Supporting Information

Optimization of the water network with single and double outlet treatment units

Kaili Zhang[*,†,‡,§], *Yuehong Zhao*[†,‡,§], *Hongbin Cao*[†,‡],*Hao Wen*[†,‡]

[†]Beijing Engineering Research Centre of Process Pollution Control, Beijing 100190, China

[‡]State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

[§]University of Chinese Academy of Sciences, Beijing 100049, China

Contents

S1. Mathematical model

S1.1 Freshwater sources

Freshwater sources can be supplied to process units, and also can be sent to treatment units for pretreatment, for example, freshwater can be used to produce desalted water that some process units require as shown in Figure S1.

The water balance at the splitting point is given by eq S1.

$$F_s = \sum_{p \in P} F_{s,p} + \sum_{dt \in DT} F_{s,dt} + \sum_{t \in T} F_{s,t}\ , \quad s \in S \tag{S1}$$

For each of the flowrates between the splitter point of the freshwater source and mixing points in the network, the lower and upper bound constraints formulated with 0-1 variables that denote the existence of these streams are given as follows.

$$F^{lo}_{s,p} \cdot y_{s,p} \le F_{s,p} \le F^{up}_{s,p} \cdot y_{s,p}\ , \quad s \in S\ , \quad p \in P \tag{S2}$$

$$F^{lo}_{s,dt} \cdot y_{s,dt} \le F_{s,dt} \le F^{up}_{s,dt} \cdot y_{s,dt}\ , \quad s \in S\ , \quad dt \in DT \tag{S3}$$

$$F^{lo}_{s,t} \cdot y_{s,t} \le F_{s,t} \le F^{up}_{s,t} \cdot y_{s,t}\ , \quad s \in S\ , \quad t \in T \tag{S4}$$

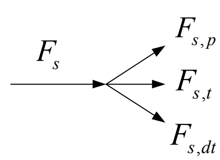

Figure S1. Splitting streams of freshwater source.

S1.2 Process units

Figure S2 shows a schematic representation of a process unit. And the balances on flows and mass loads of contaminant j at the mixing point of the process unit are given by eq S5 and eq S6, respectively.

$$\sum_{s \in S} F_{s,p} + \sum_{p' \in P} F_{p',p} + \sum_{t \in T} F_{t,p} + \sum_{dt \in DT} F^{H}_{dt,p} + \sum_{dt \in DT} F^{L}_{dt,p} = F^{in}_{p}\ , \quad p \in P \tag{S5}$$

$$\sum_{s\in S}F_{s,p}c_{s,j}+\sum_{p'\in P}F_{p',p}c_{p',j}^{out}+\sum_{t\in T}F_{t,p}c_{t,j}^{out}+\sum_{dt\in DT}F_{dt,p}^{H}c_{dt,j}^{H}+\sum_{dt\in DT}F_{dt,p}^{L}c_{dt,j}^{L}=F_{p}^{in}c_{p,j}^{in}$$

$$p\in P,\, j\in J \tag{S6}$$

The flow balance at the splitting point of the process unit is expressed in eq S7.

$$F_{p}^{out}=\sum_{p''\in P}F_{p,p''}+\sum_{t\in T}F_{p,t}+\sum_{dt\in DT}F_{p,dt}+F_{p,o}\,,\quad p\in P \tag{S7}$$

Additionally, the balances on flowrates and contaminant concentrations of process unit are formulated as eq S8 and eq S9:

$$F_{p}^{in}=F_{p}^{out}+F_{p}^{v\_loss}+F_{p}^{o\_loss}\,,\, p\in P \tag{S8}$$

$$F_{p}^{in}c_{p,j}^{in}=F_{p}^{out}c_{p,j}^{out}+F_{p}^{o\_loss}c_{p,j}^{o\_loss}\,,\quad p\in P,\, j\in J \tag{S9}$$

The contaminant concentration of loss flowrate can be seen equal to the outlet concentration of contaminant j, defined as eq S10.

