LES of n-dodecane spray combustion and pollutant formation using a multiple RIF model

M. Davidovic, M. Bode, T. Falkenstein, L. Cai, H. Pitsch
Introduction

Spray combustion

1. Nozzle internal flow
2. Primary break-up
3. Fuel evaporation / secondary break-up
4. Gas phase reactions / soot precursor formation
5. Soot oxidation / fragmentation / growth

Simulation Framework at ITV

1. LES
2. DNS
3./ 4./ 5. LES

Schlieren data provided by CMT (http://www.cmt.upv.es/ECN10.aspx)
Outline

- Introduction
- Numerical Framework
- Combustion Model
- Simulation Results
- Summary & Outlook
Numerical Framework
Features of CIAO Flow Solver

**Governing Equations**

- **Incompressible**
- **Low-Mach Number**
- **Compressible**

\[
\begin{align*}
\frac{\partial p}{\partial t} + \frac{\partial (pu_j)}{\partial x_j} &= 0 \\
\frac{\partial (pu_i)}{\partial t} + \frac{\partial (pu_i u_j)}{\partial x_j} &= -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} \\
\frac{\partial (pe)}{\partial t} + \frac{\partial (pu_i e)}{\partial x_i} &= -P \frac{\partial u_i}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) \\
P &= \rho \frac{R}{W} T
\end{align*}
\]

**Physical Models**

- **Multiphase**
- **SFS Model**
- **Combustion**

**Representation of Turbulence**

- **DNS**
- **RANS**
- **LES**

**Spatial Discretization**

- Momentum Eq.: Central Difference
- Scalar Eq.: WENO
**Numerical Framework**

**Features of CIAO Flow Solver**

### Governing Equations

- **Incompressible**
  - Low-Mach Number
- **Compressible**
  - \( \frac{\partial p}{\partial t} + \frac{\partial (rho u_j)}{\partial x_j} = 0 \)
  - \( \frac{\partial (rho u_j)}{\partial t} + \frac{\partial (rho u_j u_i)}{\partial x_i} = \frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_i} \)
  - \( \frac{\partial (rho \nu)}{\partial t} + \frac{\partial (rho \nu u_i)}{\partial x_i} = -\rho \frac{\partial u_i}{\partial x_i} + \tau_{ij} + \frac{}{\partial x_i} (\lambda \frac{\partial T}{\partial x_i}) \)
  - \( p = \rho \frac{\partial}{\partial x_i} \)

### Representation of Turbulence

- **DNS**
- **RANS**
- **LES**

### Physical Models

- **Multiphase**
  - Eulerian (CLSVOF)
  - Lagrangian
    - Evaporation
    - KHRT / TAB Breakup
    - Wall interaction
    - Wall film
  - Momentum Eq.: Central Difference
  - Scalar Eq.: WENO

This Study: 2nd Order Accuracy
Institute for Combustion Technology | Prof. Dr.-Ing. H. Pitsch

**Numerical Framework**

**Features of CIAO Flow Solver**

### Governing Equations
- **Incompressible**
- **Low-Mach Number**
- **Compressible**
  - \( \frac{\partial p}{\partial t} + \frac{\partial (\rho v_j)}{\partial x_j} = 0 \)
  - \( \frac{\partial (\rho v_j)}{\partial t} + \frac{\partial (\rho v_i v_j)}{\partial x_i} = -\frac{\partial P}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} \)
  - \( \frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon v_j)}{\partial x_j} = -P \frac{\partial \varepsilon}{\partial x_j} + \tau_{ij} \frac{\partial v_i}{\partial x_j} - \left( \frac{\partial \theta}{\partial x_j} \right) \)
  - \( P = P \frac{\varepsilon}{\rho} + T \)

### Representation of Turbulence
- **DNS**
- **RANS**
- **LES**

### Physical Models
- **Multiphase**
- **SFS Model**
- **Combustion**

#### SFS
- **Dynamic Smagorinsky**
- **Coherent Structure**
- **Sigma**
Numerical Framework
Features of CIAO Flow Solver

 Governing Equations

Incompressible

Low-Mach Number

Compressible

\[
\begin{align*}
\frac{\partial P}{\partial t} + \frac{\partial (P \rho)}{\partial x_i} &= 0 \\
\frac{\partial (P \rho u_j)}{\partial t} + \frac{\partial (P \rho u_j u_j)}{\partial x_i} &= \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right) \\
\frac{\partial (P \rho e)}{\partial t} + \frac{\partial (P \rho e u_j)}{\partial x_i} &= -P \frac{\partial \rho u_j}{\partial x_i} + \frac{\partial \rho}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) + \frac{\partial}{\partial x_j} \left( \tau_{ij} \right)
\end{align*}
\]

\[P = \rho W T\]

 Representation of Turbulence

DNS

RANS

LES

 Physical Models

Multiphase

SFS Model

Combustion

- FPVA
- Combined Levelset/FPVA
- RIF
- Finite rate chemistry
- HMOM Soot model
Combustion Model
Representative Interactive Flamelet Model (RIF)

- Unsteady non-premixed combustion with detailed chemistry
  - No further modeling of CO / HC / NO\textsubscript{x} required

- Various pressure
  - Directly applicable to engine simulations
Combustion Model
Representative Interactive Flamelet Model (RIF)

Shortcoming at long injection events

- Different fuel residence time is not captured
  - Post ignition phase is not captured correctly (e.g. Flame lift-off)

Time: 0.485 ms

<table>
<thead>
<tr>
<th>T / K</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
</tr>
<tr>
<td>925</td>
</tr>
<tr>
<td>1350</td>
</tr>
<tr>
<td>1775</td>
</tr>
<tr>
<td>2200</td>
</tr>
</tbody>
</table>

