catalysts

an Open Access Journal by MDPI

IMPACT FACTOR 3.8

CITESCORE 6.8

Reactors and Models in Catalysis

Guest Editors:

Prof. Dr. Joris W. Thybaut
Laboratory for Chemical Technology, Ghent University, Krijgslaan 281 – S5, B-9000 Ghent, Belgium

Prof. Dr. Nikos Papayannakos
National Technical University of Athens, School of Chemical Engineering, Heroon Polytechniou 9, Zografos, 157 80 Athens, Greece

Deadline for manuscript submissions:
closed (28 February 2019)

Message from the Guest Editors

Catalysis critically relies on an adequate reactor configuration for being optimally exploited. This can range from ideal, laboratory-scale reactors aimed at intrinsic kinetics acquisition, up to realistic, industrial-scale reactors targeting a maximized productivity. Models are of strategic advantage to bridge the gap between the various scales involved. Whereas laboratory-scale data typically serve the purpose of (micro)kinetic model construction, accounting for flow pattern non-idealities and/or transport phenomena at the pellet scale allows extrapolating the laboratory kinetics to the industrially relevant scale. The latter can be reliably achieved when the model accounts for the dominant phenomena in a fundamental manner. Even with present-day computational facilities, comprehensive models accounting for all potentially occurring phenomena, represent significant challenges for being solved within an acceptable time frame. The art in 'reactors and models in catalysis' is, hence, to tailor the model complexity to the needs of the objectives that are pursued starting from molecular catalyst design and extending up to the full-fledged industrial reactor optimization.