$$c_{p,j}^{o\_loss}=c_{p,j}^{out}\quad,\, p\in P,\, j\in J \tag{S10}$$

Considering the inlet concentration cannot be greater than the maximum inlet concentration of contaminant j, a constraint is defined as eq S11.

$$c_{p,j}^{in}\le c_{p,j}^{in,\max}\,,\, p\in P,\, j\in J \tag{S11}$$

The lower and upper bound constraints that formulate flows between the splitter point of the process unit and mixing points in the network with binary variables are given as follows.

$$F_{p,p'}^{lo}\cdot y_{p,p'}\le F_{p,p'}\le F_{p,p'}^{up}\cdot y_{p,p'}\quad,\, p\in P\,,\, p'\in P \tag{S12}$$

$$F_{p,t}^{lo}\cdot y_{p,t}\le F_{p,t}\le F_{p,t}^{up}\cdot y_{p,t}\quad,\quad p\in P\,,\, t\in T \tag{S13}$$

$$F_{p,dt}^{lo}\cdot y_{p,dt}\le F_{p,dt}\le F_{p,dt}^{up}\cdot y_{p,dt}\,,\quad p\in P\,,\, dt\in DT \tag{S14}$$

$$F_{p,o}^{lo}\cdot y_{p,o}\le F_{p,o}\le F_{p,o}^{up}\cdot y_{p,o}\qquad p\in P \tag{S15}$$

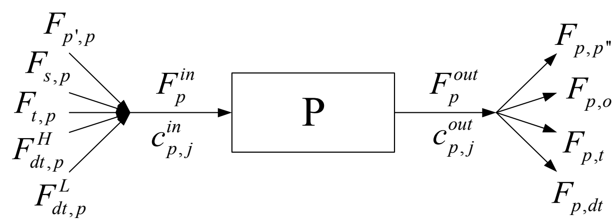

Figure S2. Inlet and outlet streams of process unit.

S1.3 Single outlet treatment units

Figure S3 shows a representation of a single outlet treatment unit, of which the outlet stream can be used by process units, other single outlet treatment units, double outlet treatment units or discharged, the inlet stream can receive water from freshwater sources, process units, other single outlet treatment units and double outlet treatment units.

The balances on flows and mass loads of contaminant j at the mixing point of the single outlet treatment unit are given by eq S16 and eq S17, respectively.

$$\sum_{s\in S} F_{s,t} + \sum_{p\in P} F_{p,t} + \sum_{t'\in T, t'\neq t} F_{t',t} + \sum_{dt\in DT} F_{dt,t}^{H} + \sum_{dt\in DT} F_{dt,t}^{L} = F_{t}^{in}, \quad t \in T \tag{S16}$$

$$\sum_{s\in S} F_{s,t} c_{s,j} + \sum_{p\in P} F_{p,t} c_{p,j}^{out} + \sum_{t'\in T, t'\neq t} F_{t',t} c_{t',j}^{out} + \sum_{dt\in DT} F_{dt,t}^{H} c_{dt,j}^{H} + \sum_{dt\in DT} F_{dt,t}^{L} c_{dt,j}^{L} = F_{t}^{in} c_{t,j}^{in} \quad ,$$

$$t \in T, \ j \in J \tag{S17}$$

The flow balance at the splitting point of the process unit is expressed by eq S18.

$$F_{t}^{out} = \sum_{p\in P} F_{t,p} + \sum_{t''\in T, t''\neq t} F_{t,t''} + \sum_{dt\in DT} F_{t,dt} + F_{t,o} \quad , \quad t \in T \tag{S18}$$

Besides, the balances on flowrates and contaminant concentrations of the single outlet treatment unit are formulated as eq S19 and eq S20:

$$F_{t}^{in} = F_{t}^{out} + F_{t}^{loss}, \quad t \in T \tag{S19}$$

$$c_{t,j}^{out} = (1 - R_{t,j}) c_{t,j}^{in} \quad t \in T \quad , j \in J \tag{S20}$$

