Supporting Information for

Simultaneous Targeting and Scheduling for Batch Water Networks

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■ APPENDIX

The necessary timing constraints for the case studies are presented below.

Timing Constraints for Case Study 1

In this case study, all water sources and sinks occur during the course of the semi-continuous water-using operations. Equations S.1a-d correlate the operation times with the sink timings. It is stated that a sink j occurs from the start to the end of its corresponding water-using operation $s_{\text{in},u}$, lasting for $\alpha(s_{\text{in},u})$ time intervals. In other words, if $y(s_{\text{in},u},t) = 1$ at a given time interval t, then $y_{j,t} = 1$ for $t = t, t + 1, \ldots, t + \alpha(s_{\text{in},u}) - 1$.

$$y\left(\text{s1}_{\text{in,U1}},t\right) \le y_{\text{SK1},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\text{s1}_{\text{in,U1}}\right) - 1 \tag{S.1a}$$

$$y\left(\text{s2}_{\text{in,U2}},t\right) \le y_{\text{SK2},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\text{s2}_{\text{in,U2}}\right) - 1 \tag{S.1b}$$

$$y\left(\text{s4}_{\text{in,U3}},t\right) \le y_{\text{SK3},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\text{s4}_{\text{in,U3}}\right) - 1 \tag{S.1c}$$

$$y\left(\text{s5}_{\text{in,U4}},t\right) \le y_{\text{SK4},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\text{s5}_{\text{in,U4}}\right) - 1 \tag{S.1d}$$

where $y(s_{\text{in},u},t)$ is a binary variable indicating if the operation starts at the beginning of time interval t, $y_{j,t}$ is a binary variable indicating if sink j occurs in time interval t, and $\alpha(s_{\text{in},u})$ is the operation duration in terms of the number of time intervals. In addition, $\text{s1}_{\text{in,U1}}$, $\text{s2}_{\text{in,U2}}$, $\text{s4}_{\text{in,U3}}$ and $\text{s5}_{\text{in,U4}}$ are effective states representing operations 1-4, respectively.

Equations S.2a-d ensure that each of the sinks has the same number of occurrences as its corresponding water-using operation.

$$\sum_{t\in\mathbf{T}} y_{\text{SK1},t} = \alpha\left(\text{s1}_{\text{in,U1}}\right) \sum_{t\in\mathbf{T}} y\left(\text{s1}_{\text{in,U1}},t\right) \tag{S.2a}$$

$$\sum_{t\in\mathbf{T}} y_{\text{SK2},t} = \alpha\left(\text{s2}_{\text{in,U2}}\right) \sum_{t\in\mathbf{T}} y\left(\text{s2}_{\text{in,U2}},t\right) \tag{S.2b}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK3},t} = \alpha\left(\mathrm{s4}_{\mathrm{in,U3}}\right)\sum_{t\in\mathbf{T}} y\left(\mathrm{s4}_{\mathrm{in,U3}},t\right) \tag{S.2c}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK4},t} = \alpha\left(\mathrm{s5}_{\mathrm{in,U4}}\right)\sum_{t\in\mathbf{T}} y\left(\mathrm{s5}_{\mathrm{in,U4}},t\right) \tag{S.2d}$$

Similarly, eqs S.3 and S.4 apply to the water sources.

$$y\left(\mathrm{s1}_{\mathrm{in,U1}},t\right) \le y_{\mathrm{SR1},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\mathrm{s1}_{\mathrm{in,U1}}\right) - 1 \tag{S.3a}$$

$$y\left(\mathrm{s2}_{\mathrm{in,U2}},t\right) \le y_{\mathrm{SR2},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\mathrm{s2}_{\mathrm{in,U2}}\right) - 1 \tag{S.3b}$$

$$y\left(\mathrm{s4}_{\mathrm{in,U3}},t\right) \le y_{\mathrm{SR3},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\mathrm{s4}_{\mathrm{in,U3}}\right) - 1 \tag{S.3c}$$

