COMPUTER-AIDED PROCESS MODELLING

Theses of Ph.D. dissertation

written by
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1 Motivation and aim

Process modelling [1] is a basic and most important activity in process system engineering. This fact is due to the growing spread of process models at all levels from process synthesis and design, through operation planning, to process control and optimization problems. Besides the above traditional application areas, process models are widely used nowadays in the fields of risk and pollution assessment, too.

It is worth mentioning that the major part of process engineering activity is the construction of process models. New process models must often be constructed even when only a minor or major modification of an existing process model would be needed. The reason for this is the often badly defined structure and documentation of the previously constructed model.

Besides the growing application of process models, more and more complex models are required. This fact explains that several advanced and high-level modelling techniques [2] have been proposed and used in the last decades. A great number of computer-aided modelling tools [3]-[11] have been developed facilitating the activities of process engineers thanks to the growing development in computer software and hardware tools.

Recently several commercial computer packages [9]-[10] have also been developed that assists process engineers in the construction of flowsheet models from predefined unit models. But these novel tools often do not assist properly the construction, testing and documentation of a new model from novel elements and/or unit connections. Therefore research groups worldwide deal with computer-aided development of process models on various levels of abstraction.

As the constructed process model sometimes is too simple or too difficult for a given problem, it may be necessary to modify it with either extension or simplification or it must be redefined in the worst case. The modification of a process model is weakly supported or not supported at all by the computer-aided modelling tools available in the literature. So the computer-aided model simplification and extension is an interesting and challenging open problem.

In order to avoid any inconsistency during model simplification and extension, it is extremely useful to know modelling assumptions applied in the construction and modification of the process model. The documentation of the model contains these modelling assumptions [12] in the ideal case, but this documentation can often be incomplete or missing. In order to complete the model documentation with all modelling assumptions, assumption-retrieval algorithms could be used. The retrieving of modelling assumptions is a reverse engineering problem where both the correct problem definition and the solution is unusual and more difficult compared to the ordinary case.

The aim of my PhD thesis work was to elaborate on and to investigate assumption-driven methods and procedures which are applicable in computer aided modelling tools. These assumption driven methods can be used for construction and simplification of process models and for the determination of modelling assumptions from two related process models. The applicability and operability of the proposed methods are illustrated on case studies constructed by our intelligent model editor. This editor is a research prototype of a computer aided modelling tool.

The main aims of my work were as follows:

- Construction of a model building procedure, which
  - builds process models applying an assumption-driven method,
  - constructs verified and minimal process models, and
  - builds process models in their canonical form which can efficiently be used for model simplification.
- Construction of a model simplification procedure, which
  - automatically determines applicable modelling assumptions to a given process model,
  - can be used for simplification of process models.
- Construction of an assumption-retrieval procedure, which
  - reconstructs the modelling assumptions which transform a given process model to a simplified one.

2 New scientific results

The main scientific contributions of the dissertation are summarized in the following theses.

1. Syntax and semantics of process models **[P1], [P6]**

   (a) It has been shown that a process model consists of not only an equation set, but contains variables and equations obeying a well-defined syntax and semantics. From this syntax and semantics various relation types between variables can be defined and variables can be grouped determined by their role in the process model.

   (b) A Prolog knowledge base has been defined for the description of model elements (balance volumes, differential and algebraic variables, balance equations and constitutive algebraic equations) of a process model.

2. The model building procedure **[P1], [P6]**

   An assumption-driven model building method has been developed for construction of verified and minimal process models. The proposed method is an incremental model building procedure resulting in a process model. The main steps of model building procedure are as follows:

   - specification of the balance volumes,
   - specification of the conserved extensive quantities for each balance volume,
   - specification of the transport terms in each balance volume,
   - generation of the conservation balances for each conserved extensive quantities in an automated way,
   - specification of the constitutive algebraic equations for all of the algebraic variables.

   The proposed model editor defines the knowledge elements of the process model with the help of a questionary-type user interface.

3. The syntax, semantics and properties of model simplification assumptions **[P1], [P4], [P5]**

   (a) Modelling assumptions have been formally described by a triplet. As the semantics of modelling assumptions defines the effects of the assumptions on a process model, the modelling assumptions have been considered as formal transformations, called model simplification transformations, encoded in the form of syntactical and semantical rules. From the model elements of a process model the set of model simplifying assumptions have been determined.

(b) The properties of model simplification transformations have been investigated. It has been shown that the applied transformations are usually related and the number of applicable transformations is usually decreasing during the model simplification process due to the inconsistency and redundancy of assumptions.

(c) A Prolog knowledge base has been defined for the description of modelling assumptions and formal model simplification transformations.

(d) The effects of model simplification assumptions are determined by forward reasoning. The model simplification itself consists of two well-separated parts, namely the execution of model simplification assumptions and that of formal algebraic transformations.

