Theses of the doctoral (PhD) dissertation

Algorithm Development for Reaction and Composition Characterization in Multicomponent Mixtures

Omar Péter Hamadi

University of Pannonia

Doctoral School of
Chemical Engineering and Material Sciences

Supervisor:

Tamás Varga, PhD

Alex Kummer, PhD

Department of Process Engineering

Veszprém

2024

1 Introduction and the aim of the work

Models are an essential part of every type of industrial activity. Based on their complexity, models can rely on a few equations or be expressed in complex mathematical terms. In the case of chemical reactors, the mathematical model should contain the proper thermodynamic and kinetic equations. The most detailed kinetic model possible, which describes the reaction system includes all the reactions that every single component in the system undergoes. When dealing with a multi-component mixture, it is a difficult task to consider all reactions of every single component, and the proper validation of this kind of complex model is simply not feasible. Even, if it is possible to measure the change in the concentration of each component, (in a complex reaction system) the isolation of the effects of the different reactions on one component concentration is possible only with a high level of uncertainty. To solve these tasks, in the past few decade researchers have been developed two main approaches (lumped and molecular models), in which model simplification and order reduction became central problems.

In this work, various approaches to modelling complex chemical processes and phenomena are investigated, drawing on mathematical models. Key aspects include the development of lumped models to describe catalytic hydrocracking experiments, providing insights into the phenomena of catalyst fouling and the development of yield distribution functions. Additionally, the study delves into the selection and optimization of thermodynamic models for hydrogen solubility in hydrocarbons, emphasizing the importance of proper model selection based on operating conditions. Furthermore, a method is proposed to address retention time drifts in gas chromatography analyses of complex mixtures, enabling easier comparability and analysis of chemical changes during processes like plastic waste pyrolysis. Moreover, computational methods integrating molecular similarities and Kovats retention index are explored to refine qualitative analysis in catalytic pyrolysis processes. Despite computational challenges, the study demonstrates significant insights into molecular composition estimation, underscoring the need for further refinement and validation of computational techniques using high-level measurement properties.

2 Theses

Thesis #1. I extended the discrete-lumped modeling approach by incorporating catalyst deactivation models to provide a more complex description of catalyst fouling.

- I have investigated catalyst deactivation phenomena in case of hydrocracking of sunflower oil and kerosene mixture. The investigation includes development of lumped models to describe the chemical system, moreover catalyst deactivation models were integrated into the kinetic model to improve estimation performance.

Related publications: 1

Thesis #2. I revised the continuous-lumped modeling approach to better describe the spatial and temporal changes in a hydrocracker reactor.

- I have developed a novel continuous lumping approach to model hydrocracking chemistry, enabling to analyze changes over time and space to optimize residence time and selectivity for enhanced process efficiency. Furthermore, I have developed a Gaussian mixture model to optimize the model selection for solubility estimation of hydrogen under varying operating conditions.

Related publications: 2, 5

Thesis #3. I developed new computational methods for qualitative analysis in catalytic pyrolysis by integrating molecular similarity measures and retention indices to refine the estimation of molecular compositions

- I have developed computational methods integrating molecular similarities and retention indices to refine the estimation of molecular compositions in catalytic pyrolysis. The first part of this development involved a fast and simple clustering algorithm to eliminate time drifts between chromatograms using easily accessible prior information.

- The second part consisted of formulating and solving a linear programming problem that applies molecular similarity measures to further refine the estimation of molecular compositions.

Related publications: 3, 4

3 Utilization of the results and future aims

Overall, the thesis underscores the importance of advanced computational techniques, and innovative modeling approaches in advancing sustainable energy production and waste management practices within the chemical engineering domain. Each chapter contributes unique insights and methodologies towards optimizing chemical processes for environmental and economic sustainability.

Further steps may include the introduction of a novel model, based on the extended continuous lumping approach and the developed approach for hydrogen solubility estimation. The combination of those two approaches would be resulted in an accurate model which can estimates the pressure dependency as well. Moreover, the developed molecular composition estimation can be the cornerstone for a new, single-event type modelling approach, in which the estimated composition would be the basis of reaction pathway identification.

4 Publications related to theses

Articles in international journals

1. Hamadi, Omar & Varga, Tamás & Till, Zoltán & Eller, Zoltán & Hancsók, Jenő. (2019). Model based investigation of catalyst fouling in case of special hydrocracking of sunflower oil and kerosene mixture. Energy & Fuels. 33. 10.1021/acs.energyfuels.8b04085.

   Scimago Journal Ranking: Q1, Impact factor: 3.74

2. Hamadi, Omar & Varga, Tamás. (2023). Novel distributed parameter model-based continuous lumping approach: An application to a pilot-plant hydrocracking reactor. Chemical Engineering Science. 271. 118572. 10.1016/j.ces.2023.118572.

   Scimago Journal Ranking: Q1, Impact factor: 4.435

3. Hamadi, Omar & Varga, Tamás. (2024). Computational Insights into Catalytic Pyrolysis: Refining Molecular Composition Estimates using Kovats Retention Index and Molecular Similarities. Industrial & Engineering Chemistry Research. 10.1021/acs.iecr.4c03040

   Scimago Journal Ranking: Q1, Impact factor: 3.914

Articles in Hungarian journals

4. Hamadi, Omar & Varga, Tamás. (2022). Semi-supervised Clustering Algorithm for Retention Time Alignment of Gas Chromatographic Data. Periodica Polytechnica Chemical Engineering. 66. 10.3311/PPch.18834.

   Scimago Journal Ranking: Q3, Impact factor: 1.573

Conference articles

5. Hamadi, Omar & Varga, Tamás & Abonyi, János. (2020). Application Domain Discovery of Thermodynamic Models by Mixture of Experts Learning. 10.1016/B978-0-12-823377-1.50066-5.

   Scimago Journal Ranking: Q4, Impact factor: 0.734