A Comparative Study of Approximate Models for a Tubular reactor Model with parametric Sensitivity

L. Özkan[1], *S. Weiland*[3], *R. Romijn*[2], *and J. Ludlage*[1]

[1] IPCOS, Boxtel, the Netherlands
[2] RWTH, Aachen, Germany
[3] Technical University of Eindhoven, Eindhoven, the Netherlands

Email: *Leyla.Ozkan@ipcos.nl*

Tubular reactors are a class of chemical systems whose dynamics are modeled by nonlinear partial differential equations that are coupled via boundary and initial conditions. The numerical solution of such models involves the discretization of the system equations using numerical techniques such as finite difference, finite volume or finite elements methods. This generally requires intensive computation, hence simulation time which is a limiting factor for online and real time implementations like model-based control, dynamic optimization, plant monitoring and parameter estimation. Therefore, the application of model reduction techniques for developing computationally efficient models is a natural procedure. Undoubtedly, any reduced model should not only be computationally efficient but also exhibit the relevant dynamical behavior. Previous investigations [1] have shown that tubular reactors exhibit parametric sensitivity in certain operating conditions. Specifically, any small change in the reactor inlet or operating conditions could lead to large variations in the dynamics of the tubular reactor. Such a behavior could cause the production of undesired side reactions and/or unsafe process operation.

The purpose of this presentation is to compare a number of reduced order models of a tubular reactor and to investigate the sensitivity of the resulting models to changes in input and operating conditions. That is, we aim to demonstrate the invariance of input sensitivity in reduced order models. In a recent work [2], we proposed a methodology that combines the proper orthogonal decomposition and grey-box modeling approach. In this methodology, the original nonlinear system is viewed as a interconnection of a known part (mechanistic part) with an unknown component (the empirical part) that is assumed to constitute the computationally intensive parts of the nonlinear system. Model reduction is performed on the mechanistic part, while empirical modeling techniques (polynomial approximation, neural networks) are applied for the approximation of the empirical component. By doing this, computationally expensive parts can be replaced by simple expressions that are faster to evaluate. In this work, we evaluate approximate models for a tubular reactor model with both diffusion and convection phenomena and a nonlinear heat generation term. The evaluation considers computational performance, accuracy, sensitivity analysis (perturbation analysis) and the performance of the approximate models in closed loop when a model based control architecture is implemented.

References

[1] M. Morbidelli, and A. Varma, "Parametric sensitivity and runaway in chemical reactors", *Sadhana Academy Proceedings in Engineering Sciences*, v. 10, p. 133-148, 1987.
[2] L. Özkan, R. Romijn, S. Weiland, W. Marquardt and J. Ludlage, "Model Reduction of Nonlinear Systems: A grey-box modeling approach", *In Proceedings of* 7^{th} *IFAC Symposium on Nonlinear Control Systems*, Pretoria, South Africa, 2007