4. The model simplification procedure **[P1], [P4], [P5]**

   A model simplification method has been developed for the simplification of process models. The main steps of the proposed method are the following:

   - collection of possible simplification assumptions,
   - selection of an assumption (*),
   - forward reasoning to find the effects of the selected assumption,
   - examination of the resulted model,
   - modification of possible assumptions,
   - return to step *.

   The model simplifier provides the simplified process model together with the set of selected simplification assumptions as result.

5. The assumption retrieval procedure **[P4], [P5]**

   An assumption retrieval method has been developed for the determination of simplification assumptions of two related process models. The proposed method finds the sequences of model simplification assumptions which are able to transform the detailed model to the simplified one. The main steps of the procedure are as follows:

- clumsy comparison of the process models,
- forward reasoning (*)
  - selection of a possible goal,
  - collection of the possible assumptions,
  - iterative deepening search (modification of possible assumption list in every step of search),
  - return to step *.

  Simplified process models are produced in the steps of iterative deepening search with the help of forward reasoning method of the model simplification procedure.

Prolog programming language has been used for the implementation of the proposed methods and algorithms on computer in the form of a research prototype intelligent model editor.

3 Publications related to the thesis

Journal papers

[P1] Lakner R., Hangos K.M. and I. T. Cameron: An assumption-driven case-specific model editor. *Comput. Chem. Engng.*, **23**, S695-S698. (1999)

Books

[P2] Hangos K., Gerzson M., Piglerné Lakner R., Gál I.: *Intelligent controlled systems* Lecture notes, University of Veszprém. (1995)

[P3] Hangos K. M., Lakner R. and Gerzson M.: *Intelligent control system - An introduction with examples,* Kluwer Academic Publishers. (2001)

Parts of books

[P4] Lakner R., Hangos K.M. and I. T. Cameron: Assumption retrieval from process models. *Computer Aided Chemical Engineering* **9** R. Gani, S.B. Jorgensen (Eds.), Elsevier 195-200. (2001)

[P5] Lakner R. and K. M. Hangos: Intelligent assumption retrieval from process models by model-based reasoning. *Engineering of Intelligent Systems (Lecture Notes in Computer Science* : *Lecture Notes in Artificial Intelligence)* **2070** L. Monostori, J. Váncza, Moonis Ali (Eds.), Springer, 145-154. (2001)

Conference papers

[P6] Lakner R. and K. M. Hangos: Computer-aided incremental model building *IASTED International Conference on Modelling, Identification and Control, MIC'2002* Innsbruck, Austria, February 18-21. pp. 426-431. (2002)

4 Publications partially related to the thesis

[E1] B. Csukás, Z. Kozár, R. Lakner: Prolog Structures and Valuated Prolog Structures in Process Synthesis. *The 5th Conference on Applied Chemistry, Unit Operations and Processes*, Balatonfüred, Vol. 2. 507-515, (1989)

[E2] B. Csukás, R. Lakner: Learning Prolog Algorithm in Process Synthesis. *10th International Congress CHISA'90*, Prague, (1990)

[E3] B. Csukás, R. Lakner, K. Varga, L. Jámbor: Intelligent Dynamic Simulation by Automatically Generated Prolog Programs. In: L. Puigjaner and A. Espuna Eds.: *Computer-Oriented Process Engineering*, Elsevier, Amsterdam, 41-46, (1991)

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[E6] Lakner R., Csukás B.: A struktúra bázisú logikai programozás és vegyészmérnöki alkalmazásai. Műszaki Kémiai Rendszerek '91. Veszprém, 39-40. (1991)

[E7] Varga K., Lakner R., Csukás B.: Irányított reaktorok dinamikus szimulációját segítő struktúra bázisú szakértői rendszer. Műszaki Kémiai Rendszerek '91. Veszprém, 46. (1991)

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[E9] Jámbor L., Lakner R., Csukás B.: Flexibilis műveleti egységeket működtető struktúra bázisú irányítási rendszer. Műszaki Kémiai Rendszerek '91. Veszprém, Kiadvány 59-60. (1991)

[E10] B. Csukás, R. Lakner, K. Varga, L. Jámbor, G. Wittinger: Prolog Representation of Structural Models and Cybernetic Structures in (Chemical)

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[E11] B. Csukás, K. Varga, R. Lakner, L. Horváth: Computer-Aided Process Synthesis by Automatically Generated Simulation Models. *11th International Congress of Chemical Engineering, Chemical Equipment Design and Automation*, Praha, D4-5. abstract, Volume D, 19, (1993)

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[E13] Csukás B., Lakner R., Horváth L.: A mesterséges evolúció modellezésének lehetőségei. Veszprémi Környezetvédelmi Kiállítás és Konferencia, Veszprém, (1993)

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