Parametric Study on Micro-Water Gas Shift Reactor

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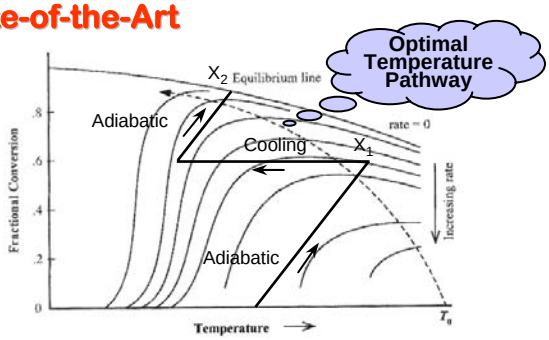
Faculty: *R. Mayor, J. Ni*

Objectives

- Develop integrated reaction and heat exchange approach to a micro-reactor design which allows the reactant stream to follow a optimal temperature path.
- Investigate sensitivity of design parameters of the integrated reaction and heat exchange design.
- Obtain design guidelines for micro-water gas shift reactor.

State-of-the-Art



- Achieving and maintaining the optimum temperature profile of the reactant stream in conventional size reactors is difficult due to complicated cooling designs and heat and mass transfer limitations. Consequently, multistage reactor schemes are often employed for practical applications as depicted in above figure in a solid line.
- With micro-scale reactors, heat and mass transfer limitations may be overcome through the beneficial scaling effects of miniaturization; at the smaller length scales, the thermal response time is significantly reduced.

Approaches

- Experimentally obtained rate laws were used for the water gas shift reaction. And, the inlet gas composition and feed were of a typical exit stream from a steam reformer.
- 1-D integrated reactor model has been developed for validation with experimental results.
- 2-D model has been developed for comparison with 1-D results and analysis of selected parameters.

$$CO + H_2O \Leftrightarrow CO_2 + H_2$$

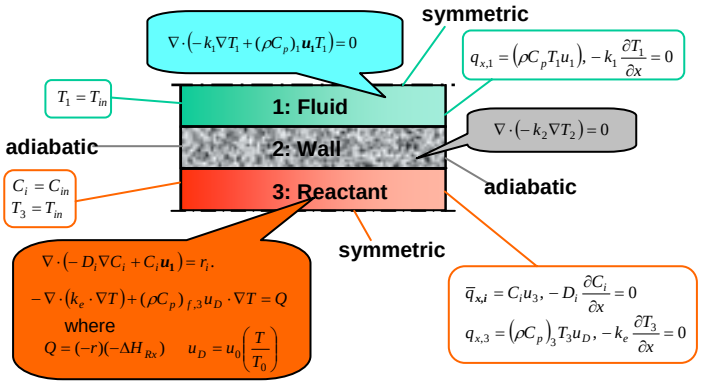
$$r_3 = k_3 P_{CO} P_{H_2O}\left(1 - \frac{P_{CO_2} P_{H_2}}{K_3 P_{CO} P_{H_2O}}\right) \quad (mol/g.s)$$

$$k_3 = 0.00225\exp(-50{,}000/RT) \quad (mol/g.s.kPa^x)$$

$$K_3 = 9.543\times10^{-3}\exp(39876/RT)$$

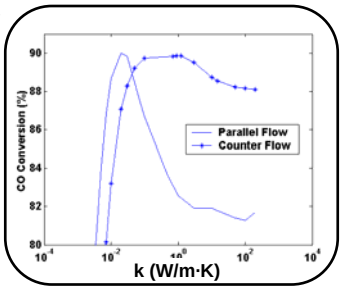
Rate equation used in the simulation (P. Mizsey)

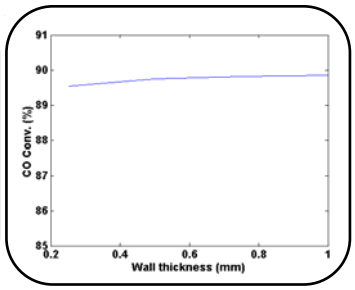
Accomplishments



Governing equations and boundary conditions for 2-D model

- Suggested operating ranges for selected design parameters (wall conductivity, heat exchange medium and inlet temperature/velocity) for counter and parallel flow configuration were obtained.
- Comparison between adiabatic and integrated design showed reduction of catalyst amount by half for integrated design.





