Differential Temperature Water-Gas Shift Reactor

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Catalyst Screening

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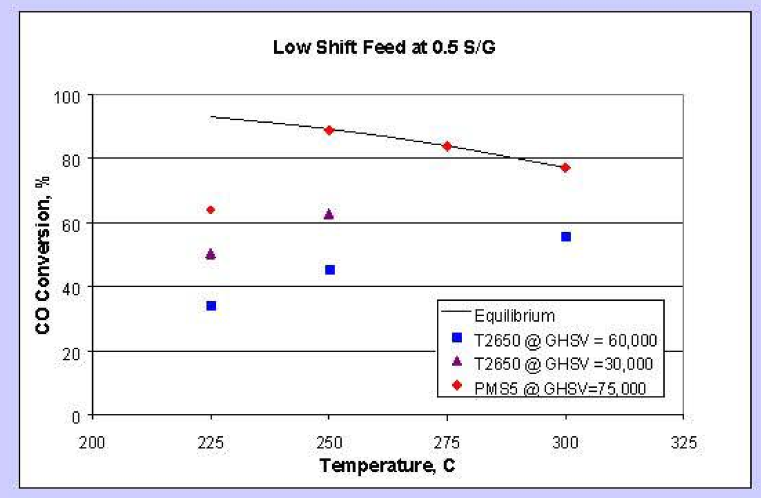
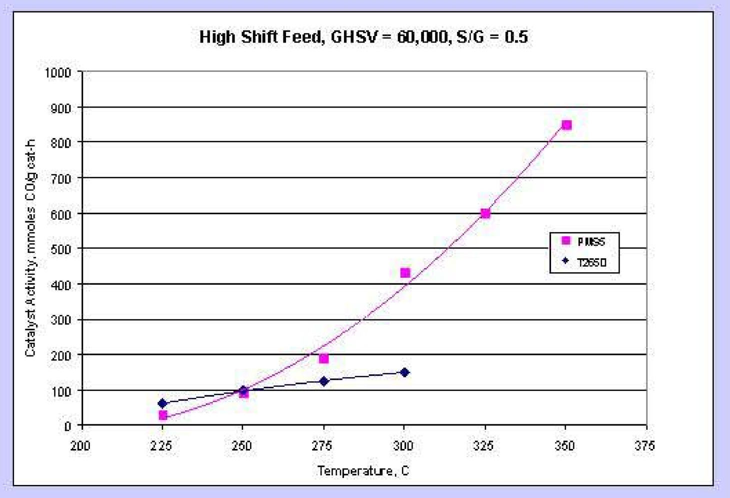
Example: Precious Metal (PMS5) vs Base Metal (T2650) WGS Activity





Kinetic Model Development

Kinetic Model Development

Single Channel Test Reactor

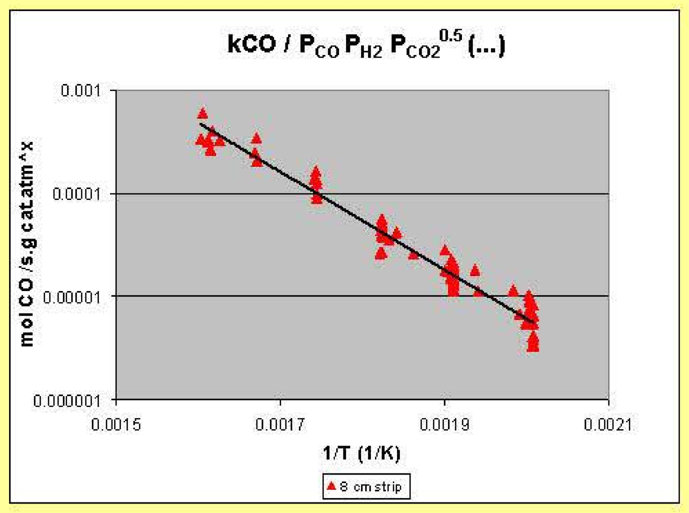
- New important research tool
  - Microchannel
  - Engineered catalyst
  - Temperature controlled
  - Easily modeled
  - High data production
  - Rapid catalyst turn-around
- Used for:
  - Kinetic model development
  - Parametric studies
  - Catalyst optimization
  - Lifetime testing
  - Benchmark performance

