13 Conclusions

13.1 OntoCAPE in a Nutshell

OntoCAPE constitutes an ontology framework designed for multiple applications in the domain of computer-aided process engineering. It comprises a top-level ontology, a domain ontology, several application ontologies as well as a generic meta-ontology that provides best-practice design patterns for various modeling problems. The individual sub-ontologies of OntoCAPE can be easily extended, customized, or integrated with other ontologies.

OntoCAPE has the objectives of being both usable and reusable. These two objectives are in a natural conflict: Usability implies specialization to match the requirements of a particular task, whereas reusability requires generality in order to facilitate an application in different contexts. Consequently, it is difficult to simultaneously achieve a high degree of usability and reusability at the same time. A reasonable compromise can only be reached partially, and it requires considerable time and effort since the ontology needs to be iteratively redesigned and tested in different applications. Contrary to numerous pseudo ontologies, which are content to support only one single application, OntoCAPE nevertheless takes up the challenge to realize a reasonable trade-off between usability and reusability.

OntoCAPE is published in form of two complementary parts, a formal specification and an informal specification. The formal specification is given by means of the modeling language OWL DL. Its current release consists of 62 OWL files comprising about 500 classes, 200 relations, and 40,000 individuals in total. The ontology terms are formally defined through a large number of axioms. Therefore, OntoCAPE can be characterized as a heavy-weight ontology. The informal specification of OntoCAPE comprises about 500 pages of natural language documentation. It serves the double purpose of (i) a user manual and (ii) a reference guide, in that it (i) explains the ontology and its handling to common users and (ii) supports applications developers in refining, extending, or changing the ontology to their particular needs.

OntoCAPE is hierarchically structured by layers, which subdivide the ontology into different levels of abstraction and thus separate general knowledge from knowledge about particular domains and even applications. The topmost Meta Layer, is the most abstract one. It holds the Meta Model, which guides ontology development and enforces design consistency when changing or extending the ontology. Next, the Upper Layer of OntoCAPE defines key concepts such as system, physical quantity, or backdrop, and introduces the principles of general systems theory according to which the ontology is organized. On the subjacent Conceptual Layer, a conceptual model of the CAPE domain is established, which covers such different areas as unit operations, equipment and machinery, materials and their

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thermophysical properties, chemical process behavior, and mathematical modeling. The two bottommost layers refine the conceptual model by adding classes and relations required for the practical application of the ontology: The Application-Oriented Layer generically extends the ontology towards certain application areas, whereas the Application-Specific Layer provides specialized classes and relations for concrete applications.

Each layer is subdivided into a number of modules. The boundaries of a module are chosen such that the module can be designed, adapted, and reused independently from the other parts of the ontology to the extent possible. Different variants of an ontology module may evolve, allowing for the coexistence of alternative knowledge representations of the same or overlapping chunks of knowledge. Modules that address closely related topics are grouped into a common partial model. Unlike modules, partial models may be nested and may stretch across several layers. Their boundaries reflect the "natural" categorization of the domain, thus providing a stable frame of orientation for the organization of the modules. Overall, the structuring of the ontology into layers, modules, and partial models follows two principal objectives, namely to facilitate the ontology's extensibility and long-term maintenance, and to enable its customization and reuse in different application contexts.

With regard to related work, OntoCAPE has incorporated certain aspects from engineering ontologies of related domains. In the chemical engineering domain, OntoCAPE is unique in the sense that it is currently the only (re)usable ontology available to support CAPE software development.

13.2 Design Rationale

Numerous recommendations for ontology design are given in the literature. They have been condensed to six major principles, which have guided the design of OntoCAPE: coherence, conciseness, intelligibility, adaptability, minimal ontological commitment, and efficiency. It has been demonstrated how OntoCAPE has put these principles into practice and, in the course of this process, significantly gained in quality. Since some of the principles are incompatible, a suitable balance between the conflicting principles had to be found. The finally realized design is a reasonable compromise between the two major objectives of usability and reusability.