- The range of acceptable thermal conductivities for the parallel flow configuration was narrow and limited to application of insulating materials. However, the counter flow arrangement shows high CO conversion for wide range of materials, enabling selection of traditional engineering materials such as stainless steel.
- The thickness of the wall does not have much influence on the CO conversion. Thus, miniaturization of the reactor may be achieved by reducing the wall thickness.

Future Work

- Experimental validation and fabrication of water gas shift reactor

Sponsors

- U.S. Department of Energy

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Development of Onboard Fuel Processing System

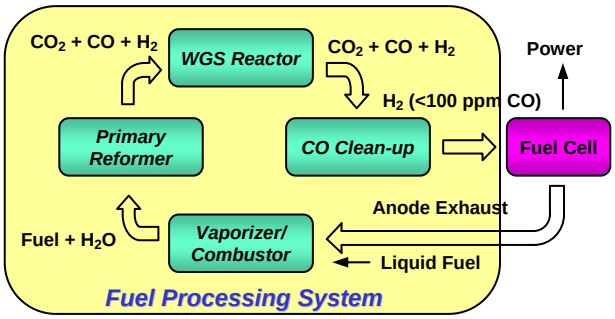
Research Assistants/Staff: *G.Y. Kim*

Faculty: *R. Mayor, M. Koc, J. Ni*

Objectives

- Demonstrate a compact fuel processor for automotive fuel cell power systems.
- Achieve miniaturization of the fuel processor by integrated design and micro-fabrication technology.

State-of-the-Art



- A typical fuel processing system consists of four reactors; vaporizer/combustor, primary reformer, WGS reactor and CO clean-up reactor. Various designs and fabrication methods are under investigation for miniaturization of the components.
- However, current technology status lags behind PNGV targets in many areas for commercialization of the onboard fuel processors due to high fabrication cost, complexities associated with integration, and transient response of the system.

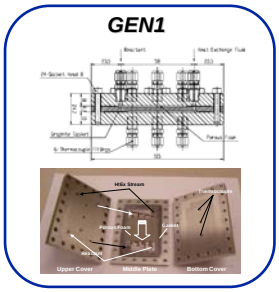
PNGV Targets for 50kW Fuel Cell System (A.D. Little)

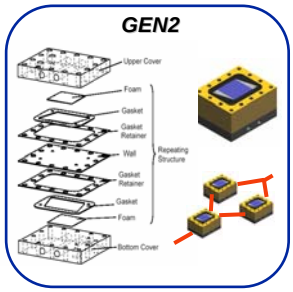
	Units	2001	2005	2010
Power density	(*W/L*)	500	700	800
Cost	($/*kW*)	85	25	10
Start-up time	(*min*)	10	1	0.5
Durability	(*hours*)	1000	4000	5000

Approaches

- **Reactor development**
  - ATR, WGS, PrOx and vaporizer investigation
  - Catalyst development for each reactor
  - Fabrication technology investigation
- **Reactor integration**
  - Mechanical integration of each reactor
  - Catalyst performance evaluation for scale-up
  - Reactor sizing
- **System integration**
  - Mechanically and thermally integrated system
  - Enhancement of transient response

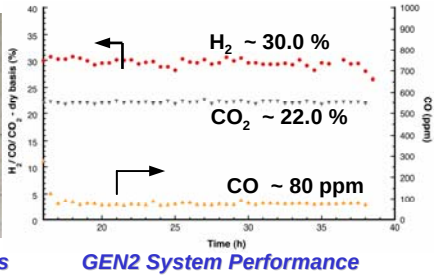
Accomplishments





- GEN1 micro-reactor is a simple layer-based design for evaluation of various catalyst for each reactor.
- GEN2 design adopts ***modular approach*** for rapid integration of the components. Enhanced manufacturability is achieved through ***layer-based design***. Flexible design also enables various flow configuration investigation.