$$y\left(\mathrm{s5}_{\mathrm{in,U4}},t\right) \le y_{\mathrm{SR4},t'} \quad \forall t,t' \in \mathbf{T}, t \le t' \le t + \alpha\left(\mathrm{s5}_{\mathrm{in,U4}}\right) - 1 \tag{S.3d}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR1},t} = \alpha\left(\mathrm{s1}_{\mathrm{in,U1}}\right)\sum_{t\in\mathbf{T}} y\left(\mathrm{s1}_{\mathrm{in,U1}},t\right) \tag{S.4a}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR2},t} = \alpha\left(\mathrm{s2}_{\mathrm{in,U2}}\right)\sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,U2}},t\right) \tag{S.4b}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR3},t} = \alpha\left(\mathrm{s4}_{\mathrm{in,U3}}\right)\sum_{t\in\mathbf{T}} y\left(\mathrm{s4}_{\mathrm{in,U3}},t\right) \tag{S.4c}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR4},t} = \alpha\left(\mathrm{s5}_{\mathrm{in,U4}}\right)\sum_{t\in\mathbf{T}} y\left(\mathrm{s5}_{\mathrm{in,U4}},t\right) \tag{S.4d}$$

where $y_{i,t}$ is a binary variable indicating if source i occurs in time interval t.

Timing Constraints for Case Study 2

In this case study, water sources and sinks arise from the washing operations for the reactors. Equations S.5a-f connect the reaction times and the sink timings. It is stated that a sink j occurs right after the end of reaction $s_{\mathrm{in},u}$ and lasts for α_j time intervals. In other words, if the reaction starts at the beginning of time interval t, then the washing operation (and hence the sink) starts after $\alpha(s_{\mathrm{in},u})$ time intervals, at the beginning of time interval $t + \alpha(s_{\mathrm{in},u})$, and finishes at the end of time interval $t + \alpha(s_{\mathrm{in},u}) + \alpha_j - 1$.

$$y\left(\mathrm{s2}_{\mathrm{in,RR1}},t\right)\le y_{\mathrm{SK1},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR1}}\right)\le t'\le t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR1}}\right)+\alpha_{\mathrm{SK1}}-1 \quad \text{(S.5a)}$$

$$y\left(\mathrm{s2}_{\mathrm{in,RR2}},t\right)\le y_{\mathrm{SK2},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR2}}\right)\le t'\le t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR2}}\right)+\alpha_{\mathrm{SK2}}-1 \quad \text{(S.5b)}$$

$$y\left(\mathrm{s6}_{\mathrm{in,RR1}},t\right)\le y_{\mathrm{SK3},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR1}}\right)\le t'\le t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR1}}\right)+\alpha_{\mathrm{SK3}}-1 \quad \text{(S.5c)}$$

$$y\left(\mathrm{s6}_{\mathrm{in,RR2}},t\right)\le y_{\mathrm{SK4},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR2}}\right)\le t'\le t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR2}}\right)+\alpha_{\mathrm{SK4}}-1 \quad \text{(S.5d)}$$

$$y\left(\mathrm{s8}_{\mathrm{in,RR1}},t\right)\le y_{\mathrm{SK5},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR1}}\right)\le t'\le t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR1}}\right)+\alpha_{\mathrm{SK5}}-1 \quad \text{(S.5e)}$$

$$y\left(\mathrm{s8}_{\mathrm{in,RR2}},t\right)\le y_{\mathrm{SK6},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR2}}\right)\le t'\le t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR2}}\right)+\alpha_{\mathrm{SK6}}-1 \quad \text{(S.5f)}$$

where RR1 denotes reactor 1 and RR2 reactor 2; α_j is the duration of sink j. In addition, $\mathrm{s2}_{\mathrm{in,RR1/2}}$, $\mathrm{s6}_{\mathrm{in,RR1/2}}$ and $\mathrm{s8}_{\mathrm{in,RR1/2}}$ are effective states representing tasks 2 (reaction 1), 3 (reaction 2) and 4 (reaction 3), respectively.

Equations S.6a-f ensure that each of the water sinks has the same number of occurrences as its corresponding reaction.

