.g., Refs. 1-9). The calculation methods can be divided into two categories. First are trial and error methods (5-9),[1] and second are Newton-Raphson iteration methods (1-4). The trial and error calculations are generally inferior to Newton-Raphson calculations for two reasons. First, they give less precision for an equivalent amount of calculation. Second, their success often depends on the intuition of the person performing the calculations in obtaining successive approximations to the solution.

The Newton-Raphson method of Eisen (1, 2) is a simultaneous solution of the continuity, energy, and momentum equations together with the equations defining chemical equilibrium in a system containing carbon, hydrogen, oxygen, and nitrogen. The procedure is to calculate the strong and weak detonation solutions for two estimates of the detonation velocity and then, using a linear interpolation based on the fact that the strong and weak detonation solutions coalesce at the Chapman-Jouguet point, to determine the Chapman-Jouguet detonation solution. The method has three difficulties. First, it combines the problem of determining equilibrium compositions in a particular chemical system with the problem of calculating the Chapman-Jouguet detonation. Second, it requires at least four, and often more, separate solutions of the detonation equations to obtain the desired Chapman-Jouguet solution. Third, the interpolation scheme can easily lead to estimates for the detonation velocity for which no solution exists.

Refs. 3 and 4 give a general Newton-Raphson iteration method. Severe oscillations were encountered during the course of iteration, and this difficulty was ascribed to the neglect of rates of change of composition and heats of reaction with respect to temperature and pressure.

The method presented in this paper is also a general Newton-Raphson iteration method, but it was developed prior to any knowledge of the work of Refs. 3 and 4. The method of this paper and that of Refs. 3 and 4 differ in several ways. First, the two equations used in the Newton-Raphson iteration are different. Second, the evaluation of the coefficients in the iteration equations used in this paper includes rates of change of composition with temperature and pressure. Third, a systematic procedure is presented in this paper for obtaining good initial estimates of detonation temperature and pressure. No difficulty has been encountered with this method for a wide variety of chemical reactants.

The effects of initial temperatures and pressures on the Chapman-Jouguet detonations have been examined by both experiment and calculation (7-10). In these references the effects of initial temperature and pressure on the calculated detonation parameters were determined by performing calculations for various initial conditions and then describing the results qualitatively. In this paper the discussion of initial conditions is extended to include the effects of initial enthalpy and to the actual evaluation of partial derivatives of detonation parameters with respect to initial temperature, pressure, and enthalpy.

Thermodynamic Calculation of Detonations

Relevant One-Dimensional Equations

In a coordinate system moving with the detonation wave front (see Fig. 1), the one-dimensional continuity, momentum, and energy equations are

$$\rho_1 u_1 = \rho_2 u_2 \qquad [1]$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \qquad [2]$$

$$h_1 + \tfrac{1}{2}u_1^2 = h_2 + \tfrac{1}{2}u_2^2 \qquad [3]$$

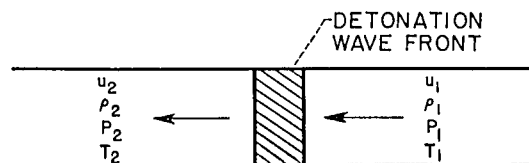[1] Numbers in parentheses indicate References at end of paper.

Fig. 1 One-dimensional flow through detonation wave (coordinate system moving with detonation wave)
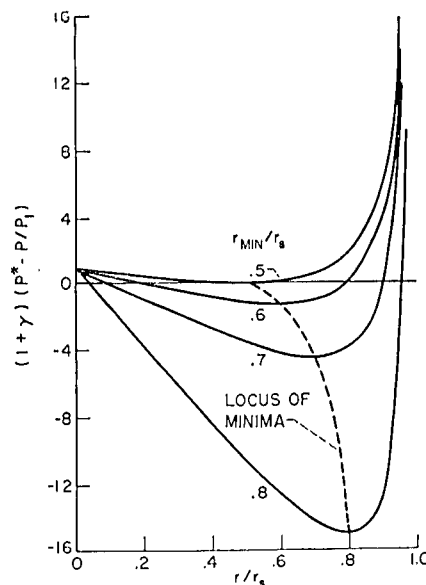

Fig. 2 Function $(1 + \gamma)(P^* - P/P_1) = 1/(1 - r/r_s) - (r/r_s)/(1 - r_{min}/r_s)^2$ vs. r/r_s with position of minimum as a parameter

Eq. 1 can be used to eliminate u_1 from Eqs. 2 and 3 to give

$$P_1 - P_2 = \rho_2 u_2^2[1 - (\rho_2/\rho_1)] \qquad [4]$$

$$h_1 - h_2 = \tfrac{1}{2}u_2^2[1 - (\rho_2/\rho_1)^2] \qquad [5]$$

Division of Eq. 5 by Eq. 4 would give the well-known Hugoniot equation; however, for detonation velocity calculations it is preferable to use Eqs. 4 and 5 rather than to use the Hugoniot equation directly.

The velocity u_2 of the products of reaction relative to the detonation wave is eliminated from Eqs. 4 and 5 by using the Chapman-Jouguet condition. This condition states that the velocity u_2 equals the velocity of sound in the burned gas (11). The analysis of Ref. 12 indicates that the equilibrium rather than the frozen speed of sound should be used. A discussion of the effect of an incorrect sonic speed on the detonation process is given in a later section of this paper. From the Chapman-Jouguet hypothesis

$$u_2^2 = a_2^2 = (\partial P_2/\partial \rho_2)_s = \gamma_2 P_2/\rho_2 \qquad [6a]$$

where

$$\gamma = (\partial \ln P/\partial \ln \rho)_s \qquad [6b]$$

It should be noted that γ is not in general equal to the ratio of specific heats. Substitution of Eq. 6a into Eqs. 4 and 5 gives, after some rearrangement, two equations relating conditions before and after the detonation wave:

$$P_2/P_1 = [1 - \gamma_2(\rho_2/\rho_1 - 1)]^{-1} \qquad [7]$$

$$h_2 = h_1 + (\gamma_2 P_2/2\rho_2)[(\rho_2/\rho_1)^2 - 1] \qquad [8]$$

Eqs. 7 and 8 suggest the definition of two functions of tem-

perature and pressure for iterative purposes:

$$P^* = [1 - \gamma(\rho/\rho_1 - 1)]^{-1} \qquad [9]$$

$$h^* = h_1 + (\gamma P/2\rho)[(\rho/\rho_1)^2 - 1] \qquad [10]$$

Eq. 10 can also be written as

$$h^* = h_1 + \frac{\gamma R T_1}{2M_1}\left(\frac{P}{P_1}\right)\frac{[(\rho/\rho_1)^2 - 1]}{\rho/\rho_1} \qquad [11]$$

where the ideal gas law

$$PM = \rho RT \qquad [12]$$

has been used. This equation of state is also applicable in situations where condensed reaction products are formed, as is pointed out in Ref. 13. The detonation process may now be defined by the simultaneous solution of

$$P^* - (P/P_1) = 0 \qquad [13]$$

$$h^* - h = 0 \qquad [14]$$

considering temperature and pressure as the independent variables.