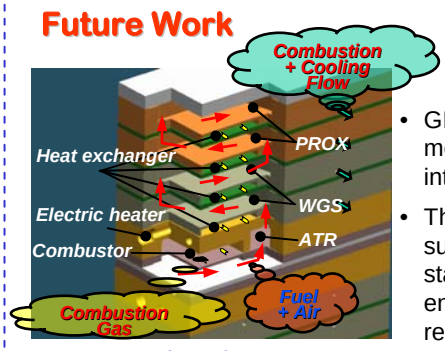
GEN2 Integrated Reactors



GEN2 System Performance

- A vaporizer/combustor, an ATR, two WGS reactors and two PrOx reactors has been integrated.
- Performance of the integrated system shows CO level below the target value of100 ppm.

Future Work



Preview of GEN3

- GEN3 design targets mechanically and thermally integrated system.
- The integrated combustor supplies heat during steady state operation. Thus, enhanced transient response is expected.

Sponsors

- U.S. Department of Energy

* The research is multidisciplinary project involving chemical eng. (Gulari, Schwank, Thompson and Yang), mechanical eng. (Assanis, Im and Ni) and aerospace eng. (Dahm).

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Micro Internal Combustion Swing Engine (MICSE)

Research Assistants/Staff: *H. Zhu*

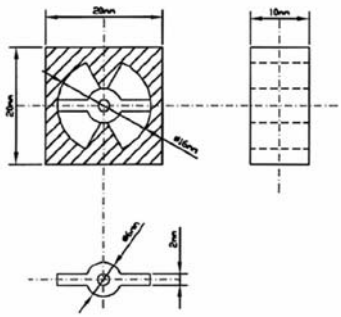
Faculty: *X. Qiao, J. Ni*

Objectives

- To develop a complete power generation system based on Micro Internal Combustion Swing Engine (MICSE) that produces 1440 Whr with a total weight less than 815g (including fuel).
- To investigate the effect of spark timing and valve timing on the thermal efficiency and further improve the engine performance through optimal controller design

State-of-the-Art

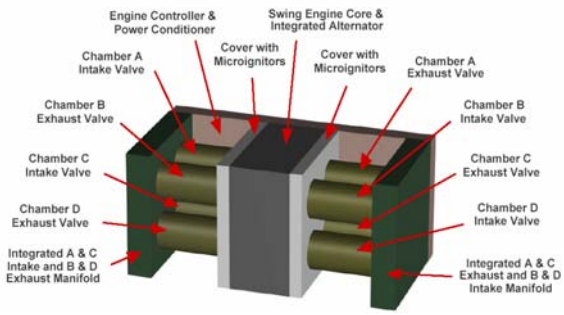
- Liquid-fueled portable power generation which has at least 25 times higher specific energy than current primary battery technologies is a major new research area with enormous potential for practical application.
- Based on combustion in four chambers separated by a rotating swing-arm, with virtually no other moving parts.
- The low mass, low moment of inertia, and angular motion of the swing-arm provides extremely low vibration and noise.



Approaches

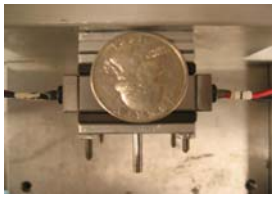
Development of the MICSE system is being done via the following subtasks

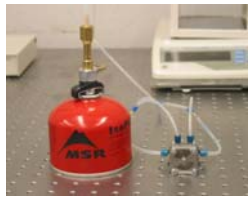
- Fuel Supply and Delivery Subtasks
- MICSE Core Subsystem Subtasks
- Electrical Power Converter Subtasks
- Micro Control Subsystem Subtasks
- System Integration

