Responses to Review of Ph.D. Dissertation: Algorithm Development to Support Reaction Characterization in Multicomponent Mixtures

Title of Dissertation: Algorithm Development to Support Reaction Characterization in Multicomponent Mixtures

Candidate: Hamadi Omar Péter

Reviewer: Dr. Szabó László

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Dear Szabó László,

I would like to sincerely thank you for your thorough and thoughtful review of my thesis. Your valuable feedback and constructive comments have greatly contributed to improving the quality of my work. I truly appreciate the time and effort you dedicated to this process.

Thank you once again for your time and support!

Your sincerely,

Hamadi Omar Péter

Budapest, 23. April 2025.

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Hamadi Omar Péter

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Question:

Chapter 3: How can you develop the model equations to describe the effect the pressure change?

Answer:

The pressure dependence of hydrocracking can be incorporated into kinetic models in several ways. One approach is empirical, often based on Langmuir-Hinshelwood-type expressions, where the reaction rate is modeled as a power function of the partial pressure of hydrogen. Another method considers the solubility of hydrogen, using the concentration of dissolved hydrogen to describe its effect on the reaction rate, which is especially relevant in liquid-phase systems. In this thesis, the estimation of hydrogen solubility is discussed, and in future work, it would be feasible to integrate both approaches into a unified kinetic model.

Question:

Chapter 4: Why identification reach α2 upper limit of the M2 model? Do you tried to expand the range of identification.

Answer:

Figure 4.2-2 shows that when the parameter reaches its upper limit of 1000, values beyond this range have no impact on the model's performance. Moreover, the parameter approaching this upper bound indicates that the only difference between the M1 and M2 models lies in the stoichiometry considered exclusively in M2.

Question:

Chapter 5: The presented method helps to identify the best thermodynamic model (TM) for process simulation. How can you identify the best TM if the required domain of the simulation is wide, and more than one TM is suggested based on the results?

Answer:

By evaluating the performance of each thermodynamic model (TM) under varying conditions such as pressure and temperature, and by calculating prediction errors like MSE and mapping application domains with Gath-Geva clustering, it becomes possible to pinpoint the optimal performance regions for each model. If selecting a single TM is preferred, the model with the lowest overall prediction error serves as a strong candidate for best overall performance.

Question:

Chapter 6, Figure 6.5-1. On right and left-hand side of figure there are sequence of points, these points could be homologous series? The developed method capable to find the homologous series?

Answer:

That's a very good observation! Indeed, if we plot the Kováts retention index on the x-axis and the carbon number on the y-axis for a homologous series, a clear linear trend can be observed in the retention indices. This linearity is a result of the normalization method inherent in the

definition of the Kováts index, which is specifically designed to provide consistent, comparable values across homologous compounds. Because of this, such linear trends become visually apparent and meaningful when analyzing retention behavior.