COMBUSTION OF RANDOM GAS-SOLID SUSPENSION.

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Work motivation
- explanation of unusual experimental fact.

Presentation is based on publications


Combustion of PMMA gas suspension (experiment).

Kobayashi H., Ono. N., Okuyama Y., and Niioka T.  
*Flame propagation experiment of PMMA particle cloud in a microgravity enviroment.*  
Experimental facts.

Shift of the maximal speed of combustion wave in the area of fuel rich mixtures.

Maximum of the combustion wave speed is shifted by 50-70% of concentration (% related to the stoichiometric concentration)

The maximum speed exceeds the speed of the combustion front at the stoichiometry by 30-50%.
Thermodynamic calculation (combustion of PMMA)

\[ \text{C}_5\text{H}_8\text{O}_2 + 6 \text{O}_2 \rightarrow 5\text{CO}_2 + 4\text{H}_2\text{O} \]

Adiabatic temperature
- Value at stoichiometry: 3045 K
- Maximal value: 3050 K

This temperature difference can change the flame front speed not more than 1%

This temperature difference can displace the concentration of maximal combustion wave speed on 2.5% in fuel rich area.
Hypothesis

The reason for the observed displacement is a random distribution of fuel particles in space.
The volume of the cell is equal to the initial volume of such a gas mixture, wherein the oxidant is sufficient for a complete combustion of the fuel particles.

"Stoichiometric" cell

\[ L_{st} \]

- \( d \approx 5 \ \mu m \)
- \( V/V_p \approx 7500 \)
- \( L_s \approx 120 \ \mu m \) (at 300 K)
- \( L_s \approx 170 \ \mu m \) (at 1000 K)
- \( U_c \approx 1 \ m/s \)
- \( \tau_c \approx 1,2 \cdot 10^{-4} \ s \)
- \( D_c \approx 1,7 \cdot 10^{-4} \ m^2/s \)
- \( L_D \approx 140 \ \mu m \)

\( L_D < L_s \)
Description of spatial structure of gas suspension.
Description of spatial structure of gas suspension.

\[ n \] is number of particles; \( N \) is number of stoichiometric cells
Application of Bose-Einstein statistics.
Main assumptions of the model

1. All the fuel particles are randomly distributed in space

2. All the fuel particles have the same size (monodisperse cloud)

3. Oxidant gas in the cell is completely consumed by the exothermic reaction (combustion), but only with the fuel particles are located in a given cell (adjacent cells do not "interact")

4. In combustion oxidant is distributed evenly among all fuel particles located in the cell.

If in the cell is \( n \) the fuel particles then the degree of conversion for each particle is \( \eta = \frac{1}{i} \).
Mathematical model.


\[ U^2 \approx \frac{2(1+b)\nu F \lambda_u B \varepsilon^2}{\rho_u C} \exp \left[ -\frac{E}{RT_f} \right] \]

\[ \varepsilon = \frac{1}{Z_e} = \frac{RT_f^2}{E(T_f - T_0)} \approx \frac{RT_f}{E} \]

Zel’dovich number

\[ V(\varphi) = \frac{U(\varphi)}{U(1)} \approx \frac{T_f(\varphi)}{T_f(1)} \exp \left[ \frac{E}{2RT_f(1)} \left( 1 - \frac{T_f(1)}{T_f(\varphi)} \right) \right] \]
**Statistical model**

\[ \phi = \frac{n}{N} \]  

is the equivalence ratio;  

\[ N = \frac{V}{V_0} \]

\[ \langle \eta(\phi) \rangle \]  
is a mean degree of fuel conversion - ???

\[ T_f(\phi) \approx T_* \phi \langle \eta(\phi) \rangle \]  
is the temperature of combustion front

\[
V(\phi) = \frac{U(\phi)}{U(1)} \approx \frac{T_f(\phi)}{T_f(1)} \exp\left[ \frac{E}{2RT_f(1)} \left( 1 - \frac{T_f(1)}{T_f(\phi)} \right) \right]
\]

\[
V(\phi) \approx \frac{\phi \langle \eta(\phi) \rangle}{\langle \eta(1) \rangle} \exp\left[ \frac{E}{2RT_f} \left( 1 - \frac{\langle \eta(1) \rangle}{\phi \langle \eta(\phi) \rangle} \right) \right]
\]

\[ \eta = \frac{1}{i} \]
The number theory
(the theory of partitions)

The Bose-Einstein distribution
in the occupation number representation

The graph theory
(Ferrers graphs)
In statistical physics traditionally is used the Bose-Einstein distribution for the \textit{grand canonical ensemble}.

\[
\langle n_k \rangle = \frac{1}{\exp\left(\frac{\epsilon_k - \mu}{T}\right) - 1}
\]

To solve this problem it is necessary the Bose-Einstein distribution for \textit{the microcanonical ensemble in the occupation number representation}.