The inlet concentration cannot be greater than the maximum inlet concentration of contaminant j, the constraint is defined as eq S21.

$$c_{t,j}^{in} \le c_{t,j}^{in,\max} \quad t \in T\ ,\ j \in J \tag{S21}$$

The lower and upper bound constraints that formulate flows between the splitter point of the single outlet treatment unit and mixing points in the network with binary variables are given as follows.

$$F_{t,p}^{lo} \cdot y_{t,p} \le F_{t,p} \le F_{t,p}^{up} \cdot y_{t,p}\ , \quad t \in T\ ,\ p \in P \tag{S22}$$

$$F_{t,t'}^{lo} \cdot y_{t,t'} \le F_{t,t'} \le F_{t,t'}^{up} \cdot y_{t,t'}\ , \quad t \in T\ ,\ t' \in T \tag{S23}$$

$$F_{t,dt}^{lo} \cdot y_{t,dt} \le F_{t,dt} \le F_{t,dt}^{up} \cdot y_{t,dt}\ , \quad t \in T\ ,\ dt \in DT \tag{S24}$$

$$F_{t,o}^{lo} \cdot y_{t,o} \le F_{t,o} \le F_{t,o}^{up} \cdot y_{t,o}\ , \quad t \in T \tag{S25}$$

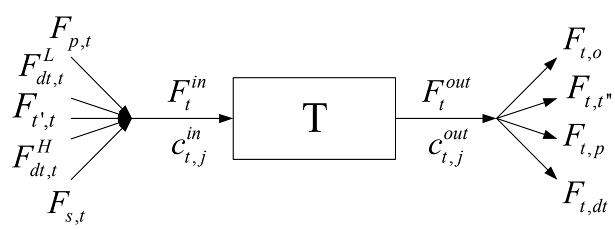

Figure S3. Inlet and outlet streams of single outlet treatment unit

S1.4 Double outlet treatment units

Figure S4 shows the diagram of a double outlet treatment unit. The process has two outflows, and both outflows can be used by process units, single outlet treatment units, other double outlet treatment units or discharged. And the double outlet treatment units can receive water from freshwater sources, process units, single outlet treatment units and other double outlet treatment units.

The balances on flows and mass loads of contaminant j at the mixing point before the double outlet treatment unit are given by eq S26 and eq S27, respectively.

$$\sum_{s\in S}F_{s,dt}+\sum_{p\in P}F_{p,dt}+\sum_{t\in T}F_{t,dt}+\sum_{dt'\in DT,dt'\neq dt}F^{H}_{dt',dt}+\sum_{dt''\in DT,dt''\neq dt}F^{L}_{dt'',dt}=F^{in}_{dt} \quad ,dt\in DT \tag{S26}$$

$$\sum_{s\in S}F_{s,dt}c_{s,j}+\sum_{p\in P}F_{p,dt}c^{out}_{p,j}+\sum_{t\in T}F_{t,dt}c^{out}_{t,j}+\sum_{dt'\in DT,dt'\neq dt}F^{H}_{dt',dt}c^{H}_{dt',j}+\sum_{dt''\in DT,dt''\neq dt}F^{L}_{dt'',dt}c^{L}_{dt'',j}=F^{in}_{dt}c^{in}_{dt,j},$$

$$dt\in DT,\ j\in J \tag{S27}$$

The flow balances at the two splitting points after the process unit are expressed by eq S28 and eq S29.

$$F^{H}_{dt}=\sum_{p\in P}F^{H}_{dt,p}+\sum_{t\in T}F^{H}_{dt,t}+\sum_{dt'''\in DT,dt'''\neq dt}F^{H}_{dt,dt'''}+F^{H}_{dt,o} \quad ,dt\in DT \tag{S28}$$

$$F^{L}_{dt}=\sum_{p\in P}F^{L}_{dt,p}+\sum_{t\in T}F^{L}_{dt,t}+\sum_{dt''''\in DT,dt''''\neq dt}F^{L}_{dt,dt''''}+F^{L}_{dt,o} \quad ,dt\in DT \tag{S29}$$

