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Water System Optimization in Coal-based Chemical Complex

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The coal chemical industry's high-water consumption has become the bottleneck for its sustainable development. Therefore, the efficient utilization of water and minimization of wastewater discharge is required. The stringent environmental regulations, as well as the escalating cost of freshwater and wastewater treatment has motivated the process and manufacturing industries to have emphasis on fresh water and waste minimization in their daily operations. In particular, optimal design and retrofit of industrial water systems provide a systematic approach for freshwater conservation. Conventional water system optimization often only considers flowrate of fresh water, but ignores flowrates of desalted water, steam and condensate water. The relationship between those types of water is lack of analysis. The minimum freshwater flowrate for the whole water system cannot be determined in one step via the conventional water system optimization model. In order to overcome such a limitation, this paper proposed a general model of a water-using process including more water types, and presented a general superstructure of water system optimization for a coal-based chemical complex. The material balance equations that relate all types of water are integrated in the model. The commercial software, GAMS, is used for modelling and solving a water system for a certain large coal-based chemical plant. A case study shows that the freshwater flowrate for the whole coal chemical plant can be calculated effectively via the proposed optimization model and it demonstrates the applicability of the model.

1. Introduction

As the substitute of petrochemical engineering, the coal chemical industry is an important part of the energy substitution strategy of China. The coal chemical industry has large water consumption, so its efficient use of water and less discharge is essential. Water system integration and optimization is a significant method that is helpful for water minimization in the coal chemical industry.

Water system integration and optimization technology can be commonly divided into the graphical Pinch Technique and Mathematical Programming Approach. The pioneering work of water pinch is proposed via Wang and Smith (1994) and the minimum fresh water consumption can be determined by generating Limiting Water Profile and plotting optimal water supply line on the concentration vs. load diagram. Later, Feng's research group extended the previous approach and proposed graphical method for targeting the water system with regeneration reuse (Bai et al., 2007) and regeneration recycling (Feng et al., 2007) schemes. There are also other representative Pinch Techniques such as Water-Surplus Diagram (Hallale, 2002), Material Recycle/Reuse Pinch Diagram (El-Halwagi et al., 2003), Water Cascade Analysis (Manan et al., 2004). The network design approaches include maximum driving force and minimum number of water sources (Wang and Smith, 1994), Water Main Approach (Feng and Seider, 2001) and Nearest Neighbour Algorithm (Prakash and Shenoy, 2005). Mathematical Programming Approaches gradually show its advantages on solving the problem with multi-contaminant and large-scale water-using processes than Pinch Techniques. The earliest research on Mathematical Programming Approach for the synthesis of refinery water system proposed via Takama et al. (1980). Later the representative work includes general superstructure for water usage and treatment network (Huang et al., 1999), the superstructure of Total Water System (Gunaratnam et al., 2005), the superstructure of Complete Water System (Faria and Bagajewicz, 2010). Mathematical Programming Approaches are also utilized for the optimization of the water network for industrial parks (Liu et al., 2016) and agricultural water network (Rubio-Castro et al., 2016).

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However, the types of water are just simply classified into fresh water, regenerated water and waste water in previous literatures, as shown in Figure 1(a). Huang et al. (1999) divided the water sources into primary water, namely fresh water; secondary water, namely discharge of production process. In fact, the types of water also include desalted water, circulating cooling water, steam and condensate water etc., shown as Figure 1(b).

