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NOMENCLATURE

$D_{F,k}$	=	Fick diffusion coefficient of component k, sq. ft./sec.
m_k	=	weight of component k added per unit area of interface, lb./sq. ft.
V_k	=	partial specific volume of component k, cu. ft./lb.
Δ	=	difference in
θ	=	time, sec.
σ_k	=	concentration of component k, lb./cu. ft.
Superscript		
*	=	average condition
Subscripts		
c	=	diffusion cell
e	=	conditions at equilibrium
g	=	gas phase
i	=	conditions at interface
j	=	component j, the stagnant component
k	=	component k, the diffusing component
l	=	liquid phase
0	=	initial conditions

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Generalized Charts of Detonation Parameters for Gaseous Mixtures

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Where detonative combustion is involved, it is frequently desirable to visualize the relationships among various detonation parameters. To fulfill this need, generalized charts of detonation parameters for all gaseous mixtures, involving only nondimensional quantities, are given. The chief usefulness of these plots of generalized equations, derived directly from the classical equations of detonation, is to provide a means for visualizing relationships among the detonation parameters for all gaseous mixtures on a small number of Mollier-type diagrams. Application of these generalized charts is illustrated by means of several examples.

There is need of simplified methods for determining and visualizing values of detonation parameters for all gaseous mixtures. Considerably more information on detonation parameters is required before the advantageous application of supersonic burning in propulsive devices can be realized. Such information may also have direct application in understanding instability phenomena (such as screech) in ramjet, turbojet, afterburner, and rocket engines. These instability phenomena and their possible association with detonative combustion have been discussed in the literature (6, 8).

To provide simplified means for analytically determining values of detonation parameters, the classical equations of detonation were previously rearranged (2), and also a calculation procedure based on the resulting generalized equations, involving only nondimensional quantities, was devised. During the process of generalizing the detonation equations it became apparent that it would be extremely useful if the detonation parameters for all gaseous mixtures could be presented in nondimensional form on a Mollier-type diagram. This would aid considerably in visualization of relationships among the various detonation parameters. It was found that the generalized detonation equations could be utilized for the graphical presentation of the detonation parameters on a small number of Mollier-type diagrams.

In this article, derivation of the generalized detonation equations is summarized, and the method of constructing the generalized charts based on these equations is described. Application of the generalized detonation charts is illustrated by means of several examples.

DERIVATION OF EQUATIONS FOR THE GENERALIZED CHARTS

The assumptions utilized in the derivation following are generally introduced where required. It is assumed that the ideal gas law holds for the reactants and their products at the initial and final conditions. This is equivalent to the assumption that the actual temperatures and pressures of the initial and final mixtures in all cases are in a region where the use of the ideal gas law results in negligible error. For the final mixture, because of the extremely high temperatures occurring in detonation, this is a reasonable assumption. It is a reasonable assumption also for the initial mixture, if the initial conditions are sufficiently far from the critical conditions of pressure and temperature for each component so that thermodynamic compressibility is a negligible factor. Thus, in all cases where an equation of state was required for describing the states of the initial and final mixtures at the initial and final conditions, the ideal gas law has been used. The usual assumption is also made that chemical equilibrium is attained in the detonation wave.

The equations of conservation across the detonation front are

Conservation of mass

$$\rho_1 V_1 = \rho_2 V_2 \tag{1}$$

Conservation of momentum, considering only normal entry into the front

$$P_1 + \rho_1 V_1^2 = P_2 + \rho_2 V_2^2 \tag{2}$$

and conservation of energy

$$Je_1 + \frac{V_1^2}{2} + \frac{P_1}{\rho_1} + Jh = Je_2 + \frac{V_2^2}{2} + \frac{P_2}{\rho_2} \tag{3}$$

The velocity of sound in the initial and final mixtures may be expressed as

$$a^2 = \gamma \frac{P}{\rho} \tag{4}$$

By definition

$$\mathbf{M} = \frac{V}{a} \tag{5}$$

and the energy release function is

$$\mathbf{B} = \frac{Jh}{a_1^2} \tag{6}$$

From the conservation of momentum Equation 2, and Equations 4 and 5, the pressure ratio across the detonation front may be expressed as

$$\frac{P_2}{P_1} = \frac{\gamma_1 \mathbf{M}_1^2 + 1}{\gamma_2 \mathbf{M}_2^2 + 1} \tag{7}$$

From the conservation of mass Equation 1, and Equations 4, 5, and 7, the density ratio may be expressed as

$$\rho_2/\rho_1 = \left(\frac{\gamma_1 \mathbf{M}_1^2}{\gamma_1 \mathbf{M}_1^2 + 1}\right) \cdot \left(\frac{\gamma_2 \mathbf{M}_2^2 + 1}{\gamma_2 \mathbf{M}_2^2}\right) \tag{8}$$

Equations 7 and 8 are the usual expressions for pressure ratio and density ratio across a normal shock.