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK1},t}=\alpha_{\mathrm{SK1}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,RR1}},t\right) \quad \text{(S.6a)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK2},t}=\alpha_{\mathrm{SK2}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,RR2}},t\right) \quad \text{(S.6b)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK3},t}=\alpha_{\mathrm{SK3}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s6}_{\mathrm{in,RR1}},t\right) \quad \text{(S.6c)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK4},t}=\alpha_{\mathrm{SK4}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s6}_{\mathrm{in,RR2}},t\right) \quad \text{(S.6d)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK5},t}=\alpha_{\mathrm{SK5}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s8}_{\mathrm{in,RR1}},t\right) \quad \text{(S.6e)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SK6},t}=\alpha_{\mathrm{SK6}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s8}_{\mathrm{in,RR2}},t\right) \quad \text{(S.6f)}$$

Similarly, eqs S.7 and S.8 apply to the water sources.

$$y\left(\mathrm{s2}_{\mathrm{in,RR1}},t\right)\le y_{\mathrm{SR1},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR1}}\right)\le t'\le t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR1}}\right)+\alpha_{\mathrm{SR1}}-1 \quad \text{(S.7a)}$$

$$y\left(\mathrm{s2}_{\mathrm{in,RR2}},t\right)\le y_{\mathrm{SR2},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR2}}\right)\le t'\le t+\alpha\left(\mathrm{s2}_{\mathrm{in,RR2}}\right)+\alpha_{\mathrm{SR2}}-1 \quad \text{(S.7b)}$$

$$y\left(\mathrm{s6}_{\mathrm{in,RR1}},t\right)\le y_{\mathrm{SR3},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR1}}\right)\le t'\le t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR1}}\right)+\alpha_{\mathrm{SR3}}-1 \quad \text{(S.7c)}$$

$$y\left(\mathrm{s6}_{\mathrm{in,RR2}},t\right)\le y_{\mathrm{SR4},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR2}}\right)\le t'\le t+\alpha\left(\mathrm{s6}_{\mathrm{in,RR2}}\right)+\alpha_{\mathrm{SR4}}-1 \quad \text{(S.7d)}$$

$$y\left(\mathrm{s8}_{\mathrm{in,RR1}},t\right)\le y_{\mathrm{SR5},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR1}}\right)\le t'\le t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR1}}\right)+\alpha_{\mathrm{SR5}}-1 \quad \text{(S.7e)}$$

$$y\left(\mathrm{s8}_{\mathrm{in,RR2}},t\right)\le y_{\mathrm{SR6},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR2}}\right)\le t'\le t+\alpha\left(\mathrm{s8}_{\mathrm{in,RR2}}\right)+\alpha_{\mathrm{SR6}}-1 \quad \text{(S.7f)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR1},t}=\alpha_{\mathrm{SR1}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,RR1}},t\right) \quad \text{(S.8a)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR2},t}=\alpha_{\mathrm{SR2}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,RR2}},t\right) \quad \text{(S.8b)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR3},t}=\alpha_{\mathrm{SR3}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s6}_{\mathrm{in,RR1}},t\right) \quad \text{(S.8c)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR4},t}=\alpha_{\mathrm{SR4}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s6}_{\mathrm{in,RR2}},t\right) \quad \text{(S.8d)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR5},t}=\alpha_{\mathrm{SR5}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s8}_{\mathrm{in,RR1}},t\right) \quad \text{(S.8e)}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR6},t}=\alpha_{\mathrm{SR6}}\sum_{t\in\mathbf{T}} y\left(\mathrm{s8}_{\mathrm{in,RR2}},t\right) \quad \text{(S.8f)}$$

where α_i is the duration of source i.

Timing Constraints for Case Study 3

In this case study, water sinks include the PVC manufacturing process (mainly for reactor feed), the utility section (boiler and cooling tower make-up) and miscellaneous usage (e.g. floor cleaning). The only water source arises from the discharge of the four parallel decanters (used to dewater the slurry effluent from the strippers).

Equations S.9a-i correlate the reactor operation time with the sink timings.

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK1},t'}\quad \forall t,t'\in\mathbf{T},t\le t'\le t+\alpha_{\mathrm{SK1}}-1 \tag{S.9a}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK2},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-\alpha_{\mathrm{SK2}}-1\le t'\le t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-2 \tag{S.9b}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK3},t}\quad \forall t\in\mathbf{T} \tag{S.9c}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK4},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-\alpha_{\mathrm{SK4}}-13\le t'\le t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-14 \tag{S.9d}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK5},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-\alpha_{\mathrm{SK5}}\le t'\le t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-1 \tag{S.9e}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK6},t'}\quad \forall t,t'\in\mathbf{T},t\le t'\le t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-1 \tag{S.9f}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK7},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-\alpha_{\mathrm{SK7}}-1\le t'\le t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-2 \tag{S.9g}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK8},t}\quad \forall t\in\mathbf{T} \tag{S.9h}$$

$$y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\le y_{\mathrm{SK9},t'}\quad \forall t,t'\in\mathbf{T},t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-\alpha_{\mathrm{SK9}}-13\le t'\le t+\alpha\left(\mathrm{s1}_{\mathrm{in,RX}}\right)-14 \tag{S.9i}$$

where RX denotes the parallel reactors; in addition, $\mathrm{s1}_{\mathrm{in,RX}}$ is the effective state for the reaction task.