Although Eq. 13 can be used as one of the two equations defining a Chapman-Jouguet detonation, it is not as suitable for use in a Newton-Raphson iteration as an alternative form to be presented later. However, an examination of Eq. 13 is useful, since its properties, which place narrow limits on the solution, can be used to obtain good initial estimates.

Considered as a function of the density ratio, Eq. 13 possesses two solutions and a first-order singularity. For simplicity of notation, the density ratio across the detonation is denoted by r. From the ideal gas law there follows

$$r = \frac{\rho}{\rho_1} = \left(\frac{P}{P_1}\right)\left(\frac{T_1}{T}\right)\left(\frac{M}{M_1}\right) = \left(\frac{P}{P_1}\right)\alpha \qquad [15]$$

Using Eq. 15 to eliminate the pressure ratio from Eq. 13 gives

$$P^* - \frac{P}{P_1} = \frac{1}{\gamma}\left[\left(\frac{1+\gamma}{\gamma}\right) - r\right]^{-1} - \frac{r}{\alpha} \qquad [16]$$

Thus a first-order singularity exists at

$$r_s = (1+\gamma)/\gamma \qquad [17]$$

Fig. 3 Function $(1/P^* - P_1/P)/(1 + \gamma) = 1 - r/r_s - [(r_{max}/r_s)^2/(r/r_s)]$ vs. r/r_s with position of maximum as a parameter

and further a minimum exists at

$$r_{min}/r_s = 1 - (\alpha\gamma)^{1/2}/(1 + \gamma) \qquad [18]$$

Eq. 16 can be rewritten in terms of the minimum and the singular point to give

$$(1+\gamma)\left(P^* - \frac{P}{P_1}\right) = \frac{1}{1 - (r/r_s)} - \frac{r/r_s}{[1 - (r_{min}/r_s)]^2} \qquad [19]$$

Fig. 2 is a plot of Eq. 19 with the location of the minimum considered as a parameter. The plot is given only for $r/r_s < 1$. For $r/r_s > 1$ the function is always negative, and therefore no solution exists.

An explicit expression can be found for the two roots of Eq. 13 by equating Eq. 19 to zero and solving the resulting quadratic equation to obtain

$$r_0/r_s = \tfrac{1}{2}\{1 \pm [1 - 4(r_{min}/r_s - 1)^2]^{1/2}\} \qquad [20]$$

The two roots will coincide for $r_{min}/r_s = \tfrac{1}{2}$. No real roots exist when $r_{min}/r_s < \tfrac{1}{2}$. As r_{min}/r_s increases corresponding to a greater energy release, the two roots separate. The lower root approaches zero as a lower limit, whereas the upper root approaches 1 as an upper limit. The smaller root represents a density ratio of less than 1 and therefore is not the desired solution.

The difficulty in the use of Eq. 13 in a Newton-Raphson iteration is that for this equation the method can safely be used only in the narrow interval $r_{min}/r_s < r/r_s < 1$. For estimates that correspond to $r/r_s < r_{min}/r_s$, the interation will converge to the smaller root. For estimates $r/r_s \geq 1$, no solution exists. These problems can be readily eliminated if, for purposes of iteration, Eq. 13 is replaced by an equivalent equation

$$1/P^* - P_1/P = \gamma[(1+\gamma)/\gamma - r] - \alpha/r = 0 \qquad [21]$$

Eq. 21 does not possess a singularity at r_s and has a maximum at

$$\frac{r_{max}}{r_s} = \left[\frac{\alpha\gamma}{(1+\gamma)^2}\right]^{1/2} \leq \left[\frac{\gamma}{(1+\gamma)^2}\right]^{1/2} \cong 0.5$$

The inequality comes from the fact that α is less than or equal to unity. A plot of

$$\frac{1}{1+\gamma}\left(\frac{1}{P^*} - \frac{P_1}{P}\right) = 1 - \frac{r}{r_s} - \frac{(r_{max}/r_s)^2}{r/r_s}$$

is given in Fig. 3 with the position of the maximum as a parameter. As is readily seen from Fig. 3, the locus of maxima is to the left of $r/r_s = 0.5$, and therefore the Newton-Raphson iteration can safely be used to the right of $r/r_s = 0.5$.

Newton-Raphson Iteration Equations

The Newton-Raphson iteration is described in Ref. 14. Applying this method to Eqs. 21 and 14 gives a set of equations linear in the corrections to the assumed values of pressure ratio and temperature ratio across the detonation:

$$\frac{\partial(1/P^* - P_1/P)}{\partial \ln(P/P_1)}\Delta\ln\frac{P}{P_1} +$$

$$\frac{\partial(1/P^* - P_1/P)}{\partial \ln(T/T_1)}\Delta\ln\frac{T}{T_1} = \frac{P_1}{P} - \frac{1}{P^*} \qquad [22a]$$

$$\frac{\partial(h^* - h)}{\partial \ln(P/P_1)}\Delta\ln\frac{P}{P_1} + \frac{\partial(h^* - h)}{\partial \ln(T/T_1)}\Delta\ln\frac{T}{T_1} = h - h^* \qquad [22b]$$

where

$$\Delta\ln\frac{P}{P_1} = \ln\left(\frac{P}{P_1}\right)_{k+1} - \ln\left(\frac{P}{P_1}\right)_k \qquad [22c]$$

