Numerical simulations of Hot-surface Ignition in Flammable Mixtures

Shyam Menon, Guillaume Blanquart
Department of Mechanical Engineering,
California Institute of Technology

Philipp Boettcher, Brian Ventura and Joseph Shepherd
Graduate Aerospace Laboratories,
California Institute of Technology

Research supported by: Boeing Company
Motivation

- **Hot-surface ignition is relevant to safety issues in:**
  - Airplanes
  - Automobiles
  - Chemical reactors
  - Underground mines
- **Aviation safety**
  - Spark ignition
    - Well characterized
    - Minimum ignition energy
  - Hot-surface ignition
    - Not as well characterized
  - Stationary hot-surface
    - Fuel tank lining/ fuel pipelines
    - Hot wires, Malfunctioning equipment, etc.
  - Moving hot-particle
    - Debris from lightning strike/ rotating machinery
- **Variables**
  - **Pressure, equivalence ratio, hot-surface temperature**
  - Hot-surface area, geometry
Hot surface ignition experiments

- **Closed 2 liter vessel**
  - Hot-surface → glow plug
    - Fixed size, zero velocity
  - Fuel → **Hexane**
  - 1 atm pressure, 294K
    - $\Phi$ between 0.6—3.0
  - 0.25, 0.40, 0.65 atm pressure, 294K
    - $\Phi = 2.15$ and $\Phi = 2.45$

- **Diagnostics**
  - Thermocouples, schlieren imaging, pressure transducer

---

Hot surface ignition experiments

- Glow plug temperature ramped at 220 K/s
- In almost all cases:
  - Ignition occurs after the formation of a thermal plume of hot gas
  - Ignition occurs right above the glow plug

\[ \Phi = 1.2, \ P = 1 \text{atm} \]

Glow plug temperature trace

\[
\begin{align*}
\text{Time [sec]} & \\
0 & 1 \quad 2 \quad 3 \quad 4 \quad 5 \\
\text{Temperature [K]} & \\
400 & 600 \quad 800 \quad 1000 \quad 1200 \quad 1400
\end{align*}
\]

Ignition at \( t \approx 2.1 \text{s} \)

Schlieren image
Numerical simulations: Governing equations

- Low-Mach number Navier-Stokes equations
  \[
  \partial_t \rho + \nabla \cdot (\rho u) = 0 \quad \partial_t (\rho u) + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot \tau + \rho g
  \]

- Chemistry modeling
  - Detailed chemistry calculations
    - Species
      \[
      \partial_t (\rho Y_i) + \nabla \cdot (\rho u Y_i) = \nabla \cdot (\rho D \nabla Y_i) + \dot{\omega}_i
      \]
    - Energy
      \[
      \partial_t (\rho C_p T) + \nabla \cdot (\rho u C_p T) = \partial_t p + \nabla \cdot (\lambda \nabla T) - \sum_i \rho C_{p,i} j_i \cdot \nabla T - \sum_i \rho h_i \dot{\omega}_i
      \]
  - Tabulated chemistry (Progress variable approach)
    - Progress variable
      \[
      \partial_t (\rho C) + \nabla \cdot (\rho u C) = \nabla \cdot (\rho D \nabla C) + \dot{\omega}_C
      \]
    - Unburned gas temperature/Enthalpy\(^1\)
      \[
      C_{p,u} \left[ \partial_t (\rho T_u) + \nabla \cdot (\rho u T_u) \right] = \nabla \left[ \lambda \nabla T_u \right]
      \]

\(^1\)S. Menon, P. Boettcher and G. Blanquart, Combust. Flame, in press
Reaction mechanism

- **Full reaction mechanism**
  - 193 species/1804 reactions
  - Reaction mechanism for engine relevant fuels\(^1\)
  - Validated for small HC fuels to aromatics\(^2\)

- **Reduced mechanism**
  - 56 species/442 reactions
  - Matches full mechanism closely at different conditions

\(\Phi=0.5, P=1, 13, 42 \text{ bar}\)
\(\Phi=1, P=1, 3, 13, 42 \text{ bar}\)
\(\Phi=2, P=1, 13, 42 \text{ bar}\)

**Tabulated chemistry**

**Detailed chemistry**

---

No experimental data for ignition delay at \(P = 1 \text{ atm}, \ \text{Temperature } \rightarrow 800 – 1500 \text{ K}\)

\(^1\)G.Blanquart, H.Pitsch et al, Combustion and Flame, 2009

\(^2\)K.Narayanaswamy, G.Blanquart, H.Pitsch, Combustion and Flame, 2010
Tabulated chemistry

- Detailed chemistry calculations for a representative model problem
  - Homogeneous, constant pressure reactor
  - Solution for constant $\Phi$, pressure, initial gas temperature
  - Set of solutions for different initial gas temperatures ($Tu$)

- Progress variable ($C$)
  - State of “reaction” of the mixture: sum of mass fractions of major product species
    - CO, CO2, H2, H2O

- Tabulate all properties as a function of $C$ and $Tu$
  - Density, Viscosity, Temperature, Species mass fractions, Source terms etc.

