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# Produktion und Logistik

## Herausgegeben von

- C. Bierwirth, Halle, Deutschland
- B. Fleischmann, Augsburg, Deutschland
- M. Fleischmann, Mannheim, Deutschland
- M. Grunow, München, Deutschland
- H.-O. Günther, Bremen, Deutschland
- S. Helber, Hannover, Deutschland
- K. Inderfurth, Magdeburg, Deutschland
- H. Kopfer, Bremen, Deutschland
- H. Meyr, Stuttgart, Deutschland
- K. Schimmelpfeng, Stuttgart, Deutschland
- Th. S. Spengler, Braunschweig, Deutschland
- H. Stadtler, Hamburg, Deutschland
- H. Tempelmeier, Köln, Deutschland
- G. Wäscher, Magdeburg, Deutschland

Diese Reihe dient der Veröffentlichung neuer Forschungsergebnisse auf den Gebieten der Produktion und Logistik. Aufgenommen werden vor allem herausragende quantitativ orientierte Dissertationen und Habilitationsschriften. Die Publikationen vermitteln innovative Beiträge zur Lösung praktischer Anwendungsprobleme der Produktion und Logistik unter Einsatz quantitativer Methoden und moderner Informationstechnologie.

**Herausgegeben von**

Professor Dr. Christian Bierwirth  
Universität Halle

Professor Dr. Herbert Kopfer  
Universität Bremen

Professor Dr. Bernhard Fleischmann  
Universität Augsburg

Professor Dr. Herbert Meyr  
Universität Hohenheim

Professor Dr. Moritz Fleischmann  
Universität Mannheim

Professor Dr. Katja Schimmelpfeng  
Universität Hohenheim

Professor Dr. Martin Grunow  
Technische Universität München

Professor Dr. Thomas S. Spengler  
Technische Universität Braunschweig

Professor Dr. Hans-Otto Günther  
Technische Universität Berlin

Professor Dr. Hartmut Stadler  
Universität Hamburg

Professor Dr. Stefan Helber  
Universität Hannover

Professor Dr. Horst Tempelmeier  
Universität Köln

Professor Dr. Karl Inderfurth  
Universität Magdeburg

Professor Dr. Gerhard Wäscher  
Universität Magdeburg

**Kontakt**

Professor Dr. Thomas S. Spengler  
Technische Universität Braunschweig  
Institut für Automobilwirtschaft  
und Industrielle Produktion  
Katharinenstraße 3  
38106 Braunschweig

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Thomas Kirschstein

# Integrated Supply Chain Planning in Chemical Industry

Potentials of Simulation  
in Network Planning

Foreword by Prof. Dr. Claudia Becker  
und Prof. Dr. Christian Bierwirth

 Springer Gabler

Thomas Kirschstein  
Halle (Saale), Germany

Dissertation University of Halle (Saale), 2014

Produktion und Logistik

ISBN 978-3-658-08432-5

ISBN 978-3-658-08433-2 (eBook)

DOI 10.1007/978-3-658-08433-2

Library of Congress Control Number: 2014958973

Springer Gabler

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## Foreword

In literature on operations management, chemical industry is primarily dealt with focused case studies. The limited flexibility of production processes as well as the volatility of customer demand were identified as the most prominent challenges for chemical supply chain management. Most chemical production assets are complex, inflexible, and incur high set-up costs. Hence, such assets can only be used in an economically reasonable way if operated continuously. Therefore, logistical processes offer substantial contributions to a chemical company's value added. E.g. logistical processes ensure the supply of downstream assets in case of asset break downs. More important, however, logistical processes allow balancing demand variations within chemical production networks. Therefore, transport and distribution planning is essential in both, intra-site logistics, mostly relying on pipeline transportation, and inter-site logistics, mostly relying on rail and ship transportation. With this book, Thomas Kirschstein covers this topic in an encompassing, profound, and general way. Starting with basic chemical production processes, which are modelled with time series methods, established and new logistical planning problems for distributed chemical production networks are presented. Finally, these components are integrated in a simulation-based planning framework which is implemented in a decision support system. The developed decision support system is validated by means of case studies relying on historical records of a real world chemical production network.

The present work is an important contribution to scientific literature from a methodological and application-oriented point of view. It develops systematically the basic elements for modelling complex chemical production networks and illustrates the benefits of advanced decision support systems in chemical supply chain management. We wish the book continued success and wide acceptance.

