Computer-Aided Modeling Framework - DTU Orbit (09/11/2017)

Computer-Aided Modeling Framework: A Generic Template as a Modeling Tool

Models are playing important roles in design and analysis of chemicals based products and the processes that manufacture them. Computer-aided methods and tools have the potential to reduce the number of experiments, which can be expensive and time consuming, and there is a benefit of working with them. As the required models may be complex and require multiple time and/or length scales, their development and application for product-process design is not trivial. Therefore, a systematic modeling framework can contribute by significantly reducing the time and resources needed for model development and application. The proposed work is a part of the project for development of methods and tools that will allow systematic generation, analysis and solution of models for various objectives. It will use the computer-aided modeling framework that is based on a modeling methodology, which combines in-depth work-flows and data-flows for different modeling tasks related to model development and application with the goal to systematize the modeling. The overall objective of this work is to allow the model developer to generate and test models systematically, efficiently and reliably. In this contribution, the concept of template-based modeling is presented and application is highlighted for the specific case of catalytic membrane fixed bed models. The modeling template is integrated in a generic computer-aided modeling framework. Furthermore, modeling templates enable the idea of model reuse as the user can then generate many problem-specific models for different applications. The templates are part of the model generation feature of the framework. Also, the model development and use for a product performance evaluation has been developed. The application of the modeling template is highlighted with a case study related to the modeling of a catalytic membrane reactor coupling dehydrogenation of ethylbenzene with hydrogenation of nitrobenzene, and, for the performance evaluation of an atomizer product. In the first case study, the reactor type is where the reactions are thermodynamically limited, such as, steam reforming and the production of olefins from inexpensive paraffins via dehydrogenation. The generated process model is based on Fickian diffusion model, which is the most widely used to account for the intraparticle mass transfer resistance. The model of the process can help to predict the yield and the quality of the output components and that will make possible to evaluate and improve the product properties. In the case of the atomizer performance, the droplet size, number and their evaporation are analyzed through a multiscale model. The mathematical equations of the model are generated through the template in ICAS-MoT and translated into a model object. Once in ICAS-MoT, the model is numerical analyzed, solved and identified. A computer-aided modeling framework integrating systematic model derivation and development tools has been developed. It includes features for model development, model identification and solution, model templates library. In this work the template based model application feature was extended with a modeling template related for catalytic membrane fixed bed reactor and a template related for product performance evaluation.

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