Thermodynamic Calculations of Hydrogen-Oxygen Detonation Parameters for Various Initial Pressures

Composition, temperature, pressure and density behind a stable detonation wave and its propagation rate have been calculated for seven hydrogen-oxygen mixtures at 1, 5, 25 and 100 atm initial pressure, and at an initial temperature of 40°C. For stoichiometric mixtures the calculations also include an initial temperature of 200°C. According to these calculations the detonation velocities of hydrogen-oxygen mixtures increase with increasing initial pressure, but decrease slightly when the initial temperature is raised from 40 to 200°C. The calculated detonation velocities agree satisfactorily with values determined experimentally. These values will be published in the near future.

The calculations are based on the assumption that complete thermodynamic and chemical equilibrium is established in the wave. Dissipating effects such as viscosity, heat transfer by conduction and radiation, and chemical reaction rate phenomena are disregarded. The calculations were carried out for hydrogen-oxygen mixtures using a rigorous method developed by Edse (1). Other gaseous reactants will be treated in a future paper.

The detonation parameters are derived from the Hugoniot equation for the reacted gas mixture in equilibrium, and from the condition that the detonation velocity is the minimum wave velocity of the possible velocities for the given state of the combustible gas. Thus the results are based on the Chapman-Jouguet point at which the velocity of the reacted gas relative to the detonation wave is equal to the equilibrium sonic speed in the reacted gas behind the wave. These conditions can be calculated more readily than those for a frozen speed of sound for which the ratio of the specific heats must be calculated (3).

Method of Calculation

Assuming that only the neutral species of H₂O, H₂, O₂, OH, O and H occur in the detonation wave of hydrogen-oxygen mixtures, the Hugoniot equation can be written

\[
\frac{p_2}{p_0} = \left[ \frac{\sum p_i (\Delta H_f/\Delta T)_i \gamma_i}{2p_{H_2O} + 2p_{H_2} + p_{OH} + p_O + p_H} \right]^{\gamma - 2} + 1
\]

where

\[
\sum p_i (\Delta H_f/\Delta T)_i \gamma_i = p_{H_2O}(\Delta H_f/\Delta T)_{H_2O} + \ldots
\]

In Equation [1] the partial pressures of H₂O, H₂, O₂, OH, O and H must satisfy the conditions for chemical equilibrium. With an assumed value for the partial pressure of molecular oxygen, the partial pressures are calculated as

\[
p_{O_2} \text{ assumed } p_0 = K_{O_2}(p_{O_2})^{1/4}
\]

\[
p_{H_2O} = \frac{K_{H_2O} \left(1 - N_0 \right) \left( p_{O_2} \right)^{1/4} - N_0 N_W K_{H_2O}}{2 \left[ (1 - 2N_0/N_W) (p_{O_2})^{1/4} - 2 N_0 N_W \right]^2}
\]

\[
p_{H_2} = \frac{K_{H_2} \left(1 - N_0 \right) \left( p_{O_2} \right)^{1/4} - N_0 N_W K_{H_2}}{2 \left[ (1 - 2N_0/N_W) (p_{O_2})^{1/4} - 2 N_0 N_W \right]^2}
\]

\[
p_{OH} = \frac{K_{OH} \left(1 - N_0 \right) \left( p_{O_2} \right)^{1/4} - N_0 N_W K_{OH}}{2 \left[ (1 - 2N_0/N_W) (p_{O_2})^{1/4} - 2 N_0 N_W \right]^2}
\]

\[
p_{O} = \frac{K_{O} \left(1 - N_0 \right) \left( p_{O_2} \right)^{1/4} - N_0 N_W K_{O}}{2 \left[ (1 - 2N_0/N_W) (p_{O_2})^{1/4} - 2 N_0 N_W \right]^2}
\]

\[
p_{H} = \frac{K_{H} \left(1 - N_0 \right) \left( p_{O_2} \right)^{1/4} - N_0 N_W K_{H}}{2 \left[ (1 - 2N_0/N_W) (p_{O_2})^{1/4} - 2 N_0 N_W \right]^2}
\]

Received Sept. 5, 1960.

1 Assistant Supervisor, Rocket Research Laboratory; also Assistant Professor, Dept. of Aeronautical Engineering. Member ARS.

