**Supplementary Material**

**Ecologically Inspired Water Network Optimization of Steel Manufacture Using Constructed Wetlands As Wastewater Treatment Process**

Kaili Zhang1, Stephen M. Malone2 , Bert Bras2, Marc Weissburg3, Yuehong Zhao1,4, Hongbin Cao1

1 Institute of Process Engineering (IPE-CAS), 1 North 2nd Street, Zhongguancun, Haidian District, Beijing, PR China

2 School of Mechanical Engineering, Georgia Institute of Technology, 801 Ferst Dr., Atlanta, Georgia 30332, USA

3 School of Biological Sciences, Georgia Institute of Technology, 950 Atlantic Dr., Atlanta, Georgia 30332, USA

4 Corresponding Author; email: yhzhao@ipe.ac.cn**S1 Mathematical models**

**S1.1 Freshwater sources**

Freshwater sources can be supplied to IO, IC, DO, OP or WD as shown in Fig. S1.

The water balance at the splitting point is given by Eq. (S1).

, (S1)

For each of the flow rates 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.

, ,  (S2)

, ,  (S3)

, ,  (S4)

, ,  (S5)

, ,  (S6)

, ,  (S7)



**Fig. S1** Splitting streams of freshwater source.

**S1.2 Once through process water systems (OP)**

Fig. S2 shows a schematic representation of a once through process water system. And the balances on flows and mass loads of contaminant j at the mixing point of the process unit are given by Eqs. (S8) and (S9) respectively.

,

 (S8)



 (S9)

The flow balance at the splitting point of the process unit is expressed in Eq. (S10).



 (S10)

Additionally, the balances on flow rates of OP are formulated as Eq. (S11):

, (S11)

Considering the inlet concentration cannot be greater than the maximum inlet concentration of contaminant j, a constraint is defined as Eq. S13.

, (S12)

The lower and upper bound constraints that formulate flows between the splitter point of the process unit and mixing points with binary variables are similar to the formulations in section S1.1.



**Fig. S2**. Inlet and outlet streams of OP.

**S1.3 Wastewater treatment systems (WT)**

Fig. S3 shows a representation of a wastewater treatment system, of which the outlet stream can be used by OP, IO, DO, WD, DS, other WT or discharged, the inlet stream can receive water from S, WS, OP, other WT, the outlet water and backwash wastewater of IO and DO, and the backwash wastewater of DS.

The balances on flows and mass loads of contaminant j at the mixing point of the WT are given by Eq. (S13) and Eq. (S14) respectively.

, (S13)



, (S14)

The flow balance at the splitting point of the system is expressed by Eq. (S15).

  (S15)

The flow rate balance and inlet concentration limit of WT are shown below.

,  (S16)

, ,  (S17)

The lower and upper bound constraints that formulate flows illustrated in Fig. S3 are similar to the formulations in section S1.1.



**Fig. S3** Inlet and outlet streams of WT.

**S1.4 Indirect open circulating cooling water systems (IO)**

Fig. S4 shows the diagram of an IO. The process has two outflows, and outlet water can be used by OP, WD, WT, DO and IO. The backwash wastewater can also be used by those systems except IO. And the system can receive water from S, WS, OP, WT, the outlet water of IO, and the soft water, desalination water and concentrate of DS.

The balances on flows and mass loads of contaminant j at the mixing point before the system are given by Eq. (S18) and Eq. (S19), respectively.

, (S18)



, (S19)

The flow balances at the two splitting points after the system are expressed by Eq. (S20) and Eq. (S21).



 (S20)

,

 (S21)

The flow rate balance and inlet concentration limit of WT are shown below.

,  (S22)

,,  (S23)

The lower and upper bound constraints are similar to the formulations in section S1.1.



**Fig. S4**. Inlet and outlet streams of IO.

**S1.5 Direct open circulating cooling water systems (DO)**

Fig. S5 shows the diagram of a DO. The process has two outflows, and outlet water can be used by OP, WD, WT, DO and IO. The backwash wastewater can also be used by those systems except IO and DO. The system can receive water from S, WS, OP, WT, both the outflows of IO, and the soft water, desalination water and concentrate of DS.

The balances on flows and mass loads of contaminant j at the mixing point before the system are given by Eq. (S24) and Eq. (S25) respectively.

 ,  (S24)



, (S25)

The flow balances at the two splitting points after the process unit are expressed by Eq. (S26) and Eq. (S27).

, (S26)

 ,  (S27)

The flow rate balance and inlet concentration limit of WT are shown below.

 ,  (S28)

, ,  (S29)

The lower and upper bound constraints are similar to the formulations in section S1.1.



**Fig. S5** Inlet and outlet streams of DO.

**S1. 6 Indirect closed circulating cooling water systems (IC)**

Fig. S6 shows the diagram of a WD. The system can receive water from S, WS, OP, WT, both the outflows of IO and DO, and the soft water, and the four outlet water of DS.

The balances on flows and mass loads of contaminant j at the mixing point before the system are given by Eq. (S30) and Eq. (S31) respectively.

 , (S30)

,,(S31)

The inlet concentration limit is shown below.

, ,  (S32)

The lower and upper bound constraints are similar to the formulations in section S1.1.



**Fig. S6** The inlet streams of IC.

**S1. 7 Water demand system (WD)**

Fig. S7 shows the diagram of a WD. The system can receive water from S, WS, OP, WT, both the outflows of IO and DO, and the soft water, and the four outlet water of DS.

