Catalysis Club of Philadelphia

Thursday, January 17th, 2018
Crowne Plaza Wilmington North
630 Naamans Road, Claymont, DE 19703

Catalysis Club of Philadelphia Award Lecture

Speaker: Dr. Carmo Pereira

Engineering Industrial Catalysts: A Personal Journey

DuPont Clean Technologies

Post-Doc Speaker: Dr. Hilal Ezgi Toraman

Multiscale Modeling for Non-Oxidative Methane Coupling over an Iron/Silica Catalyst

University of Delaware

Meeting Schedule:

Social Hour .....5:30 PM
Dinner.....6:30 PM
Meeting .....7:30 PM

Meeting Fees:

Members: $40.00
Non-Members: $45.00
Stud. & Retired Members: $25.00

Menu

A tri-colored tortellini appetizer, served with a spinach side salad, crème brulee cheesecake and your choice of 3 entrees:

1) Sliced Roast Sirloin – *Thinly sliced and served with a wild mushroom bordelaise*
2) 6 oz. Baked Flounder – *Stuffed with spinach and mushrooms, topped with creamy béchamel sauce*
3) Eggplant Parmigianino – *Eggplant parmigianino with layered mozzarella cheese and Italian bread crumbs*

Meal reservations – Please register online by ***Friday, January 11th*** at http://catalysisclubphilly.org/ or notify your company representative or our Treasurer Lifeng Wang (Lifeng.Wang@pqcorp.com) or Chair Eric Sacia (Eric.R.Sacia@dupont.com)

Membership - Dues for the 2018-19 season will be $25.00 ($5.00 for the local chapter and $20.00 for the national club). Dues for students, post-docs and retirees will be $10.00 ($5.00 for local club and $5.00 for national club).

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Dr. Carmo Pereira

Catalysis Club of Philadelphia Awardee

Engineering Industrial Catalysts: A Personal Journey

DuPont Clean Technologies

Abstract: Industrial reactors enable chemical transformations that may upgrade the quality of the feed, produce chemicals, and/or reduce process pollutants. The catalysts in these reactors are engineered to obtain the required (steady state) throughput of product over a certain time. In addition to throughput, there are additional commercialization constraints that involve cost, uptime, emissions, and project timing. The proper design of the catalyst and reactor often is key to the successful deployment of the process.

In addition to identifying the active site and the reaction mechanism, additional *application development* work is required to commercialize a catalyst. The active site must function within a range of operating conditions and in the presence of impurities that may impact activity and selectivity. Reactor pressure drop constraints can dictate the size and structure of the catalyst. The availability of active sites in a pellet is maximized by optimizing its size, shape and pore structure to minimize heat and mass transport limitations. The number of active sites in a catalyst may dramatically decrease with time due to poisoning, masking, sintering, or pore blockage. An understanding of the deactivation mechanism under operating conditions provides a basis for the reactor operating strategy and for sizing reactors that have a warranted life. A process flowsheet containing a *useful* reactor model may be subsequently value-engineered to cost-effectively meet the processing objective.

This talk will present several vignettes from the author's experience where chemical reaction engineering methodologies were used to engineer industrial catalysts used in petrochemical, chemical, and environmental applications.

Speaker Details: Carmo Pereira works in the Clean Technologies Division of the DuPont company. His prior role at DuPont was as an internal catalysis and chemical reaction engineering consultant in the Engineering Department. Before joining DuPont, he led catalyst R&D projects at the Research Division of W. R. Grace and was a process engineer at Mobil R&D Corporation.

Carmo's research contributions are in petroleum processing and environmental catalysis. He has over 80 patents and publications and has edited a book on catalyst design. His service contributions are primarily to the

American Institute of Chemical Engineers (AIChE) and to the International Symposium on Chemical Reaction Engineering (ISCRE). He has taught courses in chemical engineering opportunistically at nearby universities and for AIChE's continuing education initiative. He also has served on the external advisory boards of several chemical engineering departments.

Carmo has received several awards including the Distinguished Young Engineer Award from the Maryland Academy of Sciences (1990), the Chemical Engineer of the Year Award from the Maryland Chapter of AIChE (1991), the Practice Award from the AIChE CRE Division (2007) and the Lawrence B. Evans Award in Chemical Engineering Practice from the AIChE (2014). He is an AIChE Fellow.

Carmo obtained a bachelor's degree in chemical engineering from the Indian Institute of Technology, Bombay, and a Ph.D. from the University of Notre Dame. He has a MBA in finance from Drexel University.

Multiscale Modeling for Non-Oxidative Methane Coupling over an Iron/Silica Catalyst

Hilal Ezgi Toraman, Konstantinos Alexopoulos, and Dionisios G. Vlachos

Delaware Energy Institute, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA

Abstract: The production of large amounts of shale gas, lower overall costs, and sustainability concerns have generated interest for the production of chemicals directly from methane. Currently, methane is converted into fuels and chemicals through syngas, an energy intensive and large capital investment process. A recent study has reported that isolated iron atoms embedded in a silica matrix ($Fe@SiO_2$) enables direct conversion of methane to ethylene under non-oxidative conditions at high temperatures (1223 – 1363 K). It has been suggested that methane conversion is initiated by catalytic generation of methyl radicals and hydrogen followed by subsequent gas-phase reactions.[1] Although the concept was demonstrated experimentally, fundamental understanding of the reactions is missing. In this study, we model this process by combining detailed catalytic and gas-phase reaction mechanisms. The latter includes up to 600 species and 10,000 reactions. For the former, we investigate the C-H activation of methane and C-C coupling reactions using density functional theory (DFT) calculations. The simulations are performed using the state-of-the-art multiscale kinetic modeling software, OpenCK. The combined catalytic and gas-phase reaction mechanisms allow not only to capture the trends in terms of conversion and selectivity but also allow to assess the predictive capability of the model. Microkinetic simulations show that ethylene is the only primary product among the major species including acetylene and higher molecular weight aromatics. The complex interplay between catalytic and gas-phase reactions lead to higher hydrocarbons and acetylene whereas consumption of ethylene. Reaction path and sensitivity analyses are carried out to delineate the dominant paths, the contribution of each phase on conversion and selectivity, and how to optimize the process. Overall, the present study exemplifies the interplay between catalytic and gas phase reactions that controls selectivity.

1. Guo, X.; Fang, G.; Li, G.; Ma, H.; Fan, H.; Yu, L.; Ma, C.; Wu, X.; Deng, D.; Wei, M.et al. Direct, nonoxidative conversion of methane to ethylene, aromatics, and hydrogen. Science 2014, 344 (6184), 616.

Acknowledgments: This material is based upon work supported by the Department of Energy's Office of Energy Efficient and Renewable Energy's Advanced Manufacturing Office under Award Number DE-EE0007888-9.5.

Speaker Bio: Dr. Hilal Ezgi Toraman is a postdoctoral researcher in the Vlachos Research Group, at the University of Delaware. Her postdoctoral research focuses on experimental and computational investigation of shale gas conversion to fuels and chemicals. She received her B.Sc. and M.Sc. degree in Chemical Engineering from Middle East Technical University, Turkey. She received her Ph.D. degree in Chemical Engineering from Ghent University, Belgium under the supervision of Prof. Kevin Van Geem and Prof. Guy Marin. She was awarded a graduate research fellowship in Belgium and was the recipient of a prestigious scholarship for her M.Sc. study from the Scientific and Technological Research Council of Turkey (TUBITAK) which is awarded only to few chemical engineers in Turkey. Her research interests are in the field of chemical reaction engineering, catalysis, data science and microkinetic modeling.