The inlet concentration cannot be greater than the maximum inlet concentration of contaminant j, as shown in eq S30.

$$c^{in}_{dt,j}\le c^{in,\max}_{dt,j},dt\in DT,\ j\in J \tag{S30}$$

The lower and upper bound constraints that formulate flows between the splitter points of the double outlet treatment unit and mixing points in the network with binary variables are given as follows.

$$F^{H,lo}_{dt,p}\cdot y^{H}_{dt,p}\le F^{H}_{dt,p}\le F^{H,up}_{dt,p}\cdot y^{H}_{dt,p},\quad dt\in DT,\ p\in P \tag{S31}$$

$$F^{H,lo}_{dt,t}\cdot y^{H}_{dt,t}\le F^{H}_{dt,t}\le F^{H,up}_{dt,t}\cdot y^{H}_{dt,t},\quad dt\in DT,\ t\in T \tag{S32}$$

$$F^{H,lo}_{dt,dt'}\cdot y^{H}_{dt,dt'}\le F^{H}_{dt,dt'}\le F^{H,up}_{dt,dt'}\cdot y^{H}_{dt,dt'},\quad dt\in DT,\ dt'\in DT \tag{S33}$$

$$F^{H,lo}_{dt,o}\cdot y^{H}_{dt,o}\le F^{H}_{dt,o}\le F^{H,up}_{dt,o}\cdot y^{H}_{dt,o}\qquad dt\in DT \tag{S34}$$

$$F^{L,lo}_{dt,p}\cdot y^{L}_{dt,p}\le F^{L}_{dt,p}\le F^{L,up}_{dt,p}\cdot y^{L}_{dt,p}\qquad dt\in DT,\ p\in P \tag{S35}$$

$$F^{L,lo}_{dt,t} \cdot y^{L}_{dt,t} \le F^{L}_{dt,t} \le F^{L,up}_{dt,t} \cdot y^{L}_{dt,t} \quad dt \in DT\ , t \in T \tag{S36}$$

$$F^{L,lo}_{dt,dt'} \cdot y^{L}_{dt,dt'} \le F^{L}_{dt,dt'} \le F^{L,up}_{dt,dt'} \cdot y^{L}_{dt,dt'} \quad dt \in DT\ , dt' \in DT \tag{S37}$$

$$F^{L,lo}_{dt,o} \cdot y^{L}_{dt,o} \le F^{L}_{dt,o} \le F^{L,up}_{dt,o} \cdot y^{L}_{dt,o} \quad dt \in DT \tag{S38}$$

Other equations on a double outlet treatment unit are in main text.

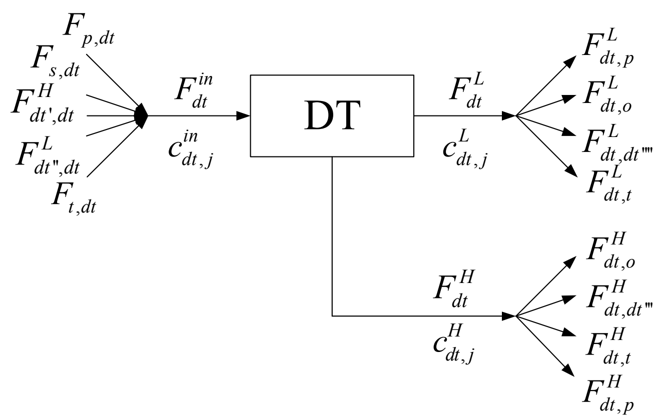

Figure S4. Inlet and outlet streams of double outlet treatment unit.