The equation of state for ideal gases may be expressed as

$$\frac{P}{\rho} = \frac{JRT}{M_w} \tag{9}$$

Applying Equation 9 to the state conditions before and after the detonation wave, and combining the resulting two equations with Equations 7 and 8, the expression for the temperature-molecular weight ratio obtained is

$$\frac{T_2 M_{w_1}}{T_1 M_{w_2}} = \frac{\gamma_2 \mathbf{M}_2^2}{(\gamma_2 \mathbf{M}_2^2 + 1)^2} \cdot \frac{(\gamma_1 \mathbf{M}_1^2 + 1)^2}{\gamma_1 \mathbf{M}_1^2} \tag{10}$$

In order to facilitate transformation of the conservation of energy Equation 3 into nondimensional form, it is assumed that both the initial and final gaseous mixtures are polytropic. It is thought that this assumption will not affect appreciably the accuracy of the final generalized equations. Based on this assumption, the expression obtained for the difference in internal energies across the detonation wave is

$$e_2 - e_1 = c_{v_2} T_2 - c_{v_1} T_1 \tag{11}$$

Utilizing Equation 11, the conservation of energy Equation 3 becomes

$$Jc_{v_1} T_1 + \frac{P_1}{\rho_1} + \frac{V_1^2}{2} + Jh = Jc_{v_2} T_2 + \frac{P_2}{\rho_2} + \frac{V_2^2}{2} \tag{12}$$

Since $c_v M_w = C_v$ and $\gamma = \frac{C_p}{C_v}$ and since, for ideal gases, $R = C_p - C_v$, the following equation is obtained from Equations 9 and 12:

$$\frac{\gamma_1}{\gamma_1 - 1} \frac{P_1}{\rho_1} + \frac{V_1^2}{2} + Jh = \frac{\gamma_2}{\gamma_2 - 1} \frac{P_2}{\rho_2} + \frac{V_2^2}{2} \tag{13}$$

Equation 13 is the approximate energy equation utilized by D. G. Samaras in his paper on endothermic and exothermic discontinuities (7), and involves approximations believed to be negligible as discussed here – e.g., assumption of polytropic gas.

From Equations 4, 5, 6, 7, 8, and 13, the following equation is obtained:

$$\mathbf{B} = \left(\frac{\gamma_2}{\gamma_2 - 1} + \frac{\gamma_2 \mathbf{M}_2^2}{2}\right) \cdot \frac{\gamma_2 \mathbf{M}_2^2}{(\gamma_2 \mathbf{M}_2^2 + 1)^2} \cdot \frac{(\gamma_1 \mathbf{M}_1^2 + 1)^2}{\gamma_1^2 \mathbf{M}_1^2} - \frac{1}{\gamma_1 - 1} - \frac{\mathbf{M}_1^2}{2} \tag{14}$$

This is a nondimensional form of the Hugoniot equation, based on the energy Equation 13.

The Chapman-Jouguet hypothesis that the product gases (final mixture) leave the detonation front at a velocity equal to the local speed of sound in those gases may be expressed as

$$\mathbf{M}_2 = 1.0 \tag{15}$$

Applying the Chapman-Jouguet hypothesis to Equations 7, 8, 10, and 14, expressions for the pressure ratio, density ratio, and temperature-molecular weight ratio across the detonation wave, and the energy release in the detonation wave, in nondimensional form, may be obtained as follows:

$$\frac{P_2}{P_1} = \frac{1}{\gamma_2 + 1} (\gamma_1 \mathbf{M}_1^2 + 1) \tag{16}$$

$$\rho_2/\rho_1 = \frac{\gamma_2 + 1}{\gamma_2} \left(\frac{\gamma_1 \mathbf{M}_1^2}{\gamma_1 \mathbf{M}_1^2 + 1}\right) \tag{17}$$

$$\frac{T_2 M_{w_1}}{T_1 M_{w_2}} = \frac{\gamma_2}{(\gamma_2 + 1)^2} \frac{(\gamma_1 \mathbf{M}_1^2 + 1)^2}{\gamma_1 \mathbf{M}_1^2} \tag{18}$$

$$\mathbf{B} = \frac{1}{\gamma_2^2 - 1} \left[\frac{\mathbf{M}_1^2}{2} + \left(\frac{\gamma_2}{\gamma_1}\right)^2 \left(\frac{1}{2\mathbf{M}_1^2} + \gamma_1\right)\right] - \frac{1}{\gamma_1 - 1} \tag{19}$$

Equation 19 is a nondimensional form of the equation commonly referred to as the Chapman-Jouguet equation, based on the energy Equation 13. The above four equations are the nondimensional generalized equations which form the basis for the graphical presentations in this article.