Sud-Chemie PMS5 WGS Catalyst Selected

- Generalized kinetic model:

$$r_{CO} = \rho_B k_{CO}(T)\, P_{CO}^{a} P_{H_2O}^{b} P_{H_2}^{c} P_{CO_2}^{d} \left(P_{H_2O} P_{CO} - \frac{P_{H_2} P_{CO_2}}{K_{eq}(T)}\right)$$

- Kinetic model fit using integral FEA model (FEMLAB©)
- Based on screened data (< 95% of equilibrium conversion)



Data Represents

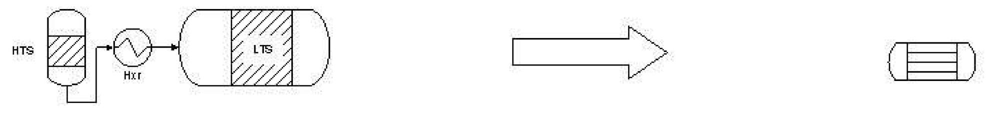
- Sud-Chemie precious metal catalyst
- HTS (14.6% CO) and LTS feed (4.5% CO)
- Temp - 225C to 450C
- Pressure - 1 to 1.3 atm
- Varied catalyst loadings
- GHSV - 23,000 to 8,000,000
- S/G - 0.2 to 0.85
- Conversions 3% - 95%
- Lowest selectivity 98.7%

Differential Temperature Approach

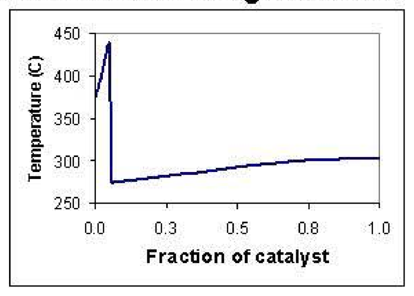
Concept: The trade-off between reaction kinetics and equilibrium with exothermic reversible reactions implies an optimal temperature profile where reaction rate is maximized, resulting in smaller reactors and optimal catalyst utilization.

Optimal temperature profiles are facilitated by integrated heat exchange in **microchannel reactors.**

Fuel Reforming Water-Gas Shift: Objective is to combine two adiabatic reactors and an intermediate heat exchanger into a single microchannel device. Size, weight, and catalyst loading further reduced by achieving a differential temperature profile. (Based on Sud-Chemie PMS5 catalyst and SR reformate.)

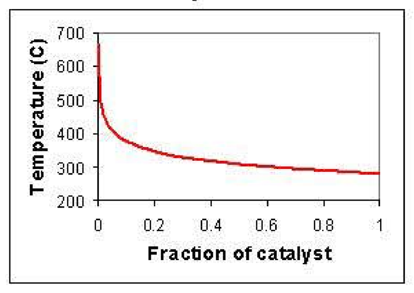


Conventional 2-stage Adiabatic



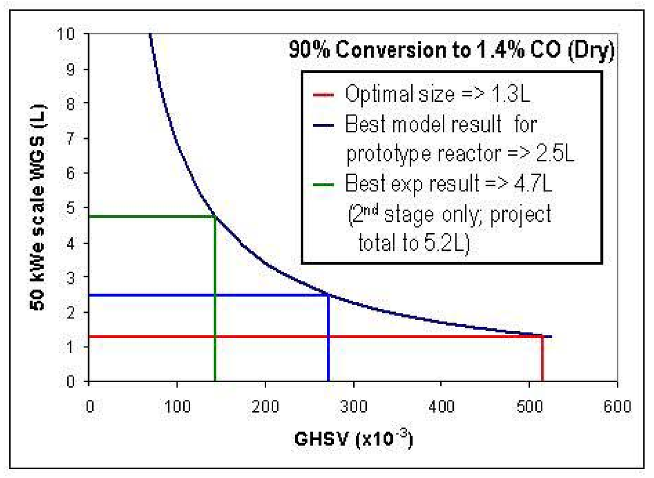
1 Integrated Unit
2.3X Less Catalyst

Ideal profile



LESS THAN 3 LITER WGS FOR 50 kWe-SCALE:

