SECA - CTP
Fuel Processing Break-out Session

Lakewood, CO

October 26, 2005

Current SECA Participants / Landscape

- Argonne National Lab
  - Perovskite materials development for catalysts – derive alternative materials – primarily for ATR-based systems
  - doing Diesel and JP-8 reforming
    - Multi-component chemistry (complicated)
  - Cool-Flame (self-sustained) combustion/pre-reforming
  - Diesel injector work (previously funded by EERE)
- Ceramatec
  - Plasma-arc reforming
- Goodrich – Fuel injection and mixing strategies
  - Pre-heated, gas-assist, piezo-electric, …
- NETL – Dave Berry, and Todd Gardner
  - Ceria and other conductive substrate materials use for introducing sulfur tolerance, …
  - Hex-alumina substrates into which substitutions of various cations can be made – combinatorial methods being applied to identify promising materials
- NETL – heterogeneous chemical kinetics
- PNNL – strontium titanate anodes for increased sulfur tolerance; on-anode reforming
- Georgia Tech (Meilin Liu) – sulfur tolerance and mechanisms of sulfur poisoning
- Franklin Fuel Cells – sulfur tolerance, internal fuel processing, impregnation tech. for anode and cathode mfg.

- Colorado School of Mines – in anode compartment fuel processing and electrochemical analyses (e.g., with CFD and detailed gas-phase and heterogenious chemical kinetics), “monster” PAH and combustion developed mechanism effectively simulated observed deposition, hex-aluminates
- Penn State and U. Mich – sulfur removal from liquid fuels (funded by ARL)
- Tufts University – novel high temperature sulfur removal materials

Initial Thoughts

- Automotive fuel processor technology – directly relevant to our challenge
  - Sprays, mixing, rapid start, preheating, coking, …
  - Much of this work may be “under wraps”
    - ANL did much work in this area
    - Automobile manufacturers, Industry (e.g., Goodrich, Delphi, …), Universities, other National Labs
- Has structure of bed been determined (foam, bed, monolith, …) – no, but much work, design dependent
- Continuous versus pulsed injection
- ACTION: conduct detailed literature review of publicly available research and development in this field (esp. University of Wisconsin, other universities conducting diesel spray/mixing research)
- Injector design and spray characterization
  - What are criteria?
  - How can criteria be met in small space over broad range of operation?
- Melting of catalyst beds observed in real diesel injection cases (droplets)
- How can methane be introduced into fuel cell by producing sufficient CH_4 in a CPOX reactor without coking?
- CO_2 reforming (perhaps with a separation membrane using anode recycle)
- Cannot count on equilibrium to be sole guide of design (kinetics can govern some processes and lead to nasty surprises)
- Turn-down requirements
- Low pressure liquid fuel (only) available, low pressure gas assist (only) available

R&D Areas that Need to be Addressed

- Fuel Handling Hardware
- Understand and enable use of synergies between fuel processing and fuel cells
- Understanding of multi-component fuel issues/differences/needs for robust fuel processor operation
- Possible use of single-component fuels (ethanol, methanol, …)
  - Think outside box – What is the desired diesel spec. – maybe simply a different standard (not cetane or octane number) would make all the difference for FC fuel processing?
- Robust, Flexible, Multi-fuel processing would be a significant market benefit
  - Same developments could handle seasonal variations, …
- Upstream sulfur management
- Downstream carbon management – how can carbon formation (if it is inevitable) be handled?
- What are the issues/barriers to achieving closer to “ideal” performance (no addition of excess steam or excess oxygen)? – intimate integration, internal reformation
- Chemical recuperation/cooling as part of an integration strategy – development of additives for delaying onset of coking in fuel stream
- Waste heat management
- Fuel Sprays and mixing
  - Including integration of such with full fuel processing system design
  - Nature of integration is fuel specific
- High temperature sulfur removal (downstream sulfur management)
- Fuel characterization

R&D Areas that Need to be Addressed (cont'd)

- Characterization and understanding of coke formation mechanisms and regimes
- Impacts of fuel additives (nitrogen-based, lubricity, other)
- Alternative sulfur removal technologies (both high and low temperature)
  - Upstream liquid
  - Low temperature, integrated
  - Low cost
  - Low maintenance
  - Variable concentrations and species
- Supported nickel catalyst work not directly applicable to anodes – fill knowledge gap

R&D Areas that Need to be Addressed (cont'd)

- Controls for high efficiency while meeting all other requirements
- Tight integration of reforming and fuel cell function
  - Design tradeoffs regarding efficiency, power density, …
  - Thermal and mechanical integration
  - Manifolding, separation membranes, mixing, recycle
  - Materials selection
- Fundamental chemistry and electrochemistry understanding and chemical mechanisms for complex fuels – especially for on-anode reformation
- A better understanding of the optimal output stream composition from a pre-reformer or external reformer
  - Controls for actually accomplishing this in the system without compromising on efficiency, coking, …
  - Strategies for achieving this composition and integration
- Development of low-cost sensing devices and strategies for fuel processing devices and systems and for multi-fuel process control
- Reactor light-up, start-up, shut-down
- Fluid mechanics, heat transfer, mixing, flow understanding and simulation
- Experimental investigation and model verification in generic reformer systems – end up with design guidelines
- Renewable fuels (bio-diesel, ethanol, etc.)
- Novel anodes and cell architectures
- Process simulation for fundamental system controls development and understanding
- Shock, vibration, relative motion, …

R&D Areas that Need to be Addressed (cont'd)

- Shock, vibration, relative motion, … impacts on performance
- Blowers, fans, pumps, and other BOP
- Assess approaches (ATR, CPOX, SR, plasma, …) for applicability, performance
- Life, durability, carbon balance (throughout system), lifetime design matching
- High temperature CO_2 and sulfur removal
- Recycle strategies and technologies
  - Condensation, cooling strategies versus hot recycle
- Pressurized reformation

Proposed Categories of R&D Areas

- Fuel Handling, Sprays and Mixing
- Fuel Reforming
- Sulfur and Carbon Management
- Reforming / Fuel Cell Integration
- System Integration, Sensors and Controls
- Modeling and Simulation