Claudia Becker and Christian Bierwirth

# Preface

This book is the product of a process which started in 2006 as a cooperation seminar between the Dow Olefinverbund GmbH and the chairs of Production & Logistics, Statistics, and Operations Research. At this time I couldn't imagine a result like this. During this time not only the project has developed and changed, also my experiences, skills, and expectations have grown. These developments would have been impossible without the support of a bunch of persons. The space provided here does not suffice to duly thank all these persons. So, the following thanks are rather exemplary than encompassing.

Special thanks are due to my supervisors Prof. Dr. Claudia Becker, Prof. Dr. Christian Bierwirth, and Prof. Dr. Taïeb Mellouli which offered invaluable support by their advices and constant commitment in all those years.

No less important was the support of all employees of Dow Olefinverbund GmbH which allowed me to study not only Dow's production and logistics processes but also their day-to-day business. In particular, I thank Wolfgang Schnabel, Andreas Kroupa, and Wubbe Prins for organizing and coordinating the practical part of this project. Without their support, this book would not exist.

Besides my direct supporters, I'd like to thank all colleagues at the department for Economics and Business Administration. Thanks to them research and teaching at the university was always a pleasant and (almost) always a productive challenge. Representative for all colleagues I thank Heidrun Rudolph, Lisiane Schnegelsberg, and Dr. Steffen Liebscher from the chair of Statistics as well as Ute Lorenz, Dorota Mańkowska, Jens Kuhpfahl, and Prof. Dr. Frank Meisel from the chair of Production & Logistics.

An important contribution to the successful completion of this book offered my family and friends. Not only by numerous discussions about the contents of the projects but also by the constant interest in its progress, I never lost sight of the goal of this project.

But, it is unthinkable that this book would exist without the support of my wife Susanne and my daughters Antonia and Emilia. All three of them are constant sources of joy, inspiration, and recuperation in particular in times of frustration and self-doubts. For their support, I'm deeply grateful.

Thomas Kirschstein

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# Contents

<b>List of Tables</b>	<b>XI</b>
<b>List of Figures</b>	<b>XV</b>
<b>List of Abbreviations</b>	<b>XVII</b>
<b>List of Notation</b>	<b>XIX</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Motivation . . . . .	1
1.2 Outline of the thesis . . . . .	3
<b>2 Chemical production processes</b>	<b>5</b>
2.1 Characterization of chemical production processes . . . . .	7
2.2 Modelling chemical production processes . . . . .	14
2.2.1 Chemical kinetics . . . . .	15
2.2.2 Modelling & simulation of chemical processes . . . . .	18
2.2.3 Process identification & control . . . . .	22
2.3 Time series methodology . . . . .	25
2.3.1 ARIMA models . . . . .	25
2.3.2 GARCH models . . . . .	29
2.3.3 Multivariate time series models . . . . .	31
2.3.4 Data preparation, model specification and residual checking . . . . .	33
<b>3 Distribution planning in chemical industry logistics</b>	<b>51</b>
3.1 Characteristics of chemical industry logistics . . . . .	52
3.2 Planning problems for pipeline operations . . . . .	54
3.2.1 Technical and organizational prerequisites . . . . .	54
3.2.2 Single-product pipelines . . . . .	56
3.2.3 Multi-product pipelines . . . . .	67
3.2.3.1 Batch flow pipelines . . . . .	68
3.2.3.2 Batch split pipelines . . . . .	81
3.2.3.3 Multi-source pipeline systems . . . . .	85
3.3 Planning problems for rail operations . . . . .	87

3.3.1	Technical and organizational prerequisites . . . . .	87
3.3.2	A short-term rail transportation problem . . . . .	90
3.3.2.1	Problem formulation . . . . .	90
3.3.2.2	Components for modelling rail transports . . . . .	91
3.3.2.3	Components for modelling turnover processes . . . . .	92
3.3.2.4	Components for modelling the objective function . . . . .	93
3.3.2.5	Mathematical model . . . . .	94
3.4	Planning problems for ship operations . . . . .	108
3.4.1	Technical and organizational prerequisites . . . . .	108
3.4.2	Maritime inventory routing problems . . . . .	110
3.4.3	Maritime inventory shipping problems . . . . .	113
<b>4</b>	<b>Integrated planning of chemical supply chains</b>	<b>123</b>
4.1	Literature review . . . . .	125
4.2	Sources and effects of uncertainty in chemical industry . . . . .	141
4.3	A framework for simulation-based integrated planning of supply chains in chemical industry . . . . .	150
4.3.1	Conceptual modelling & data analysis . . . . .	151
4.3.2	Components of chemical supply chain simulation models . . . . .	159
4.3.3	Verification & validation . . . . .	167
4.3.4	Planning of simulation experiments . . . . .	170
4.3.4.1	Performance measures in (chemical) supply chain models .	172
4.3.4.2	Experimental designs . . . . .	175
4.3.4.3	Simulation optimization . . . . .	185
4.3.5	Decision support . . . . .	196
<b>5</b>	<b>Conclusion and final remarks</b>	<b>203</b>
	<b>Bibliography</b>	<b>207</b>
	<b>Appendix</b>	<b>229</b>



