Thoughts on Surrogate Fuels for Combustion

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Surrogate Fuels

- Definition
- Purpose
- Selection
- Costs
- Test Sensitivities
- Experience
Definition

- Surrogate fuel – A mixture of a small set of individual hydrocarbon ‘species’ or components in a specific mixture ratio that when combined replicate the behavior of a real fuel

- Applications to GT (aero), IGT, Diesel, SI
Purpose

In the case of a surrogate for combustion:

- **Primary: For Modeling**
  We cannot yet capture the combustion characteristics of a real fuel – except for simplified problems in CFD simulations. Lack of accurate kinetic description is likely a contributor to this problem.
  
  Capturing the fuel chemistry of a real fuel will remain unachievable for the foreseeable future.
  
  Establishing the chemistry is one step towards a new CFD capability.

- **Secondary: For Validation**
  
  Proof. There is no guarantee that a surrogate can successfully achieve this goal. Experimental validation is a logical follow-on step.

- **Tertiary: For Sensitivities**
  
  Once surrogate is established, sensitivities to changes in the physical or chemical nature of the fuel can be examined.
Questions?

- **Modeling –**
  - Can a few components truly simulate real fuel behavior?
  - Can a reaction model be constructed that (accurately) simulates the individual components, the surrogate, let alone the real fuel?
  - Fuel interaction effects?
  - What accuracy level is required?
  - How to prove this can work?
  - how to establish accuracy requirements?
  - How to simplify for practical CFD?

- **Validation –**
  - Accuracy requirements for experiment?
  - Range of data? (P/T, f/a, spray)
  - Costs? – forces use of solvents and impose complications to kinetic models
Selection of Surrogates

- No unique solutions
- Targets:
  - Selection of components – limited by availability of kinetic models
  - Selection of targets –
    - Ideally to match combustion (entire) characteristics
    - Treatment of both physical and chemical dependencies
    - So far done by personal preference…..or limitations
- Few robust, well defined methods
More Questions

- Can we ensure that matching a few selected targets guarantees matching all combustion characteristics?
- If not what are the limits in accuracy, or inability to match certain behavior?
- What specific targets are needed to match the ‘full set’; or a reduced set of combustion characteristics
- Is it acceptable to match a limited set of combustion characteristics? Does everything need to be matched?
- Are there specific characteristics that must be matched? – What are they?
Targets – proposed (for combustion)

- Chemical classes (n-alkanes, i-alkanes, cycloalkanes, aromatics…)
- Chemical groups (-CH2-, -CH3, -iC4H9, C7H7-, C6H11-, …..)
- TSI
- Ave MW
- CN, Ignition
- Boiling point (T10, T50, T90)
- H/C
- Premixed/Nonpremixed Extinction
- Liquid density
- Viscosity, surface tension
- ……
- Various combinations thereof
- Interdependency of properties?
- Mixing rules??????

Relationship of targets to combustion characteristics?
Costs – Astronomical for High MW Pure Fuels

Catalogue Prices for 99% Purity

Solvents are the only real option for validation!
## Sensitivities

Solvents/Surrogates can explore contrasting physical and chemical changes

<table>
<thead>
<tr>
<th>JP-5 (petroleum)</th>
<th>HRJ-5 (Camelina)</th>
<th>Sasol IPK</th>
<th>Shell GTL</th>
<th>Linpar 1416</th>
<th>L-142</th>
<th>L-210</th>
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<tbody>
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<td><strong>JP-5 (petroleum)</strong></td>
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<tr>
<td><strong>Sasol IPK</strong></td>
<td>Primarily isoalkanes, some cyclo, C9-C14</td>
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<td>Similar MW (C10), different chemistry (role of n-alkanes)</td>
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<td>Similar MW (C10), different chemistry (iso vs. cyclo)</td>
<td>Similar chemistry, different MW (C10 vs. C14)</td>
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<td><strong>Shell GTL</strong></td>
<td>isoalkanes and normal alkanes, C9-C12</td>
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<td>Similar chemistry (not exact), different MW (C10 vs C14)</td>
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<td>Similar MW (C10), different chemistry (Cyclo vs. norm)</td>
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<tr>
<td><strong>Linpar 1416</strong></td>
<td>n-alkanes, C14-C16</td>
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<td>Different chemistry, different MW</td>
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<td>Similar MW (C14), different chemistry</td>
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<td><strong>L-142</strong></td>
<td>Cycloalkanes, and some isoalkanes, C8-C13</td>
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<td><strong>L-210</strong></td>
<td>Isoalkanes and some cycloalkanes, C13-C16</td>
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Experience

Encouraging results – but we have not closed the loop yet

- MURI
- Utah
- USC
- UTRC
- UC Irvine
- Europe
- UCSD
Combustor Validation Data – Fuels

Solvents and synthetic fuels explore contrasting physical/chemical changes

Wide range of chemical properties