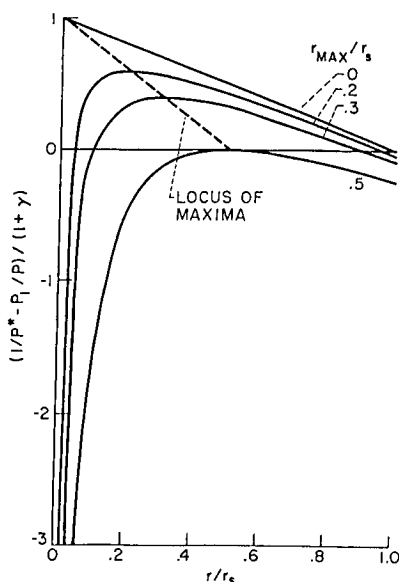$$\Delta\ln\frac{T}{T_1} = \ln\left(\frac{T}{T_1}\right)_{k+1} - \ln\left(\frac{T}{T_1}\right)_k \qquad [22d]$$

and the subscript k stands for the kth iteration. The partial derivatives appearing in Eqs. 22a and 22b can be evaluated if γ is taken to be independent of temperature and pressure. This is an excellent assumption over a moderate range of temperatures and pressures. To within the accuracy of this assumption, these partial derivatives are

$$\frac{\partial(1/P^* - P_1/P)}{\partial \ln (P/P_1)} = \frac{P_1}{P} - \gamma \left(\frac{\rho}{\rho_1}\right)\left(\frac{\partial \ln \rho}{\partial \ln P}\right)_T \quad [23a]$$

$$\frac{\partial(1/P^* - P_1/P)}{\partial \ln (T/T_1)} = - \gamma \left(\frac{\rho}{\rho_1}\right)\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P \quad [23b]$$

$$\frac{\partial(h^* - h)}{\partial \ln (P/P_1)} = \frac{\gamma}{2} \frac{P}{\rho} \left\{2 \left(\frac{\rho}{\rho_1}\right)^2 - \left[\left(\frac{\rho}{\rho_1}\right)^2 + 1\right] \times \right.$$
$$\left. \left[1 - \left(\frac{\partial \ln \rho}{\partial \ln P}\right)_T\right]\right\} - \frac{P}{\rho}\left[1 + \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P\right] \quad [23c]$$

$$\frac{\partial(h^* - h)}{\partial \ln (T/T_1)} = \frac{\gamma}{2} \frac{P}{\rho} \left[\left(\frac{\rho}{\rho_1}\right)^2 + 1\right]\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P - Tc_p \quad [23d]$$

To proceed further, the equation of state for the products of reaction must be known. Further consideration is given only to the case where the products of reaction obey the equation of state (Eq. 12). From Eq. 12 it follows that

$$\left(\frac{\partial \ln \rho}{\partial \ln P}\right)_T = \left(\frac{\partial \ln M}{\partial \ln P}\right)_T + 1 \quad [24a]$$

$$\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P = \left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1 \quad [24b]$$

The evaluation of the molecular weight derivatives appearing in Eqs. 24a and 24b is discussed in detail in Ref. 13.

Dividing Eq. 22b by P/ρ and using Eqs. 12, 23, and 24 in Eqs. 22a and 22b gives the following dimensionless iteration equations:

$$\left\{\frac{P_1}{P} - \gamma \left(\frac{\rho}{\rho_1}\right)\left[1 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right]\right\} \Delta \ln \frac{P}{P_1} + \left\{\gamma \left(\frac{\rho}{\rho_1}\right)\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]\right\} \Delta \ln \frac{T}{T_1} = \frac{P_1}{P} - \frac{1}{P^*} \quad [25a]$$

$$\left(\frac{\gamma}{2} \left\{\left(\frac{\rho}{\rho_1}\right)^2 \left[2 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right\} - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right) \Delta \ln \frac{P}{P_1} + $$
$$\left\{\frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2 + 1\right]\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right] - \frac{Mc_p}{R}\right\} \Delta \ln \frac{T}{T_1} = \frac{M}{RT}(h - h_1) - \frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2 - 1\right] \quad [25b]$$

Molecular weight derivatives cannot be neglected without appreciable effect on the convergence unless they are small relative to unity. The effect of omitting molecular weight derivatives was checked for the stoichiometric hydrogen-oxygen detonations. The omission resulted in oscillations that probably were similar to those encountered in Refs. 3 and 4.

When the iteration using Eqs. 25a and 25b has converged, the detonation velocity u_D may be calculated from the continuity equation

$$u_D \equiv u_1 = (\rho/\rho_1)u = (\rho/\rho_1)(\gamma P/\rho)^{1/2} \quad [26]$$

Initial Estimates

The computational effort involved in the iterative solution of Eqs. 21 and 14 by the Newton-Raphson method can be appreciably reduced if good initial estimates for temperature and pressure are available. These are easily obtained when one has had some previous experience with the chemical system under consideration. When the chemical system is unfamiliar, it would be useful to have some estimating scheme. An estimating scheme can be obtained for ideal gaseous detonations from Eqs. 11, 14, 15, 18, and 20.

The discussion of Eq. 13 indicated that a solution must lie in the interval $\frac{1}{2} < r_0/r_s < 1$. The following considerations show that for most systems, the solution actually lies in the

interval $0.9 < r_0/r_s < 1$. A value of $r_0/r_s > 0.9$ occurs for $r_{min}/r_s > 0.7$. From Eq. 18 for $r_{min}/r_s > 0.7$, there follows

$$\alpha = (T_1/T)(M/M_1) \le 0.09 (1 + \gamma)^2/\gamma \quad [27]$$

For a range of γ from 1.1 to 1.6 and for $M/M_1 < 1.5$, Eq. 27 gives $T/T_1 \ge 4$. Thus for even relatively weak reactions that result in temperature ratios as low as 4, the solution r_0/r_s will be greater than 0.9. The result of substituting values for r/r_s from 0.9 to 1.0 into Eqs. 11 and 14 for values of γ from 1.1 to 1.6 indicates that

$$0.6 \frac{RT_1}{M_1} \left(\frac{P}{P_1}\right) \le h - h_1 \le 0.8 \frac{RT_1}{M_1} \left(\frac{P}{P_1}\right)$$

A first approximation to enthalpy may therefore be taken as

$$h = h_1 + \tfrac{3}{4}(RT_1/M_1)(P/P_1)_0 \quad [28]$$

where $(P/P_1)_0$ is an assumed pressure ratio across the detonation wave. The temperature ratio $(T/T_1)_0$ corresponding to this enthalpy can be determined by doing an equilibrium flame temperature calculation at the assumed pressure and the enthalpy h as calculated from Eq. 28 using the method of Ref. 13 or the improved version of this method described in Ref. 15.