2 Director, Rocket Research Laboratory; also Professor, Dept. of Aeronautical Engineering. Member ARS.

3 Numbers in parentheses indicate References at end of paper.

(Reprinted from ARS JOURNAL, February, 1961)

Copyright 1961, by the American Rocket Society, Inc., and reprinted by permission of the copyright owner.
For hydrogen-rich mixtures \((N_O/N_H < 1/2)\) the assumed value of the molecular oxygen partial pressure must be less than \([2N_O/(N_H + 2N_O)]/K_{\text{H}_2}\).

Since the sum of all partial pressures must be equal to \(p_a\) as derived from Equation [1], the correct value of \(p_{\text{po}}\) can be determined by trial and error using Equations [1 through 6]. As a result of these calculations, a pair of \(p_a\) and \(p_a\) values is obtained that satisfies the Hugoniot equation.

This procedure is repeated until a pair of \(p_a\) and \(p_a\) values is found which makes this Mach number a minimum. These values and the minimum value of the wave relative to the unreacted gas

\[
k_bM^2 = \frac{(p_a/p_b) - 1}{1 - \frac{2p_a}{1 + N_O/N_H}} \cdot \frac{T_a/T_b}{2p_{\text{po}} + 2p_a + p_{\text{po}} + p_a}
\]

This is obtained using the continuity equation

\[
\frac{T_a}{T_b} = \frac{2p_{\text{po}} + 2p_a + p_{\text{po}} + p_a}{2p_{\text{po}}}
\]

where

\[
u_a = \frac{u_D}{u_D}, \quad \nu_b = \frac{u_D}{u_D}, \quad \frac{2p_a}{1 + N_O/N_H}
\]

The results of these calculations are presented in Tables 1 through 5. A small amount of scatter in the results was unavoidable because of the limited number of iterations used during these calculations, which were made with a Square Root Friden calculating machine.

Assuming that the immediate front of the detonation wave consists of a normal shock wave, propagating at the velocity \(u_D\) through the combustible gas mixture without causing any chemical reactions in the gas, we can calculate the temperature and pressure behind this wave by solving the

<table>
<thead>
<tr>
<th>Molar per cent fuel in mixture</th>
<th>(p_{\text{po}}) atm</th>
<th>(p_a) atm</th>
<th>(p_{\text{po}}) atm</th>
<th>(p_a) atm</th>
<th>(p_{\text{po}}) atm</th>
<th>(p_a) atm</th>
<th>(p_{\text{po}}) atm</th>
<th>(p_a) atm</th>
<th>(p_{\text{po}}) atm</th>
<th>(p_a) atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
<td>0.234</td>
</tr>
<tr>
<td>25</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
</tr>
<tr>
<td>45</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
<td>0.056</td>
</tr>
<tr>
<td>50</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
<td>0.029</td>
</tr>
<tr>
<td>60</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
<td>0.016</td>
</tr>
<tr>
<td>75</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
</tr>
<tr>
<td>90</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
<td>0.006</td>
</tr>
<tr>
<td>100</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
</tr>
</tbody>
</table>

* Initial temperature = 313.16 K except where noted.

* Initial temperature = 473.16 K.

ARS JOURNAL
### Table 2 Properties of a hydrogen-oxygen detonation wave, $p_0 = 1$ atm

<table>
<thead>
<tr>
<th>Molar per cent fuel in mixture</th>
<th>$T_a$</th>
<th>$T_m, a$</th>
<th>$T_m, s$</th>
<th>$P_a, a$</th>
<th>$P_m$</th>
<th>$u_a$</th>
<th>$u_p$</th>
<th>$M_D = \frac{u_p}{a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>313.16</td>
<td>2960</td>
<td>1560</td>
<td>14.38</td>
<td>24.174</td>
<td>24.096</td>
<td>1024</td>
<td>1845</td>
</tr>
<tr>
<td>45</td>
<td>313.16</td>
<td>3220</td>
<td>1795</td>
<td>16.70</td>
<td>28.660</td>
<td>29.296</td>
<td>1169</td>
<td>2182</td>
</tr>
<tr>
<td>55</td>
<td>313.16</td>
<td>3538</td>
<td>1875</td>
<td>17.50</td>
<td>31.377</td>
<td>30.459</td>
<td>1322</td>
<td>2459</td>
</tr>
<tr>
<td>66.67</td>
<td>313.16</td>
<td>3646</td>
<td>1981</td>
<td>18.00</td>
<td>32.270</td>
<td>31.752</td>
<td>1522</td>
<td>2826</td>
</tr>
<tr>
<td>66.67</td>
<td>473.16</td>
<td>3576</td>
<td>2083</td>
<td>11.20</td>
<td>20.666</td>
<td>17.290</td>
<td>1385</td>
<td>2784</td>
</tr>
<tr>
<td>75</td>
<td>313.16</td>
<td>3567</td>
<td>1976</td>
<td>17.50</td>
<td>32.060</td>
<td>29.917</td>
<td>1750</td>
<td>3173</td>
</tr>
<tr>
<td>85</td>
<td>313.16</td>
<td>3108</td>
<td>1725</td>
<td>15.61</td>
<td>27.251</td>
<td>26.260</td>
<td>2017</td>
<td>3627</td>
</tr>
<tr>
<td>90</td>
<td>313.16</td>
<td>2563</td>
<td>1512</td>
<td>13.00</td>
<td>23.215</td>
<td>21.140</td>
<td>2155</td>
<td>3796</td>
</tr>
</tbody>
</table>

