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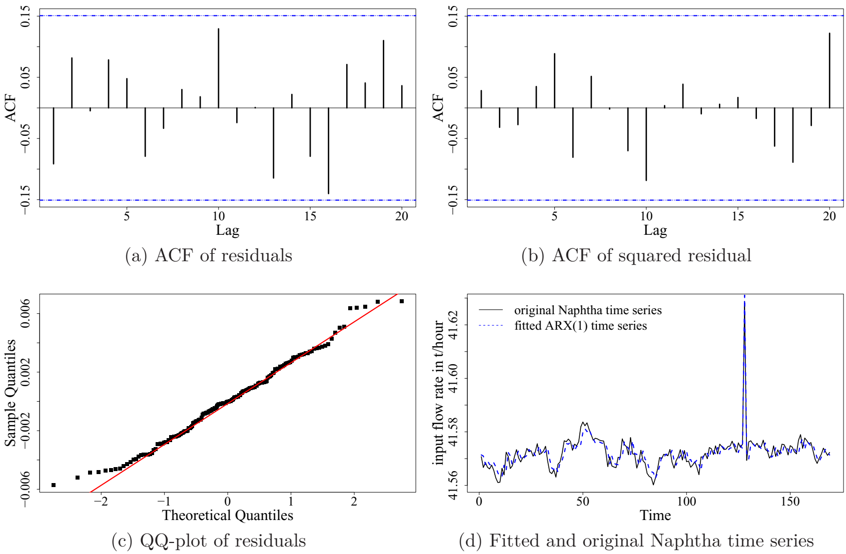
Appendix

Time series analysis



(a) ACF of residuals (b) ACF of squared residual

(c) QQ-plot of residuals (d) Fitted and original Naphtha time series

Figure A.1: Diagnostic plots for the ARX(1) model of the Naphtha time series

	VARX order					
p	1	2	3	4	5	6
AIC(p)	-3.81	-3.95	**-4.22**	-4.24	-4.23	-4.20
SIC(p)	-3.72	-3.81	**-4.04**	-4.01	-3.95	-3.88
HQIC(p)	-3.77	-3.89	**-4.15**	-4.15	-4.12	-4.08

Table A.1: Information criteria for VARX models of order 1 to 6 for the de-alkylation plant

T. Kirschstein, *Integrated Supply Chain Planning in Chemical Industry,* Produktion und Logistik,
DOI 10.1007/978-3-658-08433-2,

$\hat{\boldsymbol{\Phi}}_1$	$\hat{\boldsymbol{\Phi}}_2$	$\hat{\boldsymbol{\Phi}}_3$	$\hat{\boldsymbol{\upsilon}}_1$	$\hat{\boldsymbol{\upsilon}}_2$
$\begin{pmatrix} 0.05 & 2.76 \\ 0.04 & 0.85 \end{pmatrix}$	$\begin{pmatrix} 0.01 & -0.99 \\ 0.01 & -0.24 \end{pmatrix}$	$\begin{pmatrix} -0.14 & -2.06 \\ -0.02 & 0.18 \end{pmatrix}$	$\begin{pmatrix} 0.99 \\ -0.03 \end{pmatrix}$	$\begin{pmatrix} -0.00024 \\ -0.00004 \end{pmatrix}$

Table A.2: Coefficients of the $VARX(3)$ model with outlier correction

coefficient	**estimate**	**standard error**	**p-value**
$\hat{\Phi}_1^{11}$	0.12	0.053	0.03*
$\hat{\Phi}_1^{12}$	1.76	1.131	0.14
$\hat{\Phi}_1^{21}$	0.04	0.002	0.00***
$\hat{\Phi}_1^{22}$	0.82	0.046	0.00***
$\hat{\Phi}_2^{11}$	0.03	0.062	0.58
$\hat{\Phi}_2^{12}$	0.78	1.371	0.57
$\hat{\Phi}_2^{21}$	0.01	0.003	0.00***
$\hat{\Phi}_2^{22}$	-0.21	0.046	0.00***
$\hat{\Phi}_3^{11}$	-0.20	0.054	0.00***
$\hat{\Phi}_3^{12}$	-2.91	0.878	0.00***
$\hat{\Phi}_3^{21}$	-0.02	0.002	0.00***
$\hat{\Phi}_3^{22}$	0.15	0.036	0.00***
$\hat{\upsilon}_1^1$	0.96	0.076	0.00***
$\hat{\upsilon}_1^2$	-0.03	0.003	0.00***
$\hat{\upsilon}_2^1$	-0.00023	0.00014	0.10†
$\hat{\upsilon}_2^2$	-0.00004	0.00000	0.00***

