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Editorial overview: Fundamentals of multiphase processes toward carbon neutrality

Ning Yang, Mao Ye and Liang-Yin Chu



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Ning Yang

State Key Laboratory of Mesoscience and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

Ning Yang is a professor at the Institute of Process Engineering, Chinese Academy of Sciences. He serves as the director of State Key Laboratory of Mesoscience and Engineering, and was honored as Distinguished Young Scholar of National Natural Science Foundation of China in 2019. His research focuses on the multiscale simulation of multiphase flows in fluidization, bubble columns, and stirred tanks, involving the development of the EMMS drag model (energy-minimization multiscale), which enhances the multiphase computational fluid dynamics (CFD) simulation. Currently, his research also encompasses multiscale simulations of multiphase flow processes in pursuit of carbon neutrality, including water splitting, hydrogen metallurgy, and electric arc furnace, among others. He is a leading scientist in numerous projects involving industrial application of CFD, collaborating with organizations such as BASF, BP, TOTAL, and Unilever. He actively engages in professional societies and editorial roles, as the secretary general of International Panel of Mesoscience, and a member of Chinese Society of Particology and International Scientific Advisory Committee for International Symposium of Gas–liquid and Gas–Liquid–Solid Reactor Engineering, and a guest editor of Chemical Engineering Journal, Chemical Engineering Science, Powder Technology, and Particology.

Mao Ye

National Engineering Research Center of Low-carbon Catalysis Technology, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

Carbon neutrality is a hot topic across various fields of science and engineering. Achieving a carbon neutrality society invariably involves the integration of multiphase processes. This special issue delves into the foundational aspects of multiphase processes on the path to carbon neutrality. It covers a spectrum of topics, commencing with process intensification, spinning measurement and simulations, and exploring the core principles of established carbon neutrality technologies and novel advancements.

Process intensification: (1) Gas–liquid microreactions have emerged as a promising approach to enhance the efficiency of CO₂ capture and utilization. Sheng et al. [1] from Tsinghua University and Dalian Institute of Chemical Physics, Chinese Academy of Sciences, provide a comprehensive overview of recent advancements in gas–liquid dispersion and microflow regulation technologies within microreactors. These developments aim to intensify mass transfer processes for CO₂ absorption and utilization. (2) Fluidization is an important technology in traditional chemical industry and hydrogen metallurgy. Guo et al. [2] from Columbia University review the hydrodynamics in vibrated gas-fluidized beds and their applications to improve fluidization quality of particles that are difficult to fluidize based on gas flow alone, to control segregation and mixing among different particle types, and to enhance heat and mass transfer.

Measurement and simulation: (1) Incorporation of heat transfer into the design of heterogeneous solid-based catalyst is pivotal in reshaping conventional industrial catalysis and achieving carbon neutrality of chemical industries. Gao et al. [3] from Dalian Institute of Chemical Physics, Chinese Academy of Sciences, present a review on *in situ/operando* multiscale thermometry. This methodology is employed for monitoring the temperature of local active sites, catalyst bodies, or reactors, emphasizing innovative heating techniques coupled with online spatiotemporal-resolved thermometry. (2) Understanding the microstructure of the electrochemical interface through fluid density functional theory (FDFT) is indispensable in the research of energy storage and conversion devices such as batteries, as it directly influences their capacity and cycle performance. Cheng et al. [4] from East China University of Science and Technology provide a comprehensive summary of the development and application of FDFT across various fields. (3) Among the methods for water electrolysis in the production of green hydrogen, polymer electrolyte membrane water electrolysis (PEMWE) offers numerous advantages, including high-voltage

Mao Ye is Chair professor of chemical engineering and deputy director of the National Engineering Research Center of Low-carbon Catalysis Technology, Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences. Before joining DICP, he had been with Twente University, Eindhoven University of Technology, and Shell Global Solutions for about 10 years. His current research interests include multiphase catalytic process development and scale-up, measurement and simulations of multiphase flows, and industrial fluidized bed reactors. He has led several industrial catalytic process developments, scale-up, and commercialization, including the third-generation methanol to olefins (DMTO-III), methanol to propylene (DMTP), and methanol and naphtha coupled to aromatics. He received Hou Debang Innovation Award of Chemical Industry and Engineering Society of China, Zhang Dayu Outstanding Scholar, and Newton Advanced Fellowship of Royal Society. He is the author and co-author of more than 130 publications, and holds more than 260 Chinese, US, and EU patents.

