Ignition of \textit{n}-Hexane–Air by Moving Hot Particles: Effect of Particle Diameter

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Hot Particle Ignition Sources

- Lightning attaches to the top of the fastener and causes damage to the resin and fibers on the backface of the composite laminate
- The breakup of the composite is due to its poor electrical conductivity that leads to resistive heating


Ignition at edge of carbon fiber composite structure, Boeing
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Ignition at edge of carbon fiber composite structure, Boeing
Stationary Hot Particle Ignition


- D. Roth et al. Combustion Science and Technology, 186 (2014) 1606–1617

M. Beyer and D. Markus (2012)

Roth et al. (2014)
Moving Hot Particle Ignition

- S. Patterson. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 28 (1939) 1-22
- S. Patterson. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 30 (1940) 437-457

R. Silver (1937)

S. Patterson (1940)
### Current study

<table>
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<tr>
<th>Material</th>
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$\Phi = 0.9$
Materials and Methods

Experimental Setup

Experimental Setup: Combustion Vessel

- Combustion vessel
- Reactive mixture
- N2 line
- Pneumatic actuator
- Sphere
- Optical shutter
- Window
- Supports
- 0.1 L
- 22 L

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Optical Diagnostics: Shearing Interferometer

P: polarizer, L: lens, WP: Wollaston prism, A: Analyzer
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Finite fringe configurations
Materials and Methods
Simulation Setup

- **Grid**
  - 2D axisymmetric
  - Square of size $20d$
  - 300,000 cells
  - Sphere vicinity (40 µm cell size)

- **Boundary conditions**
  - $T_{sphere} =$ constant
  - $T_{wall} =$ 300 K
  - Inert surface
  - Neumann boundary condition for species

- **Initial conditions**
  - $P_0 =$ 100 kPa, $T_0 =$ 300 K and $\Phi =$ 0.9
  - Flow $N_2$ at $t =$ 0 – 250 ms and $u =$ $(0, gt, 0)$
  - One-step $n$-hexane$^1$–air ($R \rightarrow P$) at $t > 250$ ms

- **OpenFOAM**: Variable-density reactive Navier-Stokes equations
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N\textsubscript{2} Hot Particle Wake (Simulation)
Results

Simulation Results

N$_2$ Hot Particle Wake (Simulation)

front stagnation point

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\textbf{N}_2 \text{ Hot Particle Wake (Simulation)}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{image.png}
\caption{Simulation Results}
\end{figure}

- Front stagnation point
- Rear stagnation point
- Toroidal vortex

$\delta_T$
N$_2$ Hot Particle Wake (Simulation)

Ignition of $n$-Hexane-Air by Moving Hot Particles
$\text{N}_2$ Hot Particle Wake (Simulation)
**N₂ Hot Particle Wake (Simulation)**

The diagram illustrates the temperature (T in K) and velocity (U in m/s) fields around a moving hot particle. The color bar on the left shows a temperature range from 300 to 960 K, while the right side shows a velocity range from 0 to 2.635 m/s. A toroidal vortex is highlighted within the flow field, indicating a region of vortical motion.

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Unreacted Hot Particle Wake: $\approx 900$ K (Exp. and Sim.)

$d = 6.0$ mm

$d = 3.5$ mm

$d = 1.8$ mm
Unreacted Hot Particle Wake (Experiment)

Time averaged unwrapped optical phase
Unreacted Hot Particle Wake (Experiment)

Time averaged unwrapped optical phase

\[
\Delta \phi
\]

\[
F(x) = 2\pi \int_0^{\infty} f(r) r (r^2 - x^2)^{1/2} dr.
\]

The inverse Abel transform is given by

\[
f(r) = -\frac{1}{\pi} \int r dF dx (x^2 - r^2)^{1/2},
\]

\[
f(r) = 2\pi \lambda [n(r) - n_o(r)]
\]

and

\[
F(x) = \Delta \phi
\]
Unreacted Hot Particle Wake (Experiment)

Time averaged unwrapped optical phase

Abel transform

\[
F(x) = 2 \int_{x}^{\infty} \frac{f(r)r}{(r^2 - x^2)^{1/2}} \, dr.
\]

(1)
Unreacted Hot Particle Wake (Experiment)

Time averaged unwrapped optical phase

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\[ f(r) = -\frac{1}{\pi} \int_{r}^{\infty} \frac{dF}{dx} \frac{dx}{(x^2 - r^2)^{1/2}}, \]

(2)
Unreacted Hot Particle Wake (Experiment)