The assumed value $(P/P_1)_0$ and the estimated $(T/T_1)_0$ obtained by the method just described can be further improved by a method of successive substitutions. The equation for improving the estimate for P/P_1 may be obtained by combining Eqs. 15 and 18 with Eq. 20 using the positive sign in Eq. 20, whereas the equation for improving the estimate for T/T_1 may be obtained from Eqs. 11, 14, and 28 and the approximate relation $\Delta T = \Delta h/c_p$:

$$\left(\frac{P}{P_1}\right)_{k+1} = \frac{1 + \gamma}{2\gamma\alpha_k}\left[1 + \left(1 - \frac{4\gamma\alpha_k}{(1 + \gamma)^2}\right)^{1/2}\right] \quad [29]$$

$$\left(\frac{T}{T_1}\right)_{k+1} = \left[\left(\frac{T}{T_1}\right)_0 - \frac{3}{4}\frac{R}{M_1 c_p}\left(\frac{P}{P_1}\right)_0\right] + \frac{\gamma}{2}\frac{R}{M_1 c_p}\left(\frac{r_{k+1}^2 - 1}{r_{k+1}}\right)\left(\frac{P}{P_1}\right)_{k+1} \quad [30]$$

where

$$\alpha_k = (T_1/T)_k(M/M_1) \quad [31a]$$

$$r_{k+1} = \alpha_k(P/P_1)_{k+1} \quad [31b]$$

The quantities M, γ, and c_p in Eqs. 29-31 are the equilibrium properties for the conditions $(P/P_1)_0$ and $(T/T_1)_0$. Eqs. 29 and 30 are used successively until the corrections to the pressure and temperature ratios become sufficiently small, say 0.5%.

This procedure will generally provide excellent initial estimates for the Newton-Raphson iteration.

Convergence Rates

The convergence rate of the Newton-Raphson iteration is illustrated in Fig. 4. The square root of the sum of the squares of the corrections obtained from Eqs. 25a and 25b is plotted as a function of iteration number. The curves in Fig. 4 illustrate the behavior of the iteration for good initial

Table 1 Simultaneous equations for obtaining partial derivatives of detonation pressure, temperature, and velocity

$$\left\{ \frac{P_1}{P} - \gamma \left(\frac{\rho}{\rho_1}\right)\left[1 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right]\right\} X_1 + \left\{\gamma\left(\frac{\rho}{\rho_1}\right)\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]\right\} X_2 = C_1$$

$$\left\{\frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2\left[2 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right\} X_1 + \left\{\frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2 + 1\right]\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right] - \frac{M c_p}{R}\right\} X_2 = C_2$$

Variable	X_1	X_2	C_1	C_2	Detonation velocity derivative[a]
T_1	$\left(\dfrac{\partial \ln P}{\partial \ln T_1}\right)_{P_1}$	$\left(\dfrac{\partial \ln T}{\partial \ln T_1}\right)_{P_1}$	$\gamma\left(\dfrac{\rho}{\rho_1}\right)$	$-\gamma\left(\dfrac{\rho}{\rho_1}\right)^2 - \dfrac{M}{R}(c_p)_f \dfrac{T_1}{T}$	$\left(\dfrac{\partial u_D}{\partial \ln T_1}\right)_{P_1} = u_D[A X_1 + B X_2 + 1]$
P_1	$\left(\dfrac{\partial \ln P}{\partial \ln P_1}\right)_{T_1,h_1}$	$\left(\dfrac{\partial \ln T}{\partial \ln P_1}\right)_{T_1,h_1}$	$\dfrac{P_1}{P} - \gamma\left(\dfrac{\rho}{\rho_1}\right)$	$\gamma\left(\dfrac{\rho}{\rho_1}\right)^2$	$\left(\dfrac{\partial u_D}{\partial \ln P_1}\right)_{T_1,h_1} = u_D[A X_1 + B X_2 - 1]$
h_1	$\left(\dfrac{\partial \ln P}{\partial h_1}\right)_{P_1,T}$	$\left(\dfrac{\partial \ln T}{\partial h_1}\right)_{P_1,T_1}$	0	$-\dfrac{M}{RT}$	$\left(\dfrac{\partial u_D}{\partial h_1}\right)_{P_1,T_1} = u_D[A X_1 + B X_2]$

[a] $A = \dfrac{1}{2}\left[2 + \left(\dfrac{\partial \ln M}{\partial \ln P}\right)_T\right]$ and $B = \dfrac{1}{2}\left[\left(\dfrac{\partial \ln M}{\partial \ln T}\right)_P - 1\right]$.
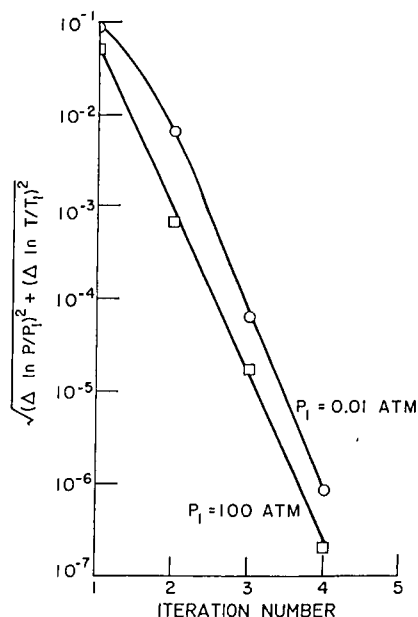

Fig. 4 Convergence rate for stoichiometric hydrogen-oxygen mixture. Initial temperature, 500° K

Table 2 Sources of thermodynamic data

Substance	Thermo-dynamic functions from Ref.	Heat of formation, $\Delta H_{298.15}$, kcal/mole	$\Delta H_{298.15}$ from Ref.
H_2	16	0	...
O_2	...[a]	0	...
H_2O	17	−57.7979	18
OH	19	9.3166	20
H	...[a]	52.1018	21
O	...[a]	59.5567	22

[a] Unpublished NASA data calculated by Gordon and McBride.

estimates obtained by the method previously described. By using these good initial estimates, approximately four figure accuracy in P/P_1, T/T_1, u_D, M/M_1, and ρ/ρ_1 can be obtained after two Newton-Raphson iterations.

Effect of Initial Conditions on Detonation Process

Choice of Independent Parameters

Several articles have described the qualitative effect of initial temperature and pressure on the detonation process (7-10). These discussions were based on both experimental results and thermodynamic calculations, almost exclusively for the stoichiometric hydrogen-oxygen system. There have not appeared, however, partial derivatives of the detonation velocity, final pressure, and final temperature with respect to the initial temperature and pressure. These partial derivatives would indicate quantitatively the effect of initial temperature and pressure on the thermodynamically calculated detonation process.