However, it is difficult to quantify the degree of quality due to the absence of generally accepted key measures assessing an agreed set of quality indicators. Thus, we decided to compensate the lack of formal measures by putting OntoCAPE to the test in a number of prototypical software applications. Even if formal measures for quality indicators were available, the degree of (re)usability can be proven ultimately only in an inductive experience-based manner by testing OntoCAPE in a (preferably large) number of different software applications.

Correspondingly, OntoCAPE has been field-tested in a number of software projects covering the chemical process modeling and simulation as well as chemical process design. Through these tests, and through the iterated application of the ontology within these projects, the quality of OntoCAPE has been systematically improved. Nevertheless, we consider it highly desirable to investigate suitable formal measures and sound procedures for checking the quality of an ontology design during ontology development prior to its use in a software project.

13.3 Ontology Evolution by a Continuous Improvement Process

Compliance with the above design principles is hard to achieve in a top-down manner. One reason is the generality, and to some degree also the vagueness, of the design principles. There are only few clear-cut and well-understood rules and guidelines to implement these design principles in a given ontology design project on the concrete level. In other words, we are still lacking validated procedures for the translation of the general design principles into concrete design and modeling decisions both on the architectural as well as on the elementary level of concepts and axioms. A second reason is the inherent complexity of the ontology design task and the lack of measurable indicators to assess quality and the degree of requirements fulfillment.

Consequently, an ontology has to be continuously improved in a systematic process. Such a strategy is comparable to the well-known and successfully applied Kaizen principle, or continuous improvement process, in management (Imai 1997). According to the Kaizen principle, reflection of the current business process constitutes the foundation for (i) the identification of suboptimal process chunks and (ii) the improvement of the business process by a series of incremental steps in an evolutionary manner, thus avoiding quantum leaps with an unpredictable outcome.

Like in business process engineering, we believe that a continuous improvement process is inevitable to achieve a good usability-reusability trade-off and thus an ontology of high quality. Reflection, as of Kaizen, is implemented in the context of ontology engineering by extensive field-testing of the ontology in a (preferably large) number of different software applications. These field tests reveal the improvement potential which is then gradually and continuously realized.

Our research and development work followed such a continuous improvement approach. The field-testing of earlier versions of OntoCAPE revealed errors, inconsistencies and opportunities for improvement. The remediation of the discovered flaws eventually led to the creation of OntoCAPE 2.0. As of this version, the ontology passed all our tests. On the one hand, our ontology proved to be applicable in different contexts, which is an indicator of reusability. On the other hand, the effort required for adapting OntoCAPE to a concrete application turned out to be moderate, which proves the usability of the ontology.

So far, OntoCAPE has not yet been tested in a real-world industrial application, but only in software prototypes and against academic usage scenarios. To close this gap, OntoCAPE is currently being put to the test in a software tool for the integration and consolidation of engineering information, which is used and produced by an interdisciplinary design team working in different organizational units during different tasks of the design lifecycle of a chemical plant. This software tool is developed in cooperation with partners from the chemical and the software industries. Extensive testing by industrial practitioners will establish whether the ontology complies with the requirements of industrial practice. The project is still in progress, but judging from our preliminary results, the ontology seems to fulfill all the requirements for industrial use. Such field-testing in an industrial context is just another and obviously essential phase of a continuous improvement process.

Yet another phase of ontology evolution requires the application and testing of the ontology by people with diverse disciplinary backgrounds and in other types of software projects, preferably in fields of application not considered so far. With respect to the latter, the areas of e-procurement and e-learning are particularly promising since they require well-structured knowledge representations, which are consensual not only across disciplinary, but in particular across institutional boundaries.

The history of OntoCAPE exemplarily shows that ontologies are dynamic information systems, which evolve and change according to the prevailing experience, context and requirements. Ontology evolution is unavoidable. Therefore, it is expected to continue in the future, in particular due to the following drivers: On the one hand, the expected advancement of ontology languages – in combination with improved algorithms resulting in reasoners with high performance for large-scale ontologies – will enable the use of more rules of more complex nature as well as the use of advanced DL constructs in the formal specification, thus allowing to further increase the level of axiomatization. On the other hand, the ontology is expected to change in scope and conceptualization in order to adopt new insights into ontology design, to extend the coverage of domain knowledge and to facilitate an increasing number and type of applications.