Equation 19 may be expressed in the form

$$\overline{\mathbf{M}}_1^2 = 2(\gamma_2^2 - 1)\,\mathbf{B} + 2\,\frac{\gamma_2^2 - \gamma_1}{\gamma_1(\gamma_1 - 1)} \tag{20}$$

where $\overline{\mathbf{M}}_1$ is the "pseudo-Mach number" (2). Thus the relationship between $\overline{\mathbf{M}}_1$ and $\mathbf{M}_1$ is

$$\overline{\mathbf{M}}_1^2 = \mathbf{M}_1^2 + \left(\frac{\gamma_2}{\gamma_1}\right)^2 \frac{1}{\mathbf{M}_1^2} \tag{21}$$

CONSTRUCTION OF THE CHARTS

Charts based on the generalized equations are given in Figures 1, 2, and 3. It was found that except for the parameter γ_1 , all the detonation parameters could be shown on one diagram. A separate chart is presented for each of three values of γ_1 – i.e., 1.2, 1.3, and 1.4, as representative values of this parameter for various gaseous mixtures. These charts show basically the variation of the pseudo-Mach number squared ($\overline{M}_1^2$) with the energy release function, **B** (dimensionless), at constant values of γ_2, the specific heat ratio for the final mixture. This relationship (Equation 20) is represented as radial lines emanating from a point near the origin.

The other detonation parameters – pressure ratio, temperature-molecular weight ratio, and density ratio across the detonation wave – are represented by cross plots on each chart, each of these parameters being a function only of the Mach number and γ_1 and γ_2. Thus, lines of constant $\frac{p_2}{p_1}$, numerically equal to the ratio P_2/P_1, together with lines of constant $\frac{T_2M_{w_1}}{T_1M_{w_2}}$ and lines of constant ρ_2/ρ_1 have been cross plotted on the generalized charts utilizing Equations 16, 17, 18 and 21.

Equation 20 was used in constructing the generalized charts rather than Equation 19. Equation 19, the Chapman-Jouguet equation, would have been the more accurate relationship but use of Equation 20 simplified the construction of the charts considerably, since the $\overline{M}_1^2$ versus **B** relationship was then simply represented by a group of straight lines emanating from a single point.

The approximation involved in the use of Equation 20 in lieu of Equation 19 is only a very slight one. The difference between these equations is given by Equation 21. A plot of Equation 21 is given in Figure 4. In Equation 21 and Figure 4, the quantities $\overline{M}_1^2$ and M_1^2 are essentially the same in the range of Mach numbers normally encountered in gaseous detonations. For all detonative Mach numbers above approximately 3.0 ($\overline{M}_1^2 \cong 9.0$), the error introduced through using $\overline{M}_1^2$ is negligible and within the reading accuracy of the chart. In the region where the detonative Mach number is 3.0 '($\overline{M}_1^2 = 9.0$), th error is still extremely small. The only appreciable error is in the region approaching a detonative Mach number equal to unity—a region of little interest in detonation studies.

It can be shown that the location of the vertex of the group of radial lines plotted from Equation 20 ($\overline{M}_1^2$ vs **B**) is given by two analytical expressions involving only γ_1:

$$\overline{M}_1^2 = -\frac{2}{\gamma_1} \tag{22}$$

$$B = -\frac{1}{\gamma_1(\gamma_1 - 1)} \tag{23}$$

A set of $\overline{M}_1^2$ versus **B** lines for any γ_1 can be plotted readily, simply by determining the point of intersection by means of Equations 22 and 23 and then plotting only one point for each desired value of γ_2.

USE OF THE CHARTS

The chief usefulness of the generalized charts (Figures 1, 2, and 3) lies in the fact that they present all of the detonation parameters for gaseous mixtures, utilizing only dimensionless quantities, on Mollier-type diagrams.

