An Ontology-based Approach to Conceptual Process Modelling

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Abstract
The development of mathematical models for process systems can start from conceptual modelling, which is defined as characterizing the process system to be modelled by physicochemical concepts. The resulting conceptual model serves as a basis to further derive a mathematical model. In this paper, we propose to develop conceptual models using an ontology that represents a conceptualization of process systems. A tool applying this approach refers to generic concepts from the ontology and presents them to the modeller in a proper manner. Specific conceptual models can then be generated by instantiating these concepts. This approach has been implemented in a prototypical software tool. The advantages of this approach include simple realization and easy processing of the resulting conceptual models, mainly due to the use of common ontology tools. This approach also holds the potential of promoting information reuse.

Keywords: computer-aided process modelling, conceptual modelling, ontology

1. Introduction
Developing mathematical models for process systems is generally a complex task, especially when the modelled object is of non-standard type. To improve the efficiency of process modelling and the quality of the resulting models, two sequential steps could be distinguished: conceptual and mathematical modelling. Keeping the purpose and performance requirements in mind, one characterizes the system being modelled with physicochemical concepts in the first step, from which one goes on to the second step to formulate and analyze mathematical equations. This idea has been previously discussed in the literature (Stephanopoulos et al., 1990; Preisig, 1995; Bieszczad, 2000; Hangos & Cameron, 2001; Bogusch et al, 2001). In this work, conceptual modelling is intended to generate the description of a process system such that this description can be mapped to variables and their mathematical relations, either automatically or with minor intervention of the human modeller. Since the step of conceptual modelling essentially addresses the creative part of process modelling, providing computed-based support to it is of remarkable significance.

In this paper, an ontology-based approach to conceptual process modelling is explored. An ontology is an explicit specification of the conceptualization of a certain domain, typically involving concepts, their relations, and axioms that represent complex constraints (Uschold & Gruninger, 1996). The development and use of ontologies are currently being extensively studied in the field of ontological engineering (Devedžić, 2002). In connection with process modelling, Bogusch et al (2001) discuss the role of

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ontologies in conceptualizing chemical processes. Batres et al. (2002) present the idea of using an ontology to enhance the exchangeability of mathematical models. The present work specifically focuses on an ontology-based approach to the generation of conceptual models. In the following, we will present the proposed approach, and then introduce a first realization of it. Thereafter, a comparison between this approach and related work will be given to reveal its advantages.

2. The Ontology-based Approach

In general, the formulation of a conceptual model involves two aspects: the provision of generic concepts needed for process modelling, and the instantiation of these concepts according to the concrete process systems to be modelled. In the following, we shall explain how the ontology-based approach addresses these two aspects.

2.1 Conceptualization of a domain

By definition, an ontology provides concepts and their relations of a target domain. For process modelling, an ontology should provide concepts about the behaviour of process systems. Besides presenting individual concepts and their relations, one can also declare in an ontology the constraints on the semantics of some concepts to clarify the intended meaning and/or usage. Such constraints, often called axioms, are especially useful in process modelling for avoiding potential modelling mistakes at the “physical level” before the derivation of mathematical equations.

Depending on the expression language used, an ontology can be either informal or formal (Uschold & Gruninger, 1996). In case automatic processing is expected, the ontology should be expressed using an artificially defined formal language. For the purpose of conceptual process modelling, a formal ontology should be used in order to facilitate processing by a modelling tool, as to be explained in Section 2.2.

2.2 Instantiation of concepts

Process modelling concepts provided in an ontology are to be instantiated to generate concrete conceptual models through the interactions between a human modeller and a conceptual modelling tool. Such a tool needs to perform four activities for proper supports:

(1) Load the ontology. This activity allows the tool to access all the contents of the ontology. An ontology parser that supports the expression language of the ontology can be employed for this purpose.

(2) Present the relevant concepts. Since the amount of concepts in an ontology can be huge, it is desirable that only the concepts relevant to the current position in the modelling process are presented to the human modeller. This can be implemented to some extent by employing an ontology querying tool which is able to determine the relations between a set of concepts.

(3) Support declaring instances of concepts. For such instantiation, the tool should provide means for the human modeller to select certain concepts, declare their instances, set up the links between them according to the ontology, and save the results. This is a task of designing and implementing a graphical user interface as well as a module performing the storage.

