

Improved Superstructural Optimisation of an Industrial Water System with Multiple Water Resources

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Most of the previous industrial water network models use freshwater as a vital water supply source without defining the origin of freshwater. However, in practice, the freshwater can be obtained from many water resources (e.g., municipal water, groundwater, surface water, municipally treated water, and seawater), after necessary Pre-treatment. Also, the effluents from the desalted water station, power station, and cooling water station can be used in other water using processes by satisfying the contaminant limits. Nevertheless, the existing water system design model does not apply directly to the design of effective industrial water systems. In order to overcome the above limitation, this paper proposed an innovative property based mathematical superstructure model for the industrial water network, consisting of water pre-treatment, water utility, water-using, and wastewater treatment systems. The proposed mathematical model provides appropriate water resource selection to acquire freshwater for the industrial water network and integrates all possible functional designs for water treatment, reuse, and recycling. The design model comprises the related equations, flow rate, and property constraints between the different water sources and sinks. The proposed model is framed as a nonlinear programming (NLP) algorithm and resolved using commercial software GAMS. The proposed model is validated by a case study of the simplified water system of the Chinese industrial chemical complex. Results show a substantial reduction of 8.39 % and 21.75 % in the total annualised cost and freshwater demand.

1. Introduction

The industrialisation has made considerable progress in recent years, and industrial production has increased rapidly worldwide. The consequence of this industrialisation is a very immediate increase in the demand for water in the industrial sector because each industry needs water for production and other essential purposes. Substantial attempts have been made to conserve water, especially in the industrial sector, but a more efficient industrial water network is still needed. Takama et al. (1980a) firstly proposed the refinery water network by implying mathematical modelling and include water treatment units/water-regeneration. The overall industrial water system superstructure presented by Gunaratnam et al. (2005) and optimised wastewater processing and water systems simultaneously. The integrated water network superstructure proposed by (Karuppiah and Grossmann, 2006), and established a global strategy for optimisation. Ng et al. (2009) proposed the direct re-use/recycling for the water system of a single contaminant via automated optimisation. Ahmetovic and Grossmann (2011) presented the global optimisation for industrial water supply by combining the water using and wastewater system into one unit. For the development of property-based industrial water network, extensive research has been carried out, which mainly includes the quality of freshwater and reuse water. Ponce Ortega et al. (2009) presented direct recycling/re-use with the wastewater treatment process. It is worth noting that in the previous models, water sources involve only regenerated water, freshwater, and wastewater, with freshwater as a source of water. Jiang et al. (2017) developed a systematic design of a water-using process involved more than one kind of water, and provided a specific superstructure of water system optimisation in a single step. Deng et al. (2018a) introduced a specific superstructure for the refinery water network by adopted a strategy for various types of water as a water source and used the replacement ratio to optimise the refinery water network. Deng et al. (2018b) proposed property-based new superstructure optimisation and used the freshwater as a water resource and split the network into other subsystems. Wang et al. (2019) proposed the integration of the

interplant water network using a multi-contaminant iterative process. Conventional water supply network resources mostly use conventional water resources such as municipal water supply. With the continuous growth of unconventional water sources (such as municipal reclaimed water and seawater), water supply networks that use conventional and unconventional water sources are more capable of, water-saving, cost reduction, and reduction in overall environmental discharge. This paper proposes a water supply network model that considers multiple water resources, and uses the non-linear programming to model industrial water network. The goal is to find the optimal selection of water resources by reducing the freshwater demand and annual cost.

2. Problem statement

Figure 1 depicts the general superstructure constitute of four subsections, which included pre-treatment, utility, water using, and wastewater treatment, systems.