### Table 3 Properties of a hydrogen-oxygen detonation wave, $p_0 = 5$ atm

<table>
<thead>
<tr>
<th>Molar per cent fuel in mixture</th>
<th>$T_a$</th>
<th>$T_m, a$</th>
<th>$T_m, s$</th>
<th>$P_a, a$</th>
<th>$P_m$</th>
<th>$u_a$</th>
<th>$u_p$</th>
<th>$M_D = \frac{u_p}{a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>313.16</td>
<td>2955</td>
<td>1586</td>
<td>74.00</td>
<td>122.96</td>
<td>124.32</td>
<td>1033</td>
<td>1861</td>
</tr>
<tr>
<td>45</td>
<td>313.16</td>
<td>3256</td>
<td>1874</td>
<td>80.20</td>
<td>151.12</td>
<td>149.14</td>
<td>1220</td>
<td>2240</td>
</tr>
<tr>
<td>55</td>
<td>313.16</td>
<td>3790</td>
<td>2018</td>
<td>91.10</td>
<td>164.37</td>
<td>158.34</td>
<td>1368</td>
<td>2517</td>
</tr>
<tr>
<td>66.67</td>
<td>313.16</td>
<td>3954</td>
<td>2102</td>
<td>92.50</td>
<td>172.10</td>
<td>157.76</td>
<td>1618</td>
<td>2918</td>
</tr>
<tr>
<td>66.67</td>
<td>473.16</td>
<td>3884</td>
<td>2193</td>
<td>58.30</td>
<td>109.76</td>
<td>92.568</td>
<td>1652</td>
<td>2869</td>
</tr>
<tr>
<td>75</td>
<td>313.16</td>
<td>3943</td>
<td>2066</td>
<td>90.50</td>
<td>169.13</td>
<td>152.79</td>
<td>1824</td>
<td>3260</td>
</tr>
<tr>
<td>85</td>
<td>313.16</td>
<td>3244</td>
<td>1777</td>
<td>80.36</td>
<td>141.26</td>
<td>135.17</td>
<td>2058</td>
<td>3692</td>
</tr>
<tr>
<td>90</td>
<td>313.16</td>
<td>2996</td>
<td>1525</td>
<td>63.50</td>
<td>117.64</td>
<td>106.19</td>
<td>2177</td>
<td>3821</td>
</tr>
</tbody>
</table>

