Production Issues and Fischer-Tropsch Commercialization

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Molecular level characterization of F-T fuels needed to establish relationships between fuel composition and

- Fischer Tropsch reaction conditions
- Fuel refining methods
- Fuel performance in engines
F-T Fuel Characterization

- No commercial methodology exists for detailed characterization of very complex hydrocarbon mixtures

- Hence, new analytical methods must be developed for F-T-fuel analysis

- These special methodologies are best implemented on ultra-high resolution mass spectrometry because of the molecular complexity of the fuels
• Most promising analytical approach:
  - Laser-induced acoustic desorption (developed at Purdue)
  - Ionization with chemical reactions specifically developed to ionize hydrocarbons without fragmentation
  - Ultra-high resolution FT-ICR mass spectrometry

• First steps:
  - Test the existing methodology (medium-resolution)
  - Use existing F-T fuels

• Goals:
  - Determine the critical areas (in addition to resolution) that need improvement for complete F-T fuel characterization
• Goals:
  - Make initial correlations between fuel’s molecular composition and performance information obtained by the engine testing group
  - This information will aid the F-T production group in optimization of the selectivity of the F-T process
  - Preliminary characterization of F-T fuels generated by the production group will lead to initial correlations between the fuel composition and F-T catalyst composition and reaction conditions

All the above correlations must be re-evaluated when analytical procedures have been developed for complete F-T fuel characterization
Production of F-T Fuels:
Four major focus areas identified

- Optimizing Selectivity
- Fischer-Tropsch Mechanism
- Integration of F-T Mechanism with reactant consumption and product distribution
- CO₂ recycle
Implications of CTL Integration

Our idea is to develop the facility to quickly add new chemistries to a full plant model so we can immediately understand their implications to the final product cost.
Optimizing Selectivity

- Selectivity: single-most important parameter
- Selectivity: complex function of various parameters
- Desired product either diesel range linear paraffins or olefins (high reactivity)

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<th>Parameter</th>
<th>Chain Length</th>
<th>Chain Branching</th>
<th>Olefin Sel</th>
<th>Alcohol Sel</th>
<th>Carbon Dep</th>
<th>Methane Sel</th>
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<td>Temperature</td>
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<td>Pressure</td>
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Integration of F-T Mechanism with Reactant Consumption and Product Distribution

• None of the available models are accurate enough
• Lack of reliable kinetic equations for all products
• Models combining overall consumption of reactants and product distribution are scarce in the literature