# List of Tables

2.1	Typology of production processes . . . . .	9
2.2	Characteristics of production processes in chemical industry . . . . .	10
2.3	EACF for $T = 100$ . . . . .	39
2.4	EACF for $T = 1000$ . . . . .	39
2.5	theoretical EACF . . . . .	39
2.6	Information criteria for both sampled time series and various model specifications . . . . .	39
2.7	Estimated parameters for the Naphtha time series . . . . .	43
2.8	Coefficients of the initial $VARX(3)$ model for de-alkylation plant . . . . .	46
2.9	Coefficients of the $VARX(3)$ model with outlier correction and variable selection . . . . .	49
3.1	Categorization of pipeline types . . . . .	55
3.2	Transition matrices and production modes for providers and consumers . . . . .	64
3.3	All combinations of plant production modes . . . . .	65
3.4	Transition matrix $\mathbf{Q}$ . . . . .	65
3.5	Comparison of problem features for Magatão et al. (2004) and Relvas et al. (2006) . . . . .	68
3.6	Set of parameters and decision variables for the sELSP . . . . .	73
3.7	Transition costs $c_{st}^{trans}$ for the PIG insertion scenario . . . . .	78
3.8	Interface quantities $d_{st}$ and transition costs $c_{st}^{trans}$ for the interface scenario . . . . .	79
3.9	Net demand rate $\omega_s$ and holding cost rates $c_s^{hold}$ for both scenarios . . . . .	79
3.10	Resulting optimal pumping cycles for the sELSP-BP and sELSP-BP-IF . . . . .	80
3.11	Pumping times and idle times of the optimal schedules for the <i>sELSP-BP</i> and <i>sELSP-BP-IF</i> . . . . .	80
3.12	Classification of literature on scheduling of one-to-many pipeline systems . . . . .	83
3.13	Sets, parameters, variables, and decision variables for the MC-RTP . . . . .	98
3.14	Exemplary assignment of RTCs to two trains . . . . .	100
3.15	Technical parameters for the rail operations planning example . . . . .	103
3.16	Consumption rate $\omega_{is}$ , stock capacities $s_{is}^{Cap}$ , initial stocks $s_{is}^{Ini}$ , and target stock levels $s_{is}^{Tar}$ for all sites $i$ and chemicals $s$ . . . . .	104
3.17	Sets, parameters, variables, and decision variables for the MISP-STA . . . . .	115
3.18	Technical specification of tankers and tanks $(n_{vk}^{Cap}, q_{sk}^{Cap}, c_v^{Trv})$ . . . . .	117