- Look up properties for the mixture as needed from the table
Test Case I : 0D reactor

- **Homogeneous isobaric reactor**
  - Initial temperature, pressure, equivalence ratio
  - Compute ignition delay in NGA\(^1\) using Tabulated & Detailed chemistry

**Graph**

N-C7H16, Φ=1.0, P = 1atm

Tabulated approach and detailed chemistry calculations are consistent

\(^1\) O.Desjardins, G.Blanquart, G.Balarac, H.Pitsch, J.Comp.Phys., 2008
Test Case II: 1D hot-surface ignition

- One-D hot surface ignition of fuel-air mixture
  - Wall temperature, initial gas temperature, pressure, equivalence ratio
  - Compute ignition delay in NGA → using Tabulated & Detailed chemistry

N-C7H16, Φ=1.0, P = 1atm, Ts=1000K, Tu=800K

- Heptane-air mixture
- Heat and species production and diffusion
- Heat conduction
- Hot surface (T_s)

Ignition delay
One-D hot surface ignition of *fuel*-air mixtures

- Fixed $\Phi$, wall temperature; varying initial gas temperature
- Calculations repeated excluding the low-temperature reaction pathways

For $Tu < 800K$ tabulated & detailed chemistry calculations are not consistent

Single definition of progress variable is unable to account for low-$T$ reaction pathways
One-D hot surface ignition of *fuel*-air mixtures

- Fixed $\Phi$, wall temperature; varying initial gas temperature

For C2H4 and H2, ignition process is well captured with current definition of progress variable.
Issues with tabulation

• **Single definition of progress variable (CO, CO2, H2 & H2O)**
  – Unable to capture low-T reaction pathways

• **Tabulation created using solutions to constant pressure homogeneous reactor**
  – Does not account for diffusion processes

• **Intelligent approach to defining progress variable**
  – Construct progress variable by assigning weights to all species in the reaction mechanism.
  – Compute weights using linear programming approach
• **Grid**
  – Axisymmetric
  – Locally refined around glow plug
  – 256 x 128 mesh points
  – Stretching factor : 1.3

• **Boundary conditions**
  – Gow plug temperature ramped at 220K/s
  – Fully transient simulation
  – Wall temperature: 294K
  – All surfaces are inert
  – Neumann boundary conditions for species.

• **Initial conditions**
  – Uniform $\Phi$, pressure, initial temperature
2D glow plug simulations

N-C7H16, P = 1 atm, Tu = 294K, phi=1.5
OD ignition of n-heptane

N-C7H16, P = 1 atm, Tu = 740K, phi=1.0, 0D reactor
2D glow plug simulations

N-C7H16, P = 1 atm, Tu = 294K, phi=1.0
2D glow plug simulations

N-C7H16, P = 1 atm, Tu = 294K
Effect of equivalence ratio

N-C7H16, P = 1 atm, Tu = 294K

Minimum glow plug temperature to cause ignition almost independent of $\Phi$
No ignition seen for $\Phi < 0.40$ (simulations), $\Phi < 0.55$ (experiments)
Effect of pressure

N-C7H16, Tu = 294K

Simulations show similar trend but values differ

Minimum hot-surface temperature for ignition [K]

Pressure [kPa]

- Experiment, Phi=2.15
- Calculations, Phi=2.15
- Experiment, Phi=2.5
- Calculations, Phi=2.5
What's missing?

- Species fluxes due to temperature gradient – Soret effect
- Enthalpy flux due to species gradient – Dufour effect
- Radiation ??
  - Compare convective flux estimated using Nu for natural convection on a cylinder with radiative heat flux
  - Estimate gas absorption coefficient - alpha (1/m)
  - Alpha*path length << 1 → Optically thin medium

![Graph showing convective and radiant fluxes vs. surface temperature](image-url)
Summary

• Hot-surface ignition simulation
  – Investigated using
    • tabulated chemistry
    • detailed chemistry
  – Currently tabulated chemistry unable to capture low-temperature reaction kinetics
  – 2D simulations to determine ignition temperature
    • Trends similar for variation in
      – Equivalence ratio
      – Pressure
    • Temperatures off by ≈200-300K

• Future Work
  – Use of second/modified progress variable to capture low-T kinetics
  – Energy balance analysis – correlate heat production and loss with ignition location

Acknowledgements:
• Funding for this research has been provided by the Boeing Company through a Strategic Research and Development Relationship Agreement CT-BA-GTA-1.