### Table 4 Properties of a hydrogen-oxygen detonation wave, $p_0 = 25$ atm

<table>
<thead>
<tr>
<th>Molar per cent fuel in mixture</th>
<th>$T_a$</th>
<th>$T_m, a$</th>
<th>$T_m, s$</th>
<th>$P_a, a$</th>
<th>$P_m$</th>
<th>$u_a$</th>
<th>$u_p$</th>
<th>$M_D = \frac{u_p}{a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>313.16</td>
<td>3049</td>
<td>1635</td>
<td>376.0</td>
<td>639.77</td>
<td>629.09</td>
<td>1061</td>
<td>1898</td>
</tr>
<tr>
<td>45</td>
<td>313.16</td>
<td>3724</td>
<td>1947</td>
<td>444.9</td>
<td>788.00</td>
<td>764.66</td>
<td>1257</td>
<td>2289</td>
</tr>
<tr>
<td>55</td>
<td>313.16</td>
<td>4064</td>
<td>2104</td>
<td>473.3</td>
<td>865.92</td>
<td>816.90</td>
<td>1417</td>
<td>2583</td>
</tr>
<tr>
<td>66.67</td>
<td>313.16</td>
<td>4296</td>
<td>2210</td>
<td>490.0</td>
<td>914.05</td>
<td>839.02</td>
<td>1627</td>
<td>3067</td>
</tr>
<tr>
<td>66.67</td>
<td>473.16</td>
<td>4241</td>
<td>2306</td>
<td>323.3</td>
<td>588.47</td>
<td>535.57</td>
<td>1653</td>
<td>2970</td>
</tr>
<tr>
<td>75</td>
<td>313.16</td>
<td>4138</td>
<td>2167</td>
<td>490.0</td>
<td>891.69</td>
<td>819.53</td>
<td>1858</td>
<td>3347</td>
</tr>
<tr>
<td>85</td>
<td>313.16</td>
<td>3349</td>
<td>1816</td>
<td>410.8</td>
<td>725.31</td>
<td>689.79</td>
<td>2062</td>
<td>3741</td>
</tr>
<tr>
<td>90</td>
<td>313.16</td>
<td>2606</td>
<td>1535</td>
<td>325.0</td>
<td>592.15</td>
<td>520.75</td>
<td>2209</td>
<td>3834</td>
</tr>
</tbody>
</table>

### Table 5 Properties of a hydrogen-oxygen detonation wave, $p_0 = 100$ atm

<table>
<thead>
<tr>
<th>Molar per cent fuel in mixture</th>
<th>$T_a$</th>
<th>$T_m, a$</th>
<th>$T_m, s$</th>
<th>$P_a, a$</th>
<th>$P_m$</th>
<th>$u_a$</th>
<th>$u_p$</th>
<th>$M_D = \frac{u_p}{a}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>313.16</td>
<td>3108</td>
<td>1663</td>
<td>1524</td>
<td>2693.2</td>
<td>2543.2</td>
<td>1072</td>
<td>1914</td>
</tr>
<tr>
<td>45</td>
<td>313.16</td>
<td>3898</td>
<td>2004</td>
<td>1885</td>
<td>3565.2</td>
<td>3327.0</td>
<td>1248</td>
<td>2328</td>
</tr>
<tr>
<td>55</td>
<td>313.16</td>
<td>4298</td>
<td>2227</td>
<td>1983</td>
<td>3396.0</td>
<td>3395.1</td>
<td>1477</td>
<td>2664</td>
</tr>
<tr>
<td>66.67</td>
<td>313.16</td>
<td>4641</td>
<td>2296</td>
<td>2070</td>
<td>3819.0</td>
<td>3597.2</td>
<td>1683</td>
<td>3573</td>
</tr>
<tr>
<td>66.67</td>
<td>473.16</td>
<td>4554</td>
<td>2387</td>
<td>1504</td>
<td>2448.5</td>
<td>2338.3</td>
<td>1674</td>
<td>3019</td>
</tr>
<tr>
<td>75</td>
<td>313.16</td>
<td>4390</td>
<td>2231</td>
<td>2000</td>
<td>3710.1</td>
<td>3431.2</td>
<td>1890</td>
<td>3413</td>
</tr>
<tr>
<td>85</td>
<td>313.16</td>
<td>3405</td>
<td>1840</td>
<td>1645</td>
<td>2945.5</td>
<td>2731.8</td>
<td>2132</td>
<td>3770</td>
</tr>
<tr>
<td>90</td>
<td>313.16</td>
<td>2622</td>
<td>1539</td>
<td>1320</td>
<td>2375.1</td>
<td>2139.7</td>
<td>2189</td>
<td>3839</td>
</tr>
</tbody>
</table>
following equations simultaneously

\[
\frac{p_{s, n.s.}}{p_b} = \frac{1}{2} + \sum_i \left[ \left( \frac{H - E_0}{\alpha T} \right)_{T_{n.s.}}^i \cdot \frac{T_{s, n.s.}}{T_b} - \left( \frac{H - E_0}{\alpha T} \right)_{T_b}^i \right] - \frac{1}{2} \frac{T_{s, n.s.}}{T_b} + \left( \frac{1}{12} + \sum_i \gamma' \times \frac{T_{s, n.s.}}{T_b} \right) \left( \frac{H - E_0}{\alpha T} \right)_{T_b}^i
\]