As a specific illustration of the usefulness of these charts in permitting immediate visualization of numerical values of all the detonation parameters for a particular case, a hypothetical example will be considered first. If the ratio of specific heats for the initial mixture is $\gamma_1 =$ 1.3, Figure 2 is the applicable generalized chart. Assuming that $p_2/p_1 = 20$ and $\gamma_2 = 1.25$, then $\rho_2/\rho_1 = 1.75$, $\overline{M}_1^2 = 33.7$, $T_2M_{w_1}/T_1M_{w_2} = 11.4$, and $B = 28.3$. Therefore, according to Figure 4, M_1^2 is also equal to 33.7.

Use of the charts can be illustrated further by considering two actual gaseous mixtures for which partial detonation data are available in the literature.

For the gaseous mixture, $C_2H_2 + O_2$ at 15° C. and a pressure of 1 atmosphere, it is found that $\gamma_1 = 1.307$. Values reported in the literature (5) for pressure ratio and final specific heat ratio are $p_2/p_1 = 50.2$ and $\gamma_2 = 1.13$, respectively. In this case, since $\gamma_1 = 1.307$, interpolation between Figure 2 ($\gamma_1 = 1.3$) and Figure 3 ($\gamma_1 = 1.4$) will be necessary. Using the literature values of p_2/p_1 and γ_2, the following values of the remaining detonation parameters may be read from Figures 2 and 3.

	Figure 2 ($\gamma_1 = 1.3$)	Figure 3 ($\gamma_1 = 1.4$)
$\overline{M}_1^2$	81.6	75.8
$\frac{\rho_2}{\rho_1}$	1.87	1.87
$\frac{T_2M_{w_1}}{T_1M_{w_2}}$	27.0	26.8
B	148	139

Interpolated values for $\gamma_1 = 1.307$ are found to be

$$\overline{M}_1^2 = 81.2 \text{ (or } \overline{M}_1 = 9.02)$$

$$\rho_2/\rho_1 = 1.87$$

$$\frac{T_2M_{w_1}}{T_1M_{w_2}} = 26.9$$

$$B = 147.4$$

For the given gaseous mixture, C_2H_2 - O_2, Manson (5) reported the detonation velocity to be 2960 meters/second. From this, the Mach number of the detonation is calculated to be

$$\overline{M}_1 = M_1 = D\sqrt{\frac{M_{w_1}}{J\gamma_1RT_1}} = 8.96,$$

or

$$\overline{M}_1^2 = M_1^2 = 80.2$$

(As stated previously, $\overline{M}_1$ and M_1 are essentially the same at Mach numbers above 3.) Manson also reported the density ratio for this case to be $\rho_2/\rho_1 = 1.87$. The values obtained from the generalized detonation charts ($\overline{M}_1^2 = 9.02$, $\rho_2/\rho_1 =$ 1.87) compare favorably with these literature values.

The second example illustrating the use of the generalized detonation charts is for the gaseous mixture, H_2 - 1/2 O_2 at 18° C. and a pressure of 1 atmosphere. For this stoichiometric mixture, it is found that $\gamma_1 = 1.4026$. Values previously calculated (2) for pressure ratio and final specific heat ratio are $p_2/p_1 = 17.22$ and $\gamma_2 = 1.2075$, respectively, assuming dissociation of the gaseous products at the detonation temperature and pressure. Since $\gamma_1 = 1.4026$, extrapolation using Figure 2 ($\gamma_1 = 1.3$) and Figure 3 ($\gamma_1 = 1.4$) will be necessary. Using the values of p_2/p_1 and γ_2 already cited, the following values of the remaining detonation parameters may be read from Figures 2 and 3:

	Figure 2 ($\gamma_1 = 1.3$)	Figure 3 ($\gamma_1 = 1.4$)
$\overline{M}_1^2$	28.5	26.5
$\frac{\rho_2}{\rho_1}$	1.77	1.78
$\frac{T_2M_{w_1}}{T_1M_{w_2}}$	9.8	9.7
B	30.0	28.7

Thus, extrapolated values for $\gamma_1 = 1.4026$, obtained from the generalized detonation charts (Figures 2 and 3), are found to be