(4) Verify the conceptual model. The conceptual model consisting of instances of concepts and their semantic links should be checked against the ontology, especially the axioms defined in it, in order to make sure the conceptual model is valid with respect to the ontology. There exist some ontology reasoners which are capable of checking the consistency between the ontology and the instances of concepts in the ontology.
3. Prototypical Realization

The above approach has been implemented in a prototypical tool for conceptual process modelling, which uses OntoCAPE as the ontology.

3.1 OntoCAPE

OntoCAPE (Yang, 2002) is developed in the COGents project (Braunschweig et al., 2004). It is based on CLiP, a comprehensive conceptual data model for process engineering (Bayer et al., 2003). The intended scope of OntoCAPE covers not only process modelling but also model-based activities such as simulation and design. To render an extensible structure, OntoCAPE has been designed to have two different parts, namely the part of common concepts sharable by different applications and the part of application-specific concepts. Each part contains a number of partial models.

For conceptual process modelling, the partial models of immediate relevance include those of “chemical process system” and “chemical process material” in the common concepts part, and that of “process model” in the application-specific part. The UML class diagram in Figure 1 gives an overview on what these OntoCAPE partial models essentially indicate: an object being modelled can be either a chemical process system or a chemical process material; the behaviour of a modelled object is characterized via its properties and/or phenomena, and is modelled by property models and laws.

Since a detailed description of all of those partial models is not possible due to space limitations, only the high level concepts in the partial model of the behavioural aspect of processing subsystem are shown in Figure 2 in the form of a UML class diagram. A processing subsystem is part of a chemical process system that reflects the perspective of physicochemical processing and complements that of control and management. According to this partial model, the behaviour of a processing subsystem is represented mainly through material amounts and material amount connections, each of which is described by a number of properties and phenomena. A material amount refers to a chemical process material which is defined in detail in a separate partial model. That partial model represents substances and phase systems which, in contrast to material amount, are irrelevant to the absolute amount or geometric shape (cf. Yang et al., 2003).

OntoCAPE provides not only concepts, but also axioms to represent constraints. As an example, one axiom states the following: if the flow pattern (a subclass of material amount phenomenon) of a material amount has been declared as “well mixed”, no intra-phase transport phenomenon (another subclass of material amount phenomenon) can be declared for the same material amount.

OntoCAPE has been formally represented using DAML+OIL, an ontology modelling language that has a solid basis in Description Logics (cf. www.daml.org). The ontology and a set of application examples will be made available on-line at www.lpt.rwth-aachen.de in early 2004.

3.2 The prototypical tool

The prototypical conceptual modelling tool (CMT for short) that can use OntoCAPE to implement the proposed approach has been developed by adapting part of an existing process modelling system called Modkit+ (Hackenberg, 2003), which itself is a re-implementation of Modkit (Bogusch et al., 2001). ModKit+ provides a framework of tools for building mathematical models of chemical processes. Within this framework, the tool generating conceptual descriptions of chemical processes is called “theory tool”, which instantiates “theories” encoded as a set of classes written in Python programming language. In this work, OntoCAPE is introduced into the “theory tool” to
replace the Python classes, and the function of instantiating concepts is adapted accordingly. The structure of the resulting CMT is shown in Figure 3.

For generating a conceptual model according to Section 2.2, the CMT first loads OntoCAPE using Jena, a popular DAML+OIL ontology parser ([www.hpl.hp.com/semweb/](http://www.hpl.hp.com/semweb/)), which can store a DAML+OIL ontology in an internal format. Thereafter, queries about the relations among different concepts and the information of individual concepts can be handled by Jena’s API.

Regarding the presentation of relevant concepts to the human modeller in a certain modelling context, this CMT assumes that a central concept denotes the current modelling context, and it presents to the human modeller only concepts that are subclasses of this concept and those that can be used as types of its properties. Meanwhile, the CMT also shows all properties of this concept. All the above classes and properties are collected from the loaded ontology using Jena.