significance codes: ***...≤ 0.001; **...≤ 0.01; *...≤ 0.05; †...≤ 0.1

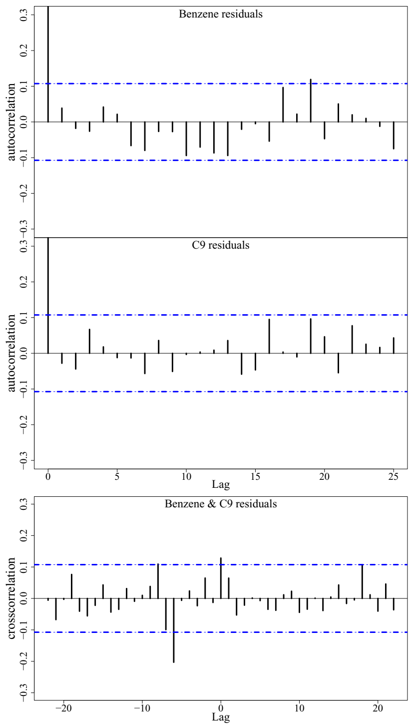
Table A.3: ANOVA table for the initial $VARX(3)$ model (without outlier correction)

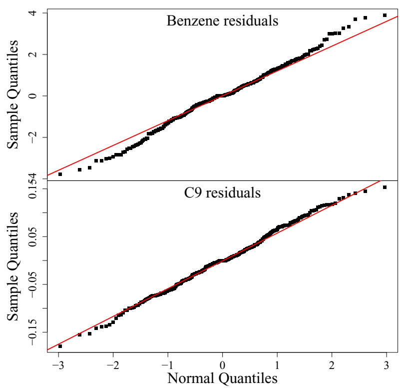
coefficient	estimate	standard error	p-value
$\hat{\Phi}_1^{11}$	–	–	–
$\hat{\Phi}_1^{12}$	2.51	0.628	0.00***
$\hat{\Phi}_1^{21}$	0.04	0.002	0.00***
$\hat{\Phi}_1^{22}$	0.85	0.043	0.00***
$\hat{\Phi}_2^{11}$	–	–	–
$\hat{\Phi}_2^{12}$	–	–	–
$\hat{\Phi}_2^{21}$	0.01	0.002	0.00***
$\hat{\Phi}_2^{22}$	-0.25	0.000	0.00***
$\hat{\Phi}_3^{11}$	-0.15	0.045	0.00***
$\hat{\Phi}_3^{12}$	-2.67	0.487	0.00***
$\hat{\Phi}_3^{21}$	-0.02	0.002	0.00***
$\hat{\Phi}_3^{22}$	0.18	0.033	0.00***
$\hat{\upsilon}_1^1$	1.05	0.041	0.00***
$\hat{\upsilon}_1^2$	-0.03	0.003	0.00***
$\hat{\upsilon}_2^1$	-0.00028	0.0002	0.01*
$\hat{\upsilon}_2^2$	-0.00003	0.000	0.00***
dummy.out.20.benz	-4.14	1.414	0.00***
dummy.out.20.c9	-0.15	0.063	0.02*
dummy.out.51.benz	-5.98	1.413	0.00***
dummy.out.51.c9	–	–	–
dummy.out.61.benz	4.02	1.411	0.00***
dummy.out.61.c9	0.16	0.063	0.01**
dummy.out.64.benz	-2.74	1.418	0.05*
dummy.out.64.c9	-0.17	0.063	0.01**
dummy.out.65.benz	-5.28	1.420	0.00***
dummy.out.65.c9	-0.17	0.064	0.01**
dummy.out.109.benz	2.96	1.426	0.04*
dummy.out.109.c9	-0.19	0.064	0.00***
dummy.out.155.benz	4.63	1.422	0.00***
dummy.out.155.c9	–	–	–
dummy.out.156.benz	2.74	1.416	0.05*
dummy.out.156.c9	-0.20	0.064	0.00***
dummy.out.158.benz	-6.43	1.433	0.00***
dummy.out.158.c9	0.16	0.064	0.01**
dummy.out.188.benz	-3.81	1.413	0.01**
dummy.out.188.c9	-0.19	0.063	0.00***

dummy.out.199.benz	2.82	1.413	0.05*
dummy.out.199.c9	0.23	0.063	0.00***
dummy.out.202.benz	–	–	–
dummy.out.202.c9	-0.20	0.064	0.00***
dummy.out.207.benz	5.85	1.414	0.00***
dummy.out.207.c9	–	–	–
dummy.out.249.benz	-4.45	1.423	0.00***
dummy.out.249.c9	0.09	0.064	0.14
dummy.out.297.benz	-6.73	1.413	0.00***
dummy.out.297.c9	-0.10	0.063	0.13
dummy.out.302.benz	5.20	1.433	0.00***
dummy.out.302.c9	0.13	0.064	0.08†

significance codes: ***...≤ 0.001; **...≤ 0.01; *...≤ 0.05; †...≤ 0.1

Table A.4: ANOVA table for the initial $VARX(3)$ model with outlier correction and variable selection





(a) Autocorrelation and cross-correlation for residuals of both outflow rates

(b) QQ-plots of residuals' marginal distributions for both outflow rates

Figure A.2: Residual diagnostic plots for $VARX(3)$ model with outlier compensation.

