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Development and Application of a Library of Elementary Model Entities for Vapor-Liquid Chemical Processes

by Odón Angeles

Abstract

The development of a library for modeling vapor-liquid chemical processes is the subject of this work. The process modeling tool, **ProMoT**, and its Model Definition Language, MDL, were used for the implementation of the library.
Focus of this contribution is on lumped systems described by ordinary differential equations of first order and algebraic equations for vapor-liquid systems.
Modeling is presented as a common activity in different scientific disciplines, with special emphasis on modeling in chemical engineering. Domain engineering activities are discussed, namely analysis domain and architecture development. These activities lead us to the software pattern proposed in this thesis and applied for the implementation of the library. The discussion emphasizes that modeling chemical engineering systems by reusing modules of a library is different than modeling from scratch and that preparing modules for reuse is a process on its own. In this context it was shown how computer-aided modeling impacts the whole modeling task.
The formulation of theoretical aspects are applied here for the development of concrete modules, namely, the network approach, the proposed phenomenological framework, and the simple-to-complex implementation strategy. This conceptual frame is proposed as a starting point for more detailed phenomenological developments of the library.
The modeler of chemical process should find a conceptually well structured knowledge space in which entities can be systematically found, used, and further developed. Although the library is a final product itself, its development would be pointless without applications associated with it. The applications consist of two different industrial chemical processes: the first one is a plant for the production of butyl acetate and the second one is a plant for the production of acetic acid. Each application is a completely independent project with the library of models as a common root. It is shown that the library can be adapted to particular requirements of the modeler and it can be further developed by either creating new modules or by modifying some others. After a validation and reuse analysis, these new models can be added to the library to make them available for different users.