FACULTY OF ENGINEERING AND ARCHITECTURE

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Technologiepark 125, 9052 Gent, Belgium

PROJECT OF KINETIC MODELING AND SIMULATION

KINETIC MODELING OF EXPERIMENTAL DATA FROM A CATALYSED REACTION

The case of "n-Hexane hydrocracking"

Report format and deadline

The report should be concise and can contain a maximum of 5 pages excluding figures, tables and references which are expected at the end of the report as an appendix (Font Arial 11 or Times New Roman 12, 1.5 spacing and normal margins). The deadline of handing in the report, presentation file and python codes is 5th of December, 2025. Send your files to Raman.Ghassemi@UGent.be and Russel.AnchamparuthySalim@UGent.be with your group members in CC.

Background

Hydrocracking is catalyzed by a bifunctional catalyst, i.e., both metallic and acid sites are available. A schematic representation of the reaction mechanism for n-hexane hydrocraking is presented in figure 1. In summary, first, the gas phase alkanes are physisorbed at the catalyst surface. Thereafter, it interacts with a metallic site by which it is dehydrogenated. The alkene formed can be protonated by an acid site after which it can react via isomerization and/or cracking. Typical isomerization reactions are the 1,2 alkyl shifts and PCP-branching. Cracking occurs via β-scission. The carbenium ions formed can be deprotonated, hydrogenated and desorb, leading to gas phase alkane products.

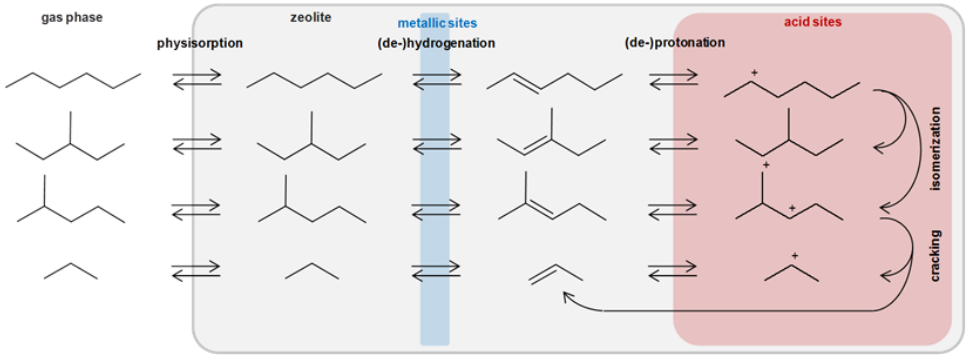


Figure 1 - Reaction scheme for n-alkane hydrocracking

Modeling

In the following section, you will find a series of tasks and steps designed to guide your analysis and modeling of the experimental results. These questions represent the minimum expected work; however, you are encouraged to explore further, investigating trends, testing additional models, and pursuing any insights you find meaningful.

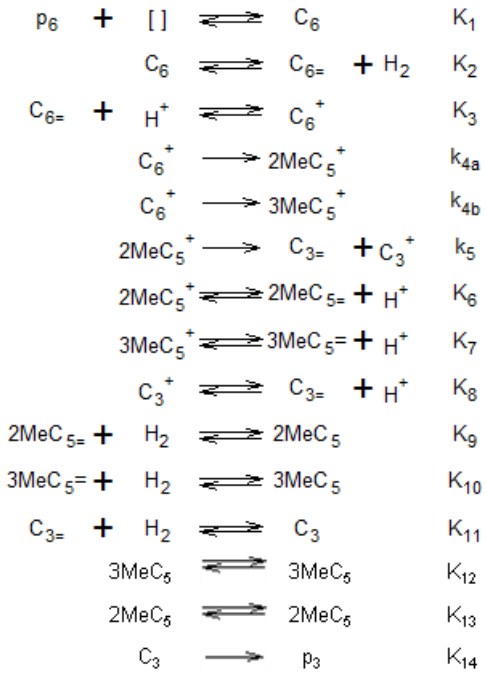
Question 1

Based on the analysis of the experimental data, what are the operating conditions that play a relevant role on the hydrocracking of n-hexane?

Hint: The key variables in catalyzed reactions are activity, selectivity, and stability.

Question 2

The reaction mechanism translates to the following elementary steps.



where:

[ ]	free site for physisorption
p	partial pressure of a molecule in the gas phase
=	alkene
+	carbenium ion

The following assumptions can be made concerning the elementary steps:

a. Physisorption is assumed to be in quasi-equilibrium and the concentrations of the physisorbed alkanes can be determined via a Langmuir isotherm. The physisorption coefficients of *n*-hexane and its isomers can be taken equal while the physisorption coefficient of propane is assumed to be zero.
b. (de-)Hydrogenation at the metallic sites is in quasi-equilibrium.
c. (de-)Protonation at the acid sites is in quasi-equilibrium.
d. The concentration of the reactive intermediates, i.e., carbenium ions, at the acid sites is negligible concerning the total concentration of active sites.

Leading to the set of equations for the rate –determining steps (steps 4a, 4b and 5).

Hint/reminder: Similar to tutorial 4, lump kinetic parameters in the reaction rate equation's numerator.

Based on this mechanism, and the given assumptions, first derive three rate equations. Then, perform the regression by implementing the kinetic model in the reactor model and estimating the model parameters.

1. First, perform an isothermal regression for every temperature, yielding estimates for the rate coefficients at every temperature.
2. Secondly, perform a non-isothermal regression. Use good initial parameter values and clarify why this is necessary.
3. For non-isothermal regression, use Arrhenius and Van't Hoff equations in their original and reparametrized formats and compare the estimated parameters and modeling results. Do you see any difference?
4. assess the model performance and statistics, and comment on the statistical and physical significance of the estimated parameters.

Question 4

Based on the parameter estimates obtained for the model,

1. Discuss the estimated parameters.
2. Is there any improvement you could propose to the model? justify briefly how the new approximation can improve the results. Performing a regression with the suggested changes is not needed.

Experimental details

Experiments are performed in a Berty-type reactor (CSTR) on a Pt/H-ZSM-5 catalyst. The following experimental results can be found in the corresponding excel sheet of the project.

F^0_{C6} [µmol s^{-1}]	F^0_{H2} [µmol s^{-1}]	Pressure [bar]	Temperature [°C]	W_{cat} [g]	F_{2MeC5} [µmol s^{-1}]	F_{3MeC5} [µmol s^{-1}]	F_{C3} [µmol s^{-1}]