Simulation model

Data for conceptual model

	site 1						site 2						
	Cr.	Hy.	EBS	Al.	PE	PS	Cr.	Hy.	EBS	B.Ex.	PP	SBR	PE
Naph.	-3,000						-2,000						
C_1	600						400						
C_2	1050		-50		-1,200		700		-120				-380
C_3	450			-195			300				-600		
C_4	300						200			-600			
C_{5+}	600	-600					400	-400					
C_{9+}		60						40					
Buta.										240		-240	
Raff.										360			
Benz.		540	-150	-390				360	-360				
Styr.			200			-600			480			-80	
Cum.				585									
PE					1,200								380
PS						600							
PP											600		
SBR												320	

Table A.5: Stationary flow rates (in t/h) for exemplary chemical production network

$\mathbf{\Phi}_1$	$\mathbf{\Phi}_2$	$\boldsymbol{\beta}$
$\begin{pmatrix} 0.50 & 0.20 & 0.10 & 0.00 & 0.00 \\ 0.20 & 0.40 & 0.30 & 0.00 & 0.00 \\ 0.00 & -0.30 & 0.50 & 0.30 & 0.00 \\ 0.00 & 0.00 & 0.20 & -0.60 & 0.30 \\ 0.00 & 0.00 & 0.00 & -0.10 & 0.40 \end{pmatrix}$	$\begin{pmatrix} 0.30 & 0.10 & 0.00 & 0.00 & 0.00 \\ 0.10 & -0.10 & 0.10 & 0.00 & 0.00 \\ 0.00 & 0.10 & -0.20 & -0.20 & 0.00 \\ 0.00 & 0.00 & 0.10 & 0.10 & 0.10 \\ 0.00 & 0.00 & 0.00 & 0.20 & -0.20 \end{pmatrix}$	$\begin{pmatrix} 0.20 \\ 0.35 \\ 0.15 \\ 0.10 \\ 0.20 \end{pmatrix}$

coefficients for input time series: $\boldsymbol{\phi} = (-0.7, -0.3, -0.15)$

Table A.6: Coefficients of the time series models for cracker at site 1 ($VARX(2) + AR(3)$)

$\mathbf{\Phi}_1$	$\mathbf{\Phi}_2$	$\boldsymbol{\beta}$
$\begin{pmatrix} 0.50 & 0.20 & -0.20 & 0.00 & 0.00 \\ 0.30 & 0.20 & 0.40 & 0.00 & 0.00 \\ 0.00 & -0.20 & 0.40 & 0.20 & 0.00 \\ 0.00 & 0.00 & 0.20 & -0.40 & 0.20 \\ 0.00 & 0.00 & 0.00 & -0.20 & 0.20 \end{pmatrix}$	$\begin{pmatrix} -0.20 & 0.00 & 0.00 & 0.00 & 0.00 \\ -0.10 & 0.10 & 0.10 & 0.00 & 0.00 \\ 0.00 & -0.10 & -0.10 & 0.10 & 0.00 \\ 0.00 & 0.00 & 0.10 & 0.10 & 0.10 \\ 0.00 & 0.00 & 0.00 & 0.10 & -0.10 \end{pmatrix}$	$\begin{pmatrix} 0.20 \\ 0.35 \\ 0.15 \\ 0.10 \\ 0.20 \end{pmatrix}$

coefficients for input time series: $\boldsymbol{\phi} = (0.5, -0.2, 0.3)$

Table A.7: Coefficients of the time series models for cracker at site 2 ($VARX(2) + AR(3)$)

$\mathbf{\Phi}_1$	$\mathbf{\Phi}_2$	$\mathbf{\Phi}_3$	$\boldsymbol{\beta}$
$\begin{pmatrix} -0.40 & 0.10 \\ 0.20 & 0.30 \end{pmatrix}$	$\begin{pmatrix} -0.10 & -0.20 \\ -0.10 & 0.15 \end{pmatrix}$	$\begin{pmatrix} 0.20 & 0.00 \\ 0.10 & 0.05 \end{pmatrix}$	$\begin{pmatrix} 0.90 \\ 0.10 \end{pmatrix}$

coefficients for input time series: $\boldsymbol{\phi} = (-0.4, 0.1)$

Table A.8: Coefficients of the time series models for hydrogenation plant at site 1 ($VARX(3) + AR(2)$)

$\mathbf{\Phi}_1$	$\mathbf{\Phi}_2$	$\mathbf{\Phi}_3$	$\boldsymbol{\beta}$
$\begin{pmatrix} 0.40 & 0.30 \\ 0.20 & 0.30 \end{pmatrix}$	$\begin{pmatrix} 0.10 & -0.20 \\ 0.10 & -0.15 \end{pmatrix}$	$\begin{pmatrix} -0.20 & 0.00 \\ 0.00 & 0.00 \end{pmatrix}$	$\begin{pmatrix} 0.90 \\ 0.10 \end{pmatrix}$

coefficients for input time series: $\boldsymbol{\phi} = (-0.6, 0.2, 0.1)$

Table A.9: Coefficients of the time series models for hydrogenation plant at site 2 ($VARX(3) + AR(3)$)

