Preface

Motivation for this Book

Ontologies have received increasing attention over the last two decades. Their roots can be traced back to the ancient philosophers, who were interested in a conceptualization of the world. In the more recent past, ontologies and ontological engineering have evolved in computer science, building on various roots such as logics, knowledge representation, information modeling and management, and (knowledge-based) information systems. Most recently, largely driven by the next generation internet, the so-called Semantic Web, ontological software engineering has developed into a scientific field of its own, which puts particular emphasis on the theoretical foundations of representation and reasoning, and on the methods and tools required for building ontology-based software applications in diverse domains. Though this field is largely dominated by computer science, close relationships have been established with its diverse areas of application, where researchers are interested in exploiting the results of ontological software engineering, particularly to build large knowledge-intensive applications at high productivity and low maintenance effort.

Consequently, a large number of scientific papers and monographs have been published in the very recent past dealing with the theory and practice of ontological software engineering. So far, the majority of those books are dedicated to the theoretical foundations of ontologies, including philosophical treatises and their relationships to established methods in information systems and ontological software engineering. Only few of these contributions deal with the topic of a concrete, formal ontology, which targets a particular application domain, and even less also include a thorough and comprehensive description of ontology design, usage, and maintenance.

The majority of the existing domain- and application-centered publications address problems in the life sciences, such as diagnostic systems in medicine or knowledge management systems in molecular and cell biology. Only little activity can be observed in the engineering sciences. In particular, very few ontologies have been elaborated for the domain of chemical engineering. And those few notable engineering ontologies available today are often found to be inappropriate for use in a context different from the one they have actually been developed for. Hence, there is hardly any ontology in the engineering sciences which can be broadly used and which is actually applicable.

The objective of this book is to contribute to closing the gap between theory and practice in ontological software engineering. In the first place, it provides a fully elaborated formal ontology for the domain of chemical engineering. This ontology provides a reasonable conceptualization of the chemical engineering domain, which is a prerequisite for establishing a shared understanding of concepts and terms in a certain scientific field and for fostering the communication in a typical cross-disciplinary engineering design team. The ontology is also supposed to support and to simplify the development of future software applications in computer-aided process engineering (CAPE), a sub-discipline of chemical engineering. The intention associated with the development of this ontology has been expressed in its name OntoCAPE, linking ontologies with computer-aided process engineering.

Besides this very concrete engineering objective, the development of OntoCAPE also aimed at the elucidation and the benchmarking of architectural principles for the design of large-scale ontologies, which can be reused in the same domain for different applications or even across related (engineering) domains. The strive for said architectural principles is closely related to the derivation of a set of guidelines, which assist the ontology engineer in capturing, structuring, formalizing, and documenting the knowledge in a complex engineering domain. Hence, we hope that the development of OntoCAPE – the process as well as the resulting architecture and design principles – can serve as a role model or at least as a best-practice example to guide related efforts in other (engineering) domains.

OntoCAPE is the result of close to two decades of research in knowledge representation and information modeling applied to chemical engineering, which was performed by the research group lead by Wolfgang Marquardt. In the first decade, the primary research objective was to find a conceptualization of the chemical engineering domain that can support the mathematical modeling of chemical process systems. In particular, the construction of phenomena-based computer-aided modeling tools has been envisioned in order to reach beyond the established equation-oriented and block-oriented modeling tools. Later, the research activities have been extended to cover the complete lifecycle of chemical process and plant design with its enormous variety of tasks and model-based solution techniques.

The development of OntoCAPE, has been conducted as part of two large, interdisciplinary research projects, the IMPROVE[1] project (Marquardt and Nagl 2004; Nagl and Marquardt 2008) funded by DFG, the German Research Foundation, as part of the collaborative research center CRC 476, and the COGents project (Braunschweig et al. 2002; Yang et al. 2008), funded by the European Commission in the 5th Framework Program as part of the Information Society Technologies track. The former has been concerned with the development of novel methods and software tools for the support of collaborative design processes in chemical engineering, while the latter has explored a future approach to numerical simulation enabling the assembly of large simulation models from model components provided by libraries distributed on the internet.

[1] IMPROVE has been continued by the Transfer Center 61 (Nagl and Marquardt 2008), the goal of which has been the transfer of selected research results obtained in IMPROVE into industrial practice.

The conceptual basis for OntoCAPE has been established by the information model CLiP (Bayer 2003). Developed in IMPROVE, CLiP itself has been built on previous work carried out prior to IMPROVE and resulting in the knowledge-base VeDa (Bogusch 2001; Baumeister 2000). Version 1.0 of OntoCAPE (Yang and Marquardt 2004; Yang et al. 2008) was developed in the COGents project using CLiP as a starting point. At that time, the development had still a quite narrow focus resulting in an overall structure and content which is very different from the current version of OntoCAPE presented in this book. After completion of the COGents project, the further development and extension of OntoCAPE was taken over by IMPROVE. In 2007, version 2.0 of OntoCAPE was released. Since then, OntoCAPE has been continuously improved to reach the status described in this book. A more extensive overview on the history of OntoCAPE can be found in Chapter 11.1 of this book.

