The Catalysis Club of Philadelphia

Thursday, October 20th, 2022

Brandywine Plaza Hotel
630 Naamans Road, Claymont, DE 19703

Speaker: Dr. William G. Borghard

Optimization and Scale-Up of Catalyst Manufacturing Unit Operations

Rutgers University

Student Speaker: Peter Corkery

Simulation of Zinc Oxide Atomic Layer Deposition in Mesoporous Substrate for Improved Zeolitic Imidazolate Framework Membrane Synthesis

Johns Hopkins University

Meeting Schedule:

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

Meeting Fees:

Members: $45.00
Non-Members: $55.00
Stud. & Retired Members: $35.00

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Meeting and Meal reservations – Please register online by ***Thursday, October 13th*** at http://catalysisclubphilly.org/meeting-registration-with-paypal/

Or contact our Treasurer Steve Hardwick (sjh.wilm.de@gmail.com) or Chair Udayshankar Singh (udayshankar.singh@grace.com)

Membership – Dues for the 2022-23 season will be $25 ($5 for the local chapter and $20 for the national club). Dues for students, post-docs and retirees will be $10 ($5 for the local club and $5 for the national club).

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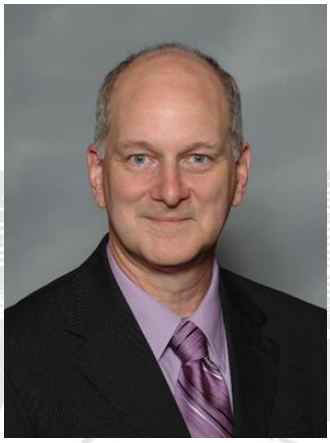


Dr. William G. Borghard

Optimization and Scale-Up of Catalyst Manufacturing Unit Operations

William G. Borghard and Benjamin J. Glasser

Department of Chemical and Biochemical Engineering, Rutgers University, NJ 08854

Abstract:

In the field of heterogeneous catalysis, much effort has focused on the identification of adsorbed species on the finished catalysts and reactive intermediates during the catalytic act. In contrast, the preparation of the solid catalysts has long been regarded as mostly technical know-how [1]. Many aspects of the various catalyst manufacturing steps are not fully understood, and in industry, the design of manufacturing processes is often based on trial and error, which can lead to sub-optimal processes and decreased quality. Poor catalyst quality may not be apparent until the latter stages of scale-up, at which point the ability to change the manufacturing process is constrained by parameters chosen early in the catalyst development. By combining the substantial level of expertise in particle technology and optimization, available at Rutgers, we are developing and promoting science-based methods for designing, scaling up and optimizing catalyst manufacturing processes as part of the Rutgers Catalyst Manufacturing Consortium. A combination of experiments and computer models has been used to improve the understanding and performance of unit operations used to make catalysts. Current projects on drying, impregnation, calcination, and powder handling and characterization will be highlighted. By way of an example, we will discuss in more detail results on scale up of rotary calcination in terms of heat transfer and residence time distribution.

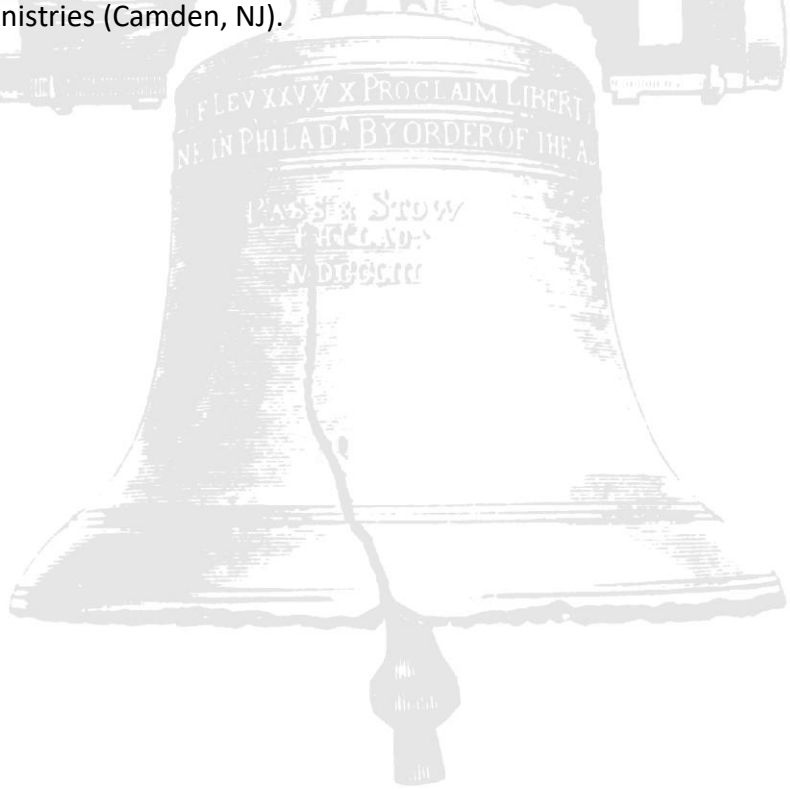
1. Lambert, J.F. and Che, M., The molecular approach to supported catalyst synthesis: state of the art and future challenges. *Journal of Molecular Catalysis A*: Chemical, 162, 5-18, (2000)