In addition to the partial derivatives with respect to T_1 and P_1, the partial derivatives with respect to h_1 were also evaluated. These latter derivatives indicate the effect produced by a change in the heat of formation of the reactants.

Evaluation of Partial Derivatives

The partial derivatives $(\partial \ln P/\partial \ln T_1)_{P_1}$ and $(\partial \ln T/\partial \ln T_1)_{P_1}$ can be obtained by solving the following set of dimensionless linear equations, which were obtained by differentiation of Eqs. 21 and 14:

$$\frac{\partial[(1/P^*) - (P_1/P)]}{\partial \ln P}\left(\frac{\partial \ln P}{\partial \ln T_1}\right)_{P_1} + \frac{\partial[(1/P^*) - (P_1/P)]}{\partial \ln T} \times$$
$$\left(\frac{\partial \ln T}{\partial \ln T_1}\right)_{P_1} = -\frac{\partial[(1/P^*) - (P_1/P)]}{\partial \ln T_1} \qquad [32a]$$

$$\frac{\rho}{P}\frac{\partial(h^* - h)}{\partial \ln P}\left(\frac{\partial \ln P}{\partial \ln T_1}\right)_{P_1} + \frac{\rho}{P}\frac{\partial(h^* - h)}{\partial \ln T}\left(\frac{\partial \ln T}{\partial \ln T_1}\right)_{P_1} =$$
$$-\frac{\rho}{P}\frac{\partial(h^* - h)}{\partial \ln T_1} - \frac{\rho}{P}T_1(c_p)_f\frac{\partial(h^* - h)}{\partial h_1} \qquad [32b]$$

In deriving Eq. 32b, the relation

$$dh_1 = T_1(c_p)_f d \ln T_1 \qquad [33]$$

was used. In Eq. 32b the ordinary partial derivative has

been used for h_1 rather than the logarithmic derivative, since the enthalpy can be positive or negative depending on the choice of enthalpy reference level.

Equations having a coefficient matrix identical to Eqs. 32a and 32b, but with different right sides, can also be obtained for either set of the partial derivatives $(\partial \ln P/\partial \ln P_1)_{T_1, h_1}$ and $(\partial \ln T/\partial \ln P_1)_{T_1, h_1}$, or $(\partial \ln P/\partial h_1)_{T_1, P_1}$ and $(\partial \ln T/\partial h_1)_{T_1, P_1}$. By using Eqs. 23, it follows that the coefficient matrix of Eqs. 32a and 32b is identical to that of the iteration equations, Eqs. 25a and 25b. Thus, the partial derivatives can be obtained by merely replacing the right side of the iteration equations with a right side appropriate to the desired partial derivatives. Table 1 summarizes the three sets of simultaneous equations for obtaining partial derivatives.

The partial derivative of the detonation velocity with respect to the initial temperature is obtained from Eq. 26 and the equation of state, Eq. 12, applied to the initial conditions

$$\frac{1}{u_D}\left(\frac{\partial u_D}{\partial \ln T_1}\right)_{P_1} = \frac{1}{2}\left[2 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right]\left(\frac{\partial \ln P}{\partial \ln T_1}\right)_{P_1} + \frac{1}{2}\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right]\left(\frac{\partial \ln T}{\partial \ln T_1}\right)_{P_1} + 1 \qquad [34]$$

In Eq. 34, $(\partial \ln P/\partial \ln T_1)_{P_1}$ and $(\partial \ln T/\partial \ln T_1)_{P_1}$ are obtained from Eqs. 32a and 32b.

The two other detonation velocity derivatives, $(\partial u_D/\partial \ln P_1)_{T_1, h_1}$ and $(\partial u_D/\partial h_1)_{P_1, T_1}$, can be expressed in the same form. These three detonation velocity derivatives are presented in Table 1.

Application to Stoichiometric Hydrogen-Oxygen Mixtures

The calculation method described in this paper was applied to a stoichiometric hydrogen-oxygen mixture for two reasons. The first was to provide a tabulation of accurately calculated detonation properties using an equilibrium γ as defined by Eq. 6b. This is contrasted with the usual calculation, where γ is replaced by either an equilibrium or frozen specific heat ratio. These three quantities can differ appreciably. In particular, it can be shown from Eqs. 58 and 61 of Ref. 13 that the ratio of equilibrium specific heat ratio κ to equilibrium γ is

$$\kappa/\gamma = 1 + (\partial \ln M/\partial \ln P)_T \qquad [35]$$

Since the molecular weight derivative appearing in Eq. 35 is never negative, κ is never less than γ. For stoichiometric hydrogen and oxygen at $P = 0.1$ atm and $T = 3000°K$, κ is about 15% larger than γ.

The second reason was to examine carefully the effect of initial temperature, pressure, and enthalpy on calculated detonation properties and to provide, if possible, a reliable method for extrapolating calculations from one set of initial conditions to another.

Thermodynamic Data

Table 2 gives the sources from which the thermodynamic data used to obtain Tables 3–7 were taken. Table 3 presents the results of the calculations using γ on a stoichiometric hydrogen-oxygen mixture from 0.01 to 100 atm and from 200° to 500°K. Tables 4–6 present the calculated partial derivatives for the same range of initial conditions. In order to insure five-figure accuracy in all the calculated data in Tables 3–7, iterations were continued until $\Delta \ln P/P_1 < 0.5 \times 10^{-5}$ and $\Delta \ln T/T_1 < 0.5 \times 10^{-5}$.

The data for H and O are essentially identical to those of Ref. 16. The data for H_2O and O_2 are only slightly different from those of Ref. 16 to 3000°K, with increasing differences over 3000°K.

