Editorial

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A multiscale science approach to the fields of catalysis science and technology offers new prospects to tackle one of the most important questions of this century; i.e., how can we make our energy carriers and materials in a more sustainable manner? There is no single answer to this question, but one thing is sure: we require understanding of all relevant chemical and physical transport processes at three critical length scales:

- Catalytic reactions at the microscale, $O(10^{-10}$ - 10^{-9} m)
- Interplay between transport and reaction inside mesoscale structures, $O(10^{-9}$ - 10^{-6} m)
- Mass and heat transfer at the macroscale, $O(10^{-4}$ - 10^{0} m)

In this special issue of Chemical Engineering Science we concentrate on processes at the mesoscopic and macroscopic scales in the context of catalytic energy conversion.

On the mesoscale, understanding of the interplay between diffusion and reaction is studied for syngas conversion by Fariduddin et al. (2019). Chemical reactions in ZSM-5 zeolites pose computational challenges because of the relatively large size of the molecular structures involved. Huang et al. (2019) discusses the mesoscale distribution of adsorbates in ZSM-5 zeolite, whereas Uslamin et al. (2019) studies biomass conversion in zeolites. New methods are proposed to perform thermometry at the mesoscale (Geitenbeek et al., 2019) and to simulate transport and chemical reactions subject to very large differences in time scales (Sengar et al., 2019).

On the macroscale, Ge et al. (2019) reviews the role of multiscale structures in particle-fluid systems. Vandewalle et al. (2019) reviews the role of heat and mass transfer in the design of chemical reactors for the specific case of oxidative coupling of methane. This is only one example showing that proper understanding of heat and mass transfer is vital for optimizing processes. This is further illustrated in the papers on mass transfer inside particles (Partopour et al., 2019) and between particles (Lu et al., 2019 and Sulaiman et al., 2019), as well as the study of wall-to-bed heat transfer in bubbly flows (Gvozdić et al., 2019). Transport of ultrafine particles inside packed beds is studied by Boccardo et al. (2019). Finally, upscaling simulations towards full-scale reactors for the purpose of real-time process control is a tremendous challenge, which is addressed by Pirker Lichtenegger (2019).

As we can learn from these studies, novel combinations of catalysts and internal reactor structure will have a large impact on future sustainable energy conversion processes. The latest developments in experimental and computational tools are presented. We hope that the topics addressed in the special issue will inspire researchers to intensify their work on sustainable energy conversion on all length scales involved.

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References

Boccardo, G., Sethi, R., Marchisio, D.L. 2019. Fine and ultrafine particle deposition in packed-bed catalytic reactors. Chem. Eng. Sci. (Vol) (Pages)

Fariduddin F., Filot I. A. W., Zijlstra B., Hensen E. J. M. 2019. Quantum-chemical-based microkinetics simulations of syngas conversion over MoS2(1 0 0) surface. Chem. Eng. Sci. (Vol) (Pages)

Ge, W., Chang, Q., Li, C., Wang, J. 2019. Multiscale structures in particle–fluid systems: Characterization, modeling, and simulation. Chem. Eng. Sci. (Vol) (Pages)

Geitenbeek, R.G., Salzmann, B.B.V., Nieuwelink, A.-E., Meijerink, A., Weckhuysen, B.M. 2019. Chemically and thermally stable lanthanide-doped Y2O3 nanoparticles for remote temperature sensing in catalytic environments. Chem. Eng. Sci. (Vol) (Pages)

Gvozdić, B., Dung, O.-Y., Alméras, E., van Gils, D.P.M., Lohse, D., Huisman, S.G., Sun, C. 2019. Experimental investigation of heat transport in inhomogeneous bubbly flow. Chem. Eng. Sci. (Vol) (Pages)

Huang. W.L., Li, J., Liu, Z., Zhou, J., Ma, C., Wen, L.-X. 2019. Mesoscale distribution of adsorbates in ZSM-5 zeolite. Chem. Eng. Sci. (Vol) (Pages)

Lu, J., Zhu, X., Peters, E.A.J.F., Verzicco, R., Lohse, D., Kuipers, J.A.M. 2019. Moving from momentum transfer to heat transfer – A comparative study of an advanced Graetz-Nusselt problem using immersed boundary methods. Chem. Eng. Sci. (Vol) (Pages)

Partopour, B., Troupel, A., Dixon, A.G. 2019. Flux-dependent anisotropic pellet diffusivity in particle-resolved CFD simulations of fixed beds. Chem. Eng. Sci. (Vol) (Pages)

Pirker, S., Lichtenegger, T. 2019. Process control of through-flow reactor operation by real-time recurrence CFD (rCFD) simulations – Proof of concept. Chem. Eng. Sci. (Vol) (Pages)

Sengar, A., Kuipers, J.A.M., van Santen, R.A., Padding, J.T. 2019. Towards a particle based approach for multiscale modeling of heterogeneous catalytic reactors. Chem. Eng. Sci. (Vol) (Pages)

Sulaiman, M., Hammouti, A., Climent, E., Wachs, A. 2019. Coupling the fictitious domain and sharp interface methods for the simulation of convective mass transfer around reactive particles: towards a reactive Sherwood number correlation for dilute systems. Chem. Eng. Sci. (Vol) (Pages)

Uslamina, E.A., Luna-Murillob, B., Kosinova, N., Bruijnincx, P.C.A., Pidkoa, E.A., Weckhuysen B.M., Hensen, E.J.M. 2019. Gallium-promoted HZSM-5 zeolites as efficient catalysts for the aromatization of biomass-derived furans. Chem. Eng. Sci. (Vol) (Pages)

Vandewalle, L.A., de Vijver, R.V., Geem, K.M.V., Marin, G.B. 2019. The role of mass and heat transfer in the design of novel reactors for oxidative coupling of methane. Chem. Eng. Sci. (Vol) (Pages)