European Symposium on Computer Aided Process Engineering – 15
L. Puigjaner and A. Espuña (Editors)

Process Modelling Goals: Concepts, Structure and Development

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Abstract

Process modelling is and should be goal-oriented. The formal statement of modelling goals in current process modelling practice is either forgotten, somehow considered implicitly, or vaguely remembered at some later point in the model building cycle. This lack of explicit goal statement greatly affects the focus, task efficiency, model parsimony and the termination of the modelling cycle, especially in model conceptualization. This practice stands in stark contrast to the building of commercial process, mechanical, electrical or software systems. Lack of explicit goals often means a model is not "fit for purpose", takes too long to develop and is either too simplistic or overly complex for the application.

The aim of this paper is to discuss the importance of defining and decomposing goal-sets for process modelling. It poses key unsolved challenges in describing and understanding goal-set development and evolution, especially in the *model conceptualization phase.* It shows how the goals can help direct the modelling effort and determine the modelling cycle termination. The paper does not provide a closed solution to this complex problem but is aimed at generating discussion across the CAPE community. This is an important aspect in the future development of intelligent multi-agent systems that can aid process modelling practice – so-called 'modelling assistants'.

Keywords: process modelling, goals, means-ends, conceptualization, multi-agent systems

1. Introduction

Goal statements together with objectives and specifications are common practice in the process, electrical and software engineering disciplines. System components and functionality go together to satisfy the ends or goals of a designer. These application areas are examples of the 'means-ends' paradigm common to the design and analysis of many socio-technical systems (Achinstein 1983, Lind 1994, Jalashgar 1999). When it comes to building process models "fit for purpose" – there has not been a serious consideration of a formal means-ends approach in the CAPE community. Is it often said "Modelling is just so different, you simply can't do it that way – it is more art than science!"

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In order to better tackle the process modelling 'means-ends' problem for new and innovative technologies or environmental systems we need to develop a clear understanding of modelling goals and their implications. A generic approach will be applicable to a wide range of modelling activities such as efficient model building for multiscale systems, providing a rational design basis for multi-agent modelling systems and generating parsimonious models. The following sections set out some of the key questions that need answering in order to make significant progress in the next phase of modelling practice. Section 2 discusses the details of modelling goals – key issues and representation.

2. Modelling Goals and Their Importance

In addressing the issue of modelling goals there are a number of key questions that need to be answered if goal-directed modelling is to be a reality. These include:

1. How do we express goal statements in a natural way that is easily understood and usable by process engineers and in intelligent systems?
2. How do we decompose a canonical goal statement into a goal tree or goal network?
3. How does the goal tree evolve with the modelling process?
4. How do we clearly relate objectives and specifications to the goals and subgoals in the tree or network?
5. How is the goal structure with its objectives and specifications linked to the model structure and the understanding of the physical reality?
6. If we adopt a "goal-driven" approach to modelling, how does that affect the workflow issues in modelling?

Ultimately all modelling has a common basis in the concept of functionality. Figure 1 shows the mapping of a physical reality to a model space. The aim is a model that encapsulates the essential functionality of the real world, appropriate for the application. The 'means-ends' paradigm applied to modelling requires the explicit statement of goals that in turn drive the means (model functionality) to achieve those goals. This is a hierarchical problem which is briefly discussed in section 2.2

2.1 Stating and representing goals

Modelling goals are statements about the *end-points* to which the modelling efforts are directed. Some typical and *real* industrial or consultancy statements of modelling goals are:

a) "We need to develop a model to help design a control system for the batch reactor"
b) "The spill of toxic liquid should be modelled to assess the potential human impacts"
c) "Modelling the sugar dryer will help us determine the best control strategy to adopt"
d) "The leaching of toxics from the processed mine material needs to be modelled to assess environmental impacts"