- **Based on:**
  - Sud-Chemie PMS5 precious metal catalyst
  - Kinetic model from single channel isothermal data
  - Predicted performance of prototype 7-channel reactor (blue line to the right)
- **Best multichannel result supports < 5L**
- **Potential for additional improvements**



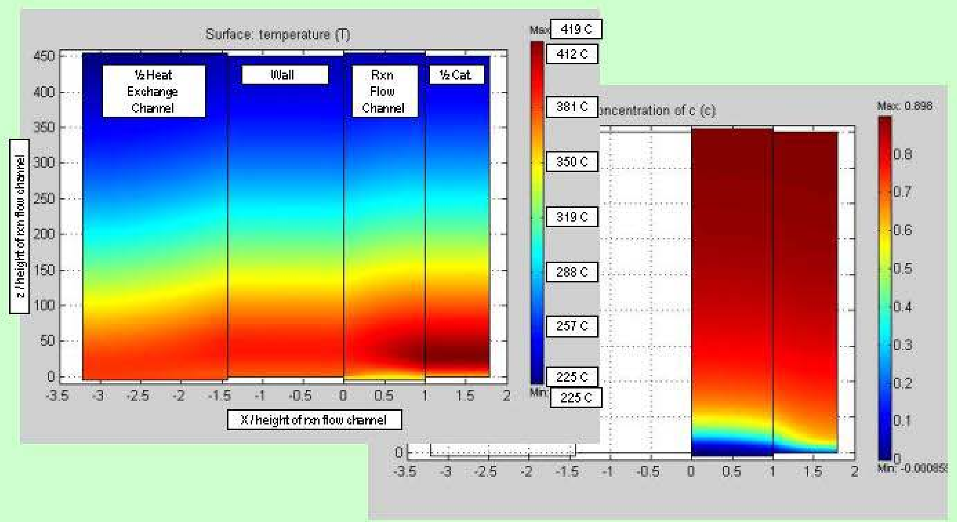
Reactor Modeling

Microchannel Reactor Modeling

- FEA Transport Modeling (FEMLAB©)
  - Mass transfer with reaction kinetics
  - Heat transfer with heat of reaction
  - Generic kinetic model
- Multi-fluid for reactor cooling / heating
  - Co-current, counter current, and cross current (3D)
- Multichannel reactors (using symmetry planes)
- Capabilities:
  - Comparison to actual performance
    - Model validation
    - Hardware diagnostics
  - Reactor design
    - To meet functional specifications
    - Optimization – catalyst activity, size, weight, or efficiency

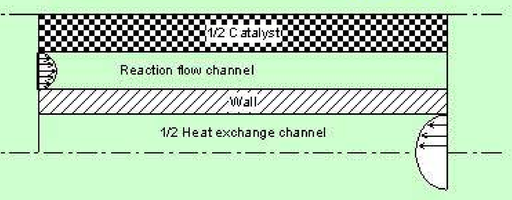
Temperature and Conversion Profiles (FEMLAB©)

- Coolant 225C Air, Reformate Inlet 350C, 285,000 GHSV (HTS feed)
- 89.7% CO conversion, 230 We power, 2.4L full-scale core volume

