Appendix E

E. Case study II: Optimisation results

Appendix E contains additional optimisation results for Case Study II which have been referred to in Chapter 7, 8 and 9. These include input uncertainty reduction optimisation results, Robustness Analysis on parameter uncertainty characterisation results and results presented for the analysis of alternative process flowsheets regarding flowsheet optimisation under uncertainty, Uncertainty and Sensitivity Analysis and optimal operating policy error tolerance results. Computational statistics are presented for the Case Study II optimisation problems.

E.1 Optimisation results for uncertainty reduction.

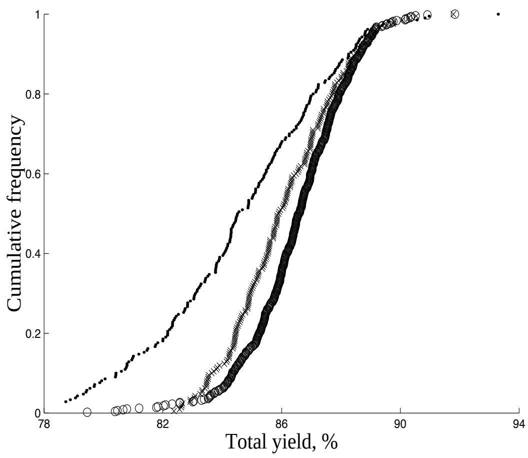
The results in Table E1 show how the optimal key input parameter uncertainties vary with parametric increases in the desired reduction in the output criteria (total yield, key and secondary endpoint impurity contents). No feasible solution was found for desired uncertainty reduction levels above 60% (of the original uncertainty in the knowledge level 6 model). Computational statistics for this problem are given in Table E6.

Table E1. Optimisation results for optimal key input parameter uncertainty reductions for knowledge level 6 Base Case flowsheet stochastic model, Case Study II.

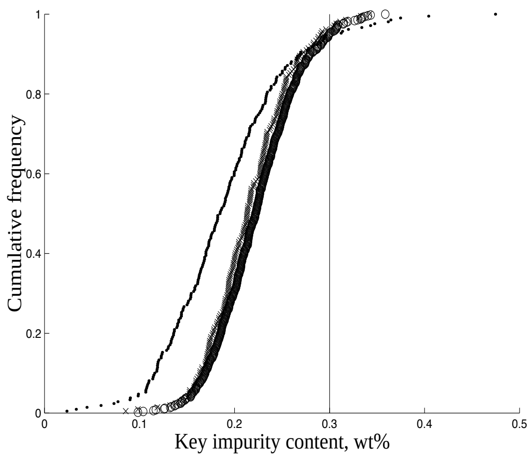
		Desired uncertainty reduction in output performance, %							
		0	10	20	30	40	50	60	70, 80, 90
Objective function, $\sum \delta_i$		7.00	6.30	5.94	5.56	4.83	3.93	1.72	-
Decisions	$\delta_{\sigma_{k_1}}$	1.00	0.93	0.73	0.64	0.47	0.28	1.0×10^{-3}	
	$\delta_{\sigma_{k_g}}$	1.00	0.82	0.81	0.56	0.50	0.40	9.1×10^{-2}	
	$\delta_{\sigma_{\sigma^*_{sl}}}$	1.00	1.00	0.72	0.98	0.58	0.39	0.34	
	$\delta_{\sigma_{k_3}}$	1.00	0.82	0.68	0.55	0.49	0.40	0.27	Infeasible
	$\delta_{\sigma_{\zeta_{actC}}}$	1.00	1.00	1.00	0.83	0.92	0.82	6.3×10^{-2}	
	$\delta_{\sigma_{\zeta_{actE}}}$	1.00	0.97	1.00	1.00	1.00	0.93	0.44	
	$\delta_{\Delta\eta_{wash}}$	1.00	0.77	1.00	1.00	0.86	0.69	1.1×10^{-2}	
5-95% Fractile width	Y_T, %	7.63	6.87	6.10	5.34	4.58	3.82	3.05	
	wt_{actC}, %	0.17	0.15	0.13	0.12	0.10	0.08	0.05	
	wt_{actE}, %	1.43	0.98	1.15	1.00	0.86	0.71	0.40	

E.2 The importance of the state of knowledge of the uncertainties results

The results of the Robustness Analysis to input uncertainty distribution, Figure E1, shows only a limited difference between output criterion distributions predicted using either normally or uniformly distributed input uncertainties (Case 2), but as expected, a significant difference when the input uncertainty spread is increased (Case 1).