These pressures are the highest that would occur in the detonation wave should complete relaxation prevail in the internal modes of motion of the unreacted gases. Completely inactive vibrational motion in the molecules of the combustible gas mixtures would lead to pressures and temperatures in the wave calculated for a normal shock at \(M_D\) with

\[
\left( \frac{H - E_0}{\alpha T} \right)_{T_b}^i \left( \frac{1 + k_0 M D_0^2}{2} - \frac{T_{s, n.s.}}{T_b} \cdot k_0 M D_0^2 \right)^{1/2}
\]

The difference between the latter values and those obtained from Equations [10 and 11] is usually quite small.

It is frequently necessary to calculate the parameters behind a steady-state detonation wave for the case where the reaction has proceeded to an arbitrarily assumed chemical composition. For such calculations a method is proposed which is based on an evaluation of the derivative \(\frac{d(p_s/p_b)}{d(T_b/T_a)}\) which, according to the Chapman-Jouguet condition

\[
d \left( \frac{\gamma_p^2}{\alpha T_b/3M_b} \right) = \langle 1 - \frac{T_s}{T_a} \rangle \cdot \frac{d(p_s/p_b)}{d(T_b/T_a)} - \frac{T_s}{T_b} \left( \frac{p_s}{p_b} - 1 \right) \frac{\Delta p_s}{\Delta T_b} \left( \frac{p_s}{p_b} - 1 \right)
\]

becomes

\[
d \left( \frac{p_s}{p_b} \right) = - \frac{T_s}{T_b} \left( \frac{p_s}{p_b} - 1 \right)
\]

Upon differentiation of the Hugoniot equation

\[
\frac{p_s}{p_b} = \frac{T_s/T_b}{\gamma_{p_b}/\gamma_{p_s}} \left[ \sum_i \frac{T_s}{T_b} \left( \frac{\Delta H_f}{\alpha T} \right)_{T_b}^i \right] - \left[ \sum_i \gamma' \left( \frac{\Delta H_f}{\alpha T} \right)_{T_b}^i \right] - \frac{T_s}{T_b} \left( \frac{p_s}{p_b} - 1 \right) \frac{\Delta p_s}{\Delta T_b} \left( \frac{p_s}{p_b} - 1 \right)
\]

this derivative becomes

\[
\frac{d(p_s/p_b)}{d(T_s/T_b)} = \frac{\sum_i \gamma' \left( (\gamma_s/\gamma_b) T_s - 1/2 \right)}{\gamma_{p_b}/\gamma_{p_s}} + \left[ \sum_i \frac{\gamma' \left( \frac{\Delta H_f}{\alpha T} \right)_{T_b}^i + 1/2}{\gamma_{p_b}/\gamma_{p_s}} \right] \left[ \sum_i \frac{\gamma' \left( \frac{\Delta H_f}{\alpha T} \right)_{T_b}^i - 1/2}{\gamma_{p_b}/\gamma_{p_s}} \right] + \frac{1}{\gamma_{p_b}/\gamma_{p_s}} \left( \frac{T_s}{T_b} \right) \left( \frac{p_s}{p_b} - 1 \right) \left( \frac{(\gamma_s/\gamma_b) T_s - 1/2}{\gamma_{p_b}/\gamma_{p_s}} \right)
\]

The detonation parameters are obtained by solving Equations [13, 14 and 15] simultaneously.

An approximate but explicit solution of the detonation problem is possible when an average value for the specific heat ratio \(k\) is introduced. According to this method, the detonation wave is considered to consist of a shock wave followed by a region in which heat is added to the gas until the Mach number becomes 1. This solution is useful primarily because it yields a quick answer, and it affords a good starting point for the exact calculations. When heat \(q\) is added to a unit mass of the subsonic flow behind the normal shock, the final Mach number \(M_3\) will be 1 if, for a given value of \(q\), the proper value of \(M_1\) is selected. The amount of heat \(q\) added to the gas is the heat of reaction of a unit mass of the gas mixture. Allowance must be made for the fact that the reaction does not go to completion in most cases. Since for the normal shock \(M_1^*\) equals 1/\(M_1^*\), and for the flow with heat addition in the present case \(M_1^*\) equals 1 which leads to

\[
[1 - (M_1^*)^2] = q \left( \frac{\alpha T_b}{3M_b} \right) = \frac{k}{k - 1} \left( \frac{1 - (M_1^*)^2}{2} \right)
\]

we obtain

\[
M_3 = \frac{k^2 - 1}{k} \left( \frac{q}{\alpha T_b/3M_b} \right) + 1 + \left[ \frac{k^2 - 1}{k} \left( \frac{q}{\alpha T_b/3M_b} \right)^2 - 1 \right]^1/2
\]