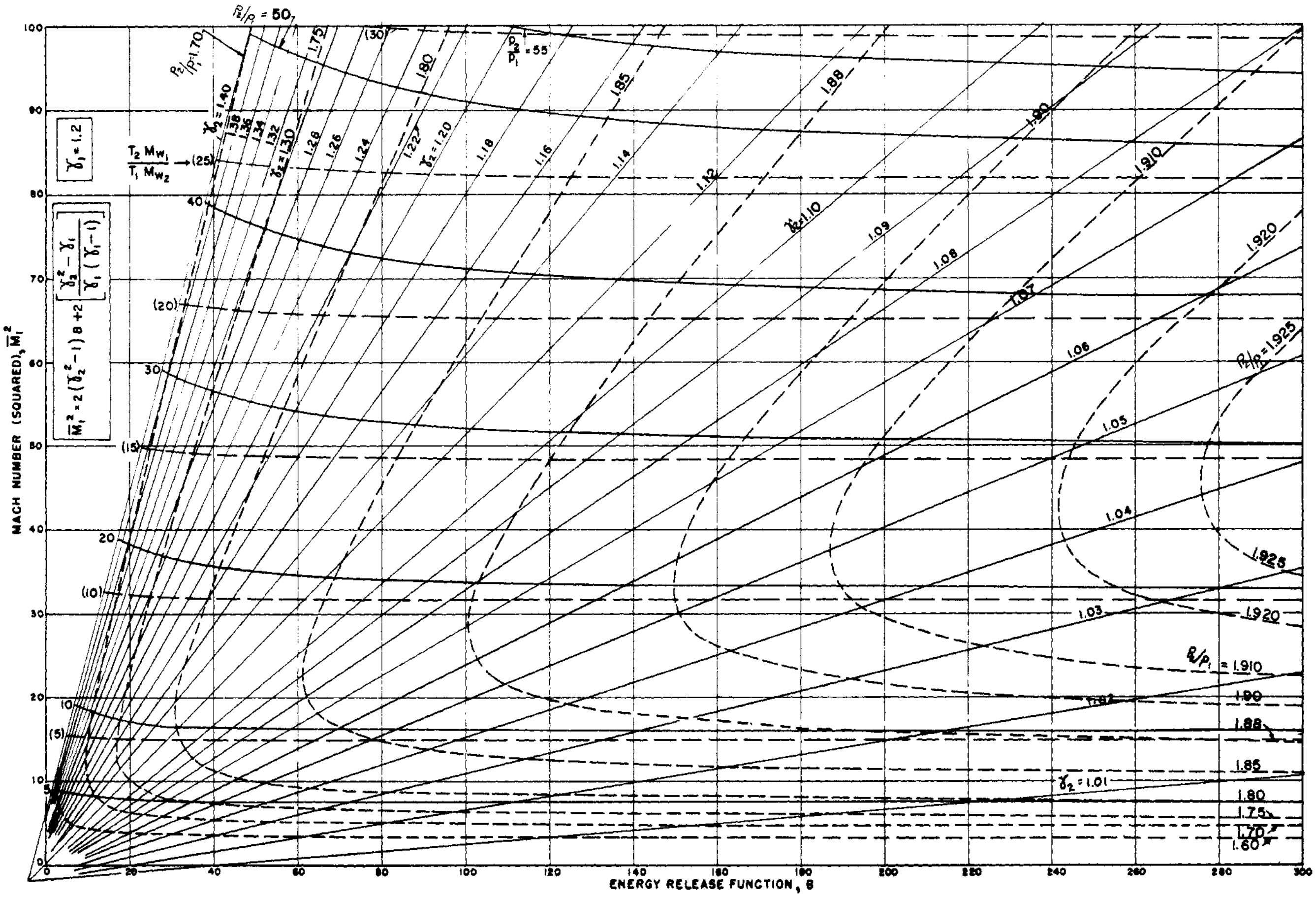

Figure 1. Generalized detonation chart for $\gamma_1 = 1.2$

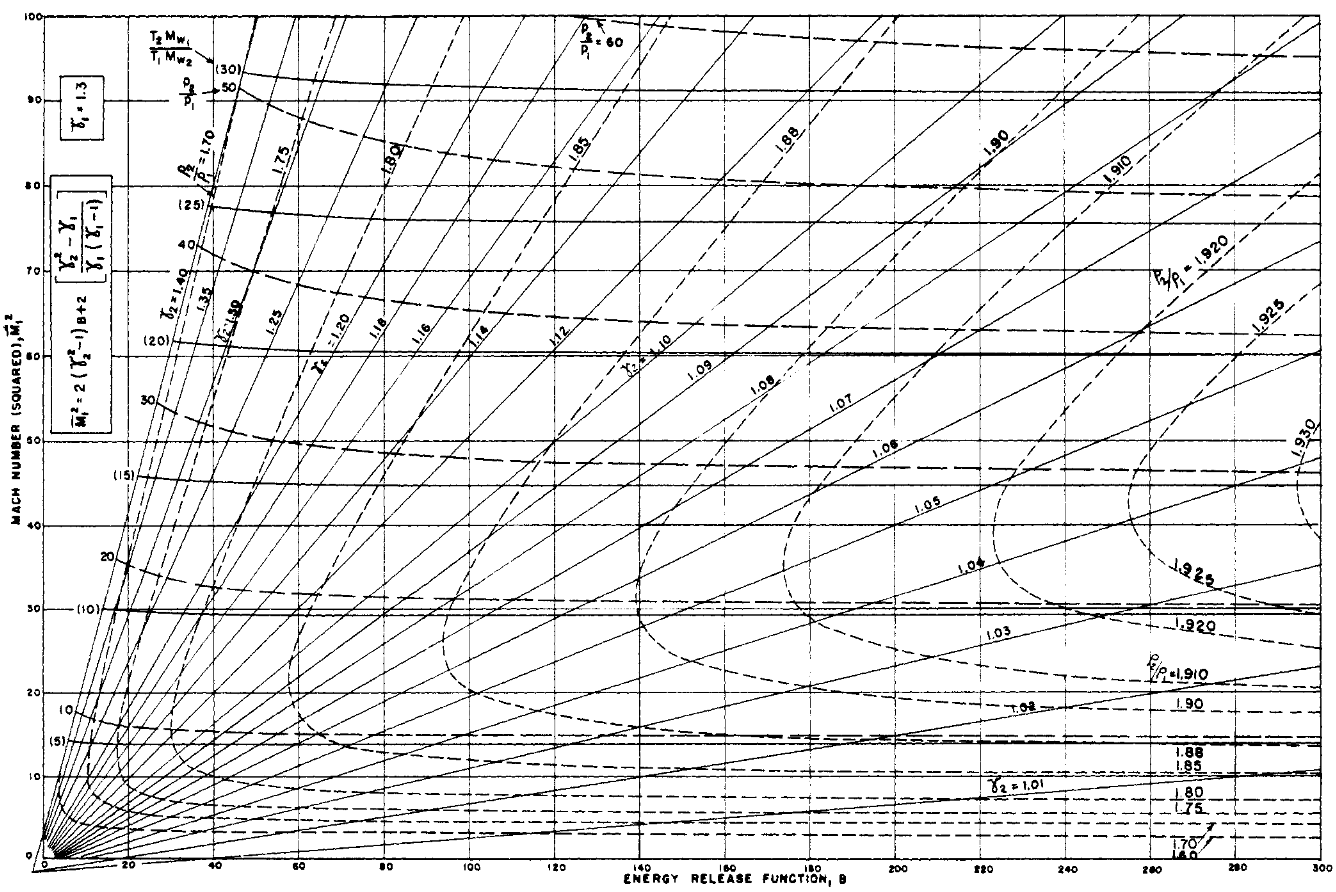

Figure 2. Generalized detonation chart for $\gamma_1 = 1.3$

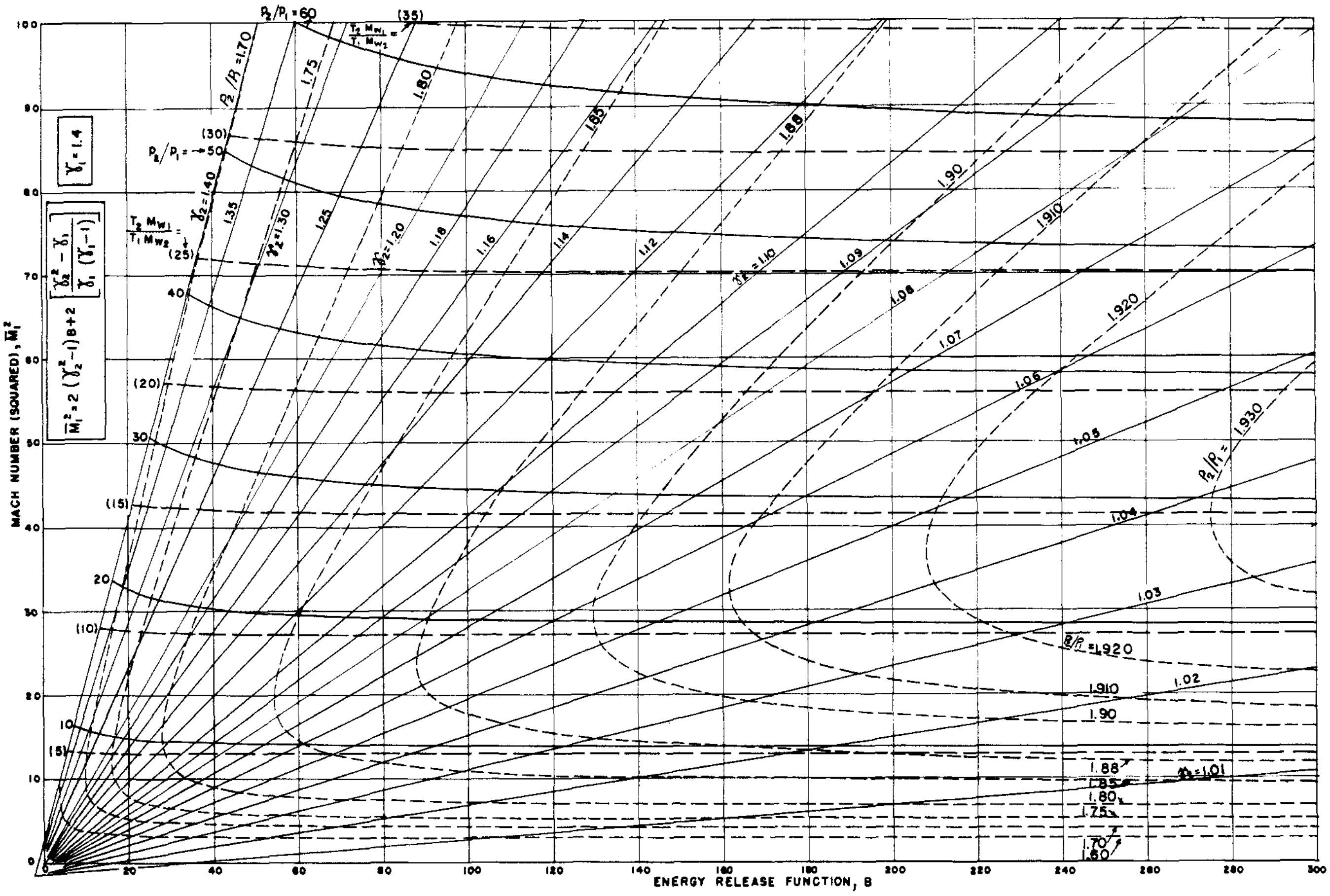

Figure 3. Generalized detonation chart for γ_1 = 1.4

$$\bar{M}_1^2 = 26.4 \text{ (or } \bar{M}_1 = 5.14)$$

$$\rho_2/\rho_1 = 1.78$$

$$\frac{T_2M_{w_1}}{T_1M_{w_2}} = 9.7$$

$$B = 28.7$$

Values of pressure ratio and final specific heat ratio found elsewhere in the literature (4, 5, 9) are p_2/p_1 = 18.05 and γ_2 = 1.214. Using these two values and that of γ_1 = 1.4026, the values which may be obtained from