(a) Total yield.



(b) Key impurity content.

Figure E1. Cumulative frequency plots for validated optimisation results under input uncertainty variations, Case Study II.
Key: o = Base Case (normally distributed), • = Case 1 (50% increase in spread, normally distributed), x = Case 2 (uniformly distributed).

E.3 Alternate flowsheet optimisation under uncertainty results.

Tables E2 and E3 and Figures E2 and E3 show the process flowsheet stochastic optimisation results for the four alternative flowsheets considered in Case Study II (Chapter 9). Alternative 2 returns the best profitability predictions under uncertainty. Only the Stage 1 reaction time ($t_{f,1}$) and Stage 12 crystallisation holding period (HP_{12}) decision variables appear sensitive to the different flowsheet configurations. Table E4 shows the main results of the Sensitivity Analysis where only SRC measures were required.

Table E2. Validated alternate process flowsheet optimisation under uncertainty results, Case Study II.

Criteria	Base Case	Alternative 1	Alternative 2	Alternative 3
E{Pty} ($ kg_{actA}^{-1} hr^{-1})	30.97	31.13	32.26	31.65
E{Ptyloss}($ kg_{actA}^{-1} hr^{-1})	3.02	2.97	3.04	3.10
Pr_{pass}	0.894	0.904	0.905	0.901
[E{wt_{actC}}, E{wt_{actE}}] (%)	[0.22, 1.42]	[0.21, 1.36]	[0.23, 1.42]	[0.23, 1.42]
[FW{wt_{actC}}, FW{wt_{actE}}] (%)	[0.14, 1.19]	[0.17, 1.36]	[0.15, 1.14]	[0.14, 1.19]
E{Y_T} (%)	86.5	89.2	86.9	85.6
FW{Y_T} (%)	5.4	5.4	6.3	5.7

Table E3. Optimal decisions for alternate process flowsheet optimisation under uncertainty, Case Study II.

Decisions	Base Case	Alternative 1	Alternative 2	Alternative 3
$t_{f,1}$ (min)	251	247	247	241
N_1 (rpm)	90.0	90.0	90.0	90.0
AF_{10}	0.40	0.40	0.40	0.40
RF_{10}	0.70	0.70	0.70	0.70
CR_{12} (ºC min^{-1})	0.50	0.50	0.50	0.50
HP_{12} (min)	54	52	47	50
	-	R_{solF_back} = 0.05	$R_{solL\_recycle}$ = 0.5	-

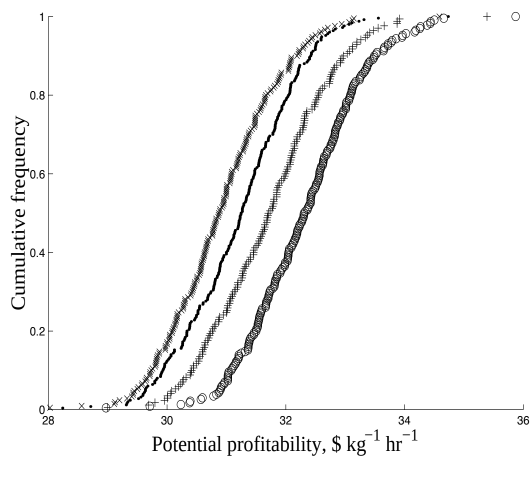
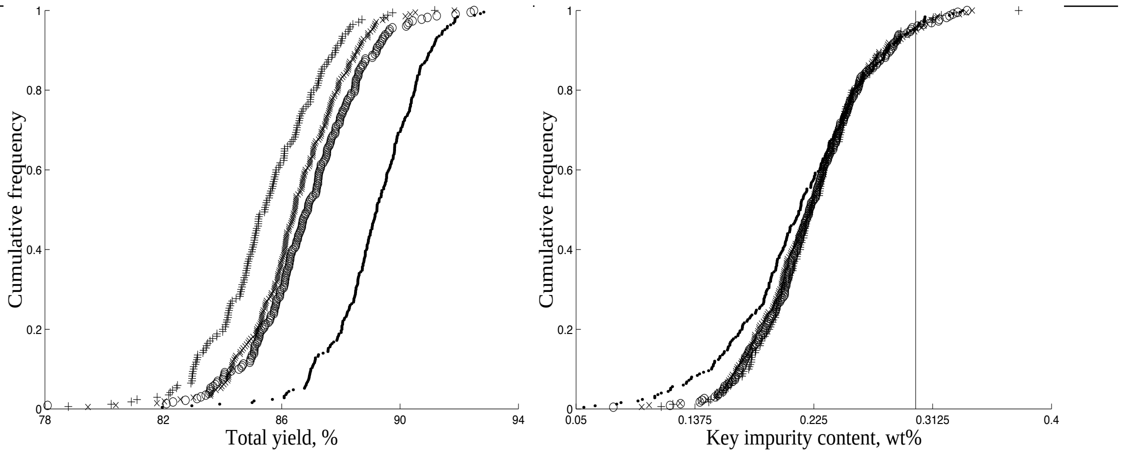