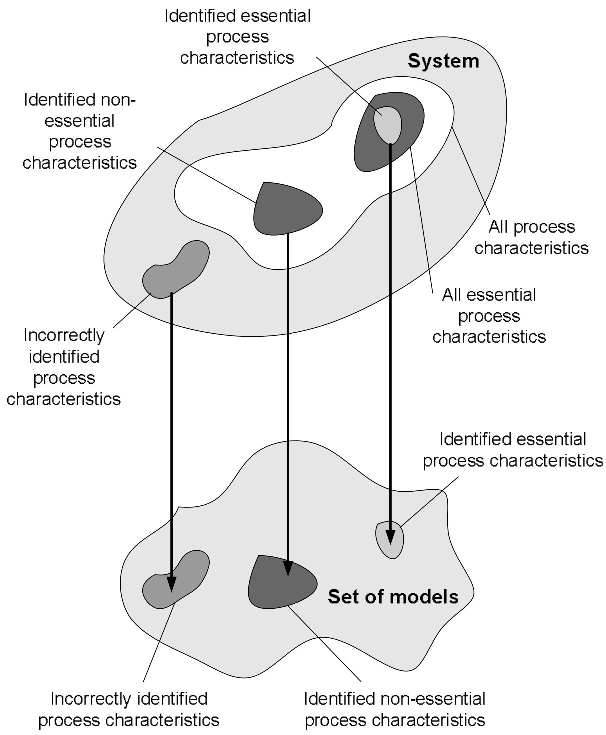

Figure 1. Mapping reality to model representation

An analysis of the above canonical goal statements leads to a well-defined modelling goal triplet: << ***Model*** >> to/for << ***Application***>> of/from/for << ***System*** >>
We define this as the <<***M-A-S***>> triplet. The <<***Application***>> component can be represented by two concepts, viz. <<***Activity***>> + <<***Outcome***>>. The model class itself can be decomposed further into a full set of related classes covering the range of empirical, mechanistic, stochastic and deterministic modelling approaches (Cameron et al. 2003).
The physical system has normally been derived from the intent of the designers, typically expressed in a hierarchical goal tree. This functional decomposition has similar representations in multi-flow modelling approaches (Lind 1994, Petersen 2000) or in safety analysis methods such as concept hazard analysis (Wells et al. 1993). Figure 2 shows such a functional description for a continuous stirred tank reactor (CSTR) system with temperature and level control. Similar functional decompositions can be performed for natural systems. These functional decompositions are not unique.

2.2 Goal decomposition

Decomposition of modelling goals is a non-trivial activity. Canonical goal statements, such as those in section 2.1 can be decomposed into sub-goals that are related to the modelling objects. In the case of process systems this ultimately involves balance volumes, phases, surfaces, convective and diffusive flows with other constitutive objects with their respective attributes. The goal decomposition is not necessarily unique since it depends on the modeller's understanding of the functions in the system under study. The model goal decomposition consists of a series of hierarchical <<***M-A-S***>> triplets. An example of this is seen in section 4.

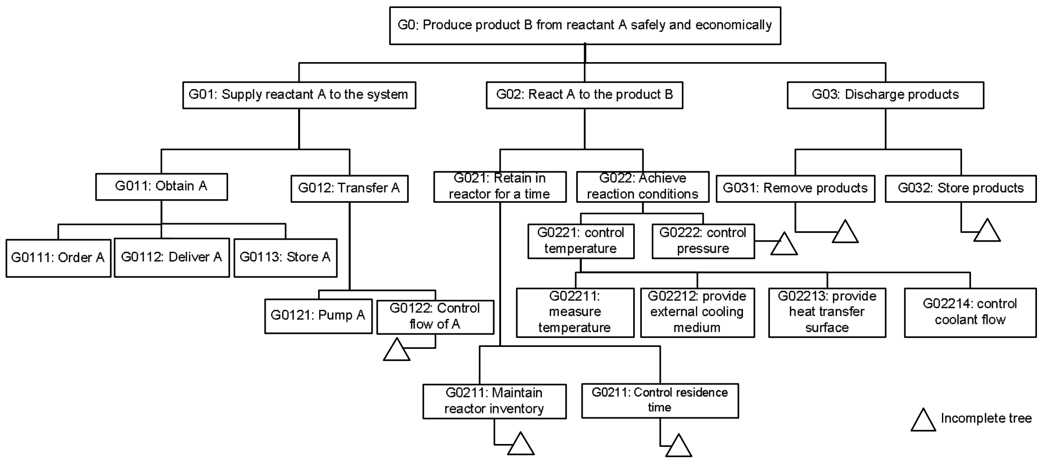

Figure 2. Part of a designer's functional description of a CSTR system – the intent