13.4 From Product to Process

Design processes in the chemical process industries, like those in many other businesses, are of a cooperative nature and involve different departments in one or more enterprises, typically at geographically distributed sites. They use and produce a vast amount of information organized in a multitude of documents with many interdependencies and overlaps stored in very different electronic formats. These documents are often called the *products* of the work *process*.

Various software tools are used to support a project team. Some of them are of a domain-specific nature (i.e., chemical process simulators, CAD or CAE systems, etc.), others are of generic type and thus independent of the requirements of chemical engineering (i.e., word processors, project management systems, etc.). An efficient support of chemical process design processes requires adequate IT support across the lifecycle of the project. Existing software tools for dedicated tasks in the project lifecycle have to be enhanced and linked to evolve into a coherent design support system, which not only offers user-interface, data, and control integration, but also integrates the distributed, collaborative, and concurrent design process carried out by interdisciplinary teams in different organizations.

To date, no satisfactory solution is available in industry. Therefore, an enormous potential exists to increase productivity of design teams, or, to put it more precisely, to reduce cost and to improve quality at the same time. Leveraging such potential constitutes a tremendous economical opportunity in particular for enterprises in high wage countries such as Europe, Japan, the US, and Canada.

Industrial work processes are complex and consequently difficult to plan, document, improve, and reuse. A fundamental understanding of these work processes is considered to be a prerequisite for their reengineering and for the development of effective support systems based on information technology. To date, the focus of semantic technologies has been mainly on the representation, integration, and retrieval of information about the *results* of work processes – sometimes called *products* – such as the specification of a chemical plant by means of documents like flow sheets and equipment lists in case of design processes. In fact, many tasks in a design process require an integrated view on work processes and their products. Examples include the monitoring of the progress in a concrete design project, the detection of inconsistencies in the design data, or even the uncovering of incomplete design tasks. Such an integration of product and process representation is crucial if we aim at software tools that reach beyond traditional data, control, and user interface integration, but provide additional functionality to support the design process more effectively.

Considerable research activity has been devoted to the modeling of work processes and to the design of supporting software systems, in particular in software engineering (e.g. Jacobson et al. 2003; ISO 12207 2008), business process (re-)engineering (e.g. Davenport 1993; Hammer and Champy 1993) and to a lesser extent in the different engineering sciences (e.g., Hubert and Houten 1999; Ullman 2002). Ontologies have also been used for the formal representation of and for the reasoning on work processes even in an engineering context (cf. Kitamura et al. 2006; Batres et al. 2000; Fuchino et al. 2005; Eggersmann et al. 2003b). A comprehensive review of this literature is obviously beyond the scope of this concluding chapter. However, we want to point to the research on ontologies for work process modeling in our group in this area, because the available and still evolving results will be integrated with OntoCAPE in the future.

As a first attempt towards the capturing and representation of work processes in chemical process design a graphical notation, C3 (Killich et al. 1999; Eggersmann et al. 2008), has been developed in the IMPROVE project (Nagl and Marquardt 2008). C3 allows a coarse-grained representation of work processes including the various *actions* (i.e., the steps of a complex work process), the *actors* (i.e., humans or software) and their *roles* in the work process, the *information* used and produced during the actions, and the *resources* required (i.e., software tools, lab equipment, etc.). The deliberately simple syntax and semantics of the notation support the participative modeling of collaborative work processes, i.e., C3 models can be created by people involved in a particular work process with little or even without any assistance of modeling experts. An iterative procedure for the creation of C3 models and the application of these models to improve industrial work processes has been established based on best-practices. An overview on the modeling procedure and its application to a number of industrial case studies has been presented by Theißen et al. (2008b; 2008c).