Figure E2. Cumulative frequency plots for potential profitability, Case Study II.

Key: + = Base Case, • = Alternative 1, o = Alternative 2, x = Alternative 3.



(a) Total yield.

(b) Key impurity content.

Figure E3. Cumulative frequency plots for validated optimisation results under input uncertainty variations, Case Study II.

Key: + = Base Case, • = Alternative 1, o = Alternative 2, x = Alternative 3.

Table E4. Key SRC contributors to predicted uncertainty for flowsheet alternatives, Case Study II.

	Base Case		Alternative 1		Alternative 2		Alternative 3	
Profitability	R^2	0.98	R^2	0.99	R^2	0.99	R^2	0.96
	DR_{15}	-0.77	DR_{15}	-0.77	DR_{15}	-0.75	DR_{14}	-0.75
	k_g	0.40	k_g	0.40	k_g	0.42	k_g	0.43
	k_1	0.30	k_1	0.31	k_1	0.28	k_1	0.32
	FR_{13}	-0.18	FR_{13}	-0.16	FR_{13}	-0.15	FR_{13}	-0.18
	σ_{sl}^*	-0.15	σ_{sl}^*	-0.10	$wt_{solL\ ml,2}$	0.11	σ_{sl}^*	-0.14
					σ_{sl}^*	-0.10		
Total yield	R^2	0.96	R^2	0.96	R^2	0.97	R^2	0.98
	k_g	0.68	k_g	0.70	k_g	0.66	k_g	0.69
	k_1	0.47	k_1	0.49	k_1	0.43	k_1	0.48
	σ_{sl}^*	-0.26	σ_{sl}^*	-0.16	σ_{sl}^*	-0.17	σ_{sl}^*	-0.24
					$wt_{solL\ ml,2}$	0.16		
Key impurity content	R^2	0.99	R^2	0.98	R^2	0.99	R^2	0.99
	k_2	0.85	k_2	0.68	k_2	0.77	k_2	0.89
	ζ_{actC}	0.45	ζ_{actC}	0.65	ζ_{actC}	0.55	ζ_{actC}	0.50
	η_{wash}	-0.32	η_{wash}	-0.27	η_{wash}	-0.36	LOD_{13}	0.14
Secondary impurity content	R^2	0.99	R^2	0.98	R^2	0.99	R^2	0.99
	k_3	0.91	k_3	0.79	k_3	0.84	k_3	0.93
	ζ_{actE}	0.33	ζ_{actE}	0.56	ζ_{actE}	0.45	ζ_{actE}	0.34
	η_{wash}	-0.19	η_{wash}	-0.17	η_{wash}	-0.22		

E.5 Alternate flowsheet operating policy tolerance optimisation results.

The optimal control variable range tolerance fraction decisions for the four process flowsheet alternatives based on 99% achievement of their respective 'here and now' optimal mean profitabilities, are given in Tables E5, E6, E7 and E8. Zero δ values indicate no tolerance in a particular policy variable deviation direction.

Table E5. Optimal decisions for the Base Case operating policy tolerance, Case Study II.

	$t_{f,1}$	N_1	AF_{10}	RF_{10}	CR_{12}	HP_{12}
$\delta_{z_d}^U$	0.110	0	0.042	0	0.006	0.153
$\delta_{z_d}^L$	0.309	0.015	0	0.081	0	0.784

Table E6. Optimal decisions and tolerance limits for Alternative 1 operating policy tolerance, Case Study II.

