Dr. Mark Saeys wins Richard A. Glenn Award

Dr. Saeys and co-workers bridged the gap between molecules and industrial processes for cheaper steam cracking and cleaner combustion

Dr. Mark Saeys of the ChemBioSys Group was honored by the American Chemical Society for his work on new, computer-discovered pathways for methane and ethane pyrolysis. The work was done in collaboration with David Matheu (National Institute of Standards and Technology), Jeffrey Grenda (ExxonMobil) and William Green (Massachusetts Institute of Technology).

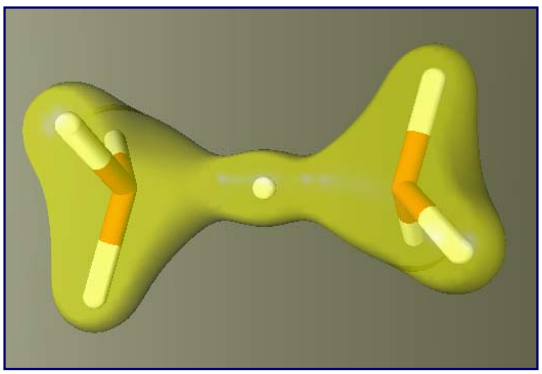

Figure 1. Quantum Chemistry: A New Tool for Chemical Engineers.

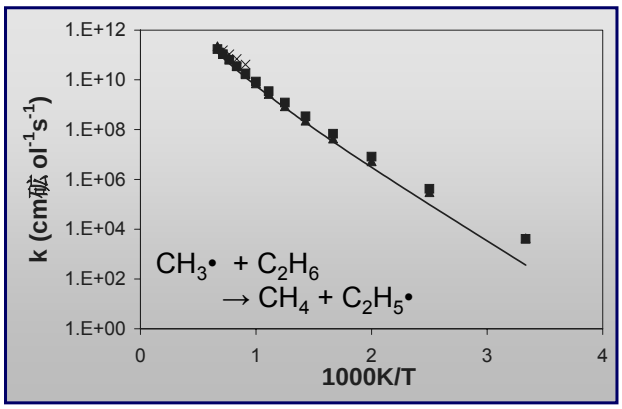

Figure 2. Quantum chemical calculations (line) can predict experimental reaction rates (data points).

Pyrolysis ("breaking up molecules by heat") is the most important process for the production of light olefins, the building blocks of the chemical, plastic and pharmaceutical industry. But pyrolysis is a very complex process that can involve thousands of reactions and products.

Modeling pyrolysis by manual means is nearly infeasible. We are developing new computer assisted techniques and algorithms to understand pyrolysis and combustion and to direct it to the products we need. With such models we have been able to explain a 30-year old problem in the pyrolysis of methane, match industrial data (Figure 3), and suggests new solutions.

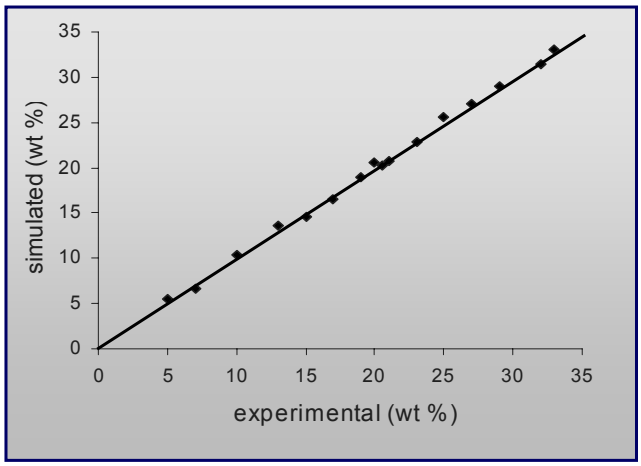

Figure 3. Comparison between industrial and simulated ethylene yields.

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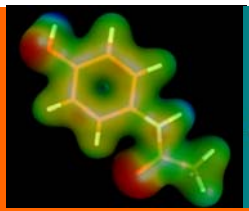

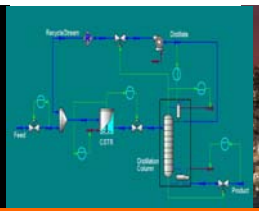

ChemBioSys @ NUS

Engineering Systems from Molecules to Multinationals