The effect of thermodynamic data on detonation parameters was determined by performing additional calculations using the data of Ref. 16. For those initial conditions that

Table 3 Stoichiometric hydrogen-oxygen detonations

P_1, atm	T_1, °K	P/P_1	T/T_1	u_D, m/sec	M/M_1 for $M_1 = 12.011$	ρ/ρ_1	$\gamma = \left(\frac{\partial \ln P}{\partial \ln \rho}\right)_s$	H_2O	H_2	OH	H	O_2	O
0.01	200.0	24.218	14.917	2631.9	1.1493	1.8659	1.1071	0.47594	0.16890	0.11816	0.12457	0.05969	0.05273
0.10		26.275	16.668	2751.1	1.1800	1.8600	1.1185	0.50477	0.16732	0.12032	0.09977	0.05373	0.04508
1.00		28.479	18.727	2874.7	1.2186	1.8532	1.1308	0.54695	0.16053	0.13375	0.07414	0.04709	0.03554
10.00		30.714	21.065	2995.6	1.2665	1.8466	1.1427	0.60690	0.14610	0.13351	0.04913	0.03955	0.02482
100.00		32.776	23.528	3102.6	1.3220	1.8417	1.1518	0.68617	0.12208	0.11875	0.02750	0.03097	0.01452
0.01	298.15	15.957	9.840	2593.8	1.1396	1.8479	1.1054	0.46585	0.16968	0.11655	0.13155	0.06095	0.05512
0.10		17.333	10.989	2714.1	1.1690	1.8439	1.1167	0.49244	0.16908	0.12883	0.10674	0.05512	0.04779
1.00		18.820	12.345	2839.6	1.2062	1.8387	1.1290	0.53160	0.16371	0.13673	0.08085	0.04866	0.03845
10.00		20.349	13.904	2964.2	1.2526	1.8332	1.1411	0.58798	0.15115	0.13675	0.05513	0.04134	0.02765
100.00		21.791	15.580	3077.0	1.3077	1.8290	1.1509	0.66430	0.12908	0.12469	0.03210	0.03297	0.01686
0.01	400.0	11.720	7.249	2559.7	1.1309	1.8283	1.1043	0.45671	0.17038	0.11605	0.13764	0.06195	0.05727
0.10		12.747	8.092	2681.4	1.1593	1.8262	1.1154	0.48162	0.17054	0.12866	0.11279	0.05622	0.05018
1.00		13.864	9.092	2809.2	1.1954	1.8228	1.1277	0.51852	0.16627	0.13768	0.08667	0.04989	0.04098
10.00		15.024	10.250	2937.1	1.2408	1.8188	1.1401	0.57216	0.15518	0.13944	0.06035	0.04275	0.03013
100.00		16.135	11.514	3054.7	1.2955	1.8154	1.1504	0.64609	0.13471	0.12951	0.03620	0.03455	0.01895
0.01	500.0	9.258	5.750	2528.8	1.1231	1.8084	1.1034	0.44848	0.17099	0.11555	0.14301	0.06276	0.05921
0.10		10.084	6.418	2652.2	1.1508	1.8083	1.1145	0.47207	0.17178	0.12867	0.11809	0.05709	0.05230
1.00		10.985	7.212	2782.2	1.1861	1.8067	1.1267	0.50720	0.16838	0.13857	0.09176	0.05088	0.04322
10.00		11.929	8.137	2913.3	1.2307	1.8042	1.1393	0.55868	0.15847	0.14171	0.06494	0.04388	0.03232
100.00		12.843	9.159	3035.1	1.2850	1.8019	1.1500	0.63064	0.13932	0.13352	0.03987	0.03584	0.02082

Table 4 Effect of initial pressure on detonation properties

P_1, atm	$\left(\dfrac{\partial u_D}{\partial \ln P_1}\right)_{T_1,h_1}$, m/sec	$\left(\dfrac{\partial \ln (P/P_1)}{\partial \ln P_1}\right)_{T_1,h_1} = \left(\dfrac{\partial \ln P}{\partial \ln P_1}\right)_{T_1,h_1} - 1$	$\left(\dfrac{\partial \ln (T/T_1)}{\partial \ln P_1}\right)_{T_1,h_1} = \left(\dfrac{\partial \ln T}{\partial \ln P_1}\right)_{T_1,h_1}$
		$T_1 = 200°\text{K}$	
0.01	50.24	0.03743	0.04689
0.10	53.06	0.03788	0.04976
1.00	53.75	0.03678	0.05148
10.00	50.43	0.03316	0.05052
100.00	41.66	0.02648	0.04506
		$T_1 = 298.15°\text{K}$	
0.01	50.59	0.03784	0.04654
0.10	53.69	0.03848	0.04958
1.00	54.94	0.03773	0.05169
10.00	52.47	0.03459	0.05145
100.00	44.52	0.02832	0.04696
		$T_1 = 400°\text{K}$	
0.01	51.13	0.03833	0.04632
0.10	54.45	0.03911	0.04949
1.00	56.10	0.03859	0.05188
10.00	54.23	0.03578	0.05217
100.00	46.91	0.02983	0.04842
		$T_1 = 500°\text{K}$	
0.01	51.81	0.03887	0.04619
0.10	55.29	0.03974	0.04947
1.00	57.24	0.03939	0.05207
10.00	55.83	0.03683	0.05276
100.00	48.97	0.03110	0.04960

Table 5 Effect of initial temperature on detonation properties

T_1, °K	$\left(\dfrac{\partial u_D}{\partial \ln T_1}\right)_{P_1}$, m/sec	$\left(\dfrac{\partial \ln (P/P_1)}{\partial \ln T_1}\right)_{P_1} = \left(\dfrac{\partial \ln P}{\partial \ln T_1}\right)_{P_1}$	$\left(\dfrac{\partial \ln (T/T_1)}{\partial \ln T_1}\right)_{P_1} = \left(\dfrac{\partial \ln T}{\partial \ln T_1}\right)_{P_1} - 1$
		$P_1 = 0.01$ atm	
200	−86.69	−1.04499	−1.04314
298.15	−105.88	−1.04945	−1.04096
400	−127.68	−1.05517	−1.03908
500	−150.52	−1.06158	−1.03743
		$P_1 = 0.1$ atm	
200	−85.03	−1.04274	−1.04491
298.15	−102.00	−1.04586	−1.04238
400	−121.27	−1.05001	−1.04014
500	−141.34	−1.05468	−1.03813
		$P_1 = 1$ atm	
200	−80.92	−1.03889	−1.04512
298.15	−95.76	−1.04080	−1.04226
400	−112.52	−1.04349	−1.03964
500	−129.83	−1.04653	−1.03722
		$P_1 = 10$ atm	
200	−72.65	−1.03257	−1.04213
298.15	−85.50	−1.03341	−1.03901
400	−99.81	−1.03475	−1.03601
500	−114.40	−1.03627	−1.03313
		$P_1 = 100$ atm	
200	−59.30	−1.02350	−1.03415
298.15	−70.17	−1.02330	−1.03073
400	−82.07	−1.02336	−1.02724
500	−93.95	−1.02345	−1.02378

