Numerical Simulation of Combustion Recession on ECN Diesel Spray A

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Introduction
→ Combustion Recession
Conditional Source-term Estimation (CSE)
→ Core Algorithms
Non-reacting Spray - Setup
Results
Reacting Spray Results
Future Plan
Introduction

- Non-premixed combustion is widely used in current diesel engine technologies
  → Automotive engines, marine engines, power generation

- Efficiency and pollution considerations
  → Low-temperature combustion (LTC), exhaust-gas recirculation (EGR), early/late injection
Motivation

- Fuel-ambient mixtures upstream of the flame lift off length (LOL) may become too lean to initiate ignition after end of injection.

- These mixtures can be a major source of unburned hydrocarbon (UHC) for LTC.

- Recent studies indicate end-of-injection (EOI) processes may support ignition recession back to injector nozzle and consumption of UHC.
Combustion Recession (CR)

**CR Schematics [4]**

**Spray A, 1000Bar, fast RD conditions [5]**
Combustion Modelling

- CFD solves transport equations of Navier-Stokes, energy etc
- Symbolic form of Favre average species transport equation:
  \[ \frac{Q_k}{\text{Rate of change}} + \frac{C_k}{\text{Convective}} = \frac{D_k}{\text{Diffusion}} + \frac{\bar{\omega}_k}{\text{Chemical source}} \]
- The focus of combustion modelling is to provide an adequate closure for the **mean chemical source term**, \( \bar{\omega}_k \)
- **Explicit** series expansion of the mean chemical source term is not viable:
  - → highly non-linear behaviour
  - → sensitivity to truncation
  - → additional term closures
Conditional Source-term Estimation (CSE)

For simulations where the scales are not fully resolved:

\[
\overline{\omega}_k \neq \dot{\omega}_k(T, Y_k, \rho) \\
\overline{\omega}_k|\eta \approx \dot{\omega}_k(T|\eta, Y_k|\eta, \rho|\eta)
\]

CSE is a combustion model for premixed and non-premixed flames:

\[
\int_0^1 \tilde{P}(\vec{x}, \eta^*) Y_k|\eta^* d\eta^* = \tilde{Y}_k(\vec{x})
\]

\[
\rightarrow A\vec{x} = \vec{b}
\]
Ensemble Selection

What is the purpose of an ensemble?

To provide the proper information for the inversion:

\[
\int_{0}^{1} \nabla P(\vec{x}, \eta^*) Y_k|\eta^*| d\eta^* = \tilde{Y}_k(\vec{x})
\]

1. A *localized* group of reactive cells:
   \[ Y_k|\eta^* \text{ homogeneous within each ensemble} \]

2. *Enough* reactive cells for a proper inversion:
   \[ \text{Overcome the problem of singularities} \]
**Implementation:**

- Pre-allocate CSE ensembles prior to runtime
- Overlapping cells between ensembles
- Each ensemble is assigned to one processor
  → Ideal for flames with clear symmetries!
- Successful implementation in Sandia methane co-flows (Sandia C, D, E, F flames)
LU-Decomposition

\[ \int_0^1 \bar{P} (\vec{x}, \eta^*) Y_k | \eta^* d\eta^* = \bar{Y}_k (\vec{x}) \rightarrow A\vec{x} = \vec{b} \]

- \( A \): \( m \times n \)
- \( \vec{b} \): \( m \times 1 \)
- \( m \): number of CSE points in ensemble (\( \mathcal{O}(10,000) \))
- \( n \): number of PDF divisions (usually 50)

Tikhonov regularization:

\[
\begin{bmatrix}
A \\
\lambda I
\end{bmatrix} \vec{x} = \begin{bmatrix}
\vec{b} \\
\lambda \vec{\alpha}_0
\end{bmatrix} \rightarrow A^* \vec{x} = \vec{b}^* ((m + n) \times n)
\]

Reduce matrix:

\[
A^*^T A^* \vec{x} = A^*^T \vec{b}^* \rightarrow A^{**} \vec{x} = \vec{b}^{**} \ (n \times n)
\]

LU-Decomposition:

\[
LU \vec{x} = \vec{b}^{**}
\]
Ensemble pre-allocation

\[ \tilde{\omega}_k \]

<table>
<thead>
<tr>
<th>CFD Module</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \tilde{Z}, \tilde{Z}''^2 ]</td>
</tr>
<tr>
<td>[ \tilde{Y}_k ]</td>
</tr>
</tbody>
</table>