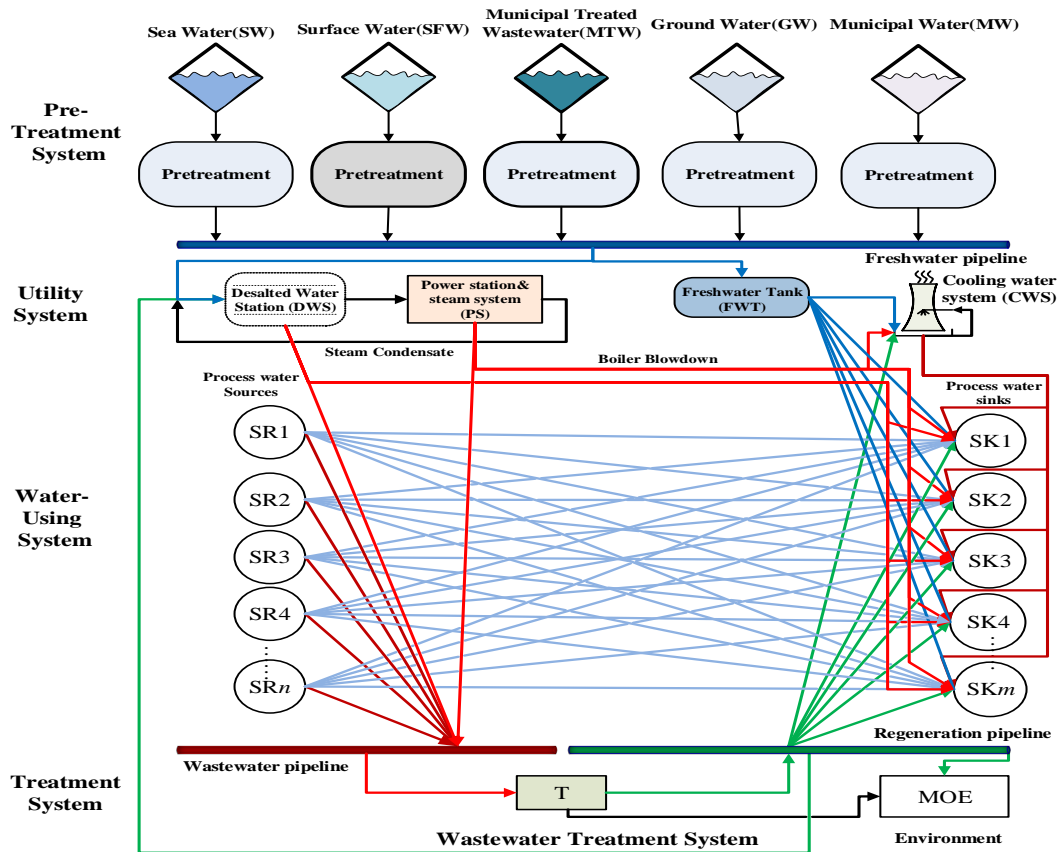


Figure 1: Industrial water network superstructure with multiple water resources

Given a series of external water resources ($i \in NI$), includes municipal water (MW), groundwater (GW), municipally treated water (MTW), surface water (SFW) (river, lake, rainwater, etc.), seawater (SW) and a series of water quality indicators (TOC, TSS... ($p \in NP$)) measure the quality of the water resource. Different water resources need to be treated with various water treatment technologies (for example, flocculation sedimentation, filtration, pH adjustment, reverse osmosis, multi-effect evaporation, etc.). The utility system primarily provides the water requirements throughout the plant site. It is consisted of a cooling water station (CWS), power and steam station (PS), desalted water station (DWS), and freshwater tank (FWT). The DWS and FWT can directly take water from the freshwater line. The effluents from the utility system used in water using system for water reuse or can be directed towards the wastewater line depending on the water quality. The water using system consists of a series of water sources ($s \in NS$) and water sinks ($k \in NK$). Water using sinks can take freshwater, utility effluents, and regenerated water. All the effluent water sources from the utility system, and water sources from water using system which does not fulfil the required water quality can go directly for further treatment in

the treatment system. The regenerated water can be used in water sinks or sent to MOE. This research intends to develop an optimal water supply network model for multiple water resource, to minimise the annual costs.

3. Mathematical model

As mentioned earlier, there are five different water resources ($i \in NI$), and every resource after passing through a particular treatment system (TS) can be allocated to the freshwater pipeline. The (FWT) and (DWS) takes water from the freshwater line. The municipal water can also go directly to a freshwater tank because it fulfils the quality of freshwater. In this model, all the variables are denoted as lower-case symbols, and all the parameters are denoted as upper-case symbols. And Indices, superscript and parameters used in this model are shown as Table 1. The flowrate balance on municipal water source is given as

$$f_i = f_{i,FWT} + f_{i,ts} \quad \forall i = MW, ts = MWTS \quad (1)$$

The water from other resources (SW, SFW, MTW, GW) can be supplied to the specified treatment system. The flowrate balance is given as.

$$f_i = \sum f_{i,ts} \quad \forall i = SFW, ts = SFWTS \quad \text{or } i = MTW, ts = MTWTS \\ \text{or } i = GW, ts = GWTS \quad \text{or } i = SW, ts = SWTS \quad (2)$$