3. Goals and Their Relationship to Model Building

Goal statements determine the necessary modelling outcomes. The important issues are to know how and when goals are satisfied in the modelling process. *Processing goals* are met when the requisite functionality exists in the design. *Modelling goals* are satisfied when correct functionality is embedded in the model. This functionality is derived from model components and their composite capabilities.

3.1 Fundamental process model building concepts

Means-end analysis for process modelling is concerned with providing a framework that allows the modeller to develop model structures that have the requisite functionality to achieve the stated goals. *Functionality includes the model representation of the basic character of the system as well as the requisite functionality for the application area.* Figure 3 shows the general concepts linking component capabilities to functional structures that meet goals. The building blocks in most process modelling are the objects seen in CAPE modelling tools such as *Model.la* (Stephanopoulos et al. 1990), *ModKit* (Bogusch et al. 2001) or *SCHEMA* (Williams et al. 2002). The suggested approach does not preclude human factors and non-process engineering capabilities from being reflected in socio-technical models.
Component capabilities, sometimes termed "primitives" can be attributed to a wide range of model building components such as balance volumes ('Hold'), surfaces('permit') and connections ('Transfer'), Chandrasekaran et al. 1986; Modarres & Cheon 1999, Cameron et al. 2003.

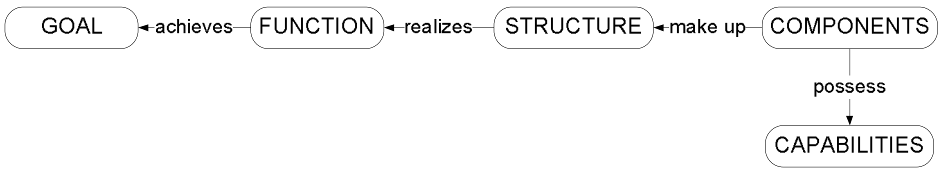

Figure 3. Principal interrelations in process modelling

Modelling, combines fundamental building blocks (balance volumes, surfaces, flows etc.) or composite components to achieve system capabilities to generate functionality. For example, the combination of two balance volumes, a shared surface and diffusive flow provides the functionality for heat transfer from one fluid to another. More complex functionality can be generated through other composite functionalities. Along with functionality it is also possible to investigate mal-functional systems for risk management studies.

4. A Modelling Goal Set Illustration

Consider a CSTR. A canonical modelling goal applied to this plant could be: "Develop a model to assess the level control performance of the CSTR". Given the plant and functional decomposition of the designer (Figure 2), a modelling goal tree can be generated for the given modelling purpose. Figure 4 gives a particular partial decomposition shown as a hierarchical <<***M-A-S***>> tree for part of the model.

