

# Devinder Mahajan

## Chemist/ Group Leader

Advanced Fuels Group, Energy Sciences & Technology Department

Tel.: (631) 344-4985; Fax: (631) 344-7905; E-mail: dmahajan@bnl.gov

B. Sc. (Honors School) (1973): Punjab University, Chandigarh, India

Ph. D. (1979): University of British Columbia, Vancouver, Canada.

### State University of New York at Stony Brook (2002 - present )

#### Research Professor

Tel.: (631) 632-1813; Fax: (631) 632- 8052; E-mail: Devinder.Mahajand@notes.cc.sunysb.edu

### Research at Chemical Engineering/Chemistry/Materials Science Interface

Research interests in design and evaluation of catalytic materials for "Future Fuels" synthesis. Synthesis of single-site and sonolysis-induced nano catalysts. Processes of interest: atom-economical methanol synthesis, methanol decomposition, H<sub>2</sub>-production for fuel-cell applications, Fischer-Tropsch (F-T) synthesis, ultra-deep hydrodesulfurization (HDS), and CO<sub>2</sub> mitigation technologies. Evaluation of materials in Batch, continuous, and mini-pilot units for process development.

## ONGOING PROJECTS

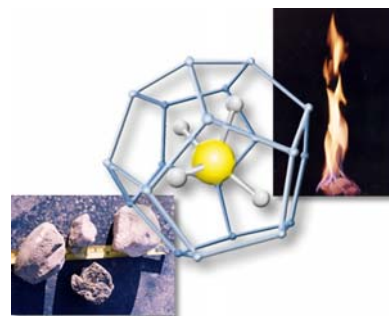
### METHANE HYDRATES

[Team: Devinder Mahajan, Keith Jones, H. Feng (Montclair State U.), T. Koetzle, G. Senum]

Our interest is in understanding fundamental issues related to methane hydrate.

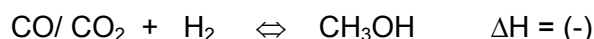
1. We have set-up a flexible unit to study hydrate Formation/Decomposition kinetics in the presence of sediments with both laboratory and natural samples.
2. We are also studying characteristics of sediments that are host to methane hydrates at X-26A/ X-27A Beamlines at the NSLS.
3. An effort is made to grow single crystals of methane hydrate that are large enough for neutron diffraction study.

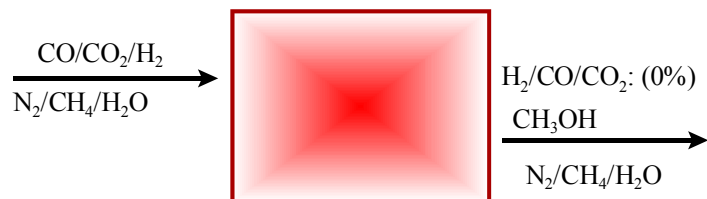
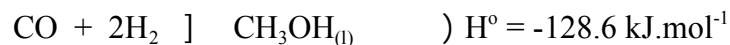
[Mahajan et al. Ann. N.Y. Acad. Sci. 912 940 (2000).



### GAS-TO-LIQUIDS: Catalytic Co-Processing of CO and CO<sub>2</sub> into Methanol

Our approach to methane conversion involves indirect route through methane-derived synthesis gas [primarily a mixture of CO, CO<sub>2</sub>, and H<sub>2</sub>] that can be catalytically converted into methanol and hydrocarbons [Fischer-Tropsch synthesis]. Since CO hydrogenation reactions are exothermic, we have developed the Liquid Phase Low Temperature [LPLT] concept to achieve atom-economical conversion at lower temperatures. Our focus is to design single-site and nano sized catalysts to affect catalytic reduction of CO. For example, methanol synthesis can be achieved with a single-site NiCl<sub>2</sub> in basic alkoxide solutions with > 95% selectivity and per pass CO conversion > 90% that eliminates gas recycle [Mahajan et al. Can. J. Chem. 79 848 (2001)].



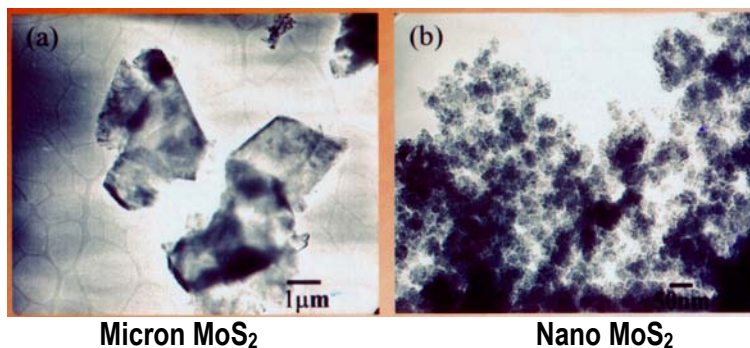


- L The “Total Carbon Utility” is a key issue to reaching the cost objectives of methanol synthesis.

We are also evaluating nano-sized catalysts for F-T synthesis [Mahajan et al. *Catal. Commun.* In press (2003)].

### HYDRODESULFURIZATION (HDS) with Nano-Phase Materials

Organic sulfur from fuels is difficult to remove. It is even more difficult to remove sulfur down to < 15 ppm. We are synthesizing unsupported and supported nano-phase materials to achieve ultra-deep sulfur removal with the premise that smaller catalyst particles can slip through sulfur-containing large aromatic rings and open the rings. We are using sonolysis (reactions catalyzed by sound waves) to synthesize nano particles of MoS<sub>2</sub> in gram quantities that are being evaluated for HDS activity to remove sulfur from transportation fuels and heavy crudes.