Table 6 Effect of initial enthalpy on detonation properties

P_1, atm	$\left(\dfrac{\partial u_D}{\partial h_1}\right)_{T_1,P_1}$, $\dfrac{\text{m/sec}}{\text{kcal/gm}}$	$\left[\dfrac{\partial \ln (P/P_1)}{\partial h_1}\right]_{T_1,P_1} = \left(\dfrac{\partial \ln P}{\partial h_1}\right)_{T_1,P_1}$, $\dfrac{\text{gm}}{\text{kcal}}$	$\left[\dfrac{\partial \ln (T/T_1)}{\partial h_1}\right]_{T_1,P_-} = \left(\dfrac{\partial \ln T}{\partial h_1}\right)_{T_1,P_1}$, $\dfrac{\text{gm}}{\text{kcal}}$
		$T_1 = 200°\mathrm{K}$	
0.01	236.4	0.17609	0.06087
0.10	262.4	0.18736	0.07474
1.00	293.9	0.20112	0.09363
10.00	329.7	0.21675	0.11869
100.00	364.9	0.23188	0.14935
		$T_1 = 298.15°\mathrm{K}$	
0.01	234.2	0.17521	0.05815
0.10	259.3	0.18587	0.07110
1.00	289.8	0.19905	0.08876
10.00	325.1	0.21429	0.11240
100.00	360.9	0.22957	0.14194
		$T_1 = 400°\mathrm{K}$	
0.01	233.4	0.17498	0.05604
0.10	257.8	0.18514	0.06830
1.00	287.6	0.19779	0.08503
10.00	322.3	0.21265	0.10755
100.00	358.4	0.22792	0.13609
		$T_1 = 500°\mathrm{K}$	
0.01	233.5	0.17518	0.05436
0.10	257.3	0.18490	0.06608
1.00	286.5	0.19710	0.08208
10.00	320.8	0.21160	0.10370
100.00	357.0	0.22676	0.13138

Table 7 Comparison of detonation properties of stoichiometric hydrogen-oxygen mixture calculated using equilibrium specific heat ratio and equilibrium γ

P_1, atm	T_1, °K	$\kappa = \dfrac{c_p}{c_v}$	$\gamma = \left(\dfrac{\partial \ln P}{\partial \ln \rho}\right)_S$	P/P_1 Using κ	P/P_1 Using γ	T/T_1 Using κ	T/T_1 Using γ	u_D, m/sec Using κ	u_D, m/sec Using γ
0.01	200.0	1.2244	1.1071	23.006	24.218	14.868	14.917	2635.7	2631.9
0.10		1.2221	1.1185	25.105	26.275	16.613	16.668	2754.2	2751.1
1.00		1.2186	1.1308	27.395	28.479	18.666	18.727	2877.0	2874.7
10.00		1.2128	1.1427	29.771	30.714	21.001	21.065	2997.1	2995.6
100.00		1.2030	1.1518	32.031	32.776	23.469	23.528	3103.5	3102.6
0.01	298.15	1.2267	1.1054	15.133	15.957	9.807	9.840	2597.8	2593.8
0.10		1.2246	1.1167	16.532	17.333	10.951	10.989	2717.4	2714.1
1.00		1.2214	1.1290	18.068	18.820	12.304	12.345	2842.2	2839.6
10.00		1.2160	1.1411	19.684	20.349	13.860	13.904	2966.0	2964.2
100.00		1.2068	1.1509	21.253	21.791	15.538	15.580	3078.0	3077.0
0.01	400.0	1.2291	1.1043	11.099	11.720	7.225	7.249	2564.0	2559.7
0.10		1.2271	1.1154	12.139	12.139	8.064	8.092	2685.0	2681.4
1.00		1.2241	1.1277	13.288	13.864	9.061	9.092	2812.0	2809.2
10.00		1.2191	1.1401	14.508	15.024	10.217	10.250	2939.1	2937.1
100.00		1.2102	1.1504	15.710	16.135	11.482	11.514	3055.9	3054.7
0.01	500.00	1.2314	1.1034	8.757	9.258	5.731	5.750	2533.4	2528.8
0.10		1.2295	1.1145	9.590	10.084	6.395	6.418	2656.1	2652.2
1.00		1.2267	1.1267	10.514	10.985	7.187	7.212	2785.3	2782.2
10.00		1.2219	1.1393	11.502	11.929	8.110	8.137	2915.4	2913.3
100.00		1.2133	1.1500	12.487	12.843	9.132	9.159	3036.4	3035.1

Table 8 Comparison of calculated detonation velocities with detonation velocities estimated from data at $P_1 = 1.0$ atm and $T_1 = 298.15°K$

| T_1, °K	u_D, m/sec		Error in u_D, m/sec
	Actual	Estimated	
	$P_1 = 0.01$ atm		
200	2632	2622	−10
298.15	2594	2587	−7
400	2560	2557	−3
500	2529	2530	1
	$P_1 = 0.10$ atm		
200	2751	2748	−3
298.15	2714	2713	−1
400	2681	2683	2
500	2652	2656	4
	$P_1 = 1.0$ atm		
200	2875	2874	−1
298.15	2840	2840	0
400	2809	2810	1
500	2782	2783	1
	$P_1 = 10$ atm		
200	2996	3001	5
298.15	2964	2966	2
400	2937	2936	−1
500	2913	2909	−4
	$P_1 = 100$ atm		
200	3103	3128	25
298.15	3077	3093	16
400	3055	3063	8
500	3035	3036	1
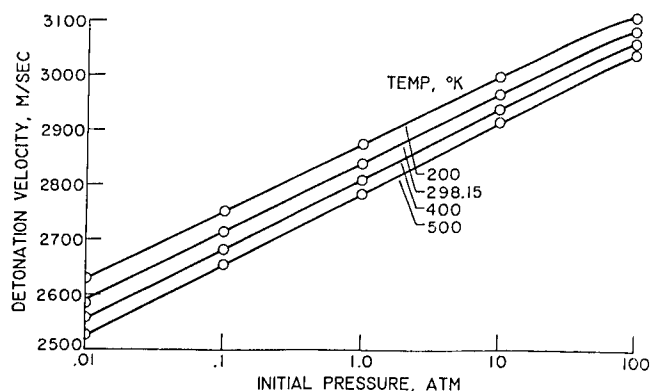
Fig. 5 Effect of initial pressure on detonation velocity