Following this principle, the CMT takes the concept *Process Model* as the default first central concept unless this is specified otherwise. Then, an instance of this concept can be generated by setting values (i.e. instances of some other classes) to its properties using a simple graphical user interface. Anyone of its properties, e.g. an instance of *processing subsystem* as the value of its “modelled object”, can be further specified in the same manner as is done for the instance of *process model*. This process recursively continues until all the intended details have been supplied. The resulting conceptual
model is saved into a DAML+OIL file by using a function offered by Jena. As the last step, an ontology reasoner called RACER (http://www.sts.tuharburg.de/~ra.moeller/racer/) is used to check the consistency of this DAML+OIL file with respect to OntoCAPE. For example, if on the one hand the material amount in a reactor is declared as well-mixed and on the other hand an intra-phase mass diffusion is specified, a warning will be raised by the reasoner according to one of the axioms defined in OntoCAPE (cf. the example of axioms in Section 3.1). To resolve this confliction, the human modeller should remove one of the two claims.

The CMT is coded using Python. It connects to Jena through COM. The reasoner RACER is connected to the CMT via the TCP/IP interface of Racer. This tool is currently being applied in the COGents project for generating descriptions of chemical processes for which mathematical models are to be obtained.

4. Comparison with Related Work

Computer-aided process modelling tools that adopt a phenomena-based approach often allow to characterize the systems to be modelled using physicochemical concepts. Some of them such as Model.la (Bieszczad, 2000) and TechTool (Linninger, 2000) do this explicitly by offering a certain phenomena-based modelling language. Drengstig et al. (1997) suggests a set of graphical symbols to represent modelling concepts. Other tools such as Modkit (Bogusch et al, 2001) and ModDev (Jensen, 1998) reflect physicochemical concepts through model building blocks which accommodate mathematical models as well. The existing tools usually provide a graphical interface for modellers to compose a conceptual model, either explicitly or implicitly. More advanced functions are also offered by some tools. For example, Model.la employs a set of model consistency operators to check the consistency of conceptual models.

The approach proposed here belongs to the category of approaches that generate explicit conceptual models apart from mathematical models. A conceptual model resulting from such approaches is not only an intermediate result of modelling, but also a perfect documentation of the mathematical model finally obtained to support model reuse. In comparison with other alternatives for generating explicit conceptual models, a distinctive feature of our approach is the use of a generic domain ontology expressed in a common and formal modelling language. Thus, the concepts employed for modelling can be processed using common ontology tools that support this ontology language. As described in the last two sections, these tools can be used during the generation of conceptual models to handle queries on the contents of the ontology and to verify a conceptual model with respect to the ontology. Therefore, conceptual modelling support can be carried out directly by using those common tools, which to a large extent simplifies the implementation. Once conceptual models are generated, common ontology tools again can be used to automatically process them for managing/accessing mathematical models of which the conceptual models are used as the documentation. The experience in the COGents project shows that such conceptual characterization of process models can be processed by ontology reasoners to select suitable models for certain process modelling tasks (Braunschweig et al., 2004).

Besides the benefits stemming from the use of common ontology tools, the use of an explicit domain ontology also holds the potential for promoting information reuse. In this work, OntoCAPE has played the role of a concepts provider. However, it is not an ontology only for process modelling. As indicated in Section 3.1, OntoCAPE well reflects the fact that process modelling and other activities share a large set of common
concepts. This makes it possible that a conceptual model may be formulated by reusing
information generated already in other tasks such as process design.

5. Conclusions and Future Work

An ontology-based approach to conceptual process modelling has been presented in this paper. This approach suggests the use of an ontology to provide physicochemical
concepts as the basis of an ontology-based conceptual modelling tool. This tool produces conceptual models through loading an ontology, presenting concepts to the
human modeller, facilitating the instantiation of concepts, and verifying the resulting
conceptual model. The development and processing of ontologies are supported by
common methods, languages, and tools from the field of ontological engineering, which
to a large extent simplifies the realization of a generic conceptual modelling tool, and
also allows automatic processing of resulting conceptual models. Certainly, the
functions currently implemented in the prototypical tool can be further extended to
incorporate specific process modelling knowledge. This could be realized in the future
through the integration of certain expert systems. Information reuse in different process
engineering activities across the life cycle (Marquardt et al., 1999) can also be
addressed, if the ontology is properly constructed. In addition, we have mentioned
earlier that the step following conceptual modelling is to derive mathematical models
from conceptual models represented by means of an ontology. Currently we are
investigating how this can be achieved by customizing and combining basic
mathematical model blocks formulated according to the same ontology; the result will
be presented elsewhere.

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