While the C3 notation is very useful for participative work process modeling, it lacks detail and the degree of formality which is required for an integrated representation of processes and products, in particular in the context of information system design and construction. Therefore, the development of formal work process models using semantic modeling and ontological technologies has been identified as a logical next step. Some first results are reported by Eggersmann et al. (2008) and Theißen and Marquardt (2008), who present an ontology for work processes extending and refining C3 and an ontology for design decisions, respectively.

In an ongoing research project (Theißen et al. 2008a; Hai et al. 2009), we aim at an extension of OntoCAPE to also provide capabilities for work process modeling. To this end, two steps are required. First, a work process ontology is developed, which does not only address the particular needs of design processes, but rather covers work processes in more general terms. This work process ontology can be integrated into the Upper Layer of OntoCAPE in the future. The second step is the refinement of the work process ontology on the Conceptual and Applications Layers of OntoCAPE to account for the characteristics of different types of work processes. The extension of OntoCAPE towards the representation of work processes of different types, including not only process design but also product design and operational processes, is a further benchmark test for the reusability of the core concepts and architecture of the ontology.

13.5 Semantic Technologies in Engineering – Dream or Reality?

Our research on the use of semantic technologies in chemical engineering has clearly revealed the enormous potential of ontology-based information modeling and of the reasoning capabilities of current semantic software technologies. A properly chosen architecture of the ontology empowers the chemical engineer to extend and modify the ontology by means of high-level modeling tools without the assistance of ontology experts. The direct access to the domain knowledge facilitates maintenance and extension of the information model and the knowledge-bases. The reasoning capabilities of semantic tools facilitate the checking of the logical consistency of the information model and the implemented knowledge. We have not only validated the concepts on academic “toy” problems, but have also implemented prototypical software systems to demonstrate advanced design support functionality in an academic environment. We are furthermore validating the methodology – OntoCAPE and the underlying semantic technologies – in ongoing industrial projects.

There are, however, also some drawbacks. In particular, the development of an extensible and widely usable ontology is by no means straightforward. Though we believe that OntoCAPE constitutes a very good foundation for a generic and widely usable ontology for chemical engineering applications, we still see a lot of room for improvement and for the extension of the ontology. In fact, we believe that an ontology is never ready for use. It cannot be complete since it is impossible to cover all the concepts in a given domain in a comprehensive manner. Even it would be complete in this sense, it would not be readily usable, because there will always be the need for adaptations and refinements to match the requirements of an envisioned application. In our opinion, this can be compared to libraries of mathematical models provided by all state-of-the-art simulation tools: These libraries provide simulation models for many standard devices. The available models can be further specialized and parameterized by a user at very little effort. Often, new models have to be created, either by deriving them from similar models available in the library or by developing them from scratch. Such a library extension may serve the purpose of extending the coverage of a certain domain in the library or of tailoring the simulation models towards the requirements of a certain model-based application. Such a library extension can be conveniently achieved only if the library is built on a sound theoretical basis.

Since OntoCAPE is primarily based on the concepts of systems engineering, we believe that its application is not restricted to the domain of chemical engineering, but it is applicable to other engineering domains, as well. Particularly the generic parts with their emphasis on reusability are conceptualized in a way to support various engineering domains.

Furthermore, the semantic technologies, in particular the ontology editors and reasoning tools, are still under development. Performance is an issue for the latter, while usability by application-domain rather than knowledge-engineering experts is the key issue for the former. The most important bottleneck at the moment is the lack of applications, which demonstrate the capabilities of semantic technologies and their advantages compared to the more established software technologies that are nowadays used for the design and construction of industrial-strength information systems. In addition, there is a lack of detailed application models, which can be used for a variety of tasks during the lifecycle of a design project or even of the plant itself.

Due to the immense workload required to come up with useful and comprehensive ontologies for chemical engineering applications, it is highly desirable that academics and industry join forces in order to develop, maintain, and gradually extend a process engineering ontology for process engineering. The open-source ontology OntoCAPE is definitely an excellent starting point for such an undertaking.

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