Graph showing temperature distribution over time.
Capturing fuel residence time

- Splitting injected fuel mass according to its injection timing
- Solving total and individual mixture fractions

\[
\frac{\partial \tilde{\rho} \tilde{Z}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{Z}}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{\rho} (D_m + D_t) \frac{\partial \tilde{Z}}{\partial x_i} \right) + \tilde{\rho}
\]

\[
\frac{\partial \tilde{\rho} \tilde{Z}_l}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{Z}_l}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{\rho} (D_m + D_t) \frac{\partial \tilde{Z}_l}{\partial x_i} \right) + \delta(n - l) \tilde{\rho}
\]

- Introducing weighting factors

\[\bar{W}_l = \frac{\tilde{Z}_l}{\tilde{Z}}\]
Model modification

- Solving multiple unsteady non-premixed flamelets
- Weighting factors considered in
  - SDS conditioning
  - Combining chemistry solutions

\[
\tilde{H}(x, t) = \sum_{\alpha} h_\alpha \left( \tilde{T} \right) \tilde{Y}_\alpha(x, t)
\]

\[
\tilde{Y}_\alpha(x, t) = \int_0^1 \tilde{P}(Z, x, t) Y_\alpha(Z, t) dZ
\]

\[
\tilde{X}(Z) = \frac{\int_V \tilde{\rho} W_i \tilde{X}_{ref}(x) f(Z) dV}{\int_V \tilde{\rho} W_i dV}
\]

1D-Flamelet Solver

1. Flamelet
2. \(i^{th}\) Flamelet
3. \(n^{th}\) Flamelet

Time: 0.408 ms
Simulation Results
Simulation Case

Spray A

- Single hole injector
- Single component fuel
- Well defined boundary conditions
- Engine relevant conditions

<table>
<thead>
<tr>
<th>Fuel</th>
<th>n-dodecane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel injection pressure</td>
<td>150 MPa</td>
</tr>
<tr>
<td>Ambient gas pressure</td>
<td>6 MPa</td>
</tr>
<tr>
<td>Ambient gas temperature</td>
<td>900 K</td>
</tr>
<tr>
<td>Ambient gas composition</td>
<td>15 % Oxygen</td>
</tr>
</tbody>
</table>

https://ecn.sandia.gov
Simulation Results
Low-Mach Solver - Reactive Case (15% O₂)

Numerical Setup

<table>
<thead>
<tr>
<th>Solver</th>
<th>Low-Mach</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical mechanism (dodecane)</td>
<td>57 Species 218 Reactions</td>
</tr>
<tr>
<td>Number of flamelets</td>
<td>each 75µs</td>
</tr>
<tr>
<td>Minimum grid spacing</td>
<td>100 µm</td>
</tr>
<tr>
<td>Time step size</td>
<td>100 ns</td>
</tr>
</tbody>
</table>

- Lagrangian spray model parameter fitted
- Ignition delay (OH based)
  - LES 0.426 ms – Exp 0.430 ms
- Flame lift-off length slightly underpredicted

Experimental data provided by Sandia National Laboratories (https://ecn.sandia.gov)
Simulation Results
Low-Mach Solver - Reactive Case (15% O₂)

Formaldehyde

- Simultaneous Schlieren and CH₂O PLIF measurements at Sandia NL [1] showed
  - Early formation of CH₂O
  - Schlieren softening due to low temperature chemistry
- CH₂O formation also observed in LES

Simulation Results
Low-Mach Solver - Reactive Case (15% O₂)

Ignition process

1. Cool flame is initiated at lean side and propagates to rich mixtures
2. Mixture ignites at rich mixtures
3. Flame propagates lean mixtures

Temperature, CH₂O and OH solution of the first flamelet
Simulation Results
Compressible Solver - Setup

Numerical Setup

<table>
<thead>
<tr>
<th>Solver</th>
<th>Compressible</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical mechanism</td>
<td>155 Species</td>
</tr>
<tr>
<td>(dodecane / NO₅ / PAH)</td>
<td>1167 Reactions</td>
</tr>
<tr>
<td>Number of flamelets</td>
<td>each 80µs</td>
</tr>
<tr>
<td>Minimum grid spacing</td>
<td>60 µm</td>
</tr>
<tr>
<td>Time step size</td>
<td>30 ns</td>
</tr>
</tbody>
</table>

Simple coupling of PB-DNS results

- Droplets initialized with nozzle diameter
- Droplet breakup enforced into DSD at coupling location (1mm)
- Spray angle obtained from PB-DNS
- KHRT model activated after PB
Simulation Results
Compressible Solver - Inert Case

Inert case

- Vapor and liquid penetration show very good agreement with experimental data
- Lagrangian spray breakup model parameter have only minor impact

Experimental data provided by Sandia National Laboratories (https://ecn.sandia.gov)
Simulation Results
Compressible Solver – Reactive Case (15% O₂)

- Schlieren softening due to low temperature ignition clearly visible in LES and experiments
- Spray penetration slightly underpredicted
- Ignition delay in good agreement

Experimental data provided by CMT (http://www.cmt.upv.es/ECN10.aspx)
Summary & Outlook

Summary

- RIF model was extended to multiple flamelets
- Low-Mach LES with fitted Lagrangian Spray Parameters
  - Very good agreement in ignition delay
  - Good agreement in lift-off and CH₂O concentration
- Compressible LES coupled with PB-DNS results
  - Reactive case agrees well in terms of combustion characteristics

Outlook

- Detailed verification of PB-DNS coupling
  - Mixture field comparison / various densities
- Dynamic control of the number of flamelets
- Coupling with HMOM soot model
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