



## Studies in Computational Intelligence, Volume 87

Editor-in-chief

Prof. Janusz Kacprzyk

Systems Research Institute

Polish Academy of Sciences

ul. Newelska 6

01-447 Warsaw

Poland

E-mail: kacprzyk@ibspan.waw.pl

---

Further volumes of this series can be found on our homepage: [springer.com](http://springer.com)

Vol. 66. Lakhmi C. Jain, Vasile Palade and Dipti Srinivasan (Eds.)

*Advances in Evolutionary Computing for System Design*, 2007

ISBN 978-3-540-72376-9

Vol. 67. Vassilis G. Kaburlasos and Gerhard X. Ritter (Eds.)

*Computational Intelligence Based on Lattice Theory*, 2007

ISBN 978-3-540-72686-9

Vol. 68. Cipriano Galindo, Juan-Antonio Fernández-Madriral and Javier Gonzalez

*A Multi-Hierarchical Symbolic Model of the Environment for Improving Mobile Robot Operation*, 2007

ISBN 978-3-540-72688-3

Vol. 69. Falko Dressler and Iacopo Carreras (Eds.)

*Advances in Biologically Inspired Information Systems: Models, Methods, and Tools*, 2007

ISBN 978-3-540-72692-0

Vol. 70. Javaan Singh Chahl, Lakhmi C. Jain, Akiko Mizutani and Mika Sato-Ilic (Eds.)

*Innovations in Intelligent Machines-1*, 2007

ISBN 978-3-540-72695-1

Vol. 71. Norio Baba, Lakhmi C. Jain and Hisashi Handa (Eds.)

*Advanced Intelligent Paradigms in Computer Games*, 2007

ISBN 978-3-540-72704-0

Vol. 72. Raymond S.T. Lee and Vincenzo Loia (Eds.)

*Computation Intelligence for Agent-based Systems*, 2007

ISBN 978-3-540-73175-7

Vol. 73. Petra Perner (Ed.)

*Case-Based Reasoning on Images and Signals*, 2008

ISBN 978-3-540-73178-8

Vol. 74. Robert Schaefer

*Foundation of Global Genetic Optimization*, 2007

ISBN 978-3-540-73191-7

Vol. 75. Crina Grosan, Ajith Abraham and Hisao Ishibuchi (Eds.)

*Hybrid Evolutionary Algorithms*, 2007

ISBN 978-3-540-73296-9

Vol. 76. Subhas Chandra Mukhopadhyay and Gourab Sen Gupta (Eds.)

*Autonomous Robots and Agents*, 2007

ISBN 978-3-540-73423-9

Vol. 77. Barbara Hammer and Pascal Hitzler (Eds.)

*Perspectives of Neural-Symbolic Integration*, 2007

ISBN 978-3-540-73953-1

Vol. 78. Costin Badica and Marcin Paprzycki (Eds.)

*Intelligent and Distributed Computing*, 2008

ISBN 978-3-540-74929-5

Vol. 79. Xing Cai and T.-C. Jim Yeh (Eds.)

*Quantitative Information Fusion for Hydrological Sciences*, 2008

ISBN 978-3-540-75383-4

Vol. 80. Joachim Diederich

*Rule Extraction from Support Vector Machines*, 2008

ISBN 978-3-540-75389-6

Vol. 81. K. Sridharan

*Robotic Exploration and Landmark Determination*, 2008

ISBN 978-3-540-75393-3

Vol. 82. Ajith Abraham, Crina Grosan and Witold Pedrycz (Eds.)

*Engineering Evolutionary Intelligent Systems*, 2008

ISBN 978-3-540-75395-7

Vol. 83. Bhanu Prasad and S.R.M. Prasanna (Eds.)

*Speech, Audio, Image and Biomedical Signal Processing using Neural Networks*, 2008

ISBN 978-3-540-75397-1

Vol. 84. Marek R. Ogiela and Ryszard Tadeusiewicz

*Modern Computational Intelligence Methods for the Interpretation of Medical Images*, 2008

ISBN 978-3-540-75399-5

Vol. 85. Arpad Kelemen, Ajith Abraham and Yulan Liang (Eds.)