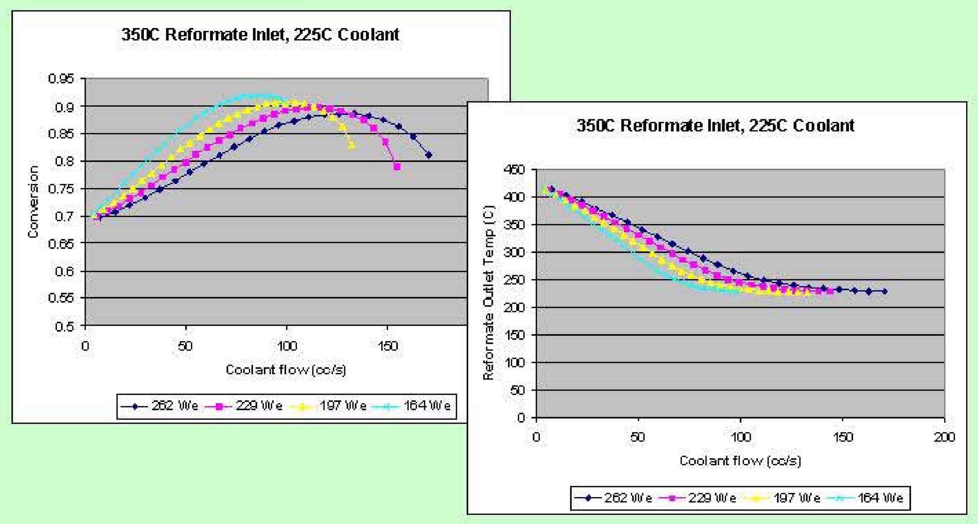


Example: Prototype 7-channel Reactor

- Predict performance
- Validate model



Parametric studies



Reactor Prototypes for Validation

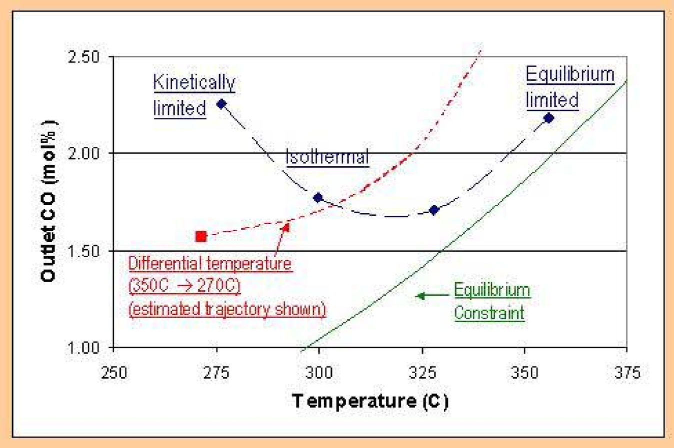
Prototype Reactor Testing

- Demonstrate concepts – differential temperature
- Support performance claims – size and weight
- Scale-up to multichannels
- Validate modeling

Example: WGS differential temperature demonstration using prototype 7-channel reactor

Isothermal to Differential Temperature Comparison

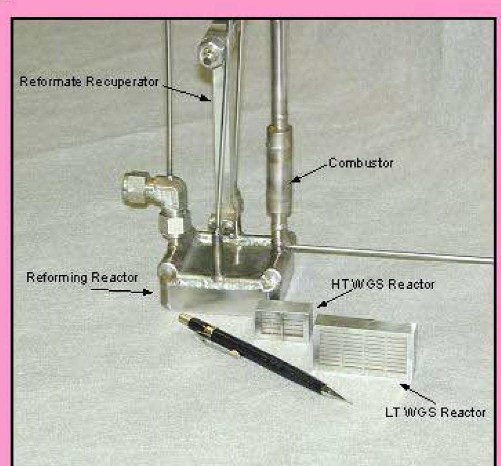
- 150,000 GHSV, 0.5 Steam/Dry Gas, 4.6% CO Feed (LTS Feed)
- Final CO concentration shown
  - Isothermal results in blue
  - Differential temperature operation (1 experiment; temperature trajectory estimated)
- **Differential temperature better than optimal isothermal or adiabatic**

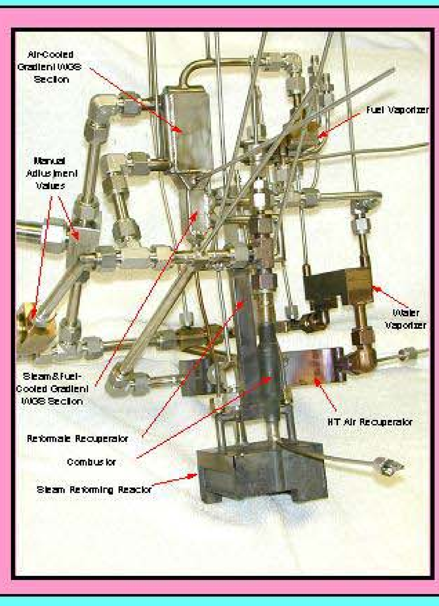


Integrate into System

Fuel Processor Integration

- Specific Design
  - Feed stream
    - HTS versus LTS
    - ATR versus SR
    - Inlet temperature
  - Efficiency - thermal integration
- Example: 200-1000 We steam reforming test stand
  - Reactant cooled front section
  - Air cooled final section





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5/15/2002