Title: Theory of Detonation Velocity in Gas (II): Effect of Inert Gases

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Abstracts of Papers

The following eighteen papers are the first part out of eighty papers, read before the semi-annual meeting of the Institute on June 6 and 7, 1952.

1. Theory of Detonation Velocity in Gas. (II)

Effect of Inert Gases

Rempei Goto and Nishio Hirai

(Goto Laboratory)

We reported previously that the propagation velocity of detonation in gas or solid explosives could be given by the velocity of transference of energy released from the flame front and reserved in the reactant systems as their kinetic energy. (This Bulletin, 23, 28 (1950).) In the stoichiometric mixture of hydrogen and oxygen (H₂ + ½O₂), the detonation velocity V₀ was given by the relation

\[ \frac{1}{2}MV₀^2 = JQ \frac{f_{H₂O}}{F_{H₂O}} \]  

(1)

where \( M \) is the total mass of reactant system, \( J \) the mechanical equivalent of heat, \( f_{H₂O} \) is the translational degrees of freedom of water molecule, and \( F_{H₂O} \) the total degrees of freedom of water molecule. It was assumed that for the energy distributed to the reactant molecules (H₂O) the equipartition law holds, but for the excess or inert gas molecules the energy of combustion may be distributed mainly to their translational degrees of freedom. Thus, for the reaction system

\[ H₂ + \frac{1}{2}O₂ + xX \rightarrow H₂O + xX + Q, \]

where \( x \) is the number of moles of inert or excess gas (X) and \( Q \) the heat of combustion, the detonation velocity \( V \) was given by the relation

\[ V = V₀ \left\{ \frac{1 + x}{(1 + 0.25x) \left( 1 + x \frac{Mx}{M_{H₂O}} \right)} \right\}^{\frac{1}{2}} \]  

(2)

where \( Mx \) and \( M_{H₂O} \) are the molecular weight of the inert gas and water molecules respectively, and \( V₀ \) the detonation velocity in the stoichiometric mixture. Calculated values of detonation velocity given by Eq. (2) showed fairly good agreement with the observed values as shown in the next table.

Table 1. Effect of inert gases on the detonation velocity in (H₂ + ½O₂) mixture.

<table>
<thead>
<tr>
<th>X</th>
<th>x mole</th>
<th>( V/V_{obs} )</th>
<th>Vcalc. m/sec.</th>
<th>Vobs. m/sec.</th>
<th>Vcalc./Vobs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>0.5</td>
<td>0.8491</td>
<td>23.68</td>
<td>23.14</td>
<td>1.02</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>0.7042</td>
<td>19.85</td>
<td>19.22</td>
<td>1.03</td>
</tr>
<tr>
<td></td>
<td>2.5</td>
<td>0.6239</td>
<td>17.72</td>
<td>17.00</td>
<td>1.04</td>
</tr>
</tbody>
</table>
2. Theory of Limit of Inflammability. (II)

Lower Limit

Rempei Goto and Nishio Hirai
(Goto Laboratory)

According to the theory proposed by Goto (Rev. Phys. Chem. Japan, 21, 152 (1942)), the correlation between lower limit of inflammability \(c_1\) and molar heat of combustion \(Q\) can be expressed by the equation

\[
\frac{1}{c_1} = \frac{k}{E} Q + k, \tag{1}
\]

where \(k\) is a constant and \(E\) the heat of activation. The linear relation found between \(\frac{1}{c_1}\) and \(Q\) suggests that the activation energy of combustion \(E\) is almost constant for most of combustible gases and vapors. By the method of least squares, we have \(k/E = 0.090, k = 1.56\) and accordingly \(E = 17\) (Kcal). Assuming that the heat of combustion are distributed equally among all degrees of freedom of excess molecules in a unit volume per one molecule of combustible and that the flame propagation can occur when the energy distributed to every one of oxygen molecule exceeds the activation energy \(E\), the condition for inflammation was given by the relation

\[
c_i(Q + E) + \frac{1}{2}fRT = E \tag{2}
\]