	$t_{f,1}$	N_1	AF_{10}	RF_{10}	CR_{12}	HP_{12}	R_{solF_back}
$\delta_{z_d}^{U}$	0.281	0	0.042	0	0.001	0.001	0.027
$\delta_{z_d}^{L}$	0.544	0.001	0	0.081	0	0.713	0.001
z_d^{UB}	290	90.0	0.41	0.70	0.50	52	0.067
z_d^{LB}	221	90.0	0.40	0.68	0.50	44	0.052

Table E7. Optimal decisions and tolerance limits for Alternative 2 operating policy tolerance, Case Study II.

	$t_{f,1}$	N_1	AF_{10}	RF_{10}	CR_{12}	HP_{12}	$R_{solL\_recycle}$
$\delta_{z_d}^{U}$	0.127	0	0.042	0	0.016	0.065	0
$\delta_{z_d}^{L}$	0.488	0.034	0	0.081	0	0.892	0.098
z_d^{UB}	266	90.0	0.41	0.70	0.56	52	0.500
z_d^{LB}	224	89.0	0.40	0.68	0.50	41	0.451

Table E8. Optimal decisions and tolerance limits for Alternative 3 operating policy tolerance, Case Study II.

	$t_{f,1}$	N_1	AF_{10}	RF_{10}	CR_{12}	HP_{12}
$\delta_{z_d}^{U}$	0.110	0	0.042	0	0.004	0.042
$\delta_{z_d}^{L}$	0.059	0.006	0	0.081	0	0.816
z_d^{UB}	258	90.0	0.41	0.70	0.51	53
z_d^{LB}	238	89.8	0.40	0.68	0.50	42

E.6 Computation statistics

These stochastic optimisation problems were solved using the MATLAB (Version 6.0) programming software and the Optimisation Toolbox function for non-linear constrained optimisation algorithm based on SQP. They were performed on a RS6000 IBM workstation. The stochastic optimisation problems involving decision variables which redefine the input uncertainty space in some way (optimal input uncertainty reduction - Problem type P1, and maximum operating policy tolerance - Problem type P3) required CPU times of an order of magnitude greater than the stochastic flowsheet optimisations of fixed space definition (Problem type P2). The latter required CPU times two orders of magnitude greater than their respective nominal optimisation problems.

Table E9. Computational statistics for optimisation problems, Case Study II.

		Problem formulation	CPU time (seconds)	Optimisation iterations	Function evaluations
Input parameter uncertainty reduction: Base case	10% red'n	P8 (type P1)	2.46×10^4	53	548
	20% red'n		5.02×10^4	120	1094
	30% red'n		3.04×10^4	78	753
	40% red'n		5.45×10^4	123	1129
	50% red'n		6.12×10^4	139	1312
	60% red'n		1.01×10^4	24	221
Nominal flowsheet optimisation: Base case		P9	67	11	102
Uncertain flowsheet optimisation: Base case		P10 (type P2)	3256	11	66
Uncertain flowsheet optimisation with input uncertainty variation: Case 1		Type P10 (type P2)	3719	12	77
Uncertain flowsheet optimisation with input uncertainty variation: Case 2		Type P10 (type P2)	4149	13	85
Uncertain flowsheet optimisation with uncertain feed purity: Base Case		Type P10 (type P2)	3213	11	66
Nominal flowsheet optimisation: Alternative 1		Type P9	50	27	197
Uncertain flowsheet optimisation: Alternative 1		Type P10 (type P2)	5365	10	85
Nominal flowsheet optimisation: Alternative 2		Type P9	19	10	77
Uncertain flowsheet optimisation: Alternative 2		Type P10 (type P2)	2387	6	41
Nominal flowsheet optimisation: Alternative 3		Type P9	19	12	79
Uncertain flowsheet optimisation: Alternative 3		Type P10	3028	11	80
Operating policy tolerance optimisation: Base Case		P11 (type P3)	1.93×10^4	52	411
Operating policy tolerance optimisation: Alternative 1		Type P3	4.08×10^4	77	798
Operating policy tolerance optimisation: Alternative 2		Type P3	3.85×10^4	80	806
Operating policy tolerance optimisation: Alternative 3		Type P3	2.72×10^4	73	605