Systematic Modeling and Simulation of One-Dimensional Packed-Bed Processes

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Abstract: Process design and real-time operation of flexible Power-to-X processes require simulation models for analysis, optimization, and control under transient operating conditions (Palys and Daoutidis, 2022). We present a systematic equation-oriented framework for modeling and simulation of one-dimensional packed-bed processes. The framework provides a reusable workflow for formulating, discretizing, and analyzing rigorous process models. To this end, packed-bed models are formulated using modular thermodynamic, kinetic, transport, and transfer submodels. Conservative mass and energy balances are written in terms of molar concentrations and internal energy as state variables, while temperature and pressure are recovered from algebraic thermodynamic constraints. The modular framework allows ideal-gas and real-fluid equations of state to be interchanged within the same model formulation. The resulting system of partial differential-algebraic equations is semi-discretized using an upwind finite volume method, yielding a large sparse system of differential-algebraic equations. Its solution requires derivative information obtained by combining analytical derivatives of the discretized balances with automatic differentiation of constitutive functions. Combined with sparse linear algebra, this supports analysis via Newton-based steady-state simulation, pseudo-arclength continuation, stiff implicit Runge-Kutta integration, and shooting-based cyclic steady-state computation. The framework is demonstrated on two packed-bed processes relevant to Power-to-Ammonia production. For nitrogen generation, an adsorption column model is developed to simulate cyclic operation and cyclic steady states (Schytt et al., 2026). For ammonia synthesis, fixed-bed and direct-cooled reactor models are developed for steady-state simulation, dynamic simulation, and parametric sensitivity under varying thermodynamic assumptions (Schytt and Jørgensen, 2026). Together, the examples demonstrate how our systematic modeling and simulation framework can express rigorous process models in a compact and extensible form, providing a basis for future simulation, optimization, and control studies.

Keywords: Process modeling, Process simulation, Packed-bed processes, Power-to-X.

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