The balances on flows and mass loads of contaminant j at the mixing point before the system are given by Eq. (S33) and Eq. (S34) respectively.



 (S33)

 , (S34)

The inlet concentration limit is expressed as Eq. (S35).

, , (S35)



**Fig. S7** The inlet streams of WD.

**S1. 8 Water source system (WS)**

The water from water source systems can be supplied to IO, IC, DO, OP, WD or WT as shown in Fig. S8.

The water balance at the splitting point is given by Eq. (S36).



 (S36)



**Fig. S8** The outlet streams of WS.

**S1. 9 Desalination system (DS)**

Fig.S9 shows an illustration of a desalination system with four outlets, of which the soft water termed as  can be used by IC, OP, IO, DO, and WD, the desalination water termed as  can be used by IC, OP, IO, DO, and WD, the concentrate termed as  can be used by OP, DO or discharge, and the backwash wastewater termed as  can only be sent to WT for treatment. The system can only receive water form S or WT.

The balances on flows at the mixing point of the DS are given below.

 ,  (S37)

,  (S38)

,  (S39)

,  (S40)

, (S41)



**Fig. S9** The inlet and outlet streams of DS.

**S1. 10 Discharge constraints**

The streams from OP, WT and the concentrate of DS can be discharged to the environment, as shown in Figure A5. Balances on flows and contaminants can be presented by Eq. (S42) and Eq. (S43).

 (S42)

, (S43)

The discharge limit is described as Eq. (S44).

,  (S44)



**Fig. 10**. Streams for discharge.

**S1.11 Objective function**

The objective function is formulated to minimize total annual cost.

The formulation is given by Eq. (S45).

 (S45)

Where is cost of freshwater,  is the cost of treatment units,  is cost of pumping, is the cost of discharge..

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

 (S46)

 (S47)



, (S48)

 (S49)

**Parameters in objective function**

 hours of plant operation time per year

 unit cost of freshwater source s

 cost coefficient for wastewater treatment system wt

 cost coefficient for soft water in desalination system ds

 operating cost coefficient for desalination water in desalination system ds

 cost coefficient for pumping

 cost coefficient for discharge

**Parameters**

 water flow rate of inlet stream of WD system

 maximum concentration of contaminant j in inlet stream of WD system

 water flow rate of WS system

 concentration of contaminant j of WS system

 water flow rate of inlet stream of OP system

 water flow rate of outlet stream of OP system

 water flow rate of evaporation of OP system

 water flow rate of losses of WT system

 maximum concentration of contaminant j in inlet stream of WT system

 concentration of contaminant j in outlet stream of OP system

 concentration of contaminant j in outlet stream of WT system

**Variables**

 concentration of contaminant j in inlet stream of WD system

 concentration of contaminant j in inlet stream of OP system

 water flow rate of inlet stream of WT system

 water flow rate of outlet stream of WT system

 concentration of contaminant j in inlet stream of WT system

**Superscripts**

 inlet stream

 outlet stream

 maximal

 lower bound

 upper bound

**S2 The data of water network of steel industry.**

**Table S2.1** The water flow rate of all IOs and DOs

|  |  |  |  |
| --- | --- | --- | --- |
| **All the IOs and DOs** | (m3/hr) | (m3/hr) | (m3/hr) |
| The IO in Sintering | 740 | 8 | 5 |
| The IO in CO | 11358 | 150 | 57 |
| The IO in IM | 2448 | 22 | 10 |
| The IO in SM(I)&CC(I)&HR(I) | 15810 | 150 | 240 |
| The DO of secondary cooling zone in SM(I)&CC(I)&HR(I) | 2200 | 160 | 100 |
| The DO of roller cooling in SM(I)&CC(I)&HR(I) | 8127 | 60 | 75 |
| The DO of laminar flow cooling in SM(I)&CC(I)&HR(I) | 7240 | 60 | 20 |
| The IO in SM(II)&CC(II) | 6453 | 86 | 25 |
| The DO of steel-making in SM(II)&CC(II) | 6453 | 57 | 10 |
| The DO of secondary cooling zone in SM(II)&CC(II) | 3255 | 50 | 67 |
| The IO in CR | 5800 | 40 | 10 |
| The IO in SS | 1700 | 22 | 10 |
| The DO in SS | 2044 | 23 | 20 |
| The IO in WR | 2140 | 20 | 5 |
| The DO in WR | 2450 | 22 | 20 |
| The IO in PP | 41000 | 450 | 0 |

**Table S2.2** The contaminant concentration data of IOs and DOs.

|  |  |  |
| --- | --- | --- |
|  | Cl-(mg/L) | TSS(mg/L) |
| Inlet concentration limit of IOs | 297 | 19.5 |
| Concentration of outlet water of IOs | 300 | 20 |
| Concentration of Backwash wastewater of IOs | 300 | 150 |
| Inlet concentration limit of DOs | 396 | 49 |
| Concentration of outlet water of DOs | 400 | 50 |
| Concentration of Backwash wastewater of DOs | 400 | 300 |

**Table S2.3** The cost data

|  |  |
| --- | --- |
| Types | C (RMB/m3/hr) |
| Freshwater | 2 |
| Soft water | 1 |
| Desalination water | 1.5 |
| Water treatment in WT | 0.3 |
| Discharge cost of concentrate | 2 |