*Computational Intelligence in Medical Informatics*, 2008

ISBN 978-3-540-75766-5

Vol. 86. Zbigniew Les and Magdalena Les

*Shape Understanding Systems*, 2008

ISBN 978-3-540-75768-9

Vol. 87. Yuri Avramenko and Andrzej Kraslawski

*Case Based Design*, 2008

ISBN 978-3-540-75705-4

Yuri Avramenko  
Andrzej Kraslawski

# Case Based Design

Applications in Process Engineering

With 61 Figures and 23 Tables

 Springer

Dr. Yuri Avramenko  
Lappeenranta University of Technology  
Skinnarilankatu 34  
FIN-53850, Lappeenranta  
Finland  
avramenk@lut.fi

Prof. Andrzej Kraslawski  
Lappeenranta University of Technology  
Skinnarilankatu 34  
FIN-53850, Lappeenranta  
Finland  
Andrzej.Kraslawski@lut.fi

ISBN 978-3-540-75705-4

e-ISBN 978-3-540-75707-8

Studies in Computational Intelligence ISSN 1860-949X

Library of Congress Control Number: 2007938414

© 2008 Springer-Verlag Berlin Heidelberg

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer-Verlag. Violations are liable to prosecution under the German Copyright Law.

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Cover design: Deblik, Berlin, Germany

Printed on acid-free paper

9 8 7 6 5 4 3 2 1

springer.com

---

## Foreword

The case-based reasoning (CBR) and case-based design (CBD) have been around for some time and established themselves as one of the commonly used mechanisms of approximate reasoning in intelligent systems and decision support systems, in particular. In a nutshell, the CBR mechanisms offer a powerful and general environment in which we generalize on a basis of already accumulated experience being represented in the form of a finite and relatively small collection of cases. Those cases constitute the essence of the existing domain knowledge. When encountering a new situation we invoke and eventually modify the already collected decision scenarios (cases) and arrive at the pertinent decision or a certain design alternative. Interestingly, uncertainty or granularity of resulting decision is inherently associated with the nature of the cases being used in the reasoning process and a way in which partial matching takes place between the historical findings (cases) and a current evidence.

The book by Professors Avramenko and Kraslawski is unique in several important ways. First, it is an impressive and in-depth treatment of the essence of the case-based reasoning strategy and case-based design dwelling upon the algorithmic facet of the paradigm. Second, the authors provided an excellent applied research framework by showing how this development can be effectively utilized in real word complicated environment of process engineering – a pursuit that is rarely reported in the literature in such a comprehensive manner as done in this book. In a highly authoritative and systematic manner, the authors guide the reader through the essential features of the CBR machinery. The book is structured into 10 chapters. The authors start with some useful generalities by setting up a stage and discussing the principles of the design process of products and stressing on the rapidly growing importance of decision support systems in design activities. Case-based reasoning forms the essence of the consecutive chapter which offers the reader an insight into the algorithms of the reasoning scheme. Chapter 4 is a useful compendium on the variety of concepts that are at the heart of the CBR activities, such as similarity measures and adaptation algorithms. The authors did an excellent

job here by combining the badly needed formalism with highly motivating explanatory notes present behind the genuine diversity of the ideas being used there. Chapter 5 brings us closer to the specific applications as the authors navigate the readers through the main functionality of the software environment of the CBR. Finally, the last part of the book consisting of Chaps. 6–9 deals with real-world applications such as, e.g. synthesis of wastewater treatment sequence or design of distillation systems.

While the practicality of the investigations offered in the book is the remarkable strength of the volume, the formal aspects, notation and derivations are rigorous, yet clear.

The writing is lucid and explains the fundamental ideas in a direct manner. The suite of real-word examples is a genuine asset of the book. Through such examples, be they chemical or biological processes, we are provided with a comprehensive, well-structured and clear guidance to the overall design process of the CBR systems.

All in all, the book is an interesting and valuable addition to the body of knowledge on fundamentals and practice of automated reasoning – an important and vitally essential step towards building intelligent systems.