Target Audience

The book is targeted at three major groups of readers. Firstly, the book addresses potential users of the ontology, i.e., practitioners in chemical engineering who are interested in the development and employment of intelligent software applications. They can derive a customized knowledge-base from OntoCAPE, which contains the knowledge they consider to be relevant for an intended application. Such a customization may include specializations of OntoCAPE to incorporate concepts on a more fine-grained, application-specific layer as well as extensions relating to other process engineering tasks which have not yet been addressed by the current version of OntoCAPE.

Secondly, OntoCAPE may serve as an example for knowledge engineers who are willing to develop an ontology for a related, but different (engineering) domain. Such an adaptation of (i) the architecture and of (ii) part of the concepts covered by OntoCAPE requires that the knowledge can be represented according to the principles of general systems theory (Bunge 1979) and systems engineering (Thomé 1993). Candidate domains for an adaptation of OntoCAPE are all engineering domains such as energy, automotive, aerospace, civil, or production engineering. Technical systems in various manifestations are at the heart of these engineering disciplines. Consequently, the more abstract concepts of the ontology should be transferable without the need for modification. In addition, applications in these and other domains are expected to explicitly benefit from the general design patterns employed in OntoCAPE, since they have been explicitly incorporated to support the applications developers in refining, extending, or changing the ontology to their particular needs.

Finally, this book is supposed to be of interest to experts in ontology engineering. OntoCAPE is expected to serve as a good example to illustrate how the plethora of design principles reported largely in the computer science literature can be put in practice to organize a complex ontology in an engineering domain. This book summarizes our experience gained during two decades of research in the design of engineering ontologies. We hope that it can serve as a guideline for ontology engineering experts to illustrate how the suggested design principles support and facilitate the development of a complex ontology.

Accessing and Using OntoCAPE

OntoCAPE is publicly accessible at http://www.avt.rwth-aachen.de/Ontocape, where it is distributed under the terms of the GNU General Public License. It is available as an informal and as a formal specification. Both specifications of OntoCAPE can be accessed via this website free of charge.

For the formal specification of OntoCAPE, the Ontology Web Language OWL has been chosen (OWL-DL, in particular, cf. Bechhofer et al. 2004). The model development was done by means of the ontology editor Protégé (Stanford 2008). For verification, the reasoner RacerPro (Racer Systems 2007) has been used. The current release of OntoCAPE consists of 62 OWL files, each of which includes one module of the ontology.

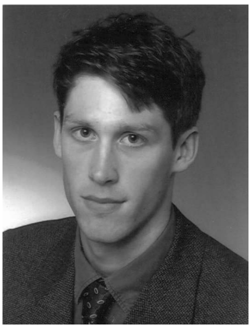
The informal specification currently takes the form of six technical reports, which jointly comprise about 500 pages. It serves the double function of (i) a users manual and (ii) a reference guide. These reports present the organization and structure of OntoCAPE; the conceptualizations of various topic areas are described in great detail. Special emphasis was placed on making OntoCAPE as user-friendly as possible by (i) providing a detailed description of concepts, relations and instances and an explanation of the corresponding interrelations in descriptive UML-like diagrams, by (ii) defining the terms of proper usage of the ontology, and by (iii) highlighting the important design decision and principles leading to the organization and structure at hand. This informal specification complements the contents of this book. While the book focuses on the design principles and architecture of OntoCAPE, concept definitions comprising class, relations and individuals definitions are only sketched and detailed in few instances for illustration purposes. In contrast, the informal specification provides all the concept definitions in a comprehensive manner for reference.

OntoCAPE complies with the two principal types of usage for an ontology that are typically mentioned in the computer science literature: Firstly, an ontology may serve as a library of knowledge components to efficiently build intelligent systems. To this aim, the generic ontology is to be transformed (i.e., extended and customized) into a knowledge-base according to the requirements of the respective application. The second type of usage refers to a shared vocabulary for communication between interacting human and/or software agents. According to their respective functions, the communicating agents may have different knowledge-bases, but all the knowledge-bases must be consistent with the ontology (Gruber

1995). Both types of usage require a consensual knowledge representation that is reusable in different application contexts.

