

Leaving Steady-State Behind: Operating Fixed-Bed Reactors for a Net-Zero Chemical Industry

Decarbonizing the chemical industry will require more than replacing fossil feedstocks—key synthesis steps must also become compatible with a power system dominated by variable renewables. Many catalytic processes, however, are still designed and operated around steady-state assumptions, while real-world Power-to-X plants must ramp up, turn down, and restart frequently. This talk presents a reactor-engineering and systems-integration perspective on how fixed-bed reactors can be redesigned and operated for flexibility without sacrificing safety, selectivity, or lifetime.

I will introduce an integrated approach that links (i) multi-scale modelling of heat and mass transfer and catalytic kinetics with (ii) efficient numerical methods and software environments that enable fast, reliable simulation of complex nonlinear reactor models, and (iii) optimization and control strategies tailored to constrained operation under fluctuating inputs. Instead of simplifying the physics, the approach focuses on making high-fidelity models computationally tractable—so they can be used repeatedly in design studies, dynamic optimization, and control-oriented analyses. A key element is the tight coupling of modelling with monitoring: advanced temperature sensing, including spatially resolved measurements, provides the data needed to detect and prevent hotspot formation, manage exothermicity, and validate dynamic models under industrially relevant transients.

As a central case study, I discuss load-flexible Power-to-Ammonia. Ammonia is an energy-dense, transportable hydrogen derivative and a potential backbone molecule for net-zero value chains. Yet conventional reactor concepts are optimized for steady operation and narrow windows. I will show how polytropic fixed-bed concepts, dynamic operating policies, and control/optimization workflows based on detailed reactor models can extend the feasible operating range, enable fast transients, and maintain conversion and thermal safety across wide turndown. The same methodology transfers to other hydrogen-based pathways such as CO₂ methanation and synthetic fuels, where dynamic heat management and operability constraints dominate performance.

Beyond technical results, the talk aims to provide actionable insights: which physical constraints most strongly limit flexibility; how to trade off catalyst/bed design against controllability and thermal robustness; how to define meaningful flexibility metrics; and how monitoring, numerical methods, and optimization can be integrated into a workflow that is useful for both academia and industrial stakeholders. Overall, the lecture argues that moving

“beyond steady-state” is not a niche control problem but a core design principle for resilient, competitive, and low-carbon chemical manufacturing in Europe and beyond.