Time averaged unwrapped optical phase

Abel transform

\[
F(x) = 2 \int_{x}^{\infty} \frac{f(r)r}{(r^2 - x^2)^{1/2}} \, dr. \tag{1}
\]

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\[
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\]

\[
f(r) = \frac{2\pi}{\lambda} [n(r) - n_o(r)] \quad \text{and} \quad F(x) = \Delta \varphi \tag{3}
\]
Gladstone-Dale relation \( n - 1 = K \rho \)
Gladstone-Dale relation

\[ n - 1 = K\rho \]

\[ P = \rho RT \]
Unreacted Hot Particle Wake: Validation

![Graph showing comparison between simulation and experiment results for temperature distribution in a hexane-air system, with temperature in Kelvin (K) and coordinates in millimeters (mm)].
Unreacted Hot Particle Wake: Validation

Simulation vs. Experiment

- Temperature (K)
- y (mm)
- x (mm)

Results
Experimental and Simulation Results

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Ignition (Experiment)

1.8 mm
Ignition (Simulation)

- $t = 1.25$ ms
- $t = 5.00$ ms
- $t = 15.0$ ms
- $t = 15.5$ ms
- $t = 16.25$ ms
Ignition (Simulation)

$t = 1.25\ ms$

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Arrival of reactive mixture (R)
Ignition (Simulation)

$t = 1.25 \text{ ms}$

Arrival of reactive mixture (R)

$t = 5.00 \text{ ms}$

Contact of reactive mixture (R) with hot sphere

$t = 15.0 \text{ ms}$

$t = 15.5 \text{ ms}$

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Creation of products (P)

Flame propagation

Flame propagation
Ignition (Simulation)

$t = 1.25 \text{ ms}$

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Results

Simulation Results

Ignition (Simulation)

- $t = 1.25\,\text{ms}$: Arrival of reactive mixture ($R$)
- $t = 5.00\,\text{ms}$: Contact of reactive mixture ($R$) with hot sphere
- $t = 15.0\,\text{ms}$: Creation of products ($P$)
- $t = 15.5\,\text{ms}$: Flame propagation
- $t = 16.25\,\text{ms}$: Flame propagation
Flame Propagation (Experiment)

Recall: $\Phi = 0.9$  
Current flame: $S_b = 2.6$ m/s  
Particle speed: $V_p = 2.3 - 2.4$ m/s

$d = 6.0$ mm

$d = 3.5$ mm

$d = 1.8$ mm

1.5 ms  3.5 ms  5.5 ms  7.5 ms  9.5 ms  11.5 ms
Ignition Thresholds (Exp. and Sim.)

![Graph showing ignition thresholds for different diameters and temperatures.]

- **Diameter (mm):** 600, 800, 1000, 1200, 1400, 1600
- **Temperature (K):** Data points with different symbols for ignition, no ignition, and simulation.

- **Symbol Key:**
  - Green circle: Ignition
  - White circle: No ignition
  - Red triangle: Simulation

- **Parameters:**
  - $\Phi = 0.9$

- **Temperature Changes:**
  - $\Delta T \approx 400$ K
  - $\Delta T \approx 100$ K
Ignition Thresholds (Exp. and Sim.)

![Graph showing ignition thresholds for different diameters and temperatures.]

- **Ignition Thresholds (Exp. and Sim.)**
- **Diameter (mm):** 600, 800, 1000, 1200, 1400, 1600
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  - $\Phi = 0.9$
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Ignition Thresholds (Exp. and Sim.)

\[ \Delta T \approx 400 \, \text{K} \]

\[ \Delta T \sim 100 \, \text{K} \]

\( \Phi = 0.9 \)

- **Ignition**
- **No ignition**
- **Simulation**
Conclusions

- Simulation predicts ignition to occur in the flow separation region

- The ignition threshold was found to be $981 \pm 10$ K, $1010 \pm 25$ K, and $1159 \pm 10$ K, for sphere diameters of 6.0 mm, 3.5 mm and 1.8 mm, respectively at $V_p = 2.3 - 2.4$ m/s for alumina spheres

- Simulations using a one-step model predicted an ignition temperature 400 K higher than the experimental thresholds
  - Similar trends predicted
  - Use of one-step model not sufficient to capture ignition behavior
  - Have not accounted for surface reactions
  - Have not accounted for species diffusion to the surface
  - Further understanding of the low-temperature oxidation of $n$-hexane needed

- Flame is affected by the presence of the sphere for the mixture composition tested
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Thank You