About the Authors

Wolfgang Marquardt, born in 1956 in Germany, studied Chemical Engineering at Stuttgart University, Germany, where he graduated in 1982. Subsequently, he joined the Institute of System Dynamics and Control of Stuttgart University where he completed his PhD dissertation in 1988. From 1989 to 1990, Wolfgang did post-doctoral research at the University of Wisconsin, Madison, USA. After returning to Stuttgart University, he completed his habilitation in the field of dynamics and operations of chemical process systems.
Wolfgang was appointed a Professor for Process Systems Engineering at RWTH Aachen University, Germany, in 1993. His research interest cover a number of areas in process systems engineering, including modeling methodologies, process synthesis, control and operations, numerical methods as well as information technologies for the support of chemical engineering design processes.
Wolfgang has been honored with a number of awards and appointments, including the Award of the Alumni Foundation of Stuttgart University in 1988, the Arnold-Eucken Award of VDI-GVC, the German national association of chemical engineers, in 1990, the appointment as a member of the North Rhine-Westphalian Academy of the Sciences in 1998, and of acatech, the German National Academy of Engineering Sciences, in 2001, the Leibniz-Preis of the German Research Foundation in 2001, the promotion to IFAC Fellow in 2007, and the distinction as the Danckwerts Lecturer of AIChE and EFCE, the US and European associations of chemical engineering, in 2008.



Jan Morbach, born in 1976 in Germany, studied Mechanical Engineering majoring Chemical Engineering at RWTH Aachen University, Germany, and Carnegie Mellon University, Pittsburgh, USA. He graduated with a Dipl.-Ing. degree from RWTH Aachen University in 2002. He worked at AVT – Process Systems Engineering, RWTH Aachen University from 2002 to 2007 as a research assistant. At AVT, his areas of interest included data integration in chemical engineering, ontology engineering, and computer-aided process design. Jan completed his PhD dissertation in 2008.

Since 2007, he works for Bayer Technology Services at Leverkusen, Germany, in the field of chemical process design.

Andreas Wiesner, born in 1981 in Germany, studied Mechanical Engineering majoring Chemical Engineering at RWTH Aachen University, Germany, and at Imperial College, London, UK. He received his Dipl.-Ing. degree in 2006 from RWTH Aachen University. Since 2006, he works as a research assistant at AVT – Process Systems Engineering, RWTH Aachen University. His areas of interest include data integration and management in chemical engineering, ontological engineering, and computer-aided process design.

Aidong Yang, born in 1971 in China, received a B. Eng. degree from Hebei University of Technology in 1992 and a Ph.D. degree from Dalian University of Technology in 1997, both in chemical engineering. During his post-doctoral career, he worked for several institutions in the area of process systems engineering, with a focus on information modeling and mathematical modeling of chemical process systems. In particular, he was a research fellow at AVT – Process Systems Engineering, RWTH Aachen University, from 1999 to 2004, where his research was mainly devoted to the development and applications of ontologies in process engineering.
Aidong is currently a lecturer in Process Systems Engineering at the Faculty of Engineering and Physical Sciences of the University of Surrey, UK. His research interests include the mathematical modeling and optimization of process systems, the application of knowledge engineering methods in process and product development and in manufacturing, and the design of engineering software systems.

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We are also indebted to a large number of individuals who directly or indirectly contributed to the results presented in this book. We enjoyed the very close and lasting collaboration with a number of research groups in computer science in areas related to ontological engineering. Most notably, we interacted with Franz Baader and his former PhD students Ulrike Sattler and Ralph Molitor, with Bertrand Braunschweig, with Matthias Jarke and his former PhD students Sebastian C. Brandt, Michalis Miatidis, Klaus Pohl and Klaus Weidenhaupt as well as with Manfred Nagl and his former PhD students Simon Becker, Markus Heller and Bernhard Westfechtel. This interdisciplinary interaction, and the sharing of the various perspectives on knowledge representation and information modeling, integration, and management contributed significantly to shape our understanding of the relevant issues. The reconciliation of the diverse schools of thought in computer science has been an important stepping stone towards OntoCAPE, its architectural principles and the design guidelines as presented in this book. This book would definitely not have been possible without the fruitful (though time-consuming) discussions with all these colleagues.

OntoCAPE 1.0 has been jointly developed by a number of colleagues under the project leadership of Aidong Yang during the CoGents projects. Contributions from Bertrand Braunschweig, Eric S. Fraga, Didier Paen, Daniel Pinol, Pascal Roux, Manel Serra and Ian Stalker are particularly acknowledged. Also we would like to thank Gabriela Henning and Horacio Leone for the good cooperation.

The OntoCAPE documentation had been sent to a number of computer scientists and experts in computer-aided process engineering and related areas for their comments. The efforts made by these external reviewers are highly appreciated. We are particularly grateful for the feedback we have received on OntoCAPE 1.0 from Rafael Batres (Tokyo Institute of Technology), Patrick Linke (University of Quatar), Michael Stollberg (University of Innsbruck), and Matthew West (Shell Information Technology International).

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We made a major effort to deliver a flawless manuscript. However, if you find any errors, or if you have any other suggestions for improvement, please do not hesitate to let us know (email: Wolfgang.Marquardt@avt.rwth-aachen.de).

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