PDF

\[ \langle \omega_k | \eta \rangle \]

Chemistry

\[ \langle Y_k | \eta \rangle \]

Tikhonov regularization, LU – Decomposition
Non-reacting Spray A Setup

**Converge 2.4.11:**

- Cylindrical domain $H, D$: 120 mm, 120 mm
- Maximum cell count: $2.95 \cdot 10^5$
- Standard ECN spray A conditions
- $2^{nd}$ order temporal/spatial schemes

<table>
<thead>
<tr>
<th>$D_{\text{nozzle}}$ ($\mu$m)</th>
<th>$T_{\text{fuel}}$ (K)</th>
<th>$\Delta t$ (s)</th>
<th>$M_{\text{fuel}}$ (mg)</th>
<th>$P_{\text{inj}}$ (Mpa)</th>
<th>$T_{\text{gas}}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>363</td>
<td>1.5</td>
<td>3.5</td>
<td>150</td>
<td>900</td>
</tr>
</tbody>
</table>

$\rightarrow$ Engine Combustion Network Spray A
Non-reacting Spray A Tests

- Grid dependency tests
- Collision model tests
  → NTC, O’Rourke, No collision
- Turbulence model tests
  → RNG $k - \epsilon$, Standard $k - \epsilon$, Realizable $k - \epsilon$
- Break up model tests
  → KHRT, Reitz-Diwakar
- Grid convergence tests
- Comparable results with both Sandia experiments and previous research

<table>
<thead>
<tr>
<th>Model Setup</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Turbulence Model</strong></td>
<td>Standard $k - \epsilon$</td>
</tr>
<tr>
<td><strong>Spray Models</strong></td>
<td></td>
</tr>
<tr>
<td>Injection models</td>
<td>Blob</td>
</tr>
<tr>
<td>Break up</td>
<td>KH-RT</td>
</tr>
<tr>
<td>Atomization</td>
<td>KH-RT</td>
</tr>
<tr>
<td>Collision</td>
<td>NTC</td>
</tr>
<tr>
<td>Drag</td>
<td>Dynamic</td>
</tr>
<tr>
<td>Evaporation</td>
<td>Frossling</td>
</tr>
<tr>
<td>Dispersion</td>
<td>Stochastic</td>
</tr>
<tr>
<td>Heat Transfer</td>
<td>Ranz-Marshall</td>
</tr>
<tr>
<td><strong>Grid</strong></td>
<td></td>
</tr>
<tr>
<td>Type</td>
<td>Structured with AMR</td>
</tr>
<tr>
<td>Dimensionality</td>
<td>3D</td>
</tr>
<tr>
<td>Smallest Grid Size</td>
<td>0.25mm</td>
</tr>
<tr>
<td><strong>Time Step</strong></td>
<td>Variable Time Step</td>
</tr>
</tbody>
</table>
Non-reacting Spray A Results

Non-reacting Spray A Standard Conditions Results

<table>
<thead>
<tr>
<th>KH size constant</th>
<th>KH time constant</th>
<th>Child velocity constant</th>
<th>$k - \epsilon$ constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_0 = 0.6$</td>
<td>$B_1 = 7$</td>
<td>$C_1 = 0.188$</td>
<td>$C_{\mu} = 1.58$</td>
</tr>
</tbody>
</table>
Reacting Spray A Tests

- Ranzi et al. CRECK 451-species detailed mechanism
- Reduced chemistry mechanism
  - Luo and Lu 106-species skeletal mechanism
  - Wang and Reitz 100-species skeletal mechanism
  - Cai and Pistch 57-species skeletal mechanism
- Combustion model tests
  - Well-Stirred Reactor (WSR/SAGE) model
  - Representative Interactive Flamelet (RIF) model
Reacting Spray Simulation Results

Objective: Implement CSE in a commercial CFD code with detailed chemistry and high spatial and temporal resolution to better represent combustion recession phenomenon.

- Evaluate the applicability of CSE for diesel fuel surrogates
- Determine the optimal analytical form to describe $\zeta$ PDF
- Incorporate second order conditional moment hypothesis to capture reignition and extinction
Thank you for your time!
References

[1] T. Poinsot and D. Veynante
_Theoretical and Numerical Combustion (2005), 2nd Edition._


[6] Sandia National Laboratories
Appendix

Scatterplot Data Source: Barlow, Frank, Karpetis, and Chen (2005).