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4.1	Classification of literature on integrated SC configuration and management planning in chemical industry . . . . .	132
4.2	Classification of literature on integrated SC management planning in chemical industry . . . . .	137
4.3	Classification of sources of uncertainties and examples (per dimension) . . .	145
4.4	Material balances (in t/hour) and storage capacities (in t) per site and chemical . . . . .	155
4.5	Examples for processors according to processor type and processing attributes	160
4.6	Relation between aggregation levels and types of processors . . . . .	162
4.7	Pseudo-code for chemical SC simulation model . . . . .	166
4.8	Classification of V&V techniques . . . . .	168
4.9	Attributes of variables . . . . .	172
4.10	Examples and classification of performance measures in SCM . . . . .	174
4.11	Values of the control variables for the experimental design . . . . .	179
4.12	Effects of input variables on responses in example 11 . . . . .	182
4.13	Overview on simulation optimization methods . . . . .	187
4.14	Optimal and baseline values for inventory parameters . . . . .	200
4.15	Performance measures for optimal and baseline values of inventory parameters	202
A.1	Information criteria for VARX models of order 1 to 6 for the de-alkylation plant . . . . .	229
A.2	Coefficients of the $VARX(3)$ model with outlier correction . . . . .	230
A.3	ANOVA table for the initial $VARX(3)$ model (without outlier correction)	230
A.4	ANOVA table for the initial $VARX(3)$ model with outlier correction and variable selection . . . . .	232
A.5	Stationary flow rates (in t/h) for exemplary chemical production network .	234
A.6	Coefficients of the time series models for cracker at site 1 ( $VARX(2)+AR(3)$ )	234
A.7	Coefficients of the time series models for cracker at site 2 ( $VARX(2)+AR(3)$ )	234
A.8	Coefficients of the time series models for hydrogenation plant at site 1 ( $VARX(3) + AR(2)$ ) . . . . .	235
A.9	Coefficients of the time series models for hydrogenation plant at site 2 ( $VARX(3) + AR(3)$ ) . . . . .	235
A.10	Coefficients of the time series models for Butex plant at site 2 ( $VARX(1) + AR(4)$ ) . . . . .	235
A.11	Coefficients of input and output time series models of SISO and MISO plants	235
A.12	Un-/loading capacities, initial stock of empty RTCs, target and initial stock levels per transported chemical at both production sites . . . . .	236
A.13	Cost rates for the MC-RTP instances . . . . .	236
A.14	Distributions of inter-arrival time and deliver quantities for external customers/suppliers . . . . .	236

---

A.15 Transition matrices for plants at site 1 . . . . .	236
A.16 Transition matrices for plants at site 2 . . . . .	237
A.17 Resolution V design for 6 dichotomous variables ("1" encodes the variable's lower level and "1" the upper level) . . . . .	238
A.18 Estimated responses for all possible configurations (dominated configura- tion gray coloured) . . . . .	239
A.19 Pseudocode for inventory system model . . . . .	243
A.20 Summary for the logistic regression model of responses of efficient settings	244

# List of Figures

1.1	Overview on the structure of the thesis . . . . .	4
2.1	Chemical SC scheme with highlighted production plants . . . . .	5
2.2	Production quantities of basic chemicals in 2008-2010 . . . . .	6
2.3	Exemplary production network of Naphtha derivatives . . . . .	11
2.4	Scheme of a distillation column . . . . .	13
2.5	Overview on chemical operations . . . . .	13
2.6	Steps in chemical process modelling & control . . . . .	14
2.7	Topics in chemical kinetic and key words/methods . . . . .	15
2.8	Schematic flow sheet of a steam cracker . . . . .	21
2.9	Chemical process control scheme . . . . .	22
2.10	Theoretical and empirical ACF and PACF for an ARMA(2,1) process . . . . .	38
2.11	ACF of residuals, ACF of squared residuals and QQ-plot of residuals for ARMA(2,0) model (small sample, $T = 100$ ) and for ARMA(2,1) model (large sample, $T = 1000$ ) . . . . .	41
2.12	Time series plot of Naphtha inflow rate . . . . .	42
2.13	ACF and PACF of corrected Naphtha time series . . . . .	43
2.14	Flowsheet of the de-alkylation plant . . . . .	44
2.15	Raw data for a de-alkylation plant . . . . .	45
2.16	Residual diagnostic plots for $VARX(3)$ model of the de-alkylation plant. . . . .	47
2.17	Scatterplot of residuals for outlier corrected $VARX(3)$ model of the de-alkylation plant . . . . .	48
2.18	Real and fitted time series of both outflow rates (outlier indices superimposed) . . . . .	50
3.1	Chemical SC scheme with highlighted inter-site transports . . . . .	51
3.2	Modal split for chemical products in Germany in 2009 (based on total transported quantity in mill. tons) . . . . .	52
3.3	Scheme of an exemplary serial multi-access pipeline . . . . .	57
3.4	Cumulative distribution function and loss function for $Y^{(4)}$ . . . . .	66
3.5	Inventory pattern in a batch flow system . . . . .	71
3.6	Illustration of interface calculation in batch pipeline systems. . . . .	76
3.7	Illustration of interface calculation in batch pipeline systems . . . . .	81
3.8	One-to-many pipeline types . . . . .	84