$\mathbf{\Phi}_1$	$\boldsymbol{\beta}$
$\begin{pmatrix} 0.70 & -0.30 \\ 0.20 & 0.50 \end{pmatrix}$	$\begin{pmatrix} 0.40 \\ 0.60 \end{pmatrix}$

coefficients for input time series:
$\boldsymbol{\phi} = (0.5, 0.3, -0.25, -0.4)$

Table A.10: Coefficients of the time series models for Butex plant at site 2 ($VARX(1) + AR(4)$)

plant	**site**	**input product**	**input process** $\boldsymbol{\phi}^i$	**output process** $\boldsymbol{\phi}^o$
PE	1	Ethylene	$(0.4, 0.1, -0.2)$	$(0.8, -0.6, 0.3, -0.15)$
PE	2	Ethylene	$(-0.3, 0.1, -0.3)$	$(0.6, -0.2)$
PS	1	Styrene	$(0.4, -0.2)$	(0.9)
PP	2	Propylene	$(-0.5, 0.2, -0.1)$	$(-0.4, -0.2)$
ESM	1	Ethylene Benzene	$(0.25, 0.1, -0.05, -0.1)$ $(0.75, -0.1, -0.2)$	$(-0.5, 0.2, -0.1)$
ESM	2	Ethylene Benzene	$(0.3, 0.2, -0.1)$ $(-0.25, 0.2, 0.1)$	$(0.25, -0.3, -0.1)$
Alkylation	1	Propylene Benzene	$(0.4, 0.3, -0.2)$ $(0.5, 0.1, -0.3)$	$(-0.45, 0.3, -0.2)$
SBR	1	Butadiene Styrene	$(0.6, 0.3, -0.1)$ $(-0.35, 0.1, 0.2)$	$(-0.25, 0.3, -0.1)$

Table A.11: Coefficients of input and output time series models of SISO and MISO plants

		C_2	C_3	C_4	Styrene
# un-/loading arms		2	3	4	3
# un-/loaded rail cars		10	15	20	15
un-/loading capacity (in t)		500	750	1,000	750
$r_{is}^{\text{E–Ini}}$	site 1	20	20	40	40
	site 2	30	30	30	30
s_{is}^{Tar}	site 1	10,000	4,000	1,000	6,000
	site 2	5,000	8,000	3,500	4,000
s_{is}^{Ini}	site 1	10,000	5,000	1,000	4,000
	site 2	5,000	5,000	2,000	4,000

Table A.12: Un-/loading capacities, initial stock of empty RTCs, target and initial stock levels per transported chemical at both production sites

c^{Os}	c^{Us}	c^{Trn}	c^{Tr}	c^{Add}
1,000	1,000	100	10,000	1

Table A.13: Cost rates for the MC-RTP instances

	site 1			**site 2**				
	PE	PS	Cum.	C_4	PE	Raff.	PP	SBR
inter-arrival time	E(2.5)	E(1.25)	E(0.488)	E(1/12)	E(0.8)	E(3/10)	E(1.25)	E(2/3)
order quantity	$\mathrm{N}(20,5)$	$\mathrm{N}(20,5)$	$\mathrm{N}(50,5)$	$\mathrm{N}(50,2)$	$\mathrm{N}(20,5)$	$\mathrm{N}(50,2)$	$\mathrm{N}(20,5)$	$\mathrm{N}(20,5)$

Table A.14: Distributions of inter-arrival time and deliver quantities for external customers/suppliers

$$Q^1_{Cracker} = \begin{array}{r} \\ 3,000 \\ 1,500 \\ 0 \end{array} \begin{array}{c} \begin{array}{ccc} 3,000 & 1,500 & 0 \end{array} \\ \begin{pmatrix} 0.99 & 0.005 & 0.005 \\ 0.15 & 0.8 & 0.05 \\ 0.1 & 0.01 & 0.89 \end{pmatrix} \end{array} \qquad Q^1_{PE} = \begin{array}{r} \\ 1,200 \\ 600 \\ 0 \end{array} \begin{array}{c} \begin{array}{ccc} 1,200 & 600 & 0 \end{array} \\ \begin{pmatrix} 0.95 & 0.03 & 0.02 \\ 0.15 & 0.80 & 0.05 \\ 0.15 & 0.01 & 0.84 \end{pmatrix} \end{array}$$

