ISCRE25 FLORENCE 2018
BRIDGING SCIENCE & TECHNOLOGY
The 25th International Symposium on Chemical Reaction Engineering
20-23 May 2018
Florence, Italy
www.aidic.it/iscre25

Development of a hierarchical methodology for the analysis of novel catalytic reactors: an application to micro packed bed reactors.

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Highlights

- Development of a hierarchical methodology enabling fundamental multi-scale modeling
- Application of the hierarchical method to study transport phenomena in micro packed beds
- Analysis of micro packed bed reactors for high exothermic processes

1. Introduction

The first-principles reactor engineering is becoming a very promising tool for the analysis of catalytic reactors [1]. It relies on a fundamental description of all the phenomena occurring in the reactor, where each scale is represented by means of its own governing equations. In heterogeneous catalysis, this approach would theoretically allow for the accurate description of the interplay between chemistry and transport processes. Despite this potential, the first-principles reactor engineering is still hampered by numerical challenges and computational costs, even for simple reactor geometries. To enable its application even to complex reactor geometries, during my PhD activities in the groups of Prof. Maestri and Prof. Dixon, I developed a specific numerical method based on a hierarchical approach [2]. This methodology couples simplified/classical models (e.g. 1D models) with multi-scale models (e.g. Computational Fluid Dynamics (CFD)) allowing a detailed and fundamental analysis of unconventional and complex reactor configurations with an affordable computational cost. In particular, in this work the hierarchical modeling is applied to micro packed bed reactors as a show-case. This reactor configuration consists of catalytic particles packed into the channel of a metallic honeycomb matrix, which leads to an unusual and complex configuration, which is different from well-established reactor geometries. For this reason, this configuration is a representative case study to test the capabilities of the proposed hierarchical methodology.

2. Methods

The application of the fundamental multi-scale modeling is limited by the dimension of the problems of practical relevance [3], which leads to impractical computational costs. A reasonable solution to this issue is to determine the controlling event at each scale.

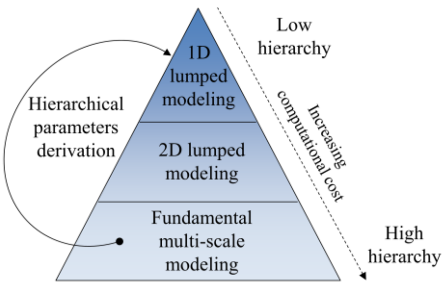

Figure 1. Schematic description of the hierarchical modeling applied to novel reactor configurations.

In this way, instead of attempting to simulate all phenomena at each scale with the highest accuracy, only the relevant events are simulated with a first principles model. This is the basis of hierarchical multiscale modeling, where the full multi-scale problem is tackled with an increasing level of complexity and

computational cost to identify the most important and governing parameters at each scale. In this work, this technique is applied to the transport phenomena following the approach reported in Figure 1. In essence, it consists of using the first principles multi-scale model to analyze a selected and limited number of operating conditions. Then, the results of these simulations are used to derive lumped parameters, which are then implemented in simplified/classical models. The generated hierarchical derived model fully retains all the information of the fundamental multi-scale model. Therefore, it enables a fundamental and multi-scale description of complex reactor geometries with an affordable computational cost.

3. Results and discussion

The hierarchical approach is, herein, applied to investigate (i) the gas-to-particle heat and mass transfer and (ii) the wall heat transfer between the packed channel and the honeycomb matrix. Figure 2 show the j-factors (a) and wall heat transfer coefficient (b) derived from CFD simulations compared with common literature correlations. Figure 2(b) illustrates the overall heat transfer. These comparisons demonstrate that only correlations derived from low Reynolds number (~70), which is the typical flow regime for micro packed bed reactors, can correctly represent the reactor behavior. Once identified and derived this correlation, they are implemented in a 2D heterogeneous reactor model to analyze the selective oxidation of o-xylene to phthalic anhydride in micro packed beds. This hierarchical derived 2D model, due to the fundamental derived correlations, enables a detailed analysis and description of the performance of the full-scale micro packed bed reactor in an affordable computational cost. This analysis shows that the micro packed bed reactor is characterized by higher heat transfer properties than a packed bed reactor. In particular, Figure 2(c) illustrates that the micro packed bed reactor is quasi-isothermal because of the enhanced heat transfer properties of the honeycomb matrix.

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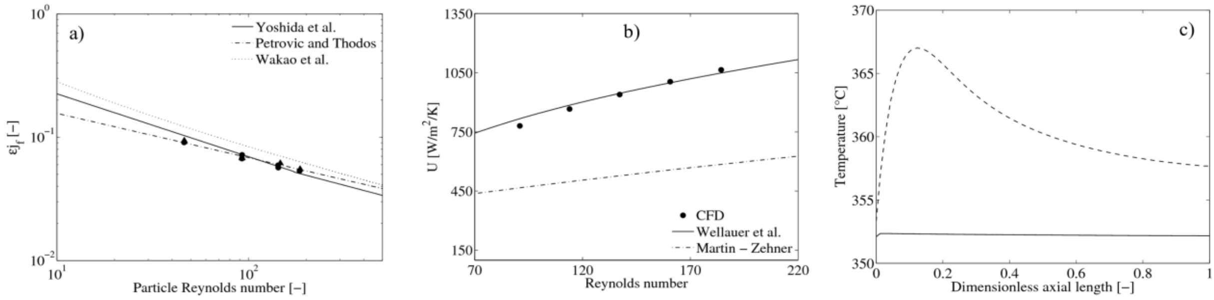

Figure 2. (a) Heat and mass transfer properties: comparison between the computer-generated packed beds and the correlations from literature; (b) Overall heat transfer coefficient as a function of the Reynolds number; (c) Temperature axial profile for the packed bed reactor (dashed line) and the micro packed bed reactor (solid line).

