# Elementary-step based kinetic modeling using KASTER: a top-down approach applied to methane steam reforming

Sébastien Siradze[1], Jeroen Poissonnier[1], Ana Rita Costa da Cruz[1], and Joris Thybaut[1]

[1]Ghent University

January 25, 2023

## Abstract

A top-down kinetic modeling methodology is proposed using the in-house developed software tool 'KASTER'. As a case study, it is applied in the assessment of methane steam reforming (MSR) kinetics on a Ni catalyst, including water-gas shift (WGS) as a side-reaction. The complexity of the reaction mechanism is gradually enhanced, leading ultimately, to a microkinetic model. The reactor equations are solved in a transient manner, preventing the crucial numerical challenges encountered in the steady-state solution. The model providing the best balance between detail and significance was found to be of the Langmuir-Hinshelwood-Hougen-Watson (LHHW) type accounting for dissociative adsorption. In this model, the rate-determining steps of MSR and WGS are CO formation and COOH formation, respectively. While the microkinetic variant indicated that both $CH_4$ dissociative adsorption and CO formation are kinetically relevant steps in MSR, CO formation is found to be rate determining at 923 K using the adopted methodology.

## Hosted file

`Elementary-step based kinetic modeling using KASTER.docx` available at https://authorea.com/users/579577/articles/620988-elementary-step-based-kinetic-modeling-using-kaster-a-top-down-approach-applied-to-methane-steam-reforming