Computer-aided modeling framework for efficient model development, analysis and identification - DTU Orbit (18/01/2019)

Computer-aided modeling framework for efficient model development, analysis and identification: Combustion and reactor modeling

Model-based computer aided product-process engineering has attained increased importance in a number of industries, including pharmaceuticals, petrochemicals, fine chemicals, polymers, biotechnology, food, energy, and water. This trend is set to continue due to the substantial benefits computer-aided methods introduce. The key prerequisite of computer-aided product-process engineering is however the availability of models of different types, forms, and application modes. The development of the models required for the systems under investigation tends to be a challenging and time-consuming task involving numerous steps, expert skills, and different modeling tools. This paper introduces a generic methodology that structures the process of model development, analysis, identification, and application by providing the modeler with the work-flow that needs to be followed in a systematic manner. The methodology has been implemented into a computer-aided modeling framework, which combines expert skills, tools, and database connections that are required for the different steps of the model development work-flow with the goal to increase the efficiency of the modeling process. The framework has two main branches; the first branch deals with single-scale model development while the second branch introduces features for multiscale model development to the methodology. In this paper, the emphasis is on single-scale model development and application part. The modeling framework and the supported stepwise model development is highlighted through a case study related to air pollution control, namely, the thermal treatment of the off-gas stream in adipic acid production in order to reduce its N2O content.

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