Predictive Kinetics: Examples and Challenges

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Design relies on predictive models. Historically, we had only limited ability to predict the products and rates of individual reactions, and could not predict the kinetics of complicated reacting systems, so design of new processes involving chemical reactions was forced to be incremental, relying on large numbers of experiments. This weakness in prediction slowed innovation. However, in recent decades it has become feasible, using quantum chemistry and a combination of several modern modeling methods, to build computer simulations that quantitatively predict complicated reaction systems. I will give an overview on the algorithms and extensible open-source software and databases which have made the new capability to predict kinetics available to everyone. Examples will be presented, including several models created by National Taiwan University alumni using RMG, which demonstrate how accurate the predictions can be, even for quite complicated systems. However, the predictions are never perfect. The sources of the inaccuracies are explained, with suggestions on how the models can be improved. The new capability to predict how product mixtures change as the reaction conditions or the molecules in the feed are varied opens many new opportunities. The current status of predictive chemical reaction engineering, how it can be implemented in process design, and some challenges and prospects for the future are discussed.

About the speaker: William H. Green is the Hoyt C. Hottel Professor at MIT. He earned his B.A. at Swarthmore College and his Ph.D. at the University of California. After postdocs at Cambridge University and the University of Pennsylvania, he worked at Exxon Research & Engineering for 6 years, then joined the faculty at MIT in 1997. He is the world leader in automated predictive chemical kinetics, and also a leader in the use of machine learning for chemistry. He has published more than 300 journal articles and his papers have been cited more than 20,000 times. In 2020 he co-founded Thiozen, a company commercializing a novel route to clean H_2 invented in his lab. He is a Fellow of the American Association for the Advancement of Science and a Fellow of the Combustion Institute, and has received several major awards including American Chemical Society's Glenn Award in Energy & Fuels and the American Institute of Chemical Engineers' R.H. Wilhelm Award in Reaction Engineering.