Production Issues and Fischer-Tropsch Commercialization

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The Indiana Center for Coal Technology Research

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Coal To Liquids, CTL

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 complexicity 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
- CO_2 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)

Parameter	Chain Length	Chain Branching	Olefin Sel	Alcohol Sel	Carbon Dep	Methane Sel
Temperature	↓	↑	*	↓	↑	↑
Pressure	↑	↓	*	↑	*	↓
H_2/CO	↓	↑	↓	↓	↓	↑
Conversion	*	*	↓	↓	↑	↑
Space Velocity	*	*	↑	↑	*	↓

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