Modeling Constant Volume Chamber Combustion at Diesel Engine Condition

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Objective

- Fundamental study on AUTOIGNITION due to FUEL and CONDITION.
- Study THEIR effects on MIXING AND COMBUSTION.

• TOOL: Experimental (Constant Volume Vessel) Numerical (Computational Fluid Dynamics)
n-heptane (CN~54) and iso-octane (CN~15) are used to study fuel effects

<table>
<thead>
<tr>
<th>Technical details</th>
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<tbody>
<tr>
<td>Chamber volume</td>
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<tr>
<td>Inner diameter</td>
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<tr>
<td>Inner length</td>
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<td>Injector details</td>
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<tr>
<td>Chamber temperature</td>
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<tr>
<td>Chamber pressure</td>
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<td>Injection pressure (P_i)</td>
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</table>
Fuel volume controlled by injector pressure $P_i$ and injection period.

Reference test done at $P_i=1600\text{bar}$, injection period $=1.9\text{ms}$.

Idealized profile for modeling showing on the right, when injecting n-heptane and iso-octane at $P_i=900\text{bar}$, injection period $=1.3\text{ms}$.

Solid: n-heptane; dash: iso-octane
n-heptane injection and autoignition (pressure rise v.s. time)

T=863K

P=50bar
iso-octane injection and autoignition
(pressure rise v.s. time)

T=863K
P=50bar
Mathematical Model

- Chemical Kinetics: 137 species and 633 reactions for n-heptane/iso-octane/toluene
  

- Combustion Modeling: Flamelet Generated Manifolds (FGM)
  
  * Reduced Chemistry Method; Instead of solving hundreds of species equations, only limited PDE are solved for reacting flows.
Flamelet Generated Manifolds (FGM):  

Flamelet Generated Manifolds (FGM) Concept: process described by only 2 variables: \( Z, Y \)

- Mixture fraction:
  \[
  Z = \frac{2Z_{C_1-Z_{C_2}}}{M_C} + \frac{1}{2} \frac{Z_{H_1-Z_{H_2}}}{M_H} - \frac{Z_{O_1-Z_{O_2}}}{M_O}
  \]
  *1,2 denotes fuel and oxidizer stream in reacting flows

- Reaction progress variable:
  \[
  Y = \frac{Y_{CO_2}}{M_{CO_2}} + \frac{Y_{CO}}{M_{CO}} + \frac{Y_{CH_2O}}{M_{CH_2O}}
  \]
  *species dominant in the products stream is chosen to represent reaction progress variable
Flamelet Generated Manifolds (FGM):

- Implication:
  \[ \frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_j Z}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_z \frac{\partial Z}{\partial x_j} \right) + \dot{\omega}_z \]
  \[ \frac{\partial \rho Y}{\partial t} + \frac{\partial \rho u_j Y}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_y \frac{\partial Y}{\partial x_j} \right) + \dot{\omega}_y \]

- Conservation Equations:

* + mass conservation, momentum conservation and ideal gas equation

Fuel injection

FGM pre-processing

Also for information such as temperature, species mass, etc.
FGM pre-processing

pre-processing

Flamelet calculation (diffusion)

- tabulation

- FGM

\[ f(Z, Y) \]

- PDF integration

- FGM

\[ f(\tilde{Z}, \tilde{Y}, Z'^2, Y'^2) \]

Manifolds

- Homogeneous reactor;
  Livengood-Wu, decide ignition

- Premixed flamelets

- Diffusion flamelets

Flame Index?

Dominant for diesel combustion
Solver: Star-CD

Spray model: Reitz-Diwakar/Reitz model built in STAR

Turbulence: high-Reynolds $k-\varepsilon$ RANS to account for turbulence from fuel injection, initial air in chamber is quiescent.

Combustion: FGM integrated into Star-CD via user-subroutine.
Mesh: \((r, z, \theta) = (50@1\text{mm}, 62@1\text{mm}, 180@2^\circ)\)

Time step: \(1 \times 10^{-6} \text{s}\) during injection and combustion

Injection: n-heptane / isooctane into quiescent high T, high P air corresponding to experimental cases

Injection profile: PAGE 3
n-heptane injection
(pressure trace history, solid-experiment)

- T=803K; P=30bar
- T=863K; P=30bar

Combustion starts after injection is finished, premixed but not totally premixed.
n-heptane injection: $T=803\text{K}$, $P=30\text{bar}$
(simulation results: temperature at EOI)
n-heptane injection: T=863K, P=30bar
(simulation results: temperature at EOI)
n-heptane injection
(mixture distribution at EOI; stoichiometric-grey zone)

- T=803K; P=30bar
- T=863K; P=30bar
iso-octane injection: $T=863\text{K}, P=50\text{bar}$

(Left: pressure trace, experiment: dots, simulation: line)

Temperature snapshot at the time (red line) indicates possible ignition location.
Conclusions & Future Work

- Experimental work shows the effect of fuels and conditions on autoignition and combustion.

- Modeling work shows capability of capturing features of mixing and combustion due to different conditions and fuels.

- Future work includes further identification on initiation of autoignition, both experimentally (lasers, schlieren photography, etc.) and numerically (Livengood-Wu integral, etc.); chemical kinetics for rich combustion should also be addressed.
Acknowledgements

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- Autoignition is important for diesel engines.
- Fuel autoignition property affects the engine performance.