Neural network assisted simultaneous optimization of reactor and catalyst pellet design

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Introduction

The adequate consideration of the catalyst pellet specifications play a crucial role during optimization of fixed bed reactors as they impact catalytic activity and selectivity through intraparticle transport characteristics and affect critical fixed bed properties such as heat transfer and pressure drop. Various approaches exist to account for intrapellet effects in pseudo-homogeneous reactor models. In particular, a shortcut method presented by our group a few years ago uses an analytical approximation to provide a reasonable estimate with low computational overhead [1]. However, without further discretization of the pellet, this method is limited to situations with only small degrees of transport limitations. In contrast, rigorous modeling of catalyst pellets by discretizing pellet balance equations alongside reactor balance equations provides accurate results but comes at comparably high computational costs and may lead to numerical instability. In chemical reactor modelling neural networks have recently emerged as promising tools due to their ability to act as fast and efficient surrogate models, e.g. for microkinetic models [2] and also for modeling of intrapellet effects in multiscale computational fluid dynamics simulations [3].

In our contribution, we present the application of neural network models to consider intrapellet effects in dynamic reactor optimization and particularly focus on the balance between high model accuracy and low numerical overhead. To illustrate the benefits of simultaneous reactor and catalyst pellet design using the proposed neural network method, a fixed bed reactor with a constant coolant temperature is optimized for the air-based partial oxidation of ethylene to ethylene oxide.

Optimization Study

The approach is first validated against existing methods for a simplified 1D reactor. As an objective the minimization of the pressure drop is chosen while performance constraints regarding conversion, selectivity and Space-Time-Yield as well as safety constraints regarding maximum temperature are required to be fulfilled. For this, the optimization with the neural network approach is compared against results from a

homogeneous model, i.e. without pellet consideration, a heterogeneous model with pellet discretization and the shortcut method for varying levels of resolution (Figure 1). By dynamically optimizing the pellet specifications (i.e. pellet size) along the reactor axis a significant pressure drop reduction of 50 % compared to an optimized reactor with prefixed pellet specifications is achieved. This study highlight the superior combination of accuracy (close to the heterogeneous model) with computational efficiency (close to the shortcut method) of the neural network approach.

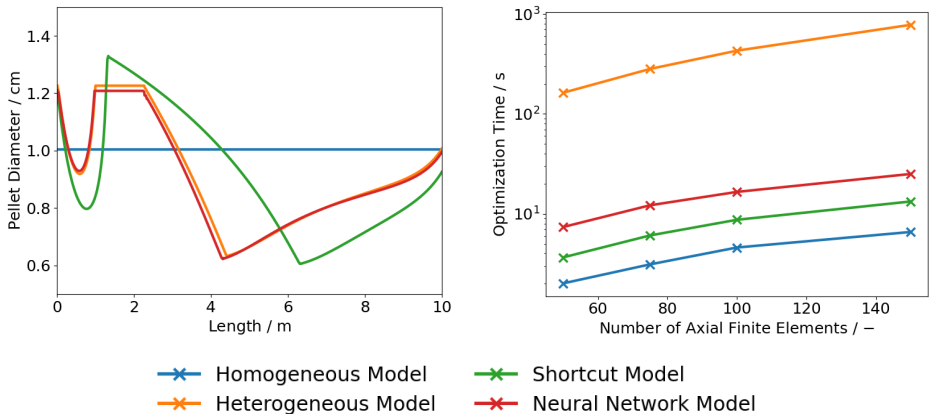

Figure 1. Left: Optimal catalyst pellet size profile resulting from different modelling approaches. Right: Resulting computational effort of different levels of model resolution for different modelling approaches.

Furthermore, the neural network approach is applied to the optimization of a more complex 2D reactor model. This provides deeper insights into the interplay between optimal reactor conditions and control variables, particularly with their now considered additional dependency on the radial coordinate. This added complexity underscores the method's robustness and ability to handle sophisticated systems at affordable computational cost.

Conclusion

By providing an efficient and accurate method for the optimization that is applicable for complex models, the presented method enables the design of tailored reactor-catalyst pellet systems and to improve the reactor performance by tuning the bed transport characteristics. Moreover, it can provide impulses for the development of novel optimal catalyst support structures and allows for an a priori numerical evaluation when embedded into technical feasible reactor concepts.

References

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