Witold Pedrycz  
President, IFSA  
May 15, 2007

---

## Preface

The growing amount of knowledge creates new opportunities as well as challenges. Unfortunately, the challenges often start to be the problems. In chemical and process engineering, the most common problems related to the huge amount of available data, information and knowledge are: difficulties with estimation of their quality, lack of efficient methods enabling the fast access to the relevant information or knowledge and “use once” model of knowledge application. The above-mentioned problems are common for all activities in chemical and process engineering: modelling, simulation, design and control. However, design phase is critical from the point of view of the satisfactory functioning of the process unit or the whole system. The wrong assumptions or errors made at this stage could be corrected only with the great amount of time and money but often it is too late for any essential change. The design is difficult as usually there is a lot of uncertainty involved. The good designers used to deal with the problem using their intuition supported by the past experience. The trouble is that industry and society are more and more innovation hungry. There is a growing demand for designs which are less and less similar to their predecessors.

There are two major approaches to deal with this situation, either to make new experiments, develop new models and on this basis build new designs or to use the existing information and knowledge. The second option is much more economically viable and less time demanding than the first one.

The use of the existing information and knowledge is performed in two ways. First method is aimed at getting new information by searching the exiting knowledge repositories. It is so-called knowledge discovery from literature. This approach usually leads to radical innovations. The second method is based on the assumption that the similar problems have the similar solutions. It is a basis of case-based reasoning. It usually leads to incremental innovations.

The objective of this book is to bridge a gap between the huge amount of available knowledge and its very small subset which is not only generated and stored but also actively used. The book is a sort of guide in a store where

## VIII Preface

knowledge is stocked up and we are invited to look for the pieces which could be useful for us in solving new problems. The authors have penetrated only a very small fragment of this huge warehouse – a room in which some elements of knowledge related to chemical and process engineering have been left.

This book is about knowledge re-use by applying of case-based reasoning to the problems typical in chemical product and process design. It is composed of three parts: description of the product and process design and decision support methods related to it, presentation of case-based design principles, issues related to adaptation of the retrieved solutions and case-based reasoning environment and finally examples of application of case-based reasoning to product and process design. The application part covers the broad spectrum of examples dealing with products formulation, synthesis of the system of processing units and mathematical models re-use.

The authors would like to thank many people for the valuable discussions, comments and advice. We are not able to mention all of them but we are particularly grateful to Dr. Tivodar Farkas and Dr. Christan Botar-Jid. We highly appreciate Professor Janusz Kacprzyk for his encouragement and constant support during the preparation of this book.

We hope that this book will contribute to a broader use of case-based design in engineering practice.

Yuri Avramenko  
Andrzej Kraslawski  
Lappeenranta, May 2007



---

## Contents

---

### Part I Design Support

---

<b>1</b>	<b>The Design Process of Product and Process Development .</b>	<b>3</b>
1.1	Design Objectives and Tasks .....	3
1.2	Design Models .....	4
1.2.1	Generic Design Models .....	5
1.2.2	Chemical Process Design Model .....	8
1.2.3	Product Design Models .....	10
1.2.4	Product Design Models Based on Abstraction Levels ...	16
1.2.5	Summary of Design Process Models .....	17
1.3	Model of the Design Process for the Development of a Chemical Product .....	17
1.3.1	Representation of a Design Activity .....	18
1.3.2	Overall Process of the Design of a Chemical Product ...	18
1.3.3	Abstraction-Level Based Model of Chemical Process Design .....	21
<b>2</b>	<b>Decision Support in Design .....</b>	<b>25</b>
2.1	Decision Making Process .....	25
2.1.1	Definition of the Problem .....	25
2.1.2	Identification of Requirements .....	26
2.1.3	Establishment of Goals .....	26
2.1.4	Generation of Alternatives .....	26
2.1.5	Determination of Criteria .....	27
2.1.6	Evaluation of Alternatives Against Criteria .....	28
2.1.7	Validation of Solution .....	28
2.2	Decision Support Methods .....	28
2.2.1	Algorithmic Approach .....	29
2.2.2	Knowledge-Based Inductive Reasoning Approach .....	30
2.2.3	Case-Based Reasoning Approach .....	33

2.3	Knowledge Engineering .....	33
2.3.1	Classification of Knowledge .....	34
2.3.2	Knowledge Acquisition .....	37
2.3.3	Software Engineering versus Knowledge Engineering ...	38
2.3.4	Knowledge Representation .....	39
2.4	Decision Supporting Systems .....	44
2.4.1	Classification of DSS .....	45
2.4.2	Architectures of DSS .....	46
2.5	Conclusions .....	47

