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Editorial: Adsorption-enhanced reactions design, engineering and optimization

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Editorial on the Research Topic
Adsorption-enhanced reactions design, engineering and optimization

In adsorption-enhanced reactions, a reaction product is selectively separated from the reaction atmosphere by means of an adsorption process. For equilibrium-limited reactions, the separation of one of the reaction products increases the conversion and selectivity by shifting the equilibrium according to Le Chatelier's principle. Moreover, it may help in preserving catalyst activity by removing an inhibiting reaction product. Recently, a wide range of exciting new scientific developments in this field have been spurred by the energy transition (Boon, 2023). These developments range from pre-combustion CO_2 capture (Martinez et al., 2019; Soria et al., 2019; Martínez et al., 2022; Capa et al., 2023; Wang and Li, 2023; Malsegna et al., 2024) to CO_2 valorisation (van Kampen et al.; Gómez et al., 2022; Jo et al., 2022; Singh et al., 2022; Peinado et al., 2024), and find applications in biomass utilisation, methanol economy and ammonia synthesis. Novel reactor concepts and hybrid materials (with adsorption and catalytic properties) have been developed, including concepts utilising membranes and adsorbents. Reactors are increasingly being tested and scaled up in technology readiness. Adsorption-enhanced reactions are by nature complex systems to design, engineer and optimise: a balance is required among the functional materials and the reactor configuration. In addition to conventional features such as catalyst activity and selectivity and heat and mass transfer phenomena, the performance of an adsorption-enhanced process is ultimately determined by kinetics, adsorbent capacity and selectivity, cyclic working capacity and regeneration conditions used. Catalysts for adsorption-enhanced processes generally work in conditions that are very different from conventional conditions. Heat and mass transfer limitations might lead to performance degradation or slip. Adsorbent capacity directly impacts the required regeneration frequency and achievable working capacity, whereas co-adsorption of reactants or of several reaction products will lead to compromising of the system performance.

As a pre-combustion CO_2 capture technique, sorption-enhanced water-gas shift (SEWGS) has seen important developments recently (Sebastiani et al., 2022; Zecca

et al., 2023; Monteiro et al., 2024). In terms of cycle design, simulations have been performed by Stadler et al. using a complex hybrid system scale model for a relatively low-temperature (250 °C) pilot plant reactor consisting of six individually accessible reaction chambers. A serial process configuration of reaction chambers was explored, indicating a significant increase in sorbent working capacity. Interestingly, the use of a novel modelling approach using a state machine (Stadler et al., 2022b), without predefined switching times allowed for further optimisation of the SEWGS cycle. In terms of the SEWGS CO_2 adsorbent, Xin et al. have investigated the long-term stability of a commercial potassium-promoted hydrotalcite-based adsorbent (KMG30) over many repetitive cycles under various operating conditions. Exposure to repetitive cycles of CO_2/N_2 (without H_2O) led to aggregation of K_2CO_3 from the adsorbent while exposure to repetitive cycles of H_2O/N_2 (without CO_2) led to a reduction in adsorption capacity due to the incomplete regeneration of one of the adsorption sites involved. In contrast, the remarkable stability of KMG30, as known from SEWGS process studies (Oliveira et al., 2008; van Selow et al., 2009; Boon et al., 2014), was confirmed during cycles of CO_2 adsorption/steam purge.

Further to the improvement of adsorption-enhanced reactions for precombustion CO_2 capture as well as oxyfuel combustion, membrane-assisted chemical looping reforming (MA-CLR) and membrane-assisted sorption-enhanced reforming (MA-SER) for CH_4 reforming were modelled by Pouw et al. In both cases, H_2 perm-selective membranes were introduced in order to allow for the production of high-purity H_2 product directly. Taking into account the increased window for carbon formation and the effect on operating conditions, MA-CLR was shown to outperform MA-SER in terms of H_2 yield, energy efficiency, and carbon capture ratio. Nevertheless, MA-SER offers advantages in terms of producing pure CO_2 product, and allowing for a lower reactor temperature.

The thermochemical conversion of CO_2 with H_2 can be enhanced by the adsorption of H_2O byproduct. In this context, the sorption-enhanced DME synthesis (SEDMES) has now been demonstrated with a multi-column test-rig by van Kampen et al., allowing for a continuous single-pass carbon yield of up to 95% well beyond the thermodynamic equilibrium.

The progress in design, engineering, and optimisation of adsorption-enhanced reactions depends on finding a delicate balance between the (intrinsic) kinetics of the individual reactions and reactor engineering. In that sense, the recent findings reported in Frontiers in Chemical Engineering Research Topic '*Adsorption-Enhanced Reactions Design, Engineering and Optimisation*' present relevant advances in the field. Experimentally, the stability conditions of potassium-promoted hydrotalcites for sorption-enhanced water-gas shift have been further elucidated under repetitive exposure to CO_2, H_2O, and mixtures thereof. On a process level, continuous multicolumn sorption-enhanced DME synthesis has been successfully validated. Modelling studies have shown how the selective removal of H_2 via membranes can affect the driving force for coking, and thus the operating window, in sorption-enhanced and chemical looping reactors. On a process level, the use of advanced Stateflow modelling techniques has led to new and improved cycle designs for the sorption-enhanced water-gas shift process that yield increased working capacity. The reported research shows that the development of adsorption-enhanced reactions is making progress, both in the field of the required materials as well as on a process level. Further development in the coming years will yield advanced, intensified process technology that enables the industrial energy transition.

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