TOWARDS COMPUTER-AIDED MODEL GENERATION

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Abstract: A crucial success factor in a technology driven market such as the chemical industry is coupled with the ability to understand and interpret new technologies fast and convert this knowledge into a competitive advantage. In search for procedures to advance corporate know-how faster, mathematical modeling is becoming an indispensable tool. The new challenge for systems research is to create a new breed of computer-based technologies for assistance and/or partial automation of the creative modeling process. Model Generation is a new modeling paradigm for rapid computer-aided model generation of large multi-scale systems in the industrial practice. It proposes model building by means of phenomena-oriented modeling languages. Using the domain-specific language concepts, users build process models by specifying the physical and chemical phenomena in a fully declarative fashion. Automatic interpretation of the high-level concepts of the model application leads to an equivalent set of system equations. Computer-aided model generation enables engineering teams to formulate highly structured process models in short amount of time. It also focuses the modeling effort onto the fundamental principles governing a process model without the need for explicit coding of all constitutive and balance equations. This article outlines solution approaches and features of a prototypical computer-assisted modeling environment entitled TechTool, which is being developed in an academic-industrial collaboration.

1. Introduction.

Background and Motivation

Phenomena-oriented modeling is a research initiative for the computer-aided support and partial automation of the creative task of process modeling. Recent reviews give a comprehensive account of the state-of-the-art and new challenges for computer-aided model building [e.g. Marquardt, 2000, VanSchijndel and Pistikopoulos, 2000]. The discourse of this presentation is limited to the computer-aided generation of mathematical models for chemical processes. This task belongs to the most challenging phases of the life-cycle of a process model. Consistency maintenance of the resulting problem formulations adds to the formidable task. It is tightly linked to structural analysis of the mathematical artifacts. Therefore model generation and structural analysis need to be addressed in conjunction. This is underscored by the fact that the generated equations lay the foundation for the mathematical solution of the process models.

Recent advances overcome some of the shortcomings pertaining to the existing modeling strategies. On-going research effort provide faster algorithms for simulation and optimization [e.g. Wright, 2000; Biegler et al, 2000; Grossman and Hooker, 2000], address dynamic simulation of continuous and discrete processes, i.e. hybrid simulation [e.g. Park and Barton, 1996; Bahl and Linninger, 2000], and point towards solution approaches in dynamic optimization [Galan and Barton, 1998, Abel and Marquardt, 2000]. Open interfaces and data sharing among commercial and academic flowsheet simulators and physical property packages are the target of initiatives such as CAPE-OPEN [e.g. Global CAPE Open, 2000]. Despite the success for the improvement of simulation environments, methodologies for the computer-aided support of the modeling activity itself have evolved at a less
spectacular pace. There is a need for automation in order to provide for expeditious, full or partial model generation. Fewer research contributions in the chemical engineering literature aim at developing solution strategies for the latter more difficult problem. It is a conservative yet common opinion to consider modeling an art not amenable to systematic treatment by information scientific approaches. This work aims at challenging some aspects of this point of view.

Several research groups have developed computer-aided process modeling and simulation tools, i.e. model generators. Stephanopoulos presented the pioneering Model.la system which presented a comprehensive library of concepts and phenomena of relevance for chemical engineering systems [Stephanopoulos et al., 1990a, 1990b]. A fully functional advanced model generator entitled of Model.la (II) was presented and demonstrated recently [e.g. Bieszczad et al., 2000, Bieszczad, 2000]. Modkit [Bogusch and Marquardt, 1997; Lohmann, 1998] also aims at computer-aided guidance for model evolution. Both environments have ample graphical features and can automatically generate gPROMS code for certain classes of processes. Modkit provides features that support the workflow of modeling process itself. The MODELLER project [Preisig and Westerweele, 2000] proposed a formal framework for declarative model building. Computer-aided approaches for improved integration of software components involved in concurrent engineering is discussed in [Batres and Naka, 2000]. Model generation is a central focus of related systems research in computer science, e.g. hardware-software co-design. The multi-graph approach supports the design and simulation of architecture and performance of electric circuits and their functionality [e.g. Karsai et al., 1997; Sztipanovits et al, 1995].

Before engaging in specific topics for computer-aided model formulation, we should like to formulate a set of goals that a new generation of computer-aided modeling environments should address. The following questions are not intended as an exhaustive list of objectives, but reflects a priority of demands expressed by practicing engineers [Linninger, 1998].