$$Q^1_{Hyd.} = \begin{array}{r} \\ 600 \\ 0 \end{array} \begin{array}{c} \begin{array}{cc} 600 & 0 \end{array} \\ \begin{pmatrix} 0.98 & 0.02 \\ 0.25 & 0.75 \end{pmatrix} \end{array} \qquad Q^1_{EBSM} = \begin{array}{r} \\ 200 \\ 0 \end{array} \begin{array}{c} \begin{array}{cc} 200 & 0 \end{array} \\ \begin{pmatrix} 0.99 & 0.01 \\ 0.15 & 0.85 \end{pmatrix} \end{array}$$

$$Q^1_{Alkyl.} = \begin{array}{r} \\ 585 \\ 0 \end{array} \begin{array}{c} \begin{array}{cc} 585 & 0 \end{array} \\ \begin{pmatrix} 0.97 & 0.03 \\ 0.20 & 0.80 \end{pmatrix} \end{array} \qquad Q^1_{PS} = \begin{array}{r} \\ 600 \\ 0 \end{array} \begin{array}{c} \begin{array}{cc} 600 & 0 \end{array} \\ \begin{pmatrix} 0.94 & 0.06 \\ 0.30 & 0.70 \end{pmatrix} \end{array}$$

Table A.15: Transition matrices for plants at site 1

$$Q^2_{Cracker} = \begin{array}{c|ccc} & 2,000 & 1,000 & 0 \\ \hline 2,000 & 0.98 & 0.01 & 0.01 \\ 1,000 & 0.20 & 0.75 & 0.05 \\ 0 & 0.08 & 0.02 & 0.90 \end{array}$$

$$Q^2_{Hyd.} = \begin{array}{c|cc} & 400 & 0 \\ \hline 400 & 0.995 & 0.005 \\ 0 & 0.30 & 0.70 \end{array}$$

$$Q^2_{EBSM} = \begin{array}{c|cc} & 480 & 0 \\ \hline 480 & 0.98 & 0.02 \\ 0 & 0.22 & 0.88 \end{array}$$

$$Q^2_{But.Ex.} = \begin{array}{c|cc} & 600 & 0 \\ \hline 600 & 0.99 & 0.01 \\ 0 & 0.25 & 0.75 \end{array}$$

$$Q^2_{PP} = \begin{array}{c|cc} & 600 & 0 \\ \hline 600 & 0.97 & 0.03 \\ 0 & 0.15 & 0.85 \end{array}$$

$$Q^2_{SBR} = \begin{array}{c|cc} & 320 & 0 \\ \hline 320 & 0.975 & 0.025 \\ 0 & 0.2 & 0.8 \end{array}$$

$$Q^2_{PE} = \begin{array}{c|cc} & 380 & 0 \\ \hline 380 & 0.95 & 0.05 \\ 0 & 0.3 & 0.7 \end{array}$$

Table A.16: Transition matrices for plants at site 2

Planning of experiments

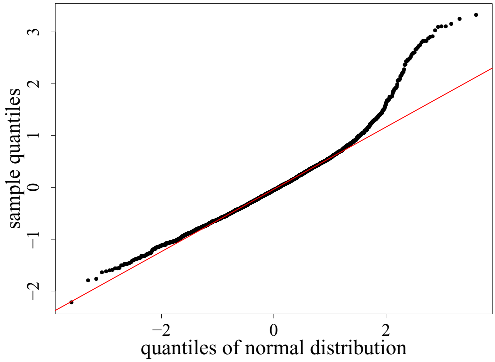
Experimental designs

# setting	# unloading arms C_2	C_3	C_4	Styrene	# trains	# handling days
1	-1	-1	-1	-1	-1	-1
2	-1	-1	-1	-1	1	1
3	-1	-1	-1	1	-1	1
4	-1	-1	-1	1	1	-1
5	-1	-1	1	-1	-1	1
6	-1	-1	1	-1	1	-1
7	-1	-1	1	1	-1	-1
8	-1	-1	1	1	1	1
9	-1	1	-1	-1	-1	1
10	-1	1	-1	-1	1	-1
11	-1	1	-1	1	-1	-1
12	-1	1	-1	1	1	1
13	-1	1	1	-1	-1	-1
14	-1	1	1	-1	1	1
15	-1	1	1	1	-1	1
16	-1	1	1	1	1	-1
17	1	-1	-1	-1	-1	1
18	1	-1	-1	-1	1	-1
19	1	-1	-1	1	-1	-1
20	1	-1	-1	1	1	1
21	1	-1	1	-1	-1	-1
22	1	-1	1	-1	1	1
23	1	-1	1	1	-1	1
24	1	-1	1	1	1	-1
25	1	1	-1	-1	-1	-1
26	1	1	-1	-1	1	1
27	1	1	-1	1	-1	1
28	1	1	-1	1	1	-1
29	1	1	1	-1	-1	1
30	1	1	1	-1	1	-1
31	1	1	1	1	-1	-1
32	1	1	1	1	1	1

