

Public summary of PhD-thesis of Aditya Sengar

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Understanding catalytic reactions for the production of cleaner gasoline

Catalysts – substances that increase the rate of a chemical reaction without being consumed - have greatly transformed the process industries that generate high quality fuels. A molecular understanding of catalyst performance under reactor conditions is the next step industries are focusing on. Researcher Aditya Sengar has developed computational methodologies that can predict products that are formed even when the activity of the catalysts has decreased. Such understanding can save industries millions of dollars in operational costs by performing reactions under optimized conditions while reducing unnecessary coproduct formation.

Our energy consumption has tremendously increased in the last hundred years. Technical revolution and industrialization, which also increase quality of human life, contributes a substantial part of this increase. From transportation to electricity, energy drives the world.

Nowadays, about 90 percent of the world energy needs are met by the combustion of fossil fuels. Not only do fossil fuels account for majority of CO₂ emissions, but they are also limited in availability. The solution to this rising energy crisis problem can only be solved by meeting short term goals with a longer term perspective in mind. Short term goals refer to the optimization of industrial processes that lead to the formation of petrochemical products and natural gas. The future, however, demands a transformation in the landscape of energy production with more focus on the production of energy by renewable sources like wind, water etc.

In this work, we focus on finding such a short-time solution. A better understanding of the chemical reaction over a catalyst and its response to the process conditions can help save petrochemical industries millions of dollars by reducing operational costs. Besides, switchover from liquid acid catalyst to solid acid catalysts itself is a field under active research because of the environment-friendly nature of such catalysts.

Understanding a chemical reaction is not an easy task because of the multiscale nature of the problem. With the huge boost in computational powers in the recent years, it has become relatively easy to write computer programs that solve these chemical reactions under different process conditions by simplifying information, for example assuming simplified kinetics for a reaction process.

In the first part of our research, we have developed a computational methodology that can simulate a large chemical reactor (1 meter) with a complex reaction occurring inside catalyst pores of micrometer size. Transport processes (convection and diffusion) are relevant at this scale as they bring reactant species near catalyst where reaction occurs. We have employed probabilistic algorithms over coarse-grained reaction mechanisms occurring at nanometer scales.

In the next part, we focus on understanding catalyst deactivation in the important alkylation reaction, which is used to produce a wide variety of petrochemical products. For the past 30 years disconnected theories have co-existed explaining the cause of a quick catalyst deactivation in the alkylation reaction. Our work brings a breakthrough in this field. Using quantum-chemical information, we were able to simplify the overall reaction into a few important steps, which were then studied under different reactor conditions.

Our theoretical framework is the first of its kind to use quantum-level information of a catalytic reaction and perform long time simulations to predict catalyst behavior. Although this has been performed for a single reaction, understanding catalyst activity for different reactions is critical to transform the process engineering landscape and improve quality of the fuel produced.

Title of PhD-thesis: Multiscale reaction kinetics in different flow regimes. Supervisor: prof.dr.ir. J.A.M. Kuipers (TU/e), Co-supervisors: prof.dr. R.A. van Santen (TU/e), prof.dr.ir. J.T. Padding (TU Delft). Other main parties involved: MCEC.