Equation S.10 ensures that each of the water sinks has the same number of occurrences as the reaction.

$$\sum_{t\in\mathbf{T}} y_{jt}=\alpha_j\sum_{t\in\mathbf{T}} y\left(\mathrm{s1}_{\mathrm{in,RX}},t\right)\quad \forall j\in\mathbf{J} \tag{S.10}$$

Similarly, eqs S.11 and S.12 apply to the water sources.

$$y\left(\mathrm{s2}_{\mathrm{in,SEP1}},t\right)\le y_{\mathrm{SR1},t'}\quad \forall t,t'\in\mathbf{T},t\le t'\le t+\alpha\left(\mathrm{s2}_{\mathrm{in,SEP1}}\right)-1 \tag{S.11a}$$

$$y\left(\mathrm{s2}_{\mathrm{in,SEP2}},t\right)\le y_{\mathrm{SR2},t'}\quad \forall t,t'\in\mathbf{T},t\le t'\le t+\alpha\left(\mathrm{s2}_{\mathrm{in,SEP2}}\right)-1 \tag{S.11b}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR1},t} = \alpha_{\mathrm{SR1}} \sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,SEP1}}, t\right) \tag{S.12a}$$

$$\sum_{t\in\mathbf{T}} y_{\mathrm{SR2},t} = \alpha_{\mathrm{SR2}} \sum_{t\in\mathbf{T}} y\left(\mathrm{s2}_{\mathrm{in,SEP2}}, t\right) \tag{S.12b}$$

where SEP1 and SEP2 denote the two downstream processing trains. In addition, $\mathrm{s2}_{\mathrm{in,SEP1/2}}$ are effective states representing the separation tasks.

Table Captions

Table S1. Computational Results for Case Study 1

Table S2. Computational Results for Case Study 2

Table S3. Computational Results for Case Study 3

Table S1. Computational Results for Case Study 1

	predefined schedule	optimised schedule	
		scenario 1	scenario 2
fresh water consumption (t/cycle)	185	185	187.5
water storage capacity (t)	30	2.86	0
water and storage cost (US$/y)	302,317*	300,844*	300,000
model solved	-	MILP	MILP
number of constraints	-	660†/721‡	726
number of variables	-	461†/467‡	473
number of binaries	-	100	106
solution time (CPU s)	-	0.2	0.2

*Calculated based on the fresh water consumption and water storage capacity.

†With the objective of minimising fresh water consumption.

‡With the objective of minimising water storage capacity.

Table S2. Computational Results for Case Study 2

	without water integration (base case)	water integration	
		without water storage	with water storage
profit ($/cycle)	1,213	1,454.75	1,511
product revenue ($/cycle)	2,280	2,633.75	2,633.75
raw material cost ($/cycle)	242	322.75	322.75
fresh water cost ($/cycle)	330	342.5	320
wastewater treatment cost ($/cycle)	495	513.75	480
model solved	MILP	MILP	MILP
number of constraints	1,078	1,366	1,366
number of variables	970	1,402	1,402
number of binaries	456	456	456
solution time (CPU s)	0.6	0.6	0.6

Table S3. Computational Results for Case Study 3

	without water integration	water integration	
		without tank emptying	with tank emptying once a cycle
TAC (US$)	187,920*	62,428	73,771
fresh water consumption (t/y)	119881.05	52479.24	59548.35
wastewater treatment (t/y)	68039.25	637.44	7706.55
water storage capacity (t)	-	85.17	33.66
model solved	-	MILP	MILP
number of constraints	-	28,820	28,820
number of variables	-	9,231	9,231
number of binaries	-	2,628	2,628
solution time (CPU s)	-	11	82

*Calculated based on the fresh water consumption and water storage capacity.