Microfluidics to Perform Hazardous Gas Phase Reactions

10.491 Presentation
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Rationale for μscale Study

• Problem
  – oxidation reactions are exothermic, explosive
  – complete combustion products have no value

• Objective
  – construct microreactor
    • improved safety through point-of-use

• Scale Up
  – improved process control, rapid implementation
Rationale for μscale Study, Cont.

• Size does Matter
  – smaller channels = smaller concentrations
  – length dimension is less than quenching distance for H₂ flame
  – enhanced process control
    • faster response time b/c surface/volume leads to efficient heat and mass transfer

• Collect data on toxic gas phase reactions
Fabrication of the Device

• Rxn: \( \text{H}_2 (g) + \text{O}_2 (g) = \text{H}_2\text{O} (g) \) \((\Delta H = -57.9 \text{ kcal/mol})\)

• Catalyst: \( \text{Al}_2\text{O}_3/\text{Pt} \) Deposition
  - \( \text{Al}_2\text{O}_3 \) deposited via Atmospheric CVD
  - Pt deposited on \( \text{Al}_2\text{O}_3 \) via wet impregnation
    @ high and low loadings

• Reactor System Design
  - Mass flow controllers, One-way valve, shut-off valves, cold trap
Microreactor/Heat Exchanger

Smaller Channel Sizes (70 µm x 100 µm) with N₂ coolant

Larger Channel Sizes (140 µm x 200 µm) with Pt/Al₂O₃ catalyst

- Stainless Steel Plates w/micromachined channels
- Stacked with 90° rotations
- Diffusion bonded
Design Concepts

- Transport Phenomena
  - Heat Transfer
    - Cross-flow heat exchangers
    - Control of reaction temperature
  - Mass Transfer
    - Concentration of reactants in nitrogen diluent
    - Mixing
- Heterogeneous catalyst options
Why Miniaturization?

- **Advantages**
  - Runaway scenario eliminated
  - More efficient heat exchange
  - Improved selectivity

- **Disadvantages**
  - Difficult to collect data
  - Equipment not readily available
  - Low production rate
Results of Study

- Concentration determines outlet gas temperature
- Low-loading of catalyst requires heaters to initiate reaction
- Induction period reduced in successive runs
- Safe operation under explosive conditions
Areas for Improvement

• Micromixers
  – Multilamination
    • $t \propto \frac{d_{sh}^2}{D}$
      – $t$ is mixing time, $d_{sh}$ is width of laminar sheets, $D$ is diffusion coefficient
    • Sinusoidal channels increase mixing area
  – Use multiple mixers in parallel
Areas for Improvement

• Heat Exchangers
  – Increase heat transfer area (diameter of coolant tubes)
  – Change coolant (increase heat capacity)
  – Change inlet temperature of coolant

• GC at end of reactor
  – Accurately determine conversion
Areas for Improvement

- Removable foils
  - Direct analysis of Pt/Alumina support
- Alumina deposition on removable foils
  - Increase response time of foils (lower heat capacity and increase reactive surface area)
  - Mimic conditions in normal reactor
Contribution of Study

- Establishes capability of safe partial oxidation for research purposes
- Provides background for further fuel cell applications
- Provides design of microfluidic device upon which better devices could be built
References