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Master Thesis
Kinetic Model Development for High-Pressure Ammonia Cracking

The Max Planck Institute for Dynamics of Complex Technical Systems is looking for a Master's student (m/f/d) in the Process Systems Engineering group.
The aim is to derive and compare reaction kinetic models for NH_3 cracking that remain thermodynamically consistent near chemical equilibrium, using published conversion data [4]. The project is purely simulative.

Motivation

Kinetic models for ammonia cracking are commonly parameterized using experimental reaction-rate data, for example for Ni/Al_2O_3 catalysts as reported in [4]. Depending on the intended application, different levels of model complexity can be employed. Empirical power-law expressions contain comparatively few parameters and can often reproduce experimental data within the investigated operating range. However, their predictive capability may deteriorate when extrapolated beyond the conditions used for parameter estimation. Mechanistically motivated rate expressions, such as Temkin-Pyzhev or Langmuir-Hinshelwood-Hougen-Watson models, account for adsorption, surface reaction, and desorption phenomena and therefore provide a stronger physical basis for extrapolation. The increased mechanistic detail, however, introduces a substantially larger number of kinetic and thermodynamic parameters, making parameter estimation and model discrimination considerably more challenging.

For this reason, this thesis therefore asks a focused modelling question:

Which reaction kinetic model, when fitted to the published conversions of [4], describes the data best and how do they compare for prediction within the fitting window and for cautious use outside it?

Work packages

1. Framing and data basis

- Survey of NH_3-cracking kinetics with emphasis on high pressure and equilibrium consistency [1–5].
- Compile the published conversion data of [4] for integral reactor fitting (steady isothermal PFR).

2. Equilibrium-consistent candidate models

Fit a small set of thermodynamically consistent rate laws to the same data, chosen from the forms standard in the NH_3-cracking literature [1,3,5]:

- Power law with equilibrium affinity term (as used for high-pressure data in [5]),
- Temkin-Pyzhev model,
- LHHW-type models (cf. [3]).

Parameters are estimated by nonlinear fitting through the integral reactor model.

3. Comparison and limits of use

Compare candidates objectively on:

- fit quality within the fitting window,
- residual structure (temperature, pressure, composition),
- behavior when used outside that window, with clear uncertainty statements.

Conclude which description is preferable for further modelling use, and where it must not be stretched.

4. Documentation and handover

Reproducible scripts, concise methods chapter, and a short recommendation for subsequent reactor modelling.

Requirements

- Completed Bachelor's degree in chemical engineering, process engineering, applied mathematics, or a comparable technical program
- Experience with scientific programming and willingness to work in Python
- Interest in mathematical modelling, parameter estimation, and chemical reaction engineering
- Ability to read kinetic papers critically and to write precisely in English
- Advantageous: previous course work in heterogeneous catalysis

Start:	by arrangement
Mode of work:	hybrid
Work language:	English or German
Thesis language:	English
Character:	simulation only; no laboratory campaign

Contact

Please send a short CV, transcript, and a few sentences on modelling/coding experience to:

bicer@mpi-magdeburg.mpg.de

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References

[1] I. Lucentini, X. Garcia, X. Vendrell, J. Llorca, Ind. Eng. Chem. Res. 60 (2021) 18560. DOI: 10.1021/acs.iecr.1c00843

[2] A.S. Chellappa, C.M. Fischer, W.J. Thomson, Appl. Catal. A 227 (2002) 231. DOI: 10.1016/S0926-860X(01)00941-3

[3] S. Armenise, E. García-Bordejé, J.L. Valverde, E. Romeo, A. Monzón, Phys. Chem. Chem. Phys. 15 (2013) 12104. DOI: 10.1039/c3cp50715g

[4] C.E. Köseoglu, M. Geske, G. Kolios, G. Podbielski, D. Kleschew, J. Pottbacker, F. Rosowski, Fuel 427 (2027) 139710. DOI: 10.1016/j.fuel.2026.139710

[5] S. Sayas, N. Morlanés, S.P. Katikaneni, A. Harale, B. Solami, J. Gascon, Catal. Sci. Technol. 10 (2020) 5027. DOI: 10.1039/d0cy00686f