Figures 2 and 3 by extrapolation are: $\bar{M}_1^2$ = 27.7 ($\bar{M}_1$ = 5.26); ρ_2/ρ_1 = 1.77; $\frac{T_2M_{w_1}}{T_1M_{w_2}}$ = 10.0; and B = 28.9.

The heat of reaction under detonation conditions may be calculated from the extrapolated value of B obtained from the generalized detonation charts. By definition

$$B = \frac{Jh}{a_1^2} = \frac{J\Delta H_R}{a_1^2 M_{w_1}} = \frac{\Delta H_R}{\gamma_1 RT_1}$$

Then, using the values of B, γ_1, and T_1 in the above example

$$\Delta H_R = B\gamma_1 RT_1 = (28.7)\ (1.4026)\ (1.98719)\ (291) = 23{,}220 \text{ cal./gram mole of initial mixture}$$

Therefore, the heat of reaction per mole of hydrogen, as calculated on the basis of data from the generalized detonation charts, is found to be 23,220 x 1.5/1 or 34,830 cal./gram mole of hydrogen. The standard heat of combustion for the mixture $H_2 + 1/2\ O_2$ as given in the literature (3) is 68,320 cal./gram mole of hydrogen (product of combustion, liquid H_2O at 18° C.). These data indicate that only 51% of the standard heat of combustion is released as available energy in the detonation process (the h in Equation 3). The energy required for vaporizing the liquid water, heating the product gases from 18° C. to the final temperature (T_2), and dissociation of the product gases accounts for the remaining 49%.

