Development of a reduced \( n \)-dodecane-PAH mechanism and its Application for \( n \)-dodecane Soot Predictions

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**Objective**
- Development of a reduced \( n \)-dodecane-PAH mechanism for \( n \)-dodecane combustion simulation and PAH prediction;
- Application of this mechanism coupled with multi-step soot model for \( n \)-dodecane combustion and soot predictions;
- Investigate the effects of the fuel molecule structure and chemical kinetic mechanism on the soot formation process.

\( n \)-dodecane (\( n \text{C}_{12} \text{H}_{26} \)) is a potential candidate to represent the paraffin class in transportation fuel surrogates and jet fuel:
- Carbon number in the middle of typical diesel range;
- Cetane number is close to diesel and \( n \)-heptane;
- Reasonable size of the molecule compared to even larger long chain alkane;

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**Table 1: Ambient conditions re-acting**

<table>
<thead>
<tr>
<th>Phenomenon</th>
<th>Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spray Breakup</td>
<td>KH-RT instability</td>
</tr>
<tr>
<td>Evaporation</td>
<td>DMC</td>
</tr>
<tr>
<td>Turbulence</td>
<td>gRNG ( k-\varepsilon )</td>
</tr>
<tr>
<td>Combustion</td>
<td>SpeedChem</td>
</tr>
<tr>
<td>Droplet collision</td>
<td>ROI collision</td>
</tr>
<tr>
<td>Near Nozzle flow</td>
<td>Gas-Jet model</td>
</tr>
</tbody>
</table>

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**n-C\textsubscript{12}H\textsubscript{26}-PAH mechanism**
- 104 species and 444 reactions
- Reduced \( n \)-dodecane mechanism
- 80 species and 299 reactions
- Reduced PAH mechanism
- 42 species and 228 reactions

\( \text{PAH mechanism} \)
- A1 formation
  \( \text{C}_6 \text{H}_5 + \text{C}_6 \text{H}_5 + \text{C}_6 \text{H}_5 \)
- \( \text{C}_6 \text{H}_5 \text{C}_6 \text{H}_5 + \text{C}_6 \text{H}_5 \text{C}_6 \text{H}_5 \)
- \( \text{C}_6 \text{H}_5 \text{C}_6 \text{H}_5 \text{C}_6 \text{H}_5 \text{C}_6 \text{H}_5 \)
- Larger PAH formation
  1. HACA sequence
  2. Small radical and molecule
  3. Addition reactions between aromatic radicals and molecules

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- The reduced mechanism performs quite well under different validation conditions;
- Species profiles from JSR and shock tube were also taken as validations for the proposed mechanism.

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**Figure 1:**
- Predicted mixture fraction distributions agree reasonable well with experimental data in both radial and axial directions by calibrating the spray model constants.

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**Table 2:**

<table>
<thead>
<tr>
<th>Injection pressure</th>
<th>150 MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection duration</td>
<td>6.0 ms</td>
</tr>
<tr>
<td>Injection fuel mass</td>
<td>13.77 mg</td>
</tr>
</tbody>
</table>

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**Figure 2:**
- A reduced \( n \)-dodecane-PAH mechanism was proposed;
- The soot formation regions and soot mass agree reasonably well with available data;
- The fuel's ignitability and the mixing process control the soot formation process, longer ignition delay longer lift-off length lower soot;
- Fuel molecule structure and mechanism do have influence on soot formation process;
- The \( \text{C}_6 \text{H}_5 \text{C}_6 \text{H}_5 \) assisted surface growth process is the most important process that affects the soot formation;