---

## Part II Case-based Design Support

---

<b>3</b>	<b>Case-Based Reasoning Approach .....</b>	<b>51</b>
3.1	Case-Based Reasoning Concept .....	51
3.1.1	Representation of Experience .....	52
3.1.2	Storage of Cases .....	53
3.1.3	Retrieval of Cases .....	54
3.1.4	Reuse of Experience .....	55
3.1.5	CBR Applications Range .....	56
3.2	Models of CBR Process .....	59
3.3	Case-Based Design Support Methodology .....	64
3.3.1	Collection of Relevant Data .....	66
3.3.2	Representation of Complex Design Cases .....	67
3.3.3	Memory Organization .....	68
3.3.4	Compilation of Case Base .....	68
3.3.5	Comparing Cases .....	69
3.3.6	Correction of Found Solution .....	69
3.3.7	Checking Obtained Solution .....	70
3.4	Summary .....	70
<b>4</b>	<b>Similarity and Adaptation Concepts .....</b>	<b>71</b>
4.1	Retrieval Method and Similarity Measures .....	71
4.1.1	Quantitative Distance .....	72
4.1.2	Qualitative Comparison .....	75
4.2	General Similarity Concept .....	76
4.2.1	Basic Notions .....	76
4.2.2	Overall and Particular Similarity .....	78
4.2.3	Difference Measurements .....	79
4.2.4	Determination of Difference for Composite Values .....	87
4.3	Concept of Adaptation .....	90
4.3.1	Foundations of Adaptation Method .....	90
4.3.2	Scaling of Solution Space .....	91
4.3.3	Solution of a Adaptation Task .....	92
4.3.4	Description of Genetic Algorithm .....	93
4.4	Summary .....	96

<b>5</b>	<b>Case-Based Reasoning Environment – Cabareen</b>	99
5.1	Introduction	99
5.2	The Core of the Environment	100
5.3	Links to the Environment	101
5.4	Work with Databases	103
5.5	Interfaces	104

---

### Part III Application to Support of Design Process

---

<b>6</b>	<b>Product Design: Food Product Formulation</b>	109
6.1	Introduction	109
6.2	Database of Fats and Oils Properties	110
6.3	Case Representation of Fats and Oils Products	111
6.4	Similarity Determination	113
6.5	Computer Assistant for Support of Food Product Formulation	113
6.6	Example: Cookie Filler Development	115
<b>7</b>	<b>Conceptual Design: Process Sequence Synthesis</b>	117
7.1	Introduction	117
7.2	Case Base of Wastewater Treatment Systems	118
7.3	Case Representation for Wastewater Treatment Problems	120
7.4	Computer Assistant for Wastewater Treatment Synthesis	122
7.4.1	Database Manager – Reference Library	123
7.4.2	Case-Based Reasoner	124
7.4.3	Treatment Builder	126
7.5	Example: Zinc-Plating Workshop Wastewater	127
<b>8</b>	<b>Pre-Detailed Design: Process Model Selection</b>	131
8.1	Introduction	131
8.2	Case Library of MINLP Model and Distillation Systems	134
8.3	Representation of Models for Synthesis of Distillation Systems	134
8.4	Similarity Calculation for Distillation Problems	139
8.5	Computer Tool for Selection of MINLP Model	141
8.6	Example: Separation of Heptane–Toluene Mixture	142
8.7	Case Representation of Forced Unsteady State Reactor Model	144
8.8	Similarity Determination Between Unsteady-State Processes	147
8.9	The Computer Tool for Model Selection of Forced Unsteady-State Reactor	147
8.10	Example: Selection of Model for Catalytic Reduction of NO <sub>x</sub> with Ammonia	149

<b>9</b>	<b>Equipment Design: Reactive Distillation Column Design . . .</b>	<b>153</b>
9.1	Introduction . . . . .	153
9.2	Representation of Design Case . . . . .	153
9.3	Description of Decision Supporting System . . . . .	155
9.3.1	Decision Supporting Module . . . . .	156
9.3.2	Case Base Editor . . . . .	158
9.3.3	Similarity Measurement Editor . . . . .	159
9.4	Similarity Determination . . . . .	160
9.5	Example: Methylpropylacetate Production . . . . .	161
	<b>Summary . . . . .</b>	<b>165</b>
	<b>References . . . . .</b>	<b>169</b>
	<b>Appendix . . . . .</b>	<b>179</b>