Operando Computational Catalysis: Microkinetic Models for COx Hydrogenation on Crowded Surfaces[1,2] – Prof. Mark Saeys

Microkinetic models are essential tools for understanding reaction mechanisms, guiding catalyst design, and optimizing chemical processes. However, traditional models often rely on low-coverage DFT calculations on idealized surfaces, which fail to capture the effects of crowded surfaces under realistic reaction conditions, leading to inaccurate predictions of activity and selectivity.

Fischer-Tropsch (FT) synthesis, a large-scale catalytic process producing long-chain hydrocarbons from syngas (CO and H_2), exemplifies reactions occurring on crowded, reconstructed surfaces. Driven by interest in sustainable aviation fuels, we developed a dual-site microkinetic model for CO-saturated surfaces. This model accurately reproduces FT activity (turnover frequency of 0.08 s^{-1}) and selectivity (chain growth probability of 0.83).

The approach was further extended to CO_2 hydrogenation over Ni and Co catalysts, demonstrating its broader applicability for realistic catalytic systems. These results highlight the importance of incorporating surface crowding effects in microkinetic modeling to improve predictions and guide the design of more efficient catalytic processes.

Curriculum vitae of Prof. Dr. Mark Saeys

Mark Saeys is a Professor at the Laboratory for Chemical Technology at Ghent University and serves as the Academic Chair of the CO_2-pipeline within the Flemish CAPTURE initiative. Previously, he was a Professor of Chemical Engineering at the National University of Singapore. In 2013, he received the Odysseus Award from the Research Foundation–Flanders to establish a research program on modelling-guided catalyst design at Ghent University.

His research integrates computational and experimental approaches, combining modelling-guided catalyst design with experimental kinetic validation and advanced characterization techniques to unravel reaction mechanisms and optimize catalytic processes.

[1] K.T. Rommens, M. Saeys, *Chem. Rev.* **123** (2023) 5798-5858.
[2] K.T. Rommens, G.T.K.K. Gunasooriya, M. Saeys, *ACS Catal.* **14** (2024), 6696–6709.