Abstract

The global transition towards sustainable energy systems necessitates the efficient thermal conversion of biomass and biogenic waste resources. Thermochemical processes like gasification and incineration are central to this effort, yet their inherent complexity, arising from coupled physical and chemical phenomena and their multiscale nature, presents a significant challenge for optimization. Mathematical modeling remains the primary suport for the development of innovative, efficient technologies, complementing often costly and time-consuming experimental research. Traditional modeling approaches focus either on detailed component-level analysis or on system-level performance, creating a gap between fundamental understanding and operational application. This thesis thus aims to develop and demonstrate a holistic, multi-scale framework for the analysis, monitoring, and optimization of thermochemical conversion systems. This involves numerical modeling of particular heat and mass transfer processes in a reactive medium and machine learning algorithms for system performance predictions.

The research is structured around three interconnected pillars. First, to advance fundamental understanding at the component level, a novel in-house Dynamic Coupled Eulerian-Lagrangian (DCEL) method is developed to model particle-scale phenomena, including fuel grain shrinkage, heat transfer and gas release within a gasifier. Producer gas can serve as a fuel for direct use in thermal and power generation systems, and as a raw material for chemicals or other energy carriers, such as hydrogen or synthetic fuels. One of the crucial factors for the feedstock conversion degree and thereby the quality and yield of syngas is the fuel movement speed. Unlike one-dimensional Eulerian-type approaches usually applied to model small-scale fixed-bed reactors, the proposed DCEL model allows for determining the fuel bed movement variable along the reactor that results from the volume change of the devolatilizing particles. Thus, the investigation focuses on the dynamics of biomass decomposition, which is critical while considering the optimal technology pathway for the specific feedstock. The DCEL model's predictive capabilities and computational efficiency are qualitatively evaluated against the advanced eXtended Discrete Element Method (XDEM), and the predictions of both are compared with experimental data. Second, the scope is expanded to system-level analysis through the application of machine learning (ML) methods. A data-driven model of an industrial sewage sludge incineration plant is elaborated, integrating Aspen Plus simulations with ML algorithms, including Gradient Boosting Machines and a novel chained-regression technique, to predict key performance indicators and identify optimal operating conditions for enhanced energy efficiency. Third, continuing the analysis of the incineration plant in terms of energy consumption optimization, the thesis culminates in the implementation of a real-time digital twin. This approach integrates physical models, analytical calculations, and operational data within a dynamic simulation

environment (AnyLogic). This digital twin enables closed-loop energy optimization through smart scenario analysis, demonstrating a validated strategy that reduces the consumption of biogas serving as an auxiliary fuel by 40% while maintaining operational compliance.

The research work carried out provides a comprehensive framework that integrates advanced numerical modeling of complex transport processes in a solid fuel bed with data-driven analytics and digital twin technology. The findings demonstrate that such a multifaceted approach is paramount for unlocking the full potential of complex energy systems, dedicated to the rational management of available biogenic fuel resources, which are difficult due to their physicochemical characteristics and diversity.