3.9	Four-layer flow network for one chemical . . . . .	95
3.10	Optimal stock levels and network flows for periods 1 to 8 of the MC-RTP example . . . . .	105
3.11	Optimal stock levels for the MC-RTP instance of example 6 . . . . .	107
3.12	Optimal stock levels and chemical flows for periods 1 to 8 of the MISP-STA example . . . . .	118
3.13	Optimal stock levels for the MISP-STA instance of example 7 . . . . .	120
4.1	Chemical SC scheme for integrated planning . . . . .	124
4.2	Adapted SCM matrix (based on Stadtler (2005)) . . . . .	127
4.3	Daily median inflow rates of aromatic hydrocarbons for a de-alkylation plant 147	
4.4	Hourly average inflow rate of aromatic hydrocarbons (including confidence intervals at a confidence level of $\alpha = 0.1\%$ ) . . . . .	148
4.5	Diagnostic plots of trimmed inflow rates of aromatic hydrocarbons for a de-alkylation plant . . . . .	149
4.6	Steps in the simulation-based planning projects . . . . .	150
4.7	Development scheme for simulation studies . . . . .	152
4.8	Exemplary chemical supply chain with two sites . . . . .	154
4.9	Flow chart of a part of the exemplary chemical SC using the notation of Table 4.5 . . . . .	164
4.10	Development scheme for simulation studies . . . . .	165
4.11	Steps in experimental planning . . . . .	171
4.12	Simulated and fitted responses per experimental configuration . . . . .	183
4.13	Loss functions for Naphtha consumption during pipeline inspection and their relation . . . . .	191
4.14	Density and loss function for total Naphtha consumption during order lead time . . . . .	192
4.15	Scatterplot of Pareto front ( $\beta$ -service level in grey scale) . . . . .	194
4.16	Grey-scaled levelplot of estimated Pareto front . . . . .	195
4.17	Example of Delaunay triangulation-based sub-sample generation . . . . .	199
4.18	Diagnostic plots of ARDs . . . . .	201
4.19	Graphical determination of optimal performance vector . . . . .	202
A.1	Diagnostic plots for the ARX(1) model of the Naphtha time series . . . . .	229
A.2	Residual diagnostic plots for VARX(3) model with outlier compensation. . . . .	233
A.3	QQ-plots of residuals for models (4.19)-(4.21) . . . . .	240
A.4	Density function of the Weibull distribution with $k = 1.5$ and $\lambda = \frac{365}{\Gamma(\frac{5}{3})}$ . . . . .	241
A.5	Loss functions for both sites during pipeline inspection . . . . .	242
A.6	Diagnostic plots for (4.22) . . . . .	245

## List of Abbreviations

AB	agent-based
ACF	auto-correlation function
AIC	Akaike information criterion
AR(X)	auto-regressive [model] (with exogenous variables)
ARCH(X)	auto-regressive conditional heteroscedasticity [model] (with exogenous variables)
ARIMA(X)	auto-regressive integrated moving average [model] (with exogenous variables)
ARMA(X)	auto-regressive moving average [model] (with exogenous variables)
ARD	average relative deviation
CV	corporate value
DE	discrete event
DSS	decision support system
EACF	extended auto-correlation function
(s)ELSP(-BP- IF)	(sequence-dependent) economic lot sequencing problem (with global stocks and interface handling)
FIR	finite impulse-response
GARCH(X)	generalized auto-regressive conditional heteroscedasticity [model] (with exogenous variables)
GA	genetic algorithm
GDP	gross domestic product
h	hour
HQIC	Hannan-Quinn information criterion
IRP	inventory routing problem
IPPSP	integrated production planning and scheduling problem
(s)LP	(stochastic) linear program
MA(X)	moving average [model] (with exogenous variables)
MAD	median absolute deviation (from median)
MC-RTP	multi-chemical rail transportation problem
(s)MILP	(stochastic) mixed-integer linear program
MIMO	multiple input, multiple output
MINLP	mixed-integer non-linear program
MIP	mixed-integer program
MIRP	maritime inventory routing problem
MIRSP	maritime inventory routing and scheduling problem