There is no such distribution in the literature...
The occupation number representation

State $\lambda$

$P(\lambda) = \frac{\Omega(\lambda, n, N)}{\Omega}$

$\Omega = \frac{(n + N - 1)!}{n!(N - 1)!}$

$\{ \lambda_1, \lambda_2, \ldots, \lambda_i, \ldots, \lambda_N \}$

$\sum_{i=1}^{N} \lambda_i = n$

$\eta(\lambda) = \sum_{\lambda_i > 0}^{N} \frac{1}{\lambda_i} \lambda_i = \sum_{\lambda_i > 0}^{N} 1$

$\langle \eta(n, N) \rangle = \sum_{\lambda} P(\lambda) \eta(\lambda)$
The additive number theory

\[ \lambda(n) = (1^{f_1} 2^{f_2} 3^{f_3} \ldots) \]

\[ \sum_{i \geq 1} f_i \cdot i = n \]

16 = 5 + 3 + 3 + 2 + 1 + 1 + 1

(1^3 2^1 3^2 4^0 5^1)

\[ f_1 = 3, \ f_2 = 1, \ f_3 = 2, \ f_4 = 0, \ f_5 = 1 \]

5 = 1 + 1 + 1 + 1 + 1

= 2 + 1 + 1 + 1

= 2 + 2 + 1

= 3 + 1 + 1

= 3 + 2

= 4 + 1

= 5.
The B.-E. distribution for the microcanonical ensemble

\[ 16 = 5 + 3 + 3 + 2 + 1 + 1 + 1 \]

\[ \lambda(n, m) = (1^{f_1}2^{f_2}3^{f_3}...\lambda_t^{f_t}) \]

\[ P(\lambda) = \frac{N!n!(N - 1)!}{(n + N - 1)!(N - m)!f_1!f_2!...f_t!} \]
Number of partitions

\[ p(5) = 7 \]

\[ p(10) = 42 \]

\[ p(50) = 204\,226 \]

\[ p(100) = 190\,569\,292 \]

\[ p(200) = 3\,972\,999\,029\,388 \approx 4 \cdot 10^{12} \]
The Boltzmann distribution

\[ \langle n \rangle \ll 1 \]

\[ \frac{\sigma}{\sqrt{\langle n \rangle}} \approx \frac{1}{\sqrt{\langle n \rangle}} \]

Normalization is performed with machine precision

\[ \sum_{\{\lambda\}} P(\lambda) = 1,0000... \]
Calculation of fuel conversion degree

\[ \phi = \frac{n}{N} \]
Comparison with experiment.
Combustion of aluminum in air.

\[ T_f = 3300 \text{ K}, \quad E = 134 \text{ kJ/mol} \]
Comparison with experiment.
Combustion of aluminum in oxygen-rich air.

\[ C_{O_2} = 28.5\% \]

\[ T_f = 2000\ K \]

\[ E = 134\ kJ/mol \]

\[ d_p = 5.7\ \mu m \]

Ageev N.D., Goroshin S.V., Solotko A. N. et al.
Comparison with experiment. Combustion of iron in air.

Sun J., Dobashi R., Hirano T.

\[ d_p = 3.0 \mu m \]

\[ T_f = 1500 \text{ K} \]

\[ E = 162 \text{ kJ/mol} \]
Limits of applicability of the model

\[ L_D < L_{st} \]

\[ L_{st} = \left( \frac{\psi \rho_p RT_{st}}{6 \rho C'_{ox} M_f} \right)^{\frac{1}{3}} d_p = \gamma_{st} d_p. \]

\[ L_D \sim \sqrt{D_c \tau_c} = \sqrt{D_c \frac{L_s}{U_c}} \]

\[ d_p > \frac{D_c}{\gamma_{st} U_c} \]
## Limits of applicability of the model

<table>
<thead>
<tr>
<th></th>
<th>Experiment</th>
<th>Estimation of $d_{cr}$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PMMA</strong></td>
<td>$d \approx 5$-$7$ μm</td>
<td>8 μm</td>
</tr>
<tr>
<td><strong>Al</strong></td>
<td>$d \approx 5$-$6$ μm</td>
<td>19 μm</td>
</tr>
<tr>
<td><strong>Fe</strong></td>
<td>$d \approx 3$ μm</td>
<td>24 μm</td>
</tr>
</tbody>
</table>

$$D = \frac{k_BT}{6\pi r \bar{\eta}}$$

$$D = \frac{k_BT}{6\pi r \bar{\eta}} \left( 1 + \frac{\partial T}{\partial x} \frac{c}{T} \right)$$

\[ d_p = 250 \text{ nm} \]
Conclusions

The statistical model was developed for the combustion gas suspensions of solid particles. The model takes into account the influence of stochastic spatial distribution of particles on the speed of the combustion front. A qualitative and satisfactory quantitative agreement was obtained between the theoretical predictions and known experimental data.

Thanks for your attention!