- Fast equation generation: Today, equation-oriented modeling and simulation is becoming a viable alternative to block-oriented flowsheet simulators, e.g. gPROMS, SPEEDUP, ASCEND, ABACUSS. However, equation-oriented process modeling is still a laborious task requiring the implementation of all constitutive equations by hand. For process models of industrial size and complexity this may amount to encoding several thousands or more equations. This effort may render the entire modeling process prohibitively time-consuming and error-prone. Could we generate mathematical artifacts without explicitly editing every single balance equation?
- Inclusion of high-level knowledge: Model equations are essential for the mathematical solution of process models. The mathematical relations alone correspond to a high level of abstractions ill-suited for conserving model intention, assumptions and simplifications. Can new model representations incorporate both phenomenological knowledge and rationale alongside the highly abstract mathematical expressions?
- Multi-disciplinary approach: Larger and more complex process models require multi-disciplinary teams of model developers. Which type of information technology will provide an electronic workbench for distributed collaborative development of large projects?
- Consistency and Structural Analysis: Consistent formulation of large-scale process models commands meticulous bookkeeping of variables, degrees of freedom and intelligence in problem scaling and initialization. Is it possible to design algorithms that can examine consistency, solvability and structural properties of mathematical artifacts?

The demands raised by industrial users call for an analysis of the difficulties in computer-assisted modeling. Before designing a computer tool to do model generation, a reflection on the thinking patterns of engineering students is in place.

Key engineering courses such as mass and energy balances, transport phenomena, thermodynamics and reaction engineering help develop the basic skills for mathematical modeling. Three significant topics appear crucial: (i) choose level of abstraction, (ii) identify fundamental quantities and apply conservation balances and (iii) select constitutive equations.

“Level of abstraction” teaches techniques for picking appropriate balance envelopes. Ubiquitous standard models surface in the form of a lumped input-output device, i.e. the continuous stirred reactor (CSTR), or as a simple distributed system in one dimension, i.e. plug flow reactor (PFR). These fundamental entities interact with each other via connections that allow exchange of matter, energy, momentum or information. Hence, we specify fundamental quantities measuring the amount of matter, their thermal and the chemical potential. Appropriate mathematical models for fundamental quantities are adopted. There are no rigorous criteria for these choices. Ambiguities may
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 occur when competing theorems are valid for the description of a single property or phenomenon. The large number of equations of states (EOS) exemplifies this situation in practice. The problem is complicated by the fact that constitutive models are state dependent, e.g. at high pressures a complex model for the fugacity coefficient in a gas mixture is needed; at moderate pressure it can be approximated as unity. The system state however can only be computed once an appropriate model is chosen. These observations elucidates the difficulty in creating a formal framework to support this fundamentally intuitive modeling activity.

Several conclusions can be drawn from these preliminary observations. (i) Computer-assisted model building should support structuring different levels of abstraction. (ii) A set of a few fundamental balances around each modeling element is expected to constitute the backbone the mathematical model. (iii) Constitutive equations quantify the specific of each balance envelope. The particular behavior of an entity and its physical and chemical properties typically depend on its level of abstraction and perhaps even on the expected state range.

Outline.

This article will outline the philosophy of an experimental phenomena-oriented modeling environment. This work is part of the TechTool project currently under development in the Laboratory for Product and Process Design (LPPD) at the University of Illinois at Chicago in collaboration with VAI, Austria. We will present the blueprint of a three-layered architecture and argue for phenomena-oriented modeling as a promising avenue for computer-aided modeling generation, analysis and simulation.

Chapter 2 introduces the principles of meta-modeling. The methodology for defining custom-built modeling languages will be discussed. Chapter 3 will illustrate model building using a declarative phenomena-oriented modeling language defined in the meta-modeling layer. A simple case study will serve as an example for evolving a process models using the high-level concepts. In chapter 4, the third layer of abstraction introduces a generic mathematical language. It will be used to map the high level concepts of the phenomena-layer into the mathematical expressions recognized by iterative solution algorithms. An argument for the importance of structural analysis will be given by means of the index analysis of differential algebraic systems. Open questions, future trends and conclusion close the presentation.

Fig. 1 depicts a scheme of TechTool’s three modeling layers. The foundation for model generation resides on its first layer entitled meta-modeling. In the