# CO Clean-up Development

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DOE 2000 Review - OTT Fuel Cells Program

June 7, 2000



#### Relevance: Meet PNGV Fuel Processor Targets



- PrOx (CO Clean-Up Device) is the last unit operation in the fuel processor process stream.
- Primary function is to remove contaminants to levels acceptable to the fuel cell stack
  - CO < 10 ppm steady-state, < 100 ppm transient</li>
  - NH<sub>3</sub>, H<sub>2</sub>S to specified levels
- Overcome critical barriers for maintaining fuel purity requirements during transient operations
- Meet fuel processor targets for energy efficiency, power density, specific power, and cost



### Technical Objective: Catalytic Clean-Up of Gas Streams

- Develop reformate clean-up technology for integration into fuel processor systems that enables them to meet the fuel purity requirements for a fuel cell stack
  - Remove trace contaminants CO, NH<sub>3</sub>, H<sub>2</sub>S, soot, HCs
  - Maintain system performance efficiency, minimum hydrogen consumption
  - Handle automotive transients power, start-up, shutdown
  - Meet automotive requirements cost, volume, weight, durability



#### Approach: Laboratory Investigation With Industrial Collaboration

- Investigate and develop Reformate clean-up technology
  - Investigate catalysts and catalyst performance
  - Use carefully instrumented and controlled experiments at the component level to measure performance
  - Develop proof-of-concept on a laboratory scale
  - Develop design tools for application
- Work with fuel processor developer(s) to integrate reformate clean-up technology into fuel processor systems and test.



PrOx operates as a series of short residence time reactors, each with thermal management, gas mixing and catalyst volume Gas distribution/mixing elements thermal management fuel stream in (up to 2% CO) fuel stream out (to fuel cell) (< 10 ppm CO) Particulate filter → very low CO air supply/metering → large turndown Catalysts selected to work  $\rightarrow$  minimal  $H_2$ together to improve transient consumption performance, minimize control requirements

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#### Laboratory PrOx Works as Baseline System for Testing Concepts



- 2% CO inlet to 10 ppm CO outlet
  - Simulated gasoline reformate
  - Natural gas system at energy partners
- Modular laboratory design gives flexibility to test:
  - Catalysts
  - Configuration options
  - Control schemes
- Design and lightweight internal components enhance transient performance
- Uniform air distribution and mixing
- Inlet temperature control



#### Work-in-Progress: Enabling an Automotive PrOx System



- Catalyst volume
  - Evaluate catalysts on foams and monoliths
  - Size
    - Evaluate configurations for reducing PrOx size
  - Air injection controls/coolant controls/sensors
    - Evaluate needs for ancillary components
    - Evaluate simplified control strategies
  - Manufacturability
    - Prepare design tools/methodology
    - Trade-off evaluations
    - Develop collaborations with fuel processor manufacturers

## **Experimental Work in Progress**



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- Catalyst/catalyst support evaluation
  - Single-stage PrOx reactor instrumented catalyst volume to measure temperature and species profiles
  - Simulated Reformate
  - Pellet, monolith, foams
  - Use microscale reactor to measure kinetics
- Transient experiments
  - Transients change in power level or change in gas composition, startup?
  - Identify need for controls target to simplify
  - Identify need for sensors, especially requirements for an online CO sensor
  - Control strategy for PrOx transients



- Single-stage PrOx- catalyst evaluation
  - Individual stage evaluation-profiles of catalyst volume of our baseline configuration
  - Initial tests on catalyzed ceramic foams
  - Tests on newly obtained catalyst/catalyst supports- June Sept 00
    - Combined particulate filter/PrOx catalyst
    - Higher density ppi monoliths
- Transient PrOx experiments
  - Conducted testing on inlet CO concentration variation
  - Power transient testing June 00
  - Start-up transient testing July 00
- Microscale catalyst evaluation
  - Kinetic data obtained on precious metal catalysts



- <u>Dec 99</u> complete testing using catalyzed foams
  - Ongoing, iterating to improve performance
- <u>March 00</u> evaluate compact gas mixers for air injection/mixing
  - Incorporated into PrOx design, working to eliminate need for separate gas mixing components
- <u>June 00</u> select industrial partner for transfer of PrOx technology and initiate joint 'design for manufacturing activities
- <u>Sept 00</u> complete design of compact gas clean-up hardware
- <u>Sept 00</u> design, fabricate, and evaluate compact gas clean-up device



- McDermott Technology/Catalytica
  - Beginning collaboration to transfer PrOx technology
  - Work together to design PrOx for commercial system
- Argonne National Laboratory
  - Collaborating to integrate a LANL PrOx design into ANL's fuel processor
- Others?
- SBIR/STTR Interactions
  - NexTech Future testing of CO sensor
  - Hydrogen Burner Technology



- Operate on real gasoline reformate
  - FY99 presentation focused on a natural gas system.
  - We test on simulated gasoline reformate identifies effects of major constituents and provides controlled experiments.
  - In-house fuel processors operate on gasoline/collaborations with fuel processor developers.
- Develop PrOx for any system, not just one system
  - PrOx technology is applicable for most systems.
  - Specific configuration will depend on the system requirements -e.G., % CO inlet and outlet,gas composition, contaminants, operating pressures and temperatures
  - Modular approach allows easy adaptation to a particular system
- Need for more work on catalysts and design-for-manufacture/ include strong effort to reduce size, weight, and cost
  - This is the focus of this year's program. Our prior focus was on a working system.
- Activity appropriate for industrial development rather than national lab
  - Technology transfer and industrial collaboration is a part of the program.
  - Gas clean-up still has major research issues transients, startup, efficiency



- Appropriate role for national laboratory research is in gaining fundamental understanding of critical aspects of the technology
- PrOx system design is system dependent, therefore
  - Focus on developing information required by developers for their own PrOx designs
  - Provide detailed information on performance of individual stages
  - Develop methodology for PrOx design along with information to model the system
- Investigate behavior of the catalytic systems on a fundamental level
  - Provide understanding that can have applicability to a wide range of systems
  - Reformate composition effects, hydrogen consumption, transients



- Continue catalyst testing and testing of multistage PrOx hardware
  - Reformate composition effects, hydrogen consumption, transients
  - Data input for PrOx reactor modeling
- Continue development of PrOx design methodology, delineate successful understanding of PrOx mechanisms
- Work on tech transfer/industrial collaborations



- Fuels effects identify fuels issues for Reformate cleanup performance
  - Lifetime, durability issues
- Catalyst development/characterization
- Minimize hydrogen consumption low stoichiometries
- PrOx geometries/operational modes that enhance catalyst performance
- Transient operation: 100:1 turndown
- CO sensor required or can the need be eliminated?
- Shift focus to other contaminants than CO
  - Soot, NH3, H2S, HCs, species identified in fuels testing



#### Gas Clean-up Future Directions Cold-start/startup Issues

- Gas clean-up operation at low temperatures
  - Catalyst operation at lower temperatures
  - Water condensation concerns
- Gas clean-up rapid start
  - Light weight catalyst supports/ reactor design
- High CO gas clean-up reactor
  - Apply PrOx concept to high inlet CO concentration (>5%)
  - Sacrifice some hydrogen consumption to obtain a fuel cell quality gas earlier in the start-up sequence



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- Laboratory PrOx configuration serves as a baseline for fundamental studies and for developing automotive configurations
  - Test bed for catalyst testing details of catalytic reactor performance
  - PrOx configuration development
  - Developing PrOx design methodology
- Tech Transfer/Collaborations starting
  - Develop and apply PrOx technology to a specific system