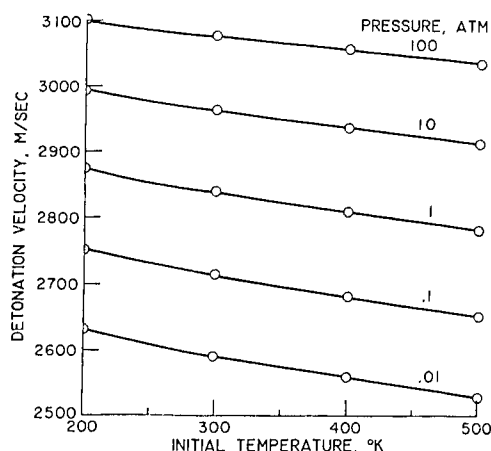

Fig. 6 Effect of initial temperature on detonation velocity

resulted in detonation temperatures less than 3000°K ($P_1 = 0.01$ atm), the thermodynamic data of Ref. 16 gave detonation velocities about 0.5 m/sec higher than the data in Table 3. For temperatures of about 3700°K ($P_1 = 1.0$ atm), the difference was about 2 m/sec, whereas for temperatures of about 4600° to 4700°K ($P_1 = 100$ atm), the difference was about 6 to 7 m/sec. Similar trends were noted in the other detonation parameters, negligible differences for detonation temperatures less than 3000°K and small but increasing differences with increasing detonation temperatures.

Effects of Initial Conditions on Stoichiometric Hydrogen-Oxygen Detonations

The data of Tables 3–6 permit the following qualitative observations: 1) increasing the initial pressure increases the detonation velocity, pressure ratio, and temperature ratio; 2) increasing the initial temperature decreases the detonation velocity, pressure ratio, and temperature ratio; and 3) increasing the initial enthalpy increases the detonation velocity, pressure ratio, and temperature ratio. Quantitative estimates of the effects can be made using the partial derivatives tabulated in Tables 4–6.

A plot of detonation velocity vs. initial pressure (Fig. 5) indicates that to a very good approximation the detonation velocity is linear with the logarithm of the initial pressure. This is substantiated by the calculated partial derivative of Table 4. The logarithmic dependence was first proposed in Ref. 10 on the basis of experimental data. If T_1^0, P_1^0, and h_1^0 are some reference initial conditions, then to a good approximation the detonation velocity for some other initial pressure P_1 will be given by

$$u_D(T_1^0, h_1^0, P_1) = u_D(T_1^0, h_1^0, P_1^0) +$$
$$(\partial u_D/\partial \ln P_1)^0_{T_1, h_1} \ln (P_1/P_1^0) \quad [36]$$

where the superscript on the partial derivative indicates that it is evaluated at T_1^0, P_1^0, h_1^0. The detonation velocity is very nearly linear with initial temperature; however, some curvature exists at the lower temperatures, as can be seen from Fig. 6. An examination of several extrapolation techniques showed that a good estimate for the effect of initial temperature can be obtained by averaging the linear and the semi-logarithmic extrapolations. Therefore

$$u_D(T_1, P_1^0) = u_D(T_1^0, P_1^0) +$$
$$\tfrac{1}{2}(\partial u_D/\partial \ln T_1)^0_{P_1}[\ln (T_1/T_1^0) + (T_1/T_1^0) - 1] \quad [37]$$

The effect of initial enthalpy can be estimated by the formula

$$u_D(T_1^0, P_1^0, h_1) = u_D(T_1^0, P_1^0, h_1^0) +$$
$$(\partial u_D/\partial h_1)^0_{T_1, P_1}(h_1 - h_1^0) \quad [38]$$

The use of these derivatives to extrapolate data can be illustrated with a typical example. Let $T_1^0 = 500°K$ and $P_1^0 = 0.01$ atm, for which $u_D = 2528.8$ m/sec (Table 3) and $(\partial u_D/\partial \ln P_1)^0_{T_1, h_1} = 51.81$ (Table 4). Using these values in Eq. 36 gives an extrapolated value of 2648.1 for $P_1 = 0.1$, which compares with the calculated value of 2652.2 (Table 3). In a similar manner, but using $(\partial u_D/\partial \ln T_1)^0_{P_1} = -150.52$ (Table 5), Eq. 37 gives 2560.6 for $T_1 = 400°K$, compared with the calculated value of 2559.7 (Table 3). For $h_1 - h_1^0 = -88.52$ cal/gm, Eq. 38 predicts 2508.2 m/sec, whereas the true value is 2508.0 m/sec.

By means of Eqs. 36 and 37, estimated detonation velocities for all initial conditions in this report were obtained using the data for only the initial condition $P_1 = 1$ atm and $T_1 = 298.15°K$. These estimated velocities are compared in Table 8 with the accurately calculated velocities of Table 3. It may be seen that for moderate changes in initial conditions, the partial derivatives of the detonation velocity permit good to excellent extrapolations. The effect of initial conditions on the pressure and temperature ratios can be estimated in a

similar manner by assuming that the tabulated partial derivatives are constant over the interval of extrapolation.

Effect of γ

As pointed out previously, many authors perform detonation calculations using a specific heat ratio in place of γ as defined by Eq. 6b. To determine what effect this has on the results, calculations were performed for the same initial conditions replacing γ by the equilibrium specific heat ratio calculated from Eq. 35. The results are given in Table 7. Comparison with the previous calculations shows that the detonation velocity is higher when using κ than when using γ, the difference being larger at the lower pressures. At the lower pressures this difference is approximately 4 m/sec. The temperature ratio is essentially unaffected, whereas the pressure ratio is invariably lower by an appreciable amount compared with that calculated using γ.

Nomenclature

a = velocity of sound

c_p = equilibrium heat capacity at constant pressure per unit mass

$(c_p)_f$ = frozen heat capacity of the reactants at constant pressure per unit mass evaluated at T_1

c_v = equilibrium heat capacity at constant volume per unit mass

h = enthalpy per unit mass

h^* = defined by Eq. 10

M = molecular weight

P = pressure

P^* = defined by Eq. 9

R = universal gas constant

r = density ratio across detonation, ρ/ρ_1

T = absolute temperature

u = velocity

u_D = detonation velocity

α = $(T_1/T)(M/M_1)$

γ = isentropic exponent defined by Eq. 6b

κ = c_p/c_v

ρ = density

Subscripts

max = maximum

min = minimum

S = constant entropy

s = singularity

0 = root or first estimates

1 = before detonation

2 = after detonation

Superscript

0 = reference initial conditions

References

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