The Mach number of the detonation wave. Results of these calculations are presented in Figs. 1 and 2 for various values of the specific heat ratio \(k\) as a function of the heat release coefficient

\[
C_q = q/\alpha T_b/3M_b
\]
Discussion of Results

The results of the calculations show that the detonation velocities of stoichiometric hydrogen-oxygen mixtures (Fig. 3) increase with initial pressure at the approximate rate of \( \frac{d(u_d)}{dp/p} = 54 \text{ m per sec} \). This coefficient becomes smaller for lean or rich mixtures. The curves of Fig. 3 also show that the detonation velocities of hydrogen-oxygen mixtures increase rather sharply with the concentration of hydrogen in mixtures up to 90 per cent. At higher hydrogen concentrations the advent of a decrease in velocity is indicated by the shape of the curves.

The pressure ratio \( \frac{p_s}{p_i} \) across the detonation wave of near stoichiometric mixtures increases rather significantly when the initial pressure is increased (Fig. 4). For very lean or very rich mixtures the effect is small. The temperature of the gas behind the detonation wave follows a similar pattern (Fig. 5). However, the density ratio \( \frac{\rho_s}{\rho_i} \) across the wave decreases as the initial pressure is increased. For lean or rich mixtures, again, the effect of pressure on this parameter is small.

Variations of the initial temperature have only a small influence on the detonation velocity, the detonation temperature and the density ratio across the wave. However, these variations affect the pressure in the wave very strongly. Whereas an increase of 160 C (50 per cent) in the initial temperature produces a decrease of the detonation velocity by less than 2 per cent, this temperature change decreases the pressure by more than 30 per cent. It is of interest to note that an increase in initial temperature leads to a lower detonation temperature.

The temperatures in the normal shock zone are almost one half the detonation temperatures, whereas the pressures behind the normal shock are almost twice the pressure of the detonation wave and slightly higher than the impact pressures.

The results of these theoretical calculations are being used in an experimental investigation to determine the detonation induction distances of hydrogen-oxygen mixtures under a variety of initial conditions. Velocity measurements and other pertinent data obtained during this experimental study will be presented later.
Acknowledgment

These studies were conducted under Contract NAw-6551 of the National Aeronautics and Space Administration, whose support is greatly appreciated.

Nomenclature

- $a$ = equilibrium sonic velocity in gas mixture
- $c_p$ = specific heat at constant pressure
- $c_v$ = heat release coefficient
- $E_0$ = zero point energy
- $H$ = absolute molar enthalpy
- $(\Delta H_f / \theta T)_i^*$ = dimensionless heat of formation of species $i$ at temperature $T$
- $k$ = ratio of specific heat at constant pressure to that at constant volume
- $K$ = equilibrium constant based on partial pressures
- $M$ = Mach number
- $M_i$ = molecular weight
- $N$ = total mole number of element in mixture
- $P$ = absolute pressure
- $P_i$ = partial pressure of species $i$
- $q$ = heat added per unit mass of gas
- $R$ = universal gas constant
- $s$ = entropy per unit mass
- $T$ = absolute temperature
- $u$ = linear velocity
- $v$ = specific volume
- $\gamma_i$ = mole fraction of reactants
- $\gamma_i^*$ = mole fraction of products
- $\rho$ = density

Subscripts

- $a$ = conditions in gas leaving detonation or shock wave
- $b$ = conditions in gas entering detonation or shock wave
- $D$ = stable detonation wave
- $i$ = $i$th species of mixture
- $imp$ = impact
- $min$ = minimum
- $N.S.$ = normal shock wave
- $1$ = initial state of gas
- $2$ = state of gas behind normal shock when initial Mach number is $M_1$
- $3$ = state of gas behind steady-state detonation wave
- $*$ = critical flow condition

References