Where i , represents the water resource and ts represent the corresponding pre-treatment system (TS), for example, the pre-treatment system for seawater resource is SFWTS. Every treatment system (TS) consists of various treatment units ($tu \in N_{tu}$) for water processing, which generates product water for the next destination and residue water with a specific production ratio. The balance on the treatment unit is given below.

$$f_{tu}^{in} = f_{tu}^{prod} + f_{tu}^{resd} \quad \forall tu \in N_{tu} \quad (3)$$

Every treatment unit is characterised to remove the impurities present in the resource water. The removal ratio of the treatment unit is defined as one minus the ratio of property ($p \in N_p$) of the produced water to the property into the treatment unit.

$$R_{tu,p} = 1 - \frac{\psi_{tu,p}^{prod}}{\psi_{tu,p}^{in}} \quad \forall tu \in N_{tu}, p \in N_p \quad (4)$$

The product water from any treatment unit can be allocated to freshwater pipeline proceeding by FWT and DWS depending on the fulfilment of the concentration of impurities present in the product water, the flow rate balance of product water from any treatment unit is given as.

$$f_{tu}^{prod} = \sum_{k=DWS \& k=FWT} f_{tu,k}^{prod} \quad \forall tu \in N_{tu} \quad (5)$$

All the residue water produced in the pre-treatment section is sent directly to MOE for further treatment to meet the environmental restrictions. The freshwater from the freshwater tank (FWT) can be delivered to the CWS and process water sinks (k). The flowrate balance for the freshwater tank is given below.

$$f_{FWT}^{out} = \sum_{k=Nk \& k \neq PS, DWS} f_{FWT,k}^{FW} \quad (6)$$

$$f_k^{in} = f_{MW,k} + \sum_{tu \in N_{tu}} f_{tu,k}^{prod} \quad \forall k = FWT \quad (7)$$

$$\psi_{k,p}^{in} \cdot f_k^{in} = \psi_{MW,p} \cdot f_{MW,k} + \sum_{p \in N_p} \psi_{tu,p}^{prod} \cdot f_{tu,k}^{prod} \quad \forall k \in FWT, p \in N_p \quad (8)$$

Desalted water station (DWS) receives water from freshwater pipeline and also can get water from the wastewater treatment section and produce desalted water bonded with quality restrictions. The equation below defines the inlet and outlet flowrate balance for DWS. Where $\psi_{k,p}^{in}$ denotes the water quality bounds.

$$\psi_{k,p}^{in} \cdot f_k^{in} = \sum_{tu \in N_{tu}} \psi_{tu,p}^{prod} \cdot f_{tu,k}^{prod} \quad \forall k = DWS, p \in N_p \quad (9)$$

$$\psi_{T,p}^{in} \cdot f_k^{in} = \sum_{t \in N_t} \psi_{T,p}^{reg} \cdot f_{T,k}^{reg} \quad \forall k = DWS, p \in N_p \quad (10)$$

The water inlet to the FWT and DWS must satisfy the water quality bounds defined in the equation below.

$$\Psi_{k,p}^{K,\min} \leq \psi_{k,p}^{K,in} \leq \Psi_{k,p}^{K,\max} \quad \forall k \in FWT, DWS \& p \in N_p \quad (11)$$

The DWS produced the desalted water and utility effluents. The overall balance of DWS is given.

$$f_k^{in} = f_{m,k}^{FW} + f_{T,k}^{prod} + f_{PS,k}^{CDW} \quad \forall k = DWS \quad (12)$$

$$f_s^{out} = \sum_{s=DWS} f_{s,k}^{DW} + \sum_{s=DWS} f_{s,k}^{ef} + f_{DWS,T}^{ef} \quad \forall k \in Nk \& k \neq FWT, CWS, DWS \quad (13)$$

Desalted water produced by the DWS linked with the inlet water flowrate by the following expression.

$$f_k^{in} = R_{DWS} \cdot f_s^{DW} \quad \forall s = k = DWS \quad (14)$$

The (PS) takes water from (DWS) to produce steam and deliver it throughout the plant site. The boiler blowdown and steam condensate (CDW) also included in PS, and can be used as a water source for other process sinks. The (CWS) is used to remove heat from the process. The cooling water circulates in a close loop and removes heat from different units; that's why cooling water is not included in this model. Still, a significant amount of water lost by evaporation. Cooling tower Blowdown can be used as a water source or directly sent to a water treatment system for further processing. The water sinks can take water from any water source (S) and wastewater treatment system (T) by fulfilling the requirement of quality ($p \in N_p$). The wastewater treatment system used to treat the water from different water sources, which cannot be used due to quality restriction. The wastewater treatment system regenerates the water and sends it to different water sinks bounded with water quality. The (MOE) can take regenerated and residue water from the treatment system, and process it according to the environmental restrictions. The mathematical equations for water using system and wastewater treatment system are taken from Deng et al. (2018b). The model objective function is the minimisation of annual costs by reducing the demand for freshwater from five different water resources.