MISP(-STA)	maritime inventory shipping problem (with ship type and tank assignment)
MISO	multiple input, single output
NACE	Nomenclature statistique des activités économiques dans la Communauté européenne
NLP	non-linear program
$\mathcal{NP}$ -hard	non-deterministic polynomial-time hard
NPV	net present value
NSGA	non-dominated sorting genetic algorithm
OLAP	on-line analytical processing
PACF	partial auto-correlation function
PE(T)	polyethylene (terephthalate)
PDP	pick-up and delivery problem
PIG	pipeline inspection gauges
PP	polypropylene
PS	polystyrene
QQ-plot	quantile-quantile plot
RMSE	root mean squared error
ROV	real-options-based value
RSA/RSM	response surface approximation/methodology
RTC	rail tank car
SBR	styrene-butadiene rubber
SC	supply chain
SCM	supply chain management
SCOR	Supply Chain Operations Reference
SD	system dynamics
SDE	stochastic differential equations
SIC	Schwarz information criterion
SIMO	single input, multiple output
SISO	single input, single output
t	ton
TSM	time series methodology
TSP	travelling salesman problem
V&V	verification and validation
VAR(X)	vector auto-regressive [model] (with exogenous variables)
VARMA(X)	vector auto-regressive moving average [model] (with exogenous variables)
VLE	vapour-liquid-equilibrium
VMA(X)	vector moving average [model] (with exogenous variables)
VRP	vehicle routing problem

## List of Notation

General notation	
$\mathbf{a}, \dots, \mathbf{z}, \boldsymbol{\alpha}, \dots, \boldsymbol{\omega}$	vectors
$\mathbf{A}, \dots, \mathbf{Z}, \boldsymbol{\Gamma}, \dots, \boldsymbol{\Omega}$	matrices
$\mathcal{A}, \dots, \mathcal{Z}$	sets
$i, j, k, b$	indices
$t, T$	time index, time horizon
$E(\cdot)/P(\cdot)/Var(\cdot)/Cov(\cdot, \cdot)$	expectation/probability/variance/covariance of $\cdot$
$\Gamma(\cdot)$	Gamma function
$\hat{\mathbf{x}}/\hat{\hat{\mathbf{x}}}$	estimate of $\mathbf{x}$ / estimate of estimate of $\mathbf{x}$
Bin ( $n, p$ )	Binomial distribution with $n$ trials and probability $p$
$N(\mu, \sigma^2)$	Normal distribution with mean $\mu$ and variance $\sigma^2$
WB ( $k, \lambda$ )	Weibull distribution with shape $k$ and scale $\lambda$
Notation of Chapter 2	
$N$	index and number of lags for exogenous variables
$L/M$	number of output/exogenous variables
$K$	number of parameters
$p/q/P/Q$	order of AR/MA/ARCH/GARCH process
$\alpha, \beta$	coefficients of (G)ARCH models
$\gamma/\rho, Corr(\cdot, \cdot)$	partial correlation/ correlation
$\phi, \theta$	AR and MA coefficients
$\Phi, \Theta$	VAR and VMA coefficient matrices
$v/v/\Upsilon$	coefficient scalars/vectors/matrices for exogenous regressors
$\delta(B), \omega(B), \theta(B), \phi(B)$	univariate lag polynomials
$\Phi(B), \Theta(B), \Upsilon(B)$	multivariate lag polynomials
$\sigma^2$	variance
$\Sigma$	covariance matrix
$\mu/\boldsymbol{\mu}$	mean scalar/vector
$\epsilon, \varepsilon, \xi, \eta/\boldsymbol{\epsilon}, \boldsymbol{\xi}/\Xi$	error scalars/vectors/matrices
$B$	back-shift operator
$C(t)$	concentration function
$X(t)$	turnover function



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$C_s$	starting concentration
$A$	reactant
$E_A$	activation energy
$R$	universal gas constant
$t_R$	Damköhler number
$m$	reaction order
$r$	reaction rate
$k$	reaction rate constant
$W(t)$	Wiener process
Notation of Chapter 3	
$\mathcal{K}, \mathcal{H}$	set of state combinations
$\mathcal{I}$	set of lot positions
$\mathcal{N}$	set of access points
$\mathcal{O}$	set of states
$\mathcal{S}$	set of modes
$\rho^{\text{Cap}}$	pumping rate capacity
$\rho$	pumping rate
$\mathbf{Q}$	transition matrix
$q_{st}$	transition probability from state $s$ to state $t$
$\boldsymbol{\pi}$	steady state vector
$\omega_s / \omega_{\mathbf{s}}$	flow level of state $s$ / state combination $\mathbf{s}$
$X_j$	flow rate at access point $j$
$y_{\mathbf{h}}$	total material balance of state combination $\mathbf{h}$
$p_{\mathbf{h}}$	probability of state combination $\mathbf{h}$
$\mu^C$	expected net deficit
$\alpha, \beta$	service level
$r$	stock level
$V(\cdot)$	expected loss function
$L / \bar{L}$	stock level / maximum stock level
$T^{\text{stock}} / T^{\text{fill}}$	stock-up time / pipeline fill time
$\tau$	time for pipeline transport
$c_s^{\text{set}} / c_s^{\text{hold}}$	set-up / holding costs for product $s$
$c_{st}^{\text{trans}}$	transition costs for a change from product $s$ to $t$
$b_{si}$	binary, 1 if at position $i = 0, \dots, I$ chemical $s$ is scheduled
$T_s$	cycle time of chemical $s \in \mathcal{S}$
$tb_i$	starting time of position $i$
$x_{sti}$	binary, 1 if from position $i - 1$ to position $i$ a transition from chemical $s$ to $t$ occurs

