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Thermal Behavior and Runaway Analysis of Exothermic Reactions in Fixed-Bed Reactors: CO_2 Methanation as a Case Study

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The catalytic methanation of CO_2 represents a key technology for Power-to-Gas applications and sustainable energy storage. However, the reaction is strongly exothermic, which poses significant challenges for reactor operation, heat management, and process safety, particularly in cooled fixed-bed reactors. Insufficient heat removal can lead to pronounced temperature gradients, hot spot formation, and, in extreme cases, thermal runaway.

This contribution investigates the impact of reactor operation and design parameters on the thermal behavior of CO_2 methanation in a packed-bed reactor. The methanation process serves as a representative case study to generally analyze thermal runaway phenomena in highly exothermic fixed-bed reactions. Special emphasis is placed on the prediction and characterization of temperature profiles within the reactor, as they are critical indicators for safe and stable operation, as well as for an accurate description of reactor performance with respect to conversion behavior.

To this end, one-dimensional (1D) and two-dimensional (2D) reactor models are developed and compared using numerical simulations for generally exothermic reactions in fixed-bed reactors. The models account for reaction kinetics, heat generation, and axial as well as radial heat transport. The one-dimensional model is augmented by an effective heat transfer correlation to enhance its predictive performance. By appropriately adjusting heat removal, the 1D model can closely reproduce the temperature profiles obtained from the 2D model, particularly regarding the onset of thermal runaway.

The results provide insights into the suitability of different modeling approaches for the analysis of exothermic fixed-bed reactors and contribute to the design and safe operation of methanation reactors and related catalytic processes.