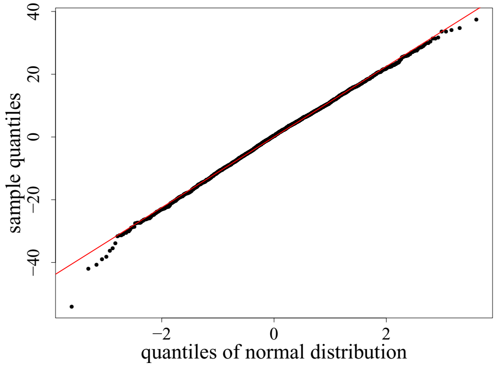
Table A.17: Resolution V design for 6 dichotomous variables ("-1" encodes the variable's lower level and "1" the upper level)

# setting	# unloading arms C_2	C_3	C_4	Styrene	# trains	# handling days	responses β	tr	r
1	2	3	4	3	6	6	0.985	264	0.540
2	4	3	4	3	6	6	0.985	261	0.524
3	2	6	4	3	6	6	0.986	263	0.547
4	4	6	4	3	6	6	0.984	261	0.532
5	2	3	8	3	6	6	0.986	263	0.541
6	4	3	8	3	6	6	0.986	260	0.531
7	2	6	8	3	6	6	0.986	262	0.546
8	4	6	8	3	6	6	0.985	259	0.536
9	2	3	4	6	6	6	0.984	264	0.543
10	4	3	4	6	6	6	0.985	260	0.526
11	2	6	4	6	6	6	0.986	263	0.549
12	4	6	4	6	6	6	0.985	260	0.532
13	2	3	8	6	6	6	0.985	263	0.543
14	4	3	8	6	6	6	0.986	260	0.532
15	2	6	8	6	6	6	0.986	262	0.547
16	4	6	8	6	6	6	0.986	259	0.536
17	2	3	4	3	7	6	0.988	283	0.509
18	4	3	4	3	7	6	0.987	280	0.496
19	2	6	4	3	7	6	0.988	282	0.510
20	4	6	4	3	7	6	0.986	280	0.496
21	2	3	8	3	7	6	0.987	282	0.511
22	4	3	8	3	7	6	0.987	279	0.503
23	2	6	8	3	7	6	0.988	281	0.509
24	4	6	8	3	7	6	0.986	279	0.502
25	2	3	4	6	7	6	0.987	282	0.514
26	4	3	4	6	7	6	0.987	278	0.499
27	2	6	4	6	7	6	0.988	282	0.513
28	4	6	4	6	7	6	0.987	279	0.498
29	2	3	8	6	7	6	0.987	281	0.514
30	4	3	8	6	7	6	0.987	278	0.506
31	2	6	8	6	7	6	0.988	281	0.511
32	4	6	8	6	7	6	0.987	278	0.503
33	2	3	4	3	6	7	0.986	263	0.542
34	4	3	4	3	6	7	0.987	260	0.527
35	2	6	4	3	6	7	0.987	262	0.548
36	4	6	4	3	6	7	0.986	259	0.533
37	2	3	8	3	6	7	0.986	263	0.540
38	4	3	8	3	6	7	0.987	260	0.531
39	2	6	8	3	6	7	0.986	262	0.543
40	4	6	8	3	6	7	0.986	259	0.534
41	2	3	4	6	6	7	0.984	264	0.539
42	4	3	4	6	6	7	0.986	260	0.523
43	2	6	4	6	6	7	0.986	263	0.543
44	4	6	4	6	6	7	0.986	260	0.527
45	2	3	8	6	6	7	0.984	264	0.536
46	4	3	8	6	6	7	0.986	261	0.526
47	2	6	8	6	6	7	0.986	263	0.538
48	4	6	8	6	6	7	0.986	260	0.528
49	2	3	4	3	7	7	0.988	282	0.512
50	4	3	4	3	7	7	0.988	279	0.499
51	2	6	4	3	7	7	0.988	282	0.510
52	4	6	4	3	7	7	0.987	279	0.498
53	2	3	8	3	7	7	0.987	283	0.510
54	4	3	8	3	7	7	0.987	279	0.503
55	2	6	8	3	7	7	0.987	282	0.506
56	4	6	8	3	7	7	0.987	279	0.500
57	2	3	4	6	7	7	0.986	283	0.510
58	4	3	4	6	7	7	0.987	279	0.496
59	2	6	4	6	7	7	0.987	283	0.507
60	4	6	4	6	7	7	0.987	279	0.494
61	2	3	8	6	7	7	0.985	283	0.507
62	4	3	8	6	7	7	0.987	279	0.500
63	2	6	8	6	7	7	0.987	283	0.503
64	4	6	8	6	7	7	0.986	279	0.495

