הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע"ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

Monday, May 16th, 2022 at 13:30

Via Zoom: https://technion.zoom.us/j/97577956516

Multiscale Hierarchical Approach and Reactive Computational Fluid Dynamics: A strategy for the analysis and design of catalytic reactors

Asst. Prof. Mauro Bracconi

Laboratory of Catalysis and Catalytic Processes, Dipartimento di Energia, Politecnico di Milano, via La Masa 34, Milano, Italy

The sustainability of the energy and chemical processes has become a priority for governments, a key challenge for the scientific community and a serious concern for society. Heterogeneous catalysis plays a fundamental role in this context, as new catalytic technologies allow for more compact, safe, energy-efficient and environmental-friendly processes. This necessarily requires fully characterising the complex chemical and physical phenomena to achieve a rational understanding of the observed catalytic functionality, eventually enabling chemical engineers to design breakthrough solutions based on first principles.

Multiscale modelling is widely acknowledged to be a promising route to achieving first-principles-based insights into the reactor and process behaviour filling the current knowledge gap in the comprehension of the physical and chemical interactions [1]. In particular, Computational Fluid Dynamics (CFD) can describe the flow field and the transport phenomena in three-dimensional complex geometries, while microkinetic modelling and kinetic Monte Carlo simulations have demonstrated unparalleled power in the detailed description of surface reactivity.

The talk will initially discuss the advanced multiscale methodologies capable of describing not only the complex fluid dynamics but also the interactions between species and heat transfer and surface reactivity in single- and multi-phase flows [2,3]. Moreover, some insights will be provided into the methodology used to reduce the computational cost, covering from conventional (e.g. in situ tabulation and agglomeration) to Machine Learning techniques [4].

Despite such advances in computational methodology, the description of the full-scale problem through a truly first-principles approach is still unsustainable in industrial-scale systems due to the huge computational cost. This hampers the adoption of multiscale CFD as a design tool for the next generation of intensified catalytic reactors. To overcome such a limitation, the multiscale hierarchical approach [5] will be presented. In brief, highly detailed multiscale CFD simulations in selected but

relevant conditions of the new design are combined with experimental measurements to achieve a fundamental understanding of the complex interplay between transport and surface reactivity. As a result, it is possible to formulate engineering correlations that can then be employed in macroscopic or high-hierarchy reactor models. They now fully retain the accuracy of the detailed simulations but provide facile and cheap design of new reactors. In this talk, the potential of the hierarchical approach in the context of the advanced design of catalytic reactors for process intensification will be disclosed through a series of examples covering micro-packed bed reactors [5] and structured catalyst supports [6].

Bibliography

[1] M. Maestri, Chem. Commun. 53 (2017) 10244–10254.
[2] D. Micale, et al., Chemie Ing. Tech. (2022).
[3] M. Bracconi, Chem. Eng. Res. Des. 179 (2022) 564–579.
[4] M. Bracconi, M. Maestri, Chem. Eng. J. (2020) 125469.
[5] S. Rebughini, et al. React. Chem. Eng. 3 (2018) 25–33.
[6] M. Bracconi, et al., Chem. Eng. J. 352 (2018) 558–571.