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Editorial

Catalytic CO_2 Methanation Reactors and Processes

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CO_2 methanation is a chemical process that involves the conversion of carbon dioxide (CO_2) and hydrogen (H_2) gases into methane (CH_4) and water (H_2O) [1–3]. This reaction plays a crucial role in carbon capture and utilization strategies, as it allows the recycling of CO_2 emissions into valuable methane, which can be used as a clean energy source or feedstock for various industries.

Catalytic CO_2 methanation requires catalysts to facilitate the reaction at reasonable temperatures and pressures. Common catalysts include nickel (Ni) [4–15], cobalt (Co) [16–19], ruthenium (Ru) [4,6,20–25], and others [26,27] supported on high-surface-area materials like Al_2O_3, ZrO_2, CeO_2, or SiO_2. Common reactor types for the CO_2 methanation process include fixed bed [28–34], monolith [35–39], fluidized bed [5,32,40–46], and microstructured [47–50]. Despite numerous studies on catalytic CO_2 methanation, reactors and processes design tasks are still limited in the current stage of process development. This Special Issue focuses on reactors and processes of catalytic CO_2 methanation, including (a) catalyst development, (b) reactor design, (c) process integrations, and (d) modeling and simulation approaches.

The significant publications featured in this Special Issue on CO_2 methanation reactors and processes include:

a. Soon Woong Chang et al. from Korea studied the deactivation and regeneration method for Ni catalyst by H_2S poisoning [4]: Catalyst poisoning is a prevalent concern in industrial applications. This research reveals that the reaction activity of the Ni-Ce-Zr catalyst significantly diminishes at 220 °C due to the toxic impact of H_2S. The study introduces a novel approach to counteract this effect by employing H_2 treatment for the generation of the Ni-Ce-Zr catalyst. Consequently, this paper provides valuable insights into the fundamentals of catalyst poisoning and offers a viable generation method for the CO_2 methanation process.
b. Son Ich Ngo et al. from Korea studied the physics-informed neural network for instant prediction of fixed-bed reactor performance [28]: Neural networks generally have advantages in instant predictions with high accuracy. Physics-informed neural networks (PINN) offer an additional advantage by incorporating governing equations within the network, enhancing extrapolation capabilities beyond sampled data. In this study, PINN was applied to the design of fixed-bed reactors for catalytic CO_2 methanation. Remarkably, even with training data covering only one sixth of the reactor length range, the forward PINN achieved an impressive 88.1% extrapolation prediction accuracy for the entire reactor length range. Moreover, the inverse PINN successfully revealed hidden reactor design parameters using only a few experimental data points. Notably, this study garnered the highest number of citations and views within this Special Issue.
c. Frances Sastre et al. from TNO in Eindhoven studied the Plasmonic Ru nanorod catalyst for sunlight-powered process [21]: At an intensity of 12.5 suns, the CO_2

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conversion rate surpassed 97%, displaying complete CH_4 selectivity and maintaining a steady production rate of 261.9 mmol/g/h for a minimum of 12 h. Notably, the CH_4 production rate exhibited an exponential rise with increasing light intensity. In a separate set of experiments conducted under 14.4 suns and a consistent bed temperature of approximately 204 °C, different flow rates were examined.

d. Daria Burova et al. from Belgium and The Netherlands made a comparison of chemical reduction in $RuCl_3$ and thermal decomposition of $Ru_3(CO)_{12}$ [20]: This study discovered that the two preparation methods yielded different particle sizes. Surprisingly, despite the variation in particle sizes, the catalysts exhibited similar activity and selectivity in the sunlight-powered process, achieving rates of 0.14–0.63 mol/g/h and >99%, respectively.

e. Byungwook Hwang et al. from Korea studied Fluidized-bed reactor design for Ni-based catalyst [5]: This study concentrated on reactor design rather than catalyst and process development. The fluidized-bed reactor, renowned for its exceptional heat and mass transfer capabilities, effectively mitigates the high endothermic Sabatier reaction's hot-spot temperatures. Nevertheless, the designs of both the reactor and the process are relatively complex due to the intricate interplay of gas hydrodynamics and solid catalyst pellets. Remarkably, in this reactor, the temperature rise is only approximately 11 °C for achieving an around 90% CO_2 conversion. Additionally, the study identified the reaction kinetics parameters for the Ni/Al_2O_3 catalyst.

f. Javier Herguido et al. from Zaragoza (Spain) presented an study about Ni-, Ni-Fe-, and Ru-based catalyst for biogas upgrading [6]: Multiple homemade catalyst types were evaluated for CO_2 methanation within the temperature range of 250 °C to 400 °C, maintaining a constant flow rate of 30,000 mL/g/h. Among them, the Ru (3.7 wt%)-based catalyst demonstrated outstanding performance, exhibiting turnover frequency (TOF) values of up to 5.1 min^{-1}. This figure was notably six times higher than that achieved with the Ni (10.3 wt%) catalyst and three times higher than that of the Ni–Fe (7.4–2.1 wt%) catalysts.

The design of CO_2 methanation reactors and processes necessitates a deep understanding of catalyst preparation, reaction kinetics mechanisms, reaction engineering, and reactor modeling. The Special Issue on "Catalytic CO_2 Methanation Reactors and Processes" gathers several articles studying different aspects as catalyst preparation, effect of feed composition, different reactor types, durability, regeneration, etc. Therefore, the issue significantly contributes to advances in the power-to-gas concept, enabling energy storage for renewable energies.

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