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# Automatic generation of kinetic models with evolving surface site densities

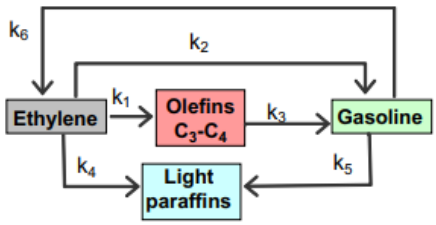
## Aim

Developing a code for kinetic modelling of catalytic reactions in which the surface site density evolves in time, i.e., the number of sites decreases as a function of time due to catalyst deactivation.

## Justification

KASTER is an in-house software tool for the generation of kinetic models [1]. Based on user-specified input information, such as a reaction network, reaction conditions and experimental data, a kinetic model is generated and the corresponding kinetic coefficients can be determined by regression to the data. The output of the tool consists of the model predictions for the dependent variables, as well as the estimated kinetic coefficients including a statistical analysis.

A novel addition to the tool would be the automatic generation of kinetic models for reactions in which the number of sites on the catalyst evolves in time. In this case, the total number of sites $L_{tot}$ is not a constant and the deactivation of catalytic sites as a function of time should be accounted for. An example of a reaction which is associated with catalyst deactivation is ethanol-to-hydrocarbons [2], which is catalyzed by acid catalysts such as zeolites and is prone to catalyst coking. In this reaction, ethanol, which includes bioethanol produced from biogas, is first dehydrated to ethylene, which is then converted to higher hydrocarbons, as in the figure below [2]. To test the developed Fortran code, it will be tested on an existing ethanol-to-hydrocarbons dataset as a case study.




## Program

- Literature study on catalyst deactivation and kinetic modelling methodologies to model changes in surface site density
- Development of a Fortran code for the estimation of kinetic parameters for catalytic reactions with changing surface site densities
- Testing of the code on an ethanol-to-hydrocarbons dataset as a case study

1. Metaxas, K., et al., Topics in Catalysis, 2010. **53**(1): p. 64-76.
2. Gayubo, A. G., et al., Chemical Engineering Journal, 2011. **167**(1): p. 262-277.