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

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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

Contents

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