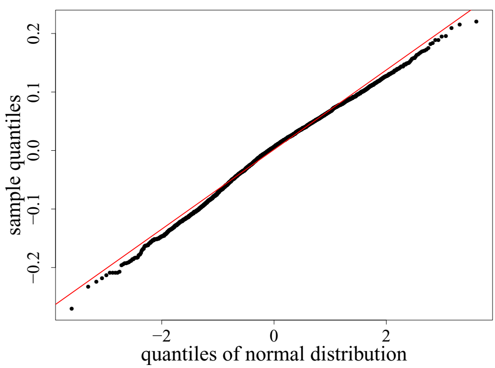
Table A.18: Estimated responses for all possible configurations (dominated configuration gray coloured)



(a) QQ-plot of residuals for (4.19)



(b) QQ-plot of residuals for (4.20)



(c) QQ-plot of residuals for (4.21)

Figure A.3: QQ-plots of residuals for models (4.19)-(4.21)

Simulation optimization

The density function of the Weibull distribution is given by

$$f(x) = \frac{k}{\lambda} \cdot \left(\frac{x}{\lambda}\right)^{(k-1)} \cdot e^{-(x/\lambda)^k}. \tag{A.1}$$

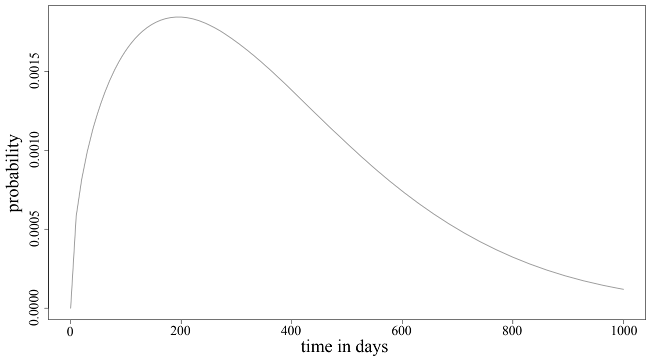
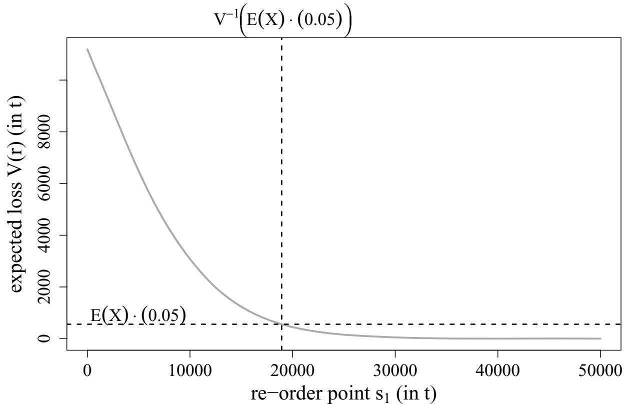
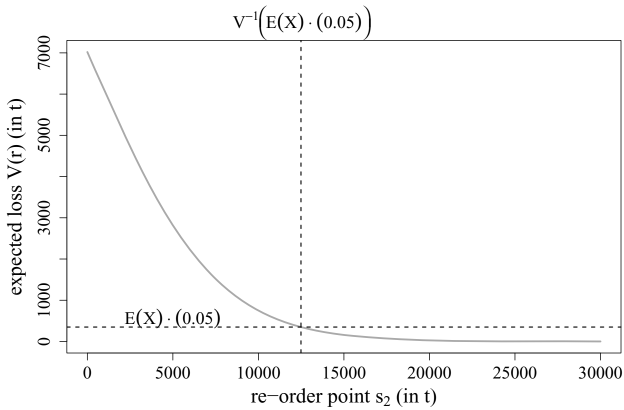


Figure A.4: Density function of the Weibull distribution with $k = 1.5$ and $\lambda = \frac{365}{\Gamma(\frac{5}{3})}$