$O_{sij}$	binary, 1 if chemical $s$ is lastly scheduled $j$ positions before $i$
$r_{si}$	binary, 1 if position $i$ is the last position where chemical $s$ is scheduled
$T_{cycle}$	fundamental cycle time
Notation of Section 3.2 summarized in Table 3.13	
Notation of Section 3.3 summarized in Table 3.17	
Notation of Chapter 4	
$\mathcal{D}$	set of Delaunay simplices
$\mathcal{I}$	set of sites
$\mathcal{O}$	set of states
$\mathcal{P}$	set of products/chemicals
$\mathcal{Y}$	set of performance vectors
$\mathcal{Z}/\mathcal{Z}^{eff}$	set of system configurations / efficient system configurations
$\omega_s$	flow level of state $s$ /state combination $\mathbf{s}$
$\mathbf{Q}$	transition matrix
$\boldsymbol{\pi}$	steady state vector
$\rho^{Cap}$	pumping rate capacity
$\rho$	pumping rate
$q^{(opt)}$	(optimal) order quantity
$t^{(opt)}$	(optimal) order interval
$c^{batch}/c^{hold}$	batch-injection / holding cost for product
$\mathbf{y}$	vector of dependent measures
$n$	number of dependent measures (length of $\mathbf{y}$ )
$\mathbf{x}$	vector of control variables
$m$	number of control variables (length of $\mathbf{x}$ )
$\mathbf{z}$	vector of performance measures (typically $\mathbf{z} = (\mathbf{x}, \mathbf{y})$ )
$H(\cdot)/\hat{H}(\cdot)/\hat{\hat{H}}(\cdot)$	real/simulation/meta-model mapping function linking $\mathbf{x}$ and $\mathbf{y}$
$C(\cdot)$	cost function
$U(\cdot)$	profit/performance function
$V(\cdot)$	(first order) loss function
$m_i$	number of levels of control variable $i$
$\mathbf{b}$	binary vector, coding a discrete system configuration
$\boldsymbol{\mu}$	intercept vector/basic performance
$\boldsymbol{\gamma}/\boldsymbol{\gamma}/\boldsymbol{\Gamma}$	coefficient scalar/vector/matrix of linear model
$r_{ip}$	relative average target stock deviation at site $i$ for product $p$

$r$	total average relative target stock deviation for all sites and all products
$s_{ip}^{\text{Tar}}$	target stock level for product $p$ at site $i$
$s_{ip}^{\text{Cap}}$	inventory capacity for product $p$ at site $i$
$s_{itp}$	stock level for product $p$ at site $i$ in period $t$
$tr$	total number of trains dispatched
$tr_{ijt}$	number of trains dispatched from $i$ to $j$ in period $t$
$\beta_{ip}$	service level for product $p$ at site $i$
$\beta$	average service level for all products and sites
$\omega_{ipt}^{\text{real}}$	realized chemical flow of product $p$ at site $i$ in period $t$
$\omega_{ipt}^{\text{plan}}$	planned/required chemical flow of product $p$ at site $i$ in period $t$
$(s_i, S_i)$	inventory parameters (re-order level and stock-up level)
$l_{it}$	(Naphtha) stock level at location $i$ in period $t$
$\bar{l}$	average total stock level ( $\frac{\sum_t \sum_i l_{it}}{T}$ )
$\delta$	number of shipments
$t^{\text{alarm}}$	time interval between successive pipeline inspections
$t^{\text{insp}}$	duration of pipeline inspections
$t^{\text{ship}}$	order lead time
<b>d</b>	Delaunay simplex (set of points constituting the simplex)
<b>e/e</b>	relative performance deviation vector / average relative performance deviation