

Development and Application of a Library of Elementary Model Entities for Vapor-Liquid Chemical Processes

Dissertation

zur Erlangung des akademischen Grades

**Doktoringenieur
(Dr.-Ing.)**

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geb. am 31. Oktober 1966 in Omitlán de Juárez, Hidalgo, Mexiko

genehmigt durch die Fakultät für Elektrotechnik und Informationstechnik
der Otto-von-Guericke-Universität Magdeburg

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Promotionskolloquium am 17. November 2005

Forschungsberichte aus dem Max-Planck-Institut
für Dynamik komplexer technischer Systeme

Band 13

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Shaker Verlag
Aachen 2006

Bibliographic information published by Die Deutsche Bibliothek

Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data is available in the internet at <http://dnb.ddb.de>.

Zugl.: Magdeburg, Univ., Diss., 2005

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Printed in Germany.

ISBN 3-8322-4765-3
ISSN 1439-4804

Shaker Verlag GmbH • P.O. BOX 101818 • D-52018 Aachen
Phone: 0049/2407/9596-0 • Telefax: 0049/2407/9596-9
Internet: www.shaker.de • eMail: info@shaker.de

Acknowledgments

I express my gratitude to the German people for giving me the opportunity of working in the Max-Planck-Institut für Dynamik komplexer technischer Systeme in Magdeburg under ideal scientific conditions. In the institute I met the most brilliant colleagues I have ever known and I was favored by stimulating discussions and warm friendship with some of them.

I would like to express my gratitude to Prof. Dr.-Ing. Dr.h.c. mult. E.D. Gilles, the founding director of the institute, for making possible for me to work under such ideal conditions.

I gratefully acknowledge Prof. Dr.-Ing. Achim Kienle for the enthusiastic discussions and supervising tasks during the development of this research project. I also wish to express my gratitude to Prof. Dr.-Ing. Kai Sundmacher for his accurate reading and reviewing of this work.

I wish to express my gratitude to Dr. Michael Mangold, Dr. Ulrike Krewer and Martin Ginkel for their comments and careful attention to detail. Their valuable contribution has enabled me to free the text from various errors and some inconsistencies, but the errors that remain are my sole responsibility.

For being always very near to me despite the long distance between Magdeburg and Mexico City, during my stay in Germany, I am in debt with Mr. Odón Angeles R. and Mrs. Marta Palacios D., my parents.

I express my gratitude to Mariana Domínguez, my wife, as well as Max and Ethel, my children for filling of sense my life the whole time.

For you:

My parents,

Mariana, Max and Ethel

Preface

This work was developed during my research fellowship in the Process Synthesis and Process Dynamics Group of the Max-Planck-Institut für Dynamik komplexer technischer Systeme in Magdeburg.

The development of a library for modeling vapor-liquid chemical processes is the subject of this work. Focus of this contribution is on lumped systems described by ordinary differential equations of first order and algebraic equations for vapor-liquid systems.

Modeling is presented as a common activity in different scientific disciplines, with special emphasis on modeling in chemical engineering. Domain engineering activities are discussed, namely analysis domain and architecture development. These activities lead us to the software pattern proposed in this thesis and applied for the implementation of the library. The discussion emphasizes that modeling chemical engineering systems by reusing modules of a library is different than modeling from scratch and that preparing modules for reuse is a process on its own. In this context it was shown how computer-aided modeling impacts the whole modeling task.

The formulation of theoretical aspects are applied here for the development of concrete modules, namely, the network approach, the proposed phenomenological framework, and the simple-to-complex implementation strategy.

The modeler of chemical process should find a conceptually well structured knowledge space in which entities can be systematically found, used, and further developed. For that, notational aspects for creating names are considered, a conceptual framework is developed to set phenomenological assumptions for the formulation of mass and energy balances, which find a very wide spectrum of application. This conceptual frame is proposed as a starting point for more detailed phenomenological developments of the library.

Although the library is a final product itself, its development would be pointless without

applications associated with it. The applications consist of two different industrial chemical processes: the first one is a plant for the production of butyl acetate and the second one is a plant for the production of acetic acid. Simulation scenarios serve to show the response of the plants. Each application is a completely independent project with the library of models as a common root. It is shown that the library can be adapted to particular requirements of the modeler and it can be further developed by either creating new modules or by modifying some others. After a validation and reuse analysis, these new models can be added to the library to make them available for different users.

Odón Angeles Palacios
Freiburg, December 2005

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Notation

c	Speed	m/s
c_p	Molar heat capacity	kJ/kmol
CO	Controller output	-
g	Gravitational acceleration	m/s ²
h	Molar enthalpy	kJ/kmol
H	Total enthalpy	kJ
$J[n]$	Molar flow	kmol/s
$J[q]$	Heat flow	kJ/s
n	Number of moles	kmol
P	Pressure	bar
P_d	Dew point pressure	bar
P_b	Bubble point pressure	bar
P^o	Vapor pressure	bar
PV	Process variable	-
R_g	Universal gas constant	kJ/(kmol K)
rhs_cmb	Right hand side of the component material balance	kmol/s
rhs_eb	Right hand side of the energy balance	kJ/s
rhs_tmb	Right hand side of the total material balance	kmol/s
T	Temperature	K
T_d	Dew point temperature	K
T_b	Bubble point temperature	K
t	Time	s
u	Molar internal energy	kJ/kmol
U	Total internal energy	kJ
V	Total volume	m ³
v	Molar volume	m ³ /kmol
x	Liquid mole fraction	[-]

y	Vapor or gas mole fraction	[-]
z	Overall mole fraction	[-]
z	Elevation with respect to a reference level	m

Greek Symbols

γ	Activity coefficient	[-]
ρ	Molar density	kmol/m ³
η	Murphree efficiency	[-]
τ	Integral time	[-]
ψ	Vapor fraction	[-]

Subscripts

a	Outlet
e	Inlet
i	Component
g	Generation

Superscripts

nc	Number of components
0	Pure component
'	Liquid
''	Vapor