Liang-Yin Chu

School of Chemical Engineering, Sichuan University, Chengdu 610065, China

Liang-Yin Chu is a distinguished professor of chemical engineering and a vice president at Sichuan University in China. He was a research fellow at the University of Tokyo and a visiting scholar at Harvard University, ESPCI Paris, and the University of Birmingham. He has received many honors and awards, including Natural Science Awards issued by the Ministry of Education, Distinguished Young Scholar issued by the National Natural Science Foundation of China, Distinguished Professor of Chang Jiang Scholars Program issued by the Ministry of Education, the Hou Debang Chemical Science and Technology Award – Innovation Award and Achievement Award issued by the Chemical Industry and Engineering Society of China, Fellow of Royal Society of Chemistry, National Technological Invention Award, Fellow of the Global Academy of Chinese Chemical Engineers, the Ho Leung Ho Lee Foundation Prize for Scientific and Technological Innovation, and Fellow of the Chemical Industry and Engineering Society of China. His teaching and research are focused on mass transfer and separations, membrane materials and processes, microfluidics, smart controlled-release systems, and advanced functional materials.

efficiency, gas purity, rapid response times, and the ability to operate at high pressure and current density. Guan et al. [5] from the Institute of Process Engineering, Chinese Academy of Sciences, review the current state of knowledge concerning multiphase flow in PEMWE, along with relevant modeling approaches. They also underscore the importance of regulating the microstructure of the porous transport layer (PTL) and distinguishing the effects of multiphase flow in the flow channel from those in the PTL.

Fundamentals of existing technology for carbon neutrality: (1) Autothermal operation serves as one of the key technology and essential step toward the scale-up of chemical looping combustion for efficient removal of CO₂. By focusing on the coupling of oxygen carriers and fuel, Fan et al. [6] from the University of Kentucky present a systematic analysis for the feasibility and approaches of autothermal operation. (2) The thermocatalytic decomposition of methane represents an environmentally and economically advantageous method for generating hydrogen and valuable carbon nanomaterials without the direct emission of greenhouse gases. Hadian and colleagues [7] from Eindhoven University of Technology underscore the importance of investigating deactivation mechanisms that can restrict catalyst performance over time. Additionally, they stress the significance of examining the impact of catalyst particle growth on critical reactor performance parameters. In the latter scenario, multiscale modeling, such as the integration of computational fluid dynamics with discrete element method (CFD-DEM) for fluid-particle coupling and intraparticle models, holds significant promise.

Novel advancement: In order to address the intermittent and variable nature of green electricity generated from solar energy, Yang and colleagues [8] from the Institute of Process Engineering, Chinese Academy of Sciences, introduce a pioneering solar-to-iron-adaptable production system that combines electrochemical iron-making with iron-based energy power systems. This novel technology is anticipated to significantly enhance the efficiency of renewable energy utilization.

In summary, the human endeavors in comprehending the complexity of multiphase processes for achieving carbon neutrality are boundless, calling for diverse perspectives. One recent initiative is the foundation of the State Key Laboratory of Mesoscience and Engineering and of the International Panel of Mesoscience at the Institute of Process Engineering, Chinese Academy of Sciences, aiming at exploring the mesoscale challenges in science and engineering. This may introduce a new paradigm and outlook to the exploration of fundamentals of multiphase processes toward carbon neutrality. We expect more advances in the future.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

1. Sheng L, Wang K, Deng J, Chen GW, Luo GS: **Gas-liquid microdispersion and microflow for CO₂ absorption and utilization: a review**. *Curr Opin Chem Eng* 2023100917.
2. Guo Q, Spittler C, Sanghishetty JM, Boyce CM: **Advances in vibrated gas-fluidized beds**. *Curr Opin Chem Eng* 2023100977.
3. Gao MB, Ye M, Liu ZM: **Emerging techniques to monitor temperature and supply heat for multiscale solidbased catalysis processes**. *Curr Opin Chem Eng* 2023100969.
4. Cheng J, Li JH, Lian C, Liu HL: **Development and application of fluid density functional theory for novel electrochemical interfaces**. *Curr Opin Chem Eng* 2023100946.
5. Guan XP, Bai JH, Zhang JC, Yang N: **Multiphase flow in PEM water electrolyzers: a mini-review**. *Curr Opin Chem Eng* 2023100988.
6. Fan Z, Huang N, Liu KL: **Understanding of chemical looping with auto-thermal operation**. *Curr Opin Chem Eng* 2023100970.
7. Hadian M, Buist KA, Kuipers JAM: **An overview of production of hydrogen and carbon nanomaterials via thermocatalytic decomposition of methane**. *Curr Opin Chem Eng* 2023100968.
8. Yang HT, Zhang HG, Zhu QS, Cheng JX, Yang PH, Wang Z, Xu RZ: **Flexible solar-to-iron system: a new concept and its implementation**. *Curr Opin Chem Eng* 2023100949.