Editorial: Multiphase Transportation, Conversion & Utilization of Energy in Chemical Engineering: A special issue for MTCUE-2022

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Energy is the essential basis for human survival and sustainable development. The clean, low-carbon, and efficient conversion and utilization of fossil and renewable energy have become important tasks and inevitable challenges for the current human society. In the process of energy conversion and utilization, chemical multiphase flow is a basic science to study heat and mass transfer, combustion, chemical reaction, etc. This special issue has collected 19 research papers that were presented in the 1st World Conference on Multiphase Transportation, Conversion & Utilization of Energy (MTCUE-2022) related to multiphase transportation, conversion & utilization of energy in chemical engineering. The summary of papers published in this special issue is as follows.

Molecular dynamics (MD) and computational fluid dynamics (CFD) have become powerful tools for conducting research from the microscopic and macroscopic perspectives. For the MD research in this special issue, Li et al.[1] studied nanobubble nucleation behavior on smooth and grooved hydrophilic substrates. The results revealed that nanobubbles that emerged on two- and three-groove surfaces could merge, forming a metastable nucleus via the coalescence event. The coalescence event lowered the required energy cost and accelerated the nucleation process. The influence of Na^+ and Ca^{2+} ions on wettability of rock surfaces with initially adsorbing stearic amine and pyrrole was revealed by Sun[2]. This work opens a new route for regulation of surface wettability, especially in the field of water-flooding oil recovery technology. Supercritical water (SCW) gasification is a clean and efficient utilization method of coal or biomass for hydrogen generation. Ding et al.[3] studied free radical diffusion in the SCW environment. The results illustrated that a higher temperature in the SCW environment can enhance diffusion of free radicals, especially for the •H radical, therefore facilitating and promoting reactions for hydrogen production.

For the CFD research in this special issue, Wang et al.[4] proposed a computational fluid dynamic-discrete element method (CFD-DEM) model to investigate and optimize the process of SCW biomass gasification. They studied the effects of pulsating SCW inlets on gasification and conducted artificial neural network to predict H_2 yields. In addition, the sludge thermal drying process was numerically simulated using a coupled CFD-DEM approach, and the optimal operating conditions were determined with flexibility recommendations for dryer design summarized[5]. The improvement and development of numerical methods is also one of the key topics of CFD research. Li et al.[6] developed a novel numerical method that was proposed by introducing the refined grid model and coarse-grained model into the unresolved discrete element method and volume of fluid (VOF) method to solve inflexibility of selecting grid size for the gas-liquid-flow simulations. The new approach drastically improved numerical modeling for gas-solid-liquid flows from the viewpoint of efficiency, accuracy, and flexibility. For multiphase flow systems, a smoothing method was implemented by Li et al.[7] to allow grid size to be close to or smaller than diameter of the particles, benefiting the subsequent calculations of interphase and interfacial interactions. Gas void fraction plays an important role in calculations of several multiphase flow parameters. A void fraction correlation for flow in annuli was proposed based on the drift-flux model with a new equation for the distribution parameter[8]. Furthermore, heat and mass transfer from droplets to gas phase by evaporation was modeled, and a self-similar description of the transport equations for concentration of the vapor phase from boundary-layer theory was derived[9]. Guo et al.[10] constructed a coupled CFD-DEM model to deal with the motion of flexible fibers in molten thermoplastic during fused deposition modeling (FDM) 3D printing process. This work provided insights for development and optimization of printer nozzles to enable printing of longer fibers without potential nozzle clogging.

As one of the substitutes for traditional fossil energy, biomass resource has attracted extensive attention. Shan et al.[11] summarized the catalytic routes for preparation of levulinate esters from C5/C6 carbohydrates and developed a lab-scale catalytic synthesis process of levulinate esters from biomass. It will facilitate and inspire future research on LE synthesis from biomass. Shi et al[12] studied fast pyrolysis characteristics of three main components of biomass (cellulose, hemicellulose, and lignin) in a fluidized-bed reactor by establishing a comprehensive mathematical model of multiphase flow-heat transfer-pyrolysis reaction in the fast pyrolysis process of biomass in a fluidized-bed reactor using a numerical simulation method. Deep learning (DL) is a promising method to attain both precision and speed, Zhong et al.[13] established two new DL models to predict instantaneous mass flow rates of major species for biomass fast pyrolysis in a bubbling fluidized bed. Furthermore, Zhang et al.[14] investigated biochar for post-combustion carbon capture. The results showed that a high surface area and pore volume of biochar resulted in an enhanced CO_2 capture capacity.

For the field of chemical industry, scholars in this special issue have made the following research. As an important intermediate, nitrosyl sulfuric acid (NSA) is widely used in diazotization in the fine chemical industry. A rotating packed bed (RPB) reactor was first applied for the synthesis of NSA, in which a liquid SO_2 and HNO_3 reaction occurred[15]. Transition of fluidization behavior of Geldart B particles to that of A particles induced by temperature change was investigated by a developed high-temperature electrical capacitance tomography (ECT) sensor[16]. Xiao et al.[17] developed a physics-informed transfer learning framework for modeling and control of a nonlinear process network with limited training data. Two chemical process networks were used to illustrate effectiveness of the proposed physics-informed transfer learning method. The regeneration process of fluid catalytic cracking (FCC) units produces amounts of greenhouse gases (GHGs), including carbon dioxide (CO_2), nitrous oxide (N_2O), and methane (CH_4). The on-site monitoring results showed that the regenerated form of the FCC unit has the greatest impact on CH_4, and CO_2 is the primary GHG, with total emissions of >99%, and coke content and composition on the spent catalysts can directly affect GHG emissions[18]. Fu et al.[19] developed a general correlation to predict effective density for immersed object separation in fluidized beds, and the proposed correlation not only provides an efficient way for design and operation of Gas-Solid Fluidized Bed Coal Beneficiator (GSFBCB) for coal dry beneficiation, but also is applicable for iron and copper ore pretreatment, agricultural crop cleaning, municipal solid waste classification, etc.

The chemical multiphase process in the conversion and utilization of energy has considerable potential for practical applications. We believe that the collection of these cutting-edge papers will be very beneficial to the scientific and industrial communities in tracking the state-of-the-art methods in this field. We also hope that our readers will enjoy the contents of this special issue and make greater contributions in the field of conversion and utilization of energy in chemical engineering.

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