$$\min \text{OBJ}_{\text{cost}} = (C_{\text{water}} + OC_{\text{treatment}}) \cdot AWH + Af \cdot (IC_{\text{pipe}} + IC_{\text{treatment}}) \quad (15)$$

Table 1: Indices, superscripts and parameters used in model

variables/indices	superscript	subscript	parameters
f flowrate	resd	Residual water	FW freshwater
i Water resources	ef	Effluent water	CDW Condensate water
s Water sources	In	Inlet flow	DW Desalted water
p Wate property	reg	Regenerated	min Minimum limit
k Water sinks	ts	pre-treatment system	tu treatment unit
	FW	freshwater	DW Desalted water
	CDW	Condensate water	max Maximum limit
			R Water production ratio
			OC Operational cost
			Af Annual factor
			IC Investment cost

4. Case study

The water system of a coal-based chemical complex is considered (Zhou, 2013), and data is extracted to analyse the applicability of the proposed model. The chemical coal complex consists of the utility section, which includes cooling water station (CWS), Power and steam station (PS), desalted water station (DWS). The water using section composes the water sources and sinks (gasification, ammonia, urea, formaldehyde and methanol). The wastewater treatment section (T) provides the necessary water treatment for reuse/recycle. The total freshwater consumption for the chemical complex is 1,370 t/h. The present demand for freshwater can be obtained from one or a combination of five different water resources (MW, GW, MTW, SFW, SW) and allocated directly to FWT, and DWS. Once the water pre-treatment system treats the resource water. The freshwater is

sent to a freshwater pipeline to transport in the freshwater tank or a desalinated water station. The concentrated water obtained is sent to the wastewater treatment system for more treatment to comply with environmental regulations. In this article, total suspended solids (TSS) and total organic carbon (TOC) are selected as leading indicators for assessing the quality of water. The core concept of the established model is focused on the distribution of water, based on quality parameters such as TSS and TOC. TSS is used to assess the information of suspended matter in water, and TOC is being used to gauge the level of contaminants in filtered water. As shown in Table 2, the very high-contamination effluents from the utility system are also considered for water reuse in the process water sinks. The quality constraints limits of each water sink and source determine the optimal flowrate of freshwater, effluent water, and the regenerated water. Unless the water source meets the quality requirement, it will go directly to that sink, otherwise directed towards the wastewater treatment system. In Table 2, the concentrations of TSS and TOC, matching to water sinks (SK1, SK2, SK3, SK4), are the upper bounds.

Table 2: Outlet quality constrains of water sources and sinks

Item	TSS (mg/L)	TOC (mg/L)	Item	TSS (mg/L)	TOC (mg/L)
ef(DWS)	28	35	Fresh water	5	6
ef(PS)	20	22	DW	1	0
ef(CWS)	10	8	CDW	2	2
SR1	8	5	Treated water	5	5
SR2	10	8	SK1	2	2
SR3	40	90	SK2	12	30
SR4	4	27	SK3	45	80
SR5	1	5	SK4	22	24

All the available water sources could be reused/recycle by the other water sinks only if they satisfied the water quality for that specific water sink. This is how the superstructure model optimised water allocation throughout the case study. The current flow rate scheme for various types of water in the chemical complex is shown in Table 3. In the current flowrate scheme, 343 t/h and 1,007 t/h of freshwater being directed to the DWS and CWS. The considerable amount of water from the water utility system and water using system goes directly to MOE, giving a total sum of 438.36 t/h. in this way, the significant quantity of water is wasted in the current flowrate scheme which can be reused/recycled.