4. Conclusions

The hierarchical approach, originally applied at the microscale, has been herein extended to the macroscale. The analysis of micro packed bed reactors demonstrates that the hierarchical modeling is a novel numerical methodology capable of handling the complexity of catalytic reactors and enabling their the fundamental description.

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Keywords
Hierarchical modeling; micro packed beds; transport phenomena; CFD

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CURRENT POSITION

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PhD *summa cum laude* in Industrial Chemistry and Chemical Engineering

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RESEARCH EXPERIENCE

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Prof. Matteo Maestri– Politecnico di Milano, Italy – thesis supervisor

RESEARCH INTERESTS

His research topic is the multi-scale modeling of catalytic reactor. During his research activity, he has developed interdisciplinary skills ranging from the computational fluid dynamic (CFD) to heterogeneous catalysis. In particular, coupling different hierarchies of models is his main research topic. In this view, the development of numerical methods enabling the multi-scale comprehension of the phenomena is crucial to increase the understanding of complex chemistry and transport interaction and to transfer this knowledge between different hierarchies of models.

SCIENTIFIC SERVICES

Reviewer for the following scientific journals:
Engineering Applications of Computational Fluid Mechanics

RESEARCH PUBLICATIONS

Scientific Refereed Publication:

1. Maffei, T., Rebughini, S., Gentile, G., Lipp, S., Cuoci, A., Maestri, M., 2014. "CFD Analysis of the Channel Shape Effect in Monolith Catalysts for the CH4 Partial Oxidation on Rh". Chemie Ingenieur Technik 86, 1099-1106 – Special issue: "Application of computational methods in process engineering"

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7. Rebughini, S., Cuoci, A., Groppi, G., Maestri, M., "Adequacy of lumped models for homogeneous and heterogenous chemistry interaction in honeycomb reactors" (in preparation).

Book chapter:

1. Rebughini, S., Bracconi, M., Cuoci, A., Maestri, M., 2016"Catalysis engineering: from the catalytic material to the catalytic reactor", book chapter in "Operando Studies in Heterogeneous Catalysis" Edited by Irene M.N. Groot and Joost W.M. Frenken, Leiden University, The Netherlands Springer, in press.

RESEARCH PRESENTATION AT INTERNALTIONAL CONFERENCES

8 oral presentations at international conferences and 3 poster presentations:

1. B. Partopour, S. Rebughini, A. G. Dixon, Predictive Analytics Methods for Multiscale Modeling in Chemical Reactors, 2016 AlChe Annual Meeting, November 13-18, 2016 - San Francisco, CA, USA (oral)

2. S. Rebughini, A. Cuoci, M. Maestri, Hierarchical Analysis of Gas-to-Particle Heat and Mass Transfer in Micro Packed Bed Reactors, XXII International Conference of Chemical Reactors, September 19-23, 2016 - London, UK (oral)

3. S. Rebughini, A. Cuoci, M. Maestri, Hierarchical Analysis of Gas-to-Particle Heat and Mass Transfer in Micro Packed Bed Reactors, 24th International Symposium on Chemical Reaction Engineering, June 12-15, 2016 - Minneapolis, MN, USA (oral)

4. S. Rebughini, A. Cuoci, M. Maestri, Handling contact points in reactive DEM-CFD simulations of heterogeneous catalytic fixed bed reactors, European Symposium on Chemical Reaction Engineering, October 27-30, 2015 - Veranstaltungsforum Fürstenfeld, Fürstenfeldbruck (nearby Munich), Germany (poster)

5. S. Rebughini, M. Maestri, “Review on modeling of spatially resolved transport and reaction in gas-solid chemical reactors”, EUROKIN TASK B6d, Presented at EUROKIN Workshop, October, 13, 2015 - Marl, Germany (oral)

6. G. Groppi, A. Beretta, A. Donazzi, A. Carrera, S. Rebughini and P. Forzatti, Effect of Pressure on CPO Reformers for Hydrocarbon Fuels, 24th North American Catalysis Societies Meeting, June 14-19, 2015 - Pittsburgh, PA, USA (oral)

7. T. Maffei, G. Gentile, S. Rebughini, A. Cuoci and M. Maestri, A Computational Framework for the Simulation of Gas-Solid Catalytic Reactors Based on a Multi-region Approach, 24th North American Catalysis Societies Meeting, June 14-19, 2015 - Pittsburgh, PA, USA (oral)

8. S. Rebughini, A. Cuoci, M. Maestri, Handling contact points in reactive DEM-CFD simulations of heterogeneous catalytic fixed bed reactors, Ski-Seminar organized by Karlsruher Institut für Technologie, March 14-18, 2015 - Angeberg, Austria (oral)

9. S. Rebughini, A. Cuoci, M. Maestri, Fundamental assessment of gas-to-particle mass transfer in packed bed reactor, XXV Congresso Nazionale della Società Chimica Italiana, September 7-12, 2014 - Rende, Italy (poster)

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