Chemical Reaction Engineering in Emerging Technologies

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Washington University in St. Louis, Missouri
Outline

• Introduction

• Emerging Technologies & CRE roles
  – Environmental Technology
  – Alternative Energies – Fuel Cells
  – Micro- & Nano-Technologies

• CRE Challenges
  – Critical Scale Down
  – Multiscale Integration
  – Interdisciplinary Efforts

• Concluding Remarks
Corning Incorporated

Founded:
1851

Headquarters:
Corning, New York

Employees:
Approximately 26,000 worldwide

2006 Revenues:
$5.17 Billion

Fortune 500 Rank:
456
A Strategic Look Back

Glass Envelope For Light Bulb

1879
A Strategic Look Back

Heat-resistant Pyrex Glass

1879

1915

CORNING | Science & Technology
A Strategic Look Back

Panels & Funnels for CRTs

Silicones
A Strategic Look Back

Glass Ceramics

1879

1915

1947

Photo-Chromatic Glasses

1957
A Strategic Look Back

1879

Early Fiber Reel

1915

Keck, Maurer & Schultz

1947

Optical waveguides developed for use in transmitting voice, video and data signals with laser beams

1970

Low-Loss Optical Fiber

CORNING Science & Technology
A Strategic Look Back

Ceramic Substrates

1879

1915

1947

1970

1972
A Strategic Look Back

1879
Alkali Free Glass

1915
The Fusion Process

Surface of glass do not touch the furnace.

1947
LCD Glass

1970 1972

1984

CORNING  Science & Technology
Recognition: National Medal of Technology

1986  Glass Ceramics and Photochromics

1994  The Company

2000  Optical Fiber

2003  Ceramic Substrates
A Culture of Innovation at Corning

1879
Glass envelope for Thomas Edison’s light bulb

1915
Heat-resistant Pyrex® glass

1947
First low-loss optical fiber

1970
LCD glass for computers and flat panel TVs

1972
Ceramic substrates for automotive catalytic converters

1984
Growth Through Innovation

• Our Culture of Innovation is built on the foundation of Research and Development

• Our commitment to innovation distinguishes Corning as a true technology leader

• Our near term growth has been fueled by three distinctly different market opportunities
  – **LCD glass** used in flat panel displays for computers, communications and entertainment
  – **Diesel emissions-control technology** for light-, medium- and heavy-duty vehicles
  – **Optical fiber**, cable and hardware for Fiber-to-the X applications
Core of CRE

Catalysis
Chemical Kinetics

Transport Phenomena

Applied Mathematics
Where Are CRE

Apply CRE core principles to new problems in emerging technologies

Apply new techniques to the more effective solution of traditional problems

Integrate the widely varied CRE activities into broad, powerful systems descriptions

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Corning Environmental Technologies

- Leading **global supplier of cellular ceramic technologies** and solutions for mobile and stationary emissions control

- New generation of **thin-wall and ultra-thin wall substrates** provide extremely high geometric surface area for improved conversion efficiency

- **Tighter diesel emission standards** worldwide drive dramatic market growth for filters and substrates

- Expanding our state-of-the-art manufacturing facility in Erwin, NY further demonstrates our commitment to meeting the demands of the burgeoning diesel market
Engine Pollutants & Substrate Products

Pollutants

- $C_mH_n$
- CO
- $NO_x$
- Soot

Three-Way Catalyst (TWC)

Diesel Particulate Filter (DPF)

Diesel Oxidation Catalyst
- LNT Catalyst
- SCR Catalyst

STOICHIOMETRIC
Gasoline Engine

FUEL LEAN
Diesel Engine
Diesel Aftertreatment Challenges

BMW Diesel.
13th DEER Conference, 13-16th August 2007 Detroit
CRE in Cellular Catalytic Converters

S. Tischer, Y. Jiang, K. W. Hughes, M. D. Patil, M. Murtagh, SAE 2007-01-1071
Toyota DPNR

(Diesel Particulate-NOx Reduction System)

NOx Storage Reduction Catalyst

Solid Oxide Fuel Cell (SOFC) R&D: CRE Roles

- Novel catalysts for fossil fuels, biomass-derived fuels
- Comprehensive models for integrated system design (heat exchanger-catalytic burner)
- Electrochemical characterization of fuel cell behaviors,
- Fundamental electrochemical kinetic studies of solid oxide cathode reactions

System description for energy balance

Single cell and fuel cell stack
A. M. Al-Qattan et al., CES, 59 (2004) 131-137
SOFC Using H₂ Fuel

Anode reaction: \( H_2 + O^{2-} \rightarrow H_2O + 2e^- \)

Cathode reaction: \( \frac{1}{2} O_2 + 2e^- \rightarrow O^{2-} \)