Table 3: Comparison of current flowrate and optimised flowrate

Current flowrate (t/h)			After optimisation (t/h) (Groundwater best economic resource)										
Item	flowrate	MOE	Item	FWT	DWS	PS	CWS	SK1	SK2	SK3	SK4	T	MOE
DWS	343(Re*)	76.58	Resourc	747.98	324.4								
PS		23.33	FWT				747.9						
CWS	1,007(Re*)	250.45	DWS			233.3		26.25				64.89	
SR1	15.5	15.5	PS				23.33						
SR2	2.0	2.0	CWS									250.4	
SR3	20	20	SR1						12	3.5			
SR4	30	30	SR2							2.0			
SR5	20.5	20.5	SR3										20.0
SK1	35		SR4						.682		28.0	1.25	
SK2	20(Re*)		SR5					8.75	7.31		4.43		
SK3	5.5		T				235.6						100.97
SK4	32.5												

Re* denotes water coming directly from water Resource

The optimisation results show that most process water sources with good water quality can be reused directly in process water sinks. However, the process water source SR3 with a high level of contaminants sent to wastewater treatment. Similarly, the effluent of PS with low contaminant used by the cooling water system while effluent of DWS and CWS goes to wastewater treatment for further treatment. The desalted water quantity allocated to process water sinks decrease from 71 t/h to 26.25 t/h. The freshwater demand for cooling water

station reduced significantly and replaced by the regenerated water. In the optimal design, 747.98 t/h of freshwater is directed to FWT and 324.47 t/h allocated to DWS. As a result of this reduction, the demand for freshwater declined, which significantly decreases the total cost. The optimisation results also show that the best possible and economic freshwater demand obtained from groundwater. The strategy of non-linear programming is used to solve the developed mathematical model by using commercially available software, General Algebraic Modeling System (GAMS). The BARON Solver is used for the solution on a computer (Intel Core i5-3550 CPU@3.0 GHZ, x64 Windows 10). The statistics of model output give a relative gap equal to zero and contain 283 single variables and 160 constraints. After optimisation, the total freshwater demand decreased from 1,370 t/h to 1,072 t/h, and the total annual cost is also reduced significantly from 7.58×10^7 CNY/y to 6.944×10^7 CNY/y.

5. Conclusions

The paper presented a superstructure based mathematical model, and provide the best possible economical freshwater source from different possible options for the chemical complex. A nonlinear programming problem is framed for the solution of the extensive superstructure model. The developed model comprises of different flowrate balance equation and other quality constraints. In the case study, the best possible and economical freshwater source can be obtained from groundwater and the freshwater intake optimised from 1,370 t/h to 1,072 t/h with annual cost reduced from 7.58×10^7 CNY/y to 6.944×10^7 CNY/y. The potential limitation of the model is that, it is not applicable to the variations of flowrates and properties. At present, the model contains only one wastewater treatment unit, the detailed modeling of wastewater treatment units will be included in our future work. The model will be applied for the optimisation of water network of real industrial plant (i.e. refinery) with multiple contaminants and water resources.

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References

- Ahmetović E., Grossmann I.E., 2011, Global superstructure optimization for the design of integrated process water networks, *AIChE Journal*, 57, 434–457.
- Deng C., Jiang W., Feng X., 2018a, Deciphering refinery water system design and optimization superstructure and generalized mathematical model, *ACS Sustainable Chemistry and Engineering*, 6, 2302–2315.
- Deng C., Jiang W., Zhou W., Feng X., 2018b, New superstructure-based optimization of property-based industrial water system, *Journal of Cleaner Production*, 189, 878–886.
- Gunaratnam M., Alva Arguez A., Kokossis A., Kim J.K., Smith R., 2005, Automated design of total water systems, *Industrial & Engineering Chemistry Research*, 44, 588–599.
- Jiang W., Deng C., Feng X., 2017, Water system optimization in coal-based chemical complex, *Chemical Engineering Transactions*, 61, 355–360.
- Karuppiyah R., Grossmann I.E., 2006, Global optimization for the synthesis of integrated water systems in chemical processes, *Computers & Chemical Engineering*, 30, 650–673.
- Ng D.K.S., Foo D.C.Y., Tan R.R., 2009, Automated targeting technique for single-impurity resource conservation networks, Part 1, direct reuse/recycle, *Industrial & Engineering Chemistry Research*, 48, 7637–7646.
- Ponce Ortega J.M., Hortua A.C., El Halwagi M., Jiménez Gutiérrez A., 2009, A property-based optimization of direct recycle networks and wastewater treatment processes, *AIChE Journal*, 55, 2329–2344.
- Takama N., Kuriyama T., Shiroko K., Umeda T., 1980a, Optimal water allocation in a petroleum refinery, *Computers & Chemical Engineering*, 4, 251–258.
- Wang X., Fan X., Liu Z.Y., 2019, Design of interplant water network of multiple contaminants with an interplant water main, *Chemical Engineering Transactions*, 72, 295–300.
- Zhou Q., 2013, Optimization of water resources utilization in typical coal chemical plant (Chinese), Master Dissertation, East China University of Science and Technology, Shanghai, China.