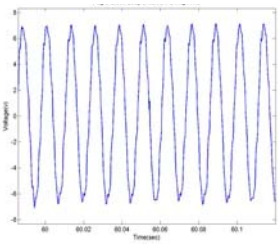


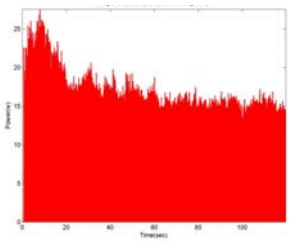
Accomplishments

- MICSE has been designed at “mini-scale” (30x30x60 mm^3, 20W) and successfully fabricated using wire EDM technique.
- Fuel induction system has been implemented with internal fuel-air mixing and external fuel-air premixing using Methane fuel and Butane fuel.
- Fully functional Micro engine control system has been successfully implemented
- Tests performed to date on MICSE have demonstrated successful long-time closed-loop operations .
- Power generation has been successfully demonstrated with external shaft-coupled DC generator with variable mass load and electrical load.









Future Work

- Optimize the whole system design in an integrated fashion that gives minimum mass and size and maximum efficiency
- Design and develop advanced control algorithms to improve the engine performance

Sponsors

- DARPA Defense Sciences Office

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Development of Miniature Ceramic Engine Components

Research Assistants/Staff: *K. Park, H.Y. Kuo, G.Y. Kim*

Faculty: *J. Ni, A. Shih*

Objectives

- Fabricate ceramic engine component for Micro-Internal Combustion Swing Engine (MICSE) for improved thermal efficiency.
- Establish optimal procedures and parameters to achieve high quality ceramic engine component.

State-of-the-Art

- The current engineering material for the engine is metallic materials, which exhibit performance losses due to thermal power loss and gas leakage at high temperatures.

Approaches

Die Design – Calculation of die dimensions; Preliminary tests for die configuration

↓

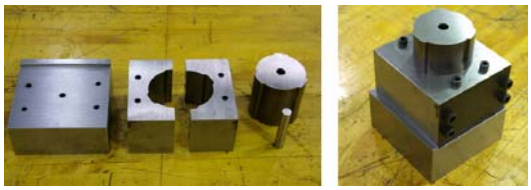
Powder Compaction – Identification of critical parameters; Obtain optimal process parameter

↓

Sintering – Investigate effect of various curing curves on the final part

Accomplishments

- The split die body design was adopted to reduce the possibility of cracking during ejection. Also, the core rod was designed to produce the inner hole. Both the die body and core rod were assembled by screw on the base plate, and a punch fitting into the die body was needed.
- In die fabrication, each part underwent machining process prior to heat treatment, which increased the hardness of die to HRC58. The hardened material was shaped into the complicated profile by the Wire-EDM process, and then precisely ground for assembly.

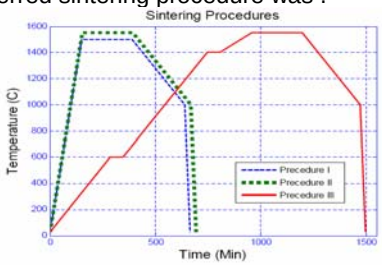


Die assembly for the intake and exhaust plate

- A compaction pressure range of 30-75 MPa is preferred for the compaction of zirconia powder using uniaxial die compaction.
- Effect of the use of different oils

Unsuccessful and successful formed green parts

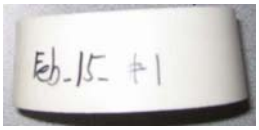
- A preferred sintering procedure was .



Temperature profile for sintering

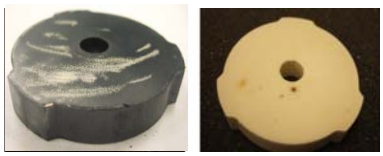
- Conical shape after sintering due to the anisotropy could be offset by the friction drag of the support substrate.
- Crack-free ceramic intake and exhaust plates have been made with the use of 50 Mpa, 0.1 in/min pressing speed and 0.005 in/min releasing speed.

Tradeoff between shrinkage Anisotropy and friction drag



Conical shape due to the friction drag and shrinkage anisotrypy

Part with Crack



Successful compacted and sintered part

Future Work

- Whisker reinforced ceramic composites will be tested for improved toughness. Optimal procedures for successful compaction and sintering need to be developed.
- Ceramic engine performance will be evaluated.

Sponsors

Powerix Technologies, LLC.

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