Net Reaction @ 650-900 C:

\[ H_2 + \frac{1}{2} O_2 \rightarrow H_2O + kWe + Q \]

Y. Jiang, S. C. Pollard, AIChE Annual Meeting, Cincinnati, OH, USA, November 1, 2005
SOFC Using Reformate

\[
\begin{align*}
\text{Anode} & : 2\text{O}^{2-} + X \rightarrow Y + 4e^- \\
\text{Electrolyte} & : 2\text{O}^{2-} \text{ ions} \quad \text{YSZ} \\
\text{Cathode} & : \text{O}_2 + 4e^- \rightarrow 2\text{O}^{2-}
\end{align*}
\]

\[\text{CH}_4 + \text{H}_2\text{O} \rightarrow 3\text{H}_2 + \text{CO} - Q\]
\[\text{CO}_2 + \text{CH}_4 \rightarrow 2\text{H}_2 + 2\text{CO} - Q\]
\[\text{CO} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{CO}_2 + Q\]
\[2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O} + Q; \text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + Q\]

External AND/OR Internal Coupling Fuel Processing & SOFC

Y. Jiang, S. C. Pollard, AIChe Annual Meeting, Cincinnati, OH, USA, November 1, 2005
SOFC System & Integration

Hydrocarbon ➔ Fuel Reformer (Endothermic)
➔ H2 Rich-Gas ➔ SOFC Stack (Exothermic)
➔ DC Power ➔ AC Power

Multiscale, Multispecies, Multi-physics System
- Thermodynamics, Transport, Kinetics Database -

Y. Jiang, S. C. Pollard, AIChE Annual Meeting, Cincinnati, OH, USA, November 1, 2005
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Internal Reforming in Anode (SOFC)

Micro- and Nano-Technologies

Corning Glass Microreactor

Mass and heat transfer

Chemistry

Reactor engineering

System engineering

C. Guemeur, Ph. Caze, O. Lobet, P. Woehl (Corning Inc.)
The 5th International Workshop on Micro Chemical Plants
January, 29-30, 2007, KYOTO University
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Critical Scale Down

- Where does the continuum concept break down?
- Complex fluids in complex flow domain

\[ J_x^* \propto \frac{\partial \Phi^*}{\partial x^*} = \frac{\Phi_2^* - \Phi_1^*}{x_2 - x_1} \]

\[ J_x \propto \frac{\partial \Phi}{\partial x} = \frac{\Phi_2 - \Phi_1}{x_2 - x_1} \]

Microscopic space

Macroscopic space

Kn < 0.01 (in continuum), ~1.0 (slip flow), > 1.0 (Knudsen flow)

LLNL Microreactor fuel processors for generating H2, chemical synthesis, & bioreaction studies.
Multiscale Transport/Reaction Fundamentals

\[ \frac{\partial C}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( D r^2 \frac{\partial C}{\partial r} \right) \]

Particle-scale Diffusion-Reaction of NOx Storage

- NOx Storage
- NOx Reduction
- Washcoat
- Substrate web
- Channel
- Monolith

Corning Celcor® substrates

\( \gamma-Al_2O_3 \) (grey); CeO_2 (white)
Multiscale Modeling Integration

Quantum

Atomistic

Meso-scale

Macro-scale

Literature

Experiment

Technical Business needs

A  B  C

D. Chowdhury (2005)
Interdisciplinary Efforts

- We don’t really understand all the physics and chemistry of many compact devices in emerging technologies
- Coupling of chemical/mechanical/electrical properties in compact devices gives rise to complex dynamics

CRE + Advanced Materials + Solid Mechanics

Meso-Scale Modelling of Reactions and Transport in Digitally Reconstructed Porous Catalyst: CO Oxidation on Pt/Al2O3, Miloš Marek, Petr Kočí, Milan Kubíček, František Štěpánek (2005)

Microstructure & simulated CO concentration:
Gaussian porous medium, $L_{xy} = 54 \text{ nm} (d_{hM}=220 \text{ nm})$, $e_{M}=15 \%$, $C_{Pt} = 50 \text{ mol/m3}$, $D_{CO} = 6 \times 10^{-8} \text{ m}^2/\text{s}$, $T=300 \, ^{\circ}\text{C}$.

Modeling crack growth in particle reinforced composites

A. Ayyar & N. Chawla (2006)
Concluding Remarks

• CRE has been expanding in scope and breadth, the strong core of CRE, however, still plays critical roles in emerging technology R&D.

• The ability to apply CRE tools and methodology to novel emerging technologies is essential.

• Emerging technologies require a greater integration of interdisciplinary skills, and it is extremely important for CRE being involved.

• Building interdisciplinary integrations in CRE curriculum and in graduate research program are crucial for CRE playing leading roles in tomorrow’s emerging technology innovations.
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