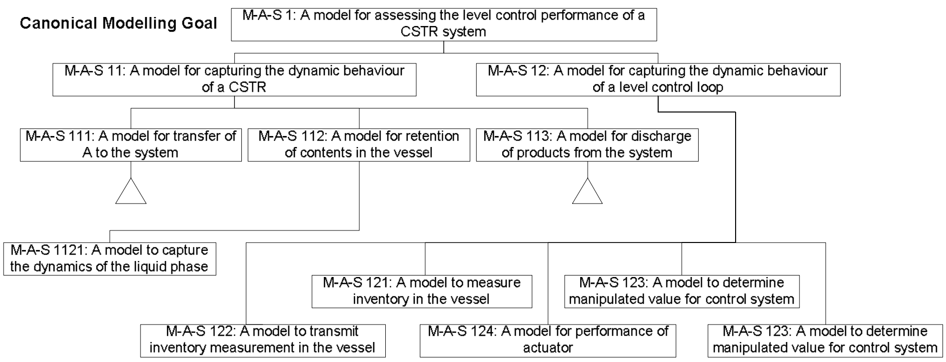

Figure 4. Modelling goal decomposition (partial) for CSTR application

In this decomposition the canonical goal has generated a set of modelling goals that excludes consideration of the temperature control system, simply because the inclusion of that functionality is considered extraneous to meeting the canonical goal. If the modelling goal involved assessment of temperature control performance then clearly that functionality would be needed as well as the level control. This is a very simple example which highlights some of the difficult issues in goal directed modelling. Many issues require attention, not the least of which is the idea of super-additivity of component capabilities – the idea that the whole is more than the sum of the parts.

5. Conclusions

In this paper we have raised some key issues with regard to goal-directed process modelling. Some of the key issues were addressed through development of a goal triplet for representation and decomposition. System and subsystem functionality that meets modelling goals is derived from composite capabilities of the fundamental modelling components. A simple illustration of the concepts is given and some observations made. There are many challenges in developing goal directed modelling strategies that can enhance process modelling and provide a robust, fundamental framework for intelligent modelling assistants. We value comments and observations from colleagues on this issue.

References

Achinstein, P., 1983, The Nature of Explanation. Oxford University Press.

Bogusch, R., B. Lohmann and W. Marquardt, 2001, Computer aided process modelling with *ModKit*, Computers and Chemical Engineering 25(7-8), pp. 963-995.

Cameron, I.T., E.S. Fraga and I.D.L. Bogle, 2003, A discussion paper on goal-set development and evolution in the conceptualization of models. Particles & System Design Centre, The University of Queensland, Australia 4072.

Chandrasekaran, B., J. Josephson and A. Keuneke, 1986, Functional representations as a basis for generating explanations, Proceedings IEEE International Conference on Systems, Man and Cybernetics, pp. 726-731.

Jalashgar, A., 1999, Goal-oriented systems modelling: Justification of the approach and overview of methods, Reliability Engineering and System Safety 64, pp. 271-278.

Lind, M., 1994, Modelling goals and functions of complex plant, Journal of Applied Artificial Intelligence 8, pp. 259-283.

Lind, M., 1999, Plant modelling for human supervisory control, Transactions of the Institute of Measurement and Control 4/5, pp. 171-180.

Modarrres, M. and S. Cheon, 1999, Function centered modelling of engineering systems using the goal tree-success tree technique and functional primitives, Reliability Engineering and System Safety 64, pp. 181-200.

Petersen, J., 2000, Causal reasoning based on multiflow modelling, Conference on Cognitive Systems Engineering in Process Control (CSEPC 2000), November 22-25, pp. 36-43.

Stepanopoulos, G., G. Henning and H. Leone, 1990, *Model.la*: A language for process engineering Parts 1 & 2, Computers and Chemical Engineering 14, pp. 813-869.

Wells, G., Wardman, M. and Whetton, C. 1993, 'Preliminary safety analysis', Journal of Loss Prevention in the Process Industries, vol. 6, no. 1, pp. 47-60

Williams, R., R. Keays, S. McGahey, I.T. Cameron and K.M. Hangos, 2002, *SCHEMA*: An object oriented modelling language for continuous and hybrid systems, Asia-Pacific Conference on Chemical Engineering (APCChE), CD-ROM, New Zealand.

Acknowledgements

Ian Cameron thanks the following people for helpful discussions on this topic: Professors Morten Lind (DTU), René Bañares-Alcantará (Oxford), Wolfgang Marquardt, Aidong Yang (RWTH-Aachen) and Katalin Hangos (HAS). ITC also acknowledges support from the UK-EPSRC during his stay at UCL and thanks Professors Fraga and Bogle for their hospitality.