Speaker Bio:

Currently, Dr. William G. Borghard is a consultant in the area of catalysis. In particular, he is the industrial liaison for the Rutgers Catalyst Manufacturing Consortium, based in the Chemical and Biochemical Engineering Department at Rutgers University.

Bill retired from ExxonMobil in 2013 after 32 years with the company. He started at the Mobil Paulsboro Lab in 1980. In 1982, Bill transferred to Mobil's lab in Princeton working in exploratory research and lab automation. In 1992, Bill returned to Paulsboro, where he had assignments in reforming, light gas upgrading, and catalyst characterization. Subsequently, he moved to the Clinton labs of ExxonMobil, where he led a number of major R&D projects, including GTL catalyst development, novel diesel catalysts, Algae BioFuels, and resid upgrading. Bill is an inventor or co-inventor on 24 U.S. patents.

Prior to joining Mobil, Bill graduated from Stanford University with a Ph.D. in chemical engineering under the tutelage of Michel Boudart. He also obtained and M.S. and B.S. in chemical engineering from the University of Connecticut where he studied under C.O. Bennett. He volunteers for Seeds of Hope Ministries (Camden, NJ).



Simulation of Zinc Oxide Atomic Layer Deposition in Mesoporous Substrate for Improved Zeolitic Imidazolate Framework Membrane Synthesis

Peter Corkery

Advisor: Prof. Michael Tsapatsis

Johns Hopkins University

Zeolitic imidazolate framework-8 (ZIF-8), a type of metal-organic framework with the topology of a sodalite zeolite, has been identified as a potential candidate for propylene-selective gas membrane systems for the separation of propane and propylene mixtures due to its effective pore aperture size of about 4Å. All-vapor phase synthesis of ZIF-8 membranes for the separation of propane/propylene mixtures with high propylene selectivity and permeance has been accomplished using the ligand-induced permselectivation (LIPS) method. This method relies on an intermediate step wherein atomic layer deposition (ALD) of zinc oxide (ZnO) is used to completely block the pores of a mesoporous substrate followed by a conversion of said layer to ZIF. In contrast to typical ALD processes on porous substrate, the LIPS method seeks to minimize the penetration depth of ALD precursors, thereby reducing the thickness of the pore-blocking ZnO layer controlling and maximizing the resulting membrane permeance. To improve the understanding of this process, a computational fluid dynamics (CFD) model was developed to determine the spatiotemporal distribution of ALD precursors within a commercial ALD reactor, and a reaction-diffusion model was used to describe the deposition and intrapore diffusion of diethylzinc. Kinetic rate constants were fit such that the modelled penetration depth of zinc surface species matched that of ZnO measured experimentally from a membrane cross-section. The reaction-diffusion process of diethylzinc was determined to be diffusion-limited due to the high rate of adsorption to hydroxyl groups relative to the rate of surface diffusion. The flux of diethylzinc into the substrate had a negligible effect on the concentration profile within the reactor, allowing the CFD model to be decoupled from the reaction-diffusion problem. Later modelling built on these results to determine the pore diameter as a function of depth and ALD cycles for different precursor dosing procedures. These results and models can be used to inform the design of scaled up membrane systems and the ALD reactor designs necessary to effectively synthesize these systems.

Speaker Bio

Peter Corkery completed bachelor's degrees in chemical engineering and chemistry at the University of Minnesota in 2018 and began his PhD in the Department of Chemical and Biomolecular Engineering under the direction of Professor Michael Tsapatsis at Johns Hopkins University in 2018. His research is focused on the vapor-phase growth of zeolitic imidazolate frameworks and their potential for use in membranes for gas separations and as a photoresist material for the synthesis of electronic devices.