CHEOPS: A tool-integration platform for chemical process modelling and simulation

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Abstract. A large number of modelling tools exist for the construction and solution of mathematical models of chemical processes. Each (chemical) process modelling tool provides its own model representation and model definition functions as well as its own solution algorithms, which are used for performing computer-aided studies for the process under consideration. However, in order to support reusability of existing models and to allow for the combined use of different modelling tools for the study of complex processes, model integration is needed. This paper presents a concept for an integration platform that allows for the integration of modelling tools, combining their models to build up a process model and performing computer-aided studies based on this integrated process model. In order to illustrate the concept without getting into complicated algorithmic issues, we focus on steady-state simulation using models comprising only algebraic equations. The concept is realized in the component-based integration platform CHEOPS, which focuses on integrating and solving existing models rather than providing its own modelling capabilities.

Keywords: Chemical process modelling – Simulation – Heterogeneous implementation – Tool integration – Co-simulation – CORBA

1 Introduction

The problem of tool integration for the modelling and simulation of technical systems is common in different application domains. The problem usually stems from the fact that different subsystems of the overall system might require different modelling and simulation tools. Therefore, for the simulation of the overall system one has to ensure that these different tools can interoper-
text the computer-aided study of the process behaviour based on the mathematical process model. This is done by applying a numerical algorithm to solve the model equations. During the design of a plant, simulation is applied to compare different design alternatives, e.g. with respect to their economics, energy consumption, environmental impact or potential hazards. During the operation of a plant, modelling and simulation are continuously used as a basis for analysing, improving and modifying the plant.

Hence, in contrast to modelling in software engineering, mathematical models are used in chemical engineering for a formal evaluation of the properties of a real (physical) manufacturing process in the sense of what-if studies. In contrast to this, in software engineering reasoning about models (e.g. using UML) is often done qualitatively, and models largely act as a blueprint of an information system to be implemented.

Due to the size and complexity of chemical processes, the resulting mathematical models are also large and complex. Up to several tens of thousands of variables and equations may be used for a rigorous description of a process. Thus, suitable software tools are needed to support the engineer in developing and simulating these models. One can distinguish two kinds of process modelling tools. General-purpose tools support the modelling and computer-aided investigation of a broad class of chemical processes. These processes have in common that the mathematical problems posed by them are similar. In contrast, special-purpose tools are designed for a specific class of problems. Their modelling capabilities and the applied numerical algorithms are tailored to the special demands of the mathematical problems posed by these process classes. Examples are tools for the investigation of particle formation in crystallization tanks [35] or the detailed simulation of flow patterns in mixing and reaction units by computational fluid dynamics (CFD) tools [10].

1.2 Case study under consideration

In this paper we consider the case study of modelling and simulating the Polyamide 6 process depicted in Fig. 1 to illustrate the capabilities of the CHEOPS platform. Polyamide 6 (PA6) is often used as a construction material in mechanical engineering (e.g. for gear wheels and boxes, tires or cases) or in the form of fibres in the textiles industry. The simplified PA6 production process considered here consists of three process parts which are modelled in three different tools. Each of these parts is included in one grey box in Fig. 1. The polymerization reaction unit, consisting of two reactors and an intermediate water separation, is modelled using PolymersPlus [1]. This is an extension of the AspenPlus [2] modelling tool, which provides a special model library for polymerization reactors. The reaction unit is followed by a separation unit which separates raw material that has not been converted in the reaction step. In our scenario, a wiped-film evaporator is used for this purpose. The model for this process unit is not available in the model libraries of process modelling tools. Therefore, an appropriate model has been developed using the general-purpose tool gPROMS, which provides a modelling language that allows for the development of user-defined models [26]. Finally, the polymer is processed in an extruder, where the polymer properties (such as the chain length distribution) are modified. The extrusion step can be simulated by a special-purpose tool called Morex [30].

1.3 Motivation and solution approach

Two major issues motivate the need for a tool-integration solution within the context of chemical process modelling. The first issue is that some process models consist of complex subsystems that cannot be modelled and simulated in a single general-purpose tool. Rather, the modelling and solution capabilities of different special-purpose tools may be required for modelling and solving different process unit models. This is exactly the case in the PA6 case study described above. Therefore, an integration platform is required that allows one to combine the models from different special-purpose tools. Such a platform should use their solution algorithms and provide a higher-level algorithm that coordinates the evaluation of the different process unit models.

The second issue is the need to support model reuse in chemical process modelling. When modelling a process at some point of its lifecycle, models for some process units are often already available from previous engineering tasks [22]. If these process unit models are not available in the same tool and if these tools are furthermore not able to interoperate, one might consider redeveloping all the models in one (new) tool. However, since chemical process models are often very complex, the cost of doing so can be very high. Hence, a solution for using the existing process unit models from different tools is desirable.

A number of issues must be addressed when designing a tool-integration solution. Different modelling tools