### Recent Publications

1. **Devinder Mahajan, Philipp Gütlich and Ulrich Stumm.** The Role of Nano-sized Iron Particles in Slurry Phase Fischer-Tropsch Synthesis. *Catal. Commun.* In press (2003).
2. **A. Naidja, C. R. Krishna, T. Butcher and D. Mahajan.** Oxidation of Fuels in the Cool Flame Regime for Combustion and Reforming for Fuel Cells. *Prog. in Energy and Combust. Sci.* In press (2003).
3. **Devinder Mahajan\* and Allen N. Goland.** Integrating Low Temperature Methanol Synthesis and CO<sub>2</sub> Sequestration Technologies: Application to IGCC Plants. *Catal. Today.* Accepted (2003).
4. **D. Mahajan, C. Song and A. W. Scaroni.** Micro-Reactor Study on Catalytic Reduction of CO<sub>2</sub> into Liquid Fuels: Simulating Reactions under Geologic Formation Conditions. International Symposium on CO<sub>2</sub> Conversion and Utilization in Refinery and Chemical Processing. Petroleum Chemistry Division. *ACS Symp. Ser. 809.* Chapter 11 (2002).
5. **D. Mahajan, V. Krisdhasima, and R. D. Sproull.** Kinetic Modeling of Homogeneous Methanol Synthesis Catalyzed by Base-promoted Nickel Complexes. *Can. J. Chem.* 79 (5/6), 848-853 (2001).
6. **D. Mahajan, T.F. Kotzle, W.T. Klooster, L. Brammer, R.K. McMullan, and A. N. Goland.** Crystal Growth, Structure Characterization, and Schemes for Economical Transport: An Integrated Approach to the Study of Natural Gas Hydrates. *Ann. N.Y. Acad. Sci.* 912 940 (2000).

7. **James E. Wegrzyn, Devinder Mahajan and Michael Gurevich.** Catalytic Routes to Transportation Fuels Utilizing Natural Gas Hydrates. *Catalysis Today*, 50 97-108 (1999).
8. **Devinder Mahajan and P. Vijayaraghavan.** Synthesis of Mixed Alcohols Catalyzed by Dissolved Base-Activated Highly Dispersed Slurried Iron. *Fuel*, 78 93-100 (1999).

## Patents

1. **D. Mahajan.** A Method for Low Temperature Catalytic Production of Hydrogen. **U.S. Patent Office Action Completed (2003).**
2. **D. Mahajan.** A Novel Liquid-Phase Low-Temperature Method for Production of Methanol from Synthesis Gas. **U.S. Patent application pending Office Action (2003).**
3. **D. Mahajan.** Sonochemical Desulfurization of Hydrocarbon Liquids Mediated by Nanometer Particles of Metals. **U.S. Patent application pending Office Action (2003).**

## Conference/Symposia Presentations

- **D. Mahajan, T. F. Koetzle, L. Brammer, W. T. Klooster, R. L. McGraw, R. K. McMullan, and G. Senum.** Structure Characterization and Sono-Stimulated Kinetic Study with Tracers in Pressure Vessels: An Integrated Approach to the Study of Gas Hydrates. Symposium on the Fundamentals of Advanced Materials for Energy Conversion, Session on Gas Clathrate Hydrates. 2002 TMS Annual Meeting, Seattle, WA, February 17-21, 2002
- **D. Mahajan.** Update of results from National Laboratories. Presented at the "Methane Hydrate Advisory Committee Meeting". Sponsored by the Office of Fossil Energy, United States Department of Energy, Woods Hole, MA. May 17-18, 2001.
- **D. Mahajan and C.L. Marshall.** Nanophase Support Materials As Catalysts for Ultra-Deep Sulfur Removal from Crude Oils and Transportation Fuels. 2000 National Laboratory Research Conference (NLCAT 2000), Argonne National Laboratory (ANL) Argonne, IL October 12-13, 2000.

## Miscellaneous

### Other Appointments

1990-93. Adjunct Professor. Department of Chemical Engineering, The University of Akron, Akron, Ohio.  
 1983-88. Adjunct Assistant Professor. Department of Natural Sciences, Baruch College, The City University of New York (CUNY), New York, NY. Taught undergraduate chemistry Lab/Lecture to business majors.  
Consultant. Power Energy Fuels, Inc., Arvada, CO (1997- present); Electric Power Research Institute (EPRI), Palo Alto, CA (1990-1993).

### Society Memberships

The American Institute of Chemical Engineers (AIChE) ; The American Chemical Society (ACS); The New York Academy of Sciences (NYAS); The American Museum of Natural History.

### Professional Recognition

2001: Secretary of Energy's 11-member National Advisory Committee on Methane Hydrate  
 2001: Chair, US DOE National Laboratories Methane Hydrate Working Group.  
 1998: Plenary Lecture, "Low temperature Methanol Synthesis" in Natural Gas Conversion Workshop, Milan, Italy.  
 1997: Annual NEDO Expert Lecture, Tokyo, Japan  
 1997: AIST Fellow, Agency of Industrial Science and Technology (AIST), Japan.  
 1992: Cited in the 1992 National Research Council (NRC) Report entitled "Catalysis Looks to the Future", National Academy Press, Washington, D. C.  
 1992- : Press releases in C&E News, Chemical Engineering, CHEMTECH, and BNL related to low temperature catalysis for clean fuels synthesis.  
 1990- : Host, various workshops related to clean fuels synthesis  
 1990-. Reviewer for Langmuir, Nano Letters, ACS Symposium Series, Energy and Fuels, Fuels, Mendeleev Communications, Annals of the New York Academy of Sciences, DOE/SBIR, OSc/DOE EPSCoR proposals, ACS-PRF grants.