S1.5 Discharge constraints

All outlet streams of processes can be discharged to the environment, as shown in Figure S5. Balances on flows and contaminants can be presented by eq S39 and eq S40.

$$F_{out} = \sum_{p \in P} F_{p,o} + \sum_{t \in T} F_{t,o} + \sum_{dt \in DT} F^{H}_{dt,o} + \sum_{dt' \in DT} F^{L}_{dt',o} \tag{S39}$$

$$F_{out} c_{out,j} = \sum_{p \in P} F_{p,o} c^{out}_{p,j} + \sum_{t \in T} F_{t,o} c^{out}_{t,j} + \sum_{dt \in DT} F^{H}_{dt,o} c^{H}_{dt,j} + \sum_{dt' \in DT} F^{L}_{dt',o} c^{L}_{dt',j}\ , \ j \in J \tag{S40}$$

The discharge limit is described as eq 41.

$$c_{out,j} \le c^{\max}_{out,j}, \quad j \in J \tag{S41}$$

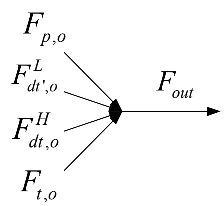

Figure S5. Streams for discharge.

S1.6 Objective function

The objective function is formulated to minimize total annual cost, instead of minimizing freshwater consumption, because the latter type of objective function may lead to increase in cost, especially in the cost of water treatment systems, which then would reduce the economic benefits of the plant.

The formulation is given by eq S42.

$$\min Z = \mathrm{C_{water}} + \mathrm{IC_{treatment}} + \mathrm{OC_{treatment}} + \mathrm{IC_{pipes}} + \mathrm{OC_{pumping}} \tag{S42}$$

Where $\mathrm{C_{water}}$ is cost of freshwater, $\mathrm{IC_{treatment}}$ is investment cost of all treatment units, $\mathrm{OC_{treatment}}$ is the operating cost of treatment units, $\mathrm{IC_{pipes}}$ and $\mathrm{OC_{pumping}}$ are investment and operating cost of piping connections.

The annualized expressions for the four cost components are defined as follows:

$$\mathrm{C_{water}} = H\sum_{s\in S}\mathrm{C}_s F_s \tag{S43}$$

$$\mathrm{IC_{treatment}} = \mathrm{AR}[\sum_{t\in T}\mathrm{IC}_t (F_t^{out})^{\beta} + \sum_{dt\in DT}\mathrm{IC}_{dt}(F_{dt}^{L})^{\beta}] \tag{S44}$$

$$\mathrm{OC_{treatment}} = \mathrm{H}(\sum_{t\in T}\mathrm{OC}_t F_t^{out} + \sum_{dt\in DT}\mathrm{OC}_{dt} F_{dt}^{L}) \tag{S45}$$

