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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.

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Integrated Supply Chain Planning in Chemical Industry

Potentials of Simulation in Network Planning

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

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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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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	
$\mathbf{a}, ..., \mathbf{z}, \boldsymbol{\alpha}, ..., \boldsymbol{\omega}$	vectors
$\mathbf{A}, ..., \mathbf{Z}, \boldsymbol{\Gamma}, ..., \boldsymbol{\Omega}$	matrices
$\mathcal{A}, ..., \mathcal{Z}$	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 $\mathbf{x}$
$\mathrm{Bin}\,(\mathrm{n}, \mathrm{p})$	Binomial distribution with n trials and probability p
$\mathrm{N}\,(\mu, \sigma^2)$	Normal distribution with mean μ and variance σ^2
$\mathrm{WB}\,(\mathrm{k}, \lambda)$	Weibull distribution with shape k and scale λ
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
α, β	coefficients of (G)ARCH models
$\gamma/\rho, Corr(\cdot,\cdot)$	partial correlation/ correlation
ϕ, θ	AR and MA coefficients
$\boldsymbol{\Phi}$, $\boldsymbol{\Theta}$	VAR and VMA coefficient matrices
$\upsilon/\boldsymbol{\upsilon}/\boldsymbol{\Upsilon}$	coefficient scalars/vectors/matrices for exogenous regressors
$\delta(B), \omega(B), \theta(B), \phi(B)$	univariate lag polynomials
$\boldsymbol{\Phi}(B), \boldsymbol{\Theta}(B), \boldsymbol{\Upsilon}(B)$	multivariate lag polynomials
σ^2	variance
$\boldsymbol{\Sigma}$	covariance matrix
$\mu/\boldsymbol{\mu}$	mean scalar/vector
ϵ, ε, ξ, $\eta/\boldsymbol{\epsilon}$, $\boldsymbol{\xi}/\boldsymbol{\Xi}$	error scalars/vectors/matrices
B	back-shift operator
$C(t)$	concentration function
$X(t)$	turnover function

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
ρ^{Cap}	pumping rate capacity
ρ	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 $\mathbf{h}$
μ^C	expected net deficit
α, β	service level
r	stock level
$V(\cdot)$	expected loss function
$L/\bar{L}$	stock level / maximum stock level
T^{stock}/T^{fill}	stock-up time/pipeline fill time
τ	time for pipeline transport
c_s^{set}/c_s^{hold}	set-up / holding costs for product s
c_{st}^{trans}	transition costs for a change from product s to t
b_{si}	binary, 1 if at position $i = 0, ..., I$ 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
ω_s	flow level of state s/state combination $\mathbf{s}$
$\mathbf{Q}$	transition matrix
$\boldsymbol{\pi}$	steady state vector
ρ^{Cap}	pumping rate capacity
ρ	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
$\gamma/\boldsymbol{\gamma}/\boldsymbol{\Gamma}$	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}^{Tar}	target stock level for product p at site i
s_{ip}^{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
β_{ip}	service level for product p at site i
β	average service level for all products and sites
ω_{ipt}^{real}	realized chemical flow of product p at site i in period t
ω_{ipt}^{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 ($\frac{\sum_t \sum_i l_{it}}{T}$)
δ	number of shipments
t^{alarm}	time interval between successive pipeline inspections
t^{insp}	duration of pipeline inspections
t^{ship}	order lead time
$\mathbf{d}$	Delaunay simplex (set of points constituting the simplex)
$\mathbf{e}/e$	relative performance deviation vector / average relative performance deviation