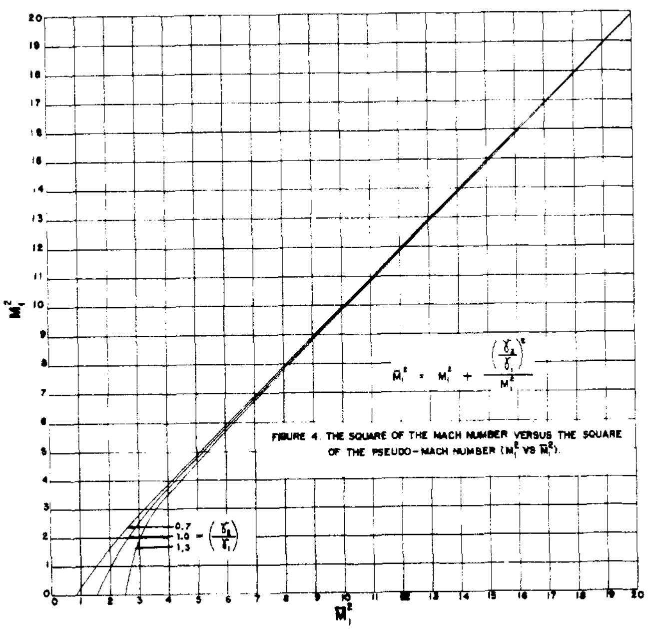

Figure 4. Caption included on drawing

For the given gaseous mixture, $H_2+1/2O_2$, data previously reported (2) gave the calculated detonated velocity as 2731.5 meters/second, the Mach number of detonation as $\overline{M}_1 = 5.138$ ($\overline{M}_1^2 = 26.40$), the density ratio as $\rho_2/\rho_1 = 1.780$, the temperature-molecular weight ratio as $T_2M_{w_1}/T_1M_{w_2} = 9.68$, and the energy release function as $\mathbf{B} = 28.60$ (assuming dissociation of the gaseous products at the detonation pressure and temperature). It will be noted that the values obtained from the generalized detonation charts,

$$\overline{M}_1^2 = 5.14,\ \rho_2/\rho_1 = 1.78,\ T_2M_{w_1}/T_1M_{w_2} = 9.7, \text{ and } \mathbf{B} = 28.7$$

are essentially the same as these calculated values. Calculated values of these detonation parameters reported elsewhere in the literature (4, 5, 9) for this case are detonation velocity of 2806 meters/second and $\rho_2/\rho_1 = 1.78$. This detonation velocity corresponds to a value of $\overline{M}_1 = 5.28$ ($\overline{M}_1^2 = 27.8$).

It should be emphasized that, although accurate values of some detonation parameters may be obtained directly from the generalized detonation charts if certain minimum data are available, the chief usefulness of these charts is to provide a means for visualizing on a small number of charts all relationships among the detonation parameters for gaseous mixtures.

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NOMENCLATURE

a = velocity of sound, cm./second

$\mathbf{B}$ = energy release function. Dimensionless

c_v = specific heat at constant volume, cal./gram, °K.

C_p = molal heat capacity at constant pressure, cal./gram mole, °K.

C_v = molal heat capacity at constant volume, cal./ gram mole, °K.

D = detonation velocity—velocity of the detonation wave with respect to the initial mixture—cm./second

e = specific internal energy, cal./gram

h = energy release per unit mass of mixture, cal./gram

ΔH_R = heat of reaction—energy release per mole of initial mixture—cal./gram mole

J = mechanical equivalent of heat, dyne-cm./cal. or ergs/cal.

$\mathbf{M}$ = Mach number. Dimensionless

$\mathbf{M}_1$ = detonative Mach number—the Mach number of the detonation wave with respect to the initial mixture. Dimensionless

$\mathbf{M}_2$ = Mach number of the detonation wave with respect to the final mixture. Dimensionless

$\overline{M}_1$ = pseudo-Mach number, close approximation to the detonative Mach number ($\mathbf{M}_1$); used for convenience only. Dimensionless

M_w = molecular weight, grams/gram mole

p = pressure, atm.

P = pressure, dynes/sq. cm.

R = universal gas constant, cal./gram mole, °K.

T = absolute temperature, °K.

V = velocity, cm./second

V_1 = velocity of detonation wave with respect to the initial mixture, cm./second

V_2 = velocity of the detonation wave with respect to the final mixture, cm./second

γ = specific heat or molal heat capacity ratio. Dimensionless

ρ = density, grams/cc.

Subscripts

1 pertains to the initial mixture at the initial conditions

2 pertains to the final mixture immediately behind the detonation wave at the final conditions

p pertains to constant pressure

v pertains to constant volume

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