$$
\begin{aligned}
\mathrm{OC_{pumping}} = \mathrm{H}[&\sum_{s\in S}\sum_{p\in P}\mathrm{PM}_{s,p}F_{s,p} + \sum_{s\in S}\sum_{t\in T}\mathrm{PM}_{s,t}F_{s,t} + \sum_{s\in S}\sum_{dt\in DT}\mathrm{PM}_{s,dt}F_{s,dt} \\
&+\sum_{p\in P}\sum_{p'\in P}\mathrm{PM}_{p,p'}F_{p,p'} + \sum_{p\in P}\sum_{t\in T}\mathrm{PM}_{p,t}F_{p,t} + \sum_{p\in P}\sum_{dt\in DT}\mathrm{PM}_{p,dt}F_{p,dt} \\
&+\sum_{p\in P}\mathrm{PM}_{p,o}F_{p,o} + \sum_{t\in T}\sum_{p\in P}\mathrm{PM}_{t,p}F_{t,p} + \sum_{t\in T}\sum_{t'\in T,t'\neq t}\mathrm{PM}_{t,t'}F_{t,t'} \\
&+\sum_{t\in T}\sum_{dt\in DT}\mathrm{PM}_{t,dt}F_{t,dt} + \sum_{t\in T}\mathrm{PM}_{t,o}F_{t,o} + \sum_{dt\in DT}\sum_{p\in P}\mathrm{PM}_{dt,p}F^{H}_{dt,p} \\
&+\sum_{dt\in DT}\sum_{t\in T}\mathrm{PM}_{dt,t}F^{H}_{dt,t} + \sum_{dt\in DT}\sum_{dt'\in DT,dt'\neq dt}\mathrm{PM}_{dt,dt'}F^{H}_{dt,dt'} \\
&+\sum_{dt\in DT}\mathrm{PM}_{dt,o}F^{H}_{dt,o} + \sum_{dt\in DT}\sum_{p\in P}\mathrm{PM}_{dt,p}F^{L}_{dt,p} + \sum_{dt\in DT}\sum_{t\in T}\mathrm{PM}_{dt,t}F^{L}_{dt,t} \\
&+\sum_{dt\in DT}\sum_{dt'\in DT,dt'\neq dt}\mathrm{PM}_{dt,dt'}F^{L}_{dt,dt'} + \sum_{dt\in DT}\mathrm{PM}_{dt,o}F^{L}_{dt,o}]
\end{aligned}
\tag{S46}
$$

$$
\begin{aligned}
\mathrm{IC_{pipes}} = \mathrm{AR}[&\sum_{s\in S}\sum_{p\in P}(\mathrm{CP}_{s,p}y_{s,p}+\mathrm{IP}_{s,p}(F_{s,p})^{\gamma}) + \sum_{s\in S}\sum_{t\in T}(\mathrm{CP}_{s,t}y_{s,t}+\mathrm{IP}_{s,t}(F_{s,t})^{\gamma}) \\
&+\sum_{s\in S}\sum_{dt\in DT}(\mathrm{CP}_{s,dt}y_{s,dt}+\mathrm{IP}_{s,dt}(F_{s,dt})^{\gamma}) + \sum_{p\in P}\sum_{p'\in P}(\mathrm{CP}_{p,p'}y_{p,p'}+\mathrm{IP}_{p,p'}(F_{p,p'})^{\gamma}) \\
&+\sum_{p\in P}\sum_{t\in T}(\mathrm{CP}_{p,t}y_{p,t}+\mathrm{IP}_{p,t}(F_{p,t})^{\gamma}) + \sum_{p\in P}\sum_{dt\in DT}(\mathrm{CP}_{p,dt}y_{p,dt}+\mathrm{IP}_{p,dt}(F_{p,dt})^{\gamma}) \\
&+\sum_{p\in P}(\mathrm{CP}_{p,o}y_{p,o}+\mathrm{IP}_{p,o}(F_{p,o})^{\gamma}) + \sum_{t\in T}\sum_{p\in P}(\mathrm{CP}_{t,p}y_{t,p}+\mathrm{IP}_{t,p}(F_{t,p})^{\gamma}) \\
&+\sum_{t\in T}\sum_{t'\in T,t'\neq t}(\mathrm{CP}_{t,t'}y_{t,t'}+\mathrm{IP}_{t,t'}(F_{t,t'})^{\gamma}) + \sum_{t\in T}\sum_{dt\in DT}(\mathrm{CP}_{t,dt}y_{t,dt}+\mathrm{IP}_{t,dt}(F_{t,dt})^{\gamma}) \\
&+\sum_{t\in T}(\mathrm{CP}_{t,o}y_{t,o}+\mathrm{IP}_{t,o}(F_{t,o})^{\gamma}) + \sum_{dt\in DT}\sum_{p\in P}(\mathrm{CP}_{dt,p}y^{H}_{dt,p}+\mathrm{IP}_{dt,p}(F^{H}_{dt,p})^{\gamma}) \\
&+\sum_{dt\in DT}\sum_{t\in T}(\mathrm{CP}_{dt,t}y^{H}_{dt,t}+\mathrm{IP}_{dt,t}(F^{H}_{dt,t})^{\gamma}) \\
&+\sum_{dt\in DT}\sum_{dt'\in DT,dt'\neq dt}(\mathrm{CP}_{dt,dt'}y^{H}_{dt,dt'}+\mathrm{IP}_{dt,dt'}(F^{H}_{dt,dt'})^{\gamma}) \\
&+\sum_{dt\in DT}(\mathrm{CP}_{dt,o}y^{H}_{dt,o}+\mathrm{IP}_{dt,o}(F^{H}_{dt,o})^{\gamma}) + \sum_{dt\in DT}\sum_{p\in P}(\mathrm{CP}_{dt,p}y^{L}_{dt,p}+\mathrm{IP}_{dt,p}(F^{L}_{dt,p})^{\gamma}) \\
&+\sum_{dt\in DT}\sum_{t\in T}(\mathrm{CP}_{dt,t}y^{L}_{dt,t}+\mathrm{IP}_{dt,t}(F^{L}_{dt,t})^{\gamma}) \\
&+\sum_{dt\in DT}\sum_{dt'\in DT,dt'\neq dt}(\mathrm{CP}_{dt,dt'}y^{L}_{dt,dt'}+\mathrm{IP}_{dt,dt'}(F^{L}_{dt,dt'})^{\gamma}) \\
&+\sum_{dt\in DT}(\mathrm{CP}_{dt,o}y^{L}_{dt,o}+\mathrm{IP}_{dt,o}(F^{L}_{dt,o})^{\gamma})]
\end{aligned}
\tag{S47}
$$