(a) Loss function for site 1



(b) Loss function for site 2

Figure A.5: Loss functions for both sites during pipeline inspection

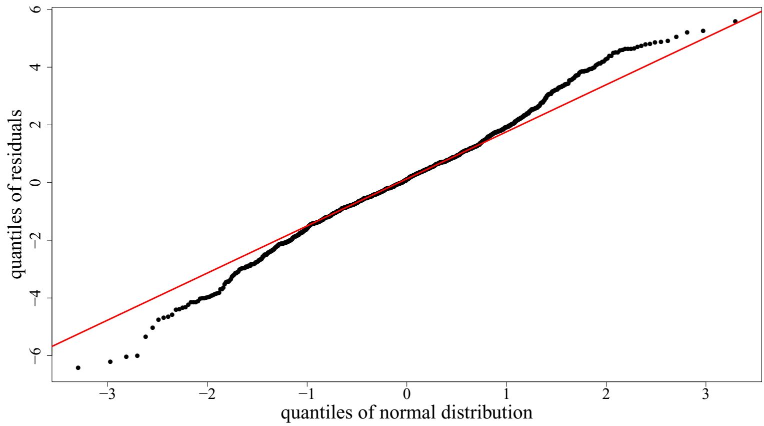
```
Function Sim.Inv.Sys(time horizon T, re-order points s_i, order-up levels S_i,
  initial stocks l_i^{ini}, inventory capacities l_i^{cap}, pumping capacities ρ_{in}^{cap}/ρ_{out}^{cap}, cracker
  models)
    generate production, flow, order & inventory matrices
    initialize inventory matrices
    for i ∈ {1,2} ∧ t = 1 → T do
        generate ω_{it}^{plan}  ▷ generate Markov chain samples
    end
    t^{alarm} ← WB(1.5, 365/Γ(5/3))  ▷ sample pipeline inspection
    t^{insp} ← 0  ▷ initial inspection time
    for t = 1 → T do
        for all locations i ∈ {1,2,h} do
            if l_{it} + Σ_{τ=t}^{T} q_{iτ} ≤ s_i then
                if i == h then
                    θ ← 2 + WB(2, 5/Γ(1.5))  ▷ sample order lead time
                    q_{i(t+θ)} ← q_{i(t+θ)} + S_i − l_{it} − Σ_{τ=t}^{T} q_{iτ}  ▷ assign order
                else
                    q_{it} ← q_{it} + S_i − l_{it} − Σ_{τ=t}^{T} q_{iτ}  ▷ assign order
                end
            end
        end
        if t == t^{alarm} then
            t^{insp} ← t + 1 + WB(1.5, 3/Γ(5/3))  ▷ sample inspection time
            t^{alarm} ← t + WB(1.5, 365/Γ(5/3))  ▷ sample next inspection
        end
        for i ∈ {h,1,2} do
            if i == h then
                f_{it} ← min(q_{it}, l_i^{cap} − l_{i(t−1)}, ρ_{out}^{cap})  ▷ calc. unloading flow
            else
                if t > t^{insp} then
                    f_{it} ← min(q_{it}, l_i^{cap} − l_{i(t−1)}, min(l_{h(t−1)} + f_{ht}, ρ_{in}^{cap}) · q_{it} / Σ_{j∈{1,2}} q_{jt})
                else
                    f_{it} ← 0  ▷ omit supply from harbour
                end
                ω_{it}^{real} ← min(ω_{it}^{plan}, l_{i(t−1)+f_{it}})  ▷ assign realized consumption
                l_{it} ← l_{i(t−1)} − ω_{it}^{real} + f_{it}  ▷ update inventory
            end
            q_{i(t+1)} ← q_{i(t+1)} + q_{it} − f_{it}  ▷ update outstanding orders
        end
        l_{ht} ← l_{h(t−1} + f_{ht} − Σ_{j∈{1,2}} f_{jt}  ▷ update harbour inventory
    end
end
```

Table A.19: Pseudocode for inventory system model

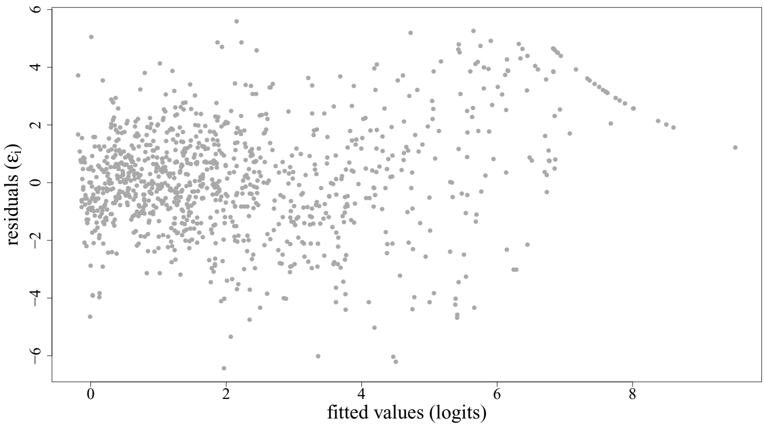
variable	Estimate	Std. Error	Pr(> $\|t\|$)
μ	-20.7348	0.2745	0.00***
$\gamma_{21}(\bar{l}^2)$	6.60E-10	2.80E-11	0.00***
$\gamma_{22}(\delta^2)$	3.92E-06	1.57E-07	0.00***
$\gamma_{11}(\bar{l})$	1.71E-05	2.05E-06	0.00***
$\gamma_{12}(\delta)$	-9.51E-03	2.79E-04	0.00***
$\gamma_{32}(\log(\delta))$	2.90	6.18E-02	0.00***
$\gamma_{31}(\log(\bar{l}))$	0.739	1.25E-02	0.00***
$\gamma_1(\bar{l} : \delta)$	9.10E-08	1.22E-09	0.00***
pseudo-R^2		0.99	

significance codes: ***...≤ 0.001; **...≤ 0.01;
*...≤ 0.05; †...≤ 0.1

Table A.20: Summary for the logistic regression model of responses of efficient settings



(a) QQ-plot of residuals for (4.22)



(b) Scatterplot of residuals vs. fitted values of (4.22)

Figure A.6: Diagnostic plots for (4.22)