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Simulation-Driven Validation and Enhancement of Reactor Models for a Technical Fixed-bed Fischer–Tropsch Synthesis

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In the context of the energy transition and the pursuit of sustainable carbon cycles, Fischer–Tropsch synthesis (FTS) is increasingly recognized as a key technology for converting CO and CO_2 into valuable hydrocarbons. When combined with renewable hydrogen in Power-to-X concepts, CO_2 can serve as a viable carbon feedstock. Iron-based catalysts, in particular, have shown significant potential for CO and CO_2 hydrogenation due to their lower methane selectivity compared to cobalt-based systems and their promotion of long-chain hydrocarbon formation. This performance arises from their ability to catalyze both the Fischer–Tropsch synthesis and the reverse water–gas shift (RWGS) reaction, thereby enabling a broader and more economically relevant product spectrum [1, 2].

At the University of Bayreuth, a pilot-scale Fischer–Tropsch facility is currently being established, operating under industrially relevant conditions, typically at pressures around 20 bar and temperatures between 200 and 300 °C. The synthesis of the catalyst at relevant scale, along with its experimental evaluation and physicochemical characterization, has already been successfully completed [2]. Results indicate favorable performance in terms of reaction rate, conversion, and selectivity. Of particular interest is the high selectivity toward paraffinic long-chain hydrocarbons (C_{20^+}), which represent the most economically valuable fraction of the Fischer–Tropsch product spectrum.

Within this framework, simulation-based optimization strategies are being developed alongside detailed reactor models. Special attention is given to heat removal and reaction kinetics, as the highly exothermic nature of Fischer–Tropsch synthesis requires advanced thermal management to prevent thermal runaway and ensure stable reactor operation. These simulations are performed using Presto Kinetics and COMSOL Multiphysics, enabling the coupling of computational fluid dynamics (CFD) with detailed chemical reaction engineering models. The primary goal of this optimization is to maximize the conversion of CO_2 within the tubular reactor while maintaining safe operation.