It should be noted that $F_{dt}^{regenerants}$ is not covered in the inlet flowrate F_{dt}^{in}, the cost of regenerants is covered in terms of the operating cost coefficient of the treatment unit.

NOTES

Parameters in objective function

H hours of plant operation time per year

C_s unit cost of freshwater source s

AR annualized factor for investment for treatment units

IC_t investment cost coefficient for single outlet treatment unit t

β cost exponent for treatment units

IC_{dt} investment cost coefficient for double outlet treatment unit dt

OC_t operating cost coefficient for single outlet treatment unit t

OC_{dt} operating cost coefficient for double outlet treatment unit dt

PM operating cost coefficient for pumping

IP variable cost for each pipe

γ cost exponent for pipes

Binary variables

$y_{s,p}$ existence of interconnection from freshwater source s to process unit p

$y_{s,t}$ existence of interconnection from freshwater source s to single outlet treatment unit t

$y_{s,dt}$ existence of interconnection from freshwater source s to double outlet treatment unit dt

$y_{p,p'}$ existence of interconnection from process unit p to process unit p'

$y_{p,t}$ existence of interconnection from process unit p to single outlet treatment unit t

$y_{p,dt}$ existence of interconnection from process unit p to double outlet treatment unit dt

$y_{p,o}$ existence of interconnection from process unit p to discharge

$y_{t,p}$ existence of interconnection from single outlet treatment unit t to process unit p

$y_{t,t'}$ existence of interconnection from single outlet treatment unit t to single outlet treatment unit t'

$y_{t,dt}$ existence of interconnection from single outlet treatment unit t to double outlet treatment unit dt

$y_{t,o}$ existence of interconnection from single outlet treatment unit t to discharge

$y_{dt,p}^{H}$ existence of interconnection from higher purity outlet of double outlet treatment unit dt to process unit p

$y_{dt,t}^{H}$ existence of interconnection from higher purity outlet of double outlet treatment unit dt to single outlet treatment unit t

$y_{dt,dt'}^{H}$ existence of interconnection from higher purity outlet of double outlet treatment unit dt to double outlet treatment unit dt'

$y_{dt,o}^{H}$ existence of interconnection from higher purity outlet of double outlet treatment unit dt to discharge

$y_{dt,p}^{L}$ existence of interconnection from lower purity outlet of double outlet treatment unit dt to process unit p

$y_{dt,t}^{L}$ existence of interconnection from lower purity outlet of double outlet treatment unit dt to single outlet treatment unit t

$y_{dt,dt'}^{L}$ existence of c interconnection from lower purity outlet of double outlet treatment unit dt to double outlet treatment unit dt'

$y_{dt,o}^{L}$ existence of interconnection from lower purity outlet of double outlet treatment unit dt to discharge

Superscripts

in inlet stream

out outlet stream

max maximal

lo lower bound

up upper bound

L lower purity outlet stream

H higher purity outlet stream

S2. The connection restrictions on multiple staged system

The connection restrictions on the multiple staged system are listed below:

$$y_{p,dt} = 0, p \in P, \quad dt \in DT \tag{S48}$$

$$y_{t,dt} = 0, t \in T, \quad dt \in DT \tag{S49}$$

$$y_{s,dt} = 0, s \in S, dt \in DT \tag{S50}$$

$$y^{H}_{dt,dt'} = 0 \quad , dt \in DT , dt' \in DT \tag{S51}$$

$$y^{L}_{dt,dt'} = 0, dt \in DT , dt' \in DT \tag{S52}$$

It should be noted that in eq. S48 and eq. S49, dt refers to all the double outlet units in the sequence except for the beginning one. And in eq. S51, dt' refers to the double outlet unit that is just after the unit that dt refers to in the sequence.

S3. Supplemental data information in case study

S3.1. Data for all units

Table S1. Water-using data in the case study.

Process units	Inlet flowrate(t/h)	Water loss_1 (t/h)	Water loss_2 (t/h)	Maximum inlet con.(ppm)	
				Cl^-	TSS
Boiler	62	52	0	1	1
Cooling system	110410	1090	110	50	30
DF	230	200	0	500	30

Table S2. Single outlet treatment units data in the case study

Single outlet treatment	Water loss(t/h)	Maximum inlet con. (ppm)		R (removal ratio)	
		Cl^-	TSS	Cl^-	TSS
DFWT	0	500	500	0	0.9
IWT	0	20000	500	0.99	0.99

Table S3. Double outlet treatment units data in the case study

Double outlet treatment units	k (flowrate coefficient)	l (load coefficient)		α (split ratio)	Maximum inlet con. (ppm)		R (removal ratio)	
		Cl^-	TSS		Cl^-	TSS	Cl^-	TSS
multi-medium filtration	0	0	0	96	500	50	0	0.85
ultrafiltration	0	0	0	87	500	50	0	0.95
reverse osmosis	0	0	0	67	500	2	0.99	0
mix-bed	0.3	1	0	86	500	2	0.95	0

Table S4. Cost data of treatment units in the case study

Treatment units	IC(investment cost coefficient)	OC(operating cost coefficient)	β
DFWT	60000	1.2	0.7
IWT	60000	0.5	0.7
multi-media filtration	20000	0.2	0.7
ultrafiltration	57000	0.8	0.7
reverse osmosis	75000	1.2	0.7
mix-bed	100800	1.5	0.7

S3.2. Illustration of data extraction for limiting concentration

All the data about limiting concentration in case study is obtained from the water quality standard, design handbook, or internal document of the plant. For example, limiting concentration (LC for abbreviation) of cooling tower is obtained from the water quality standard set for circulating cooling water. LC of other process units are set according to the design handbook or the internal document of the plant. LC of treatment units are typically obtained from design handbook.

S3.3. Adjusted data of double outlet treatment unit performing as pretreatment

Table S5. Adjusted cost data of double outlet treatment units performing as pretreatment.

Treatment units	IC(investment cost coefficient)	OC(operating cost coefficient)	β
multi-media filtration	20000	0.05	0.7
ultrafiltration	57000	0.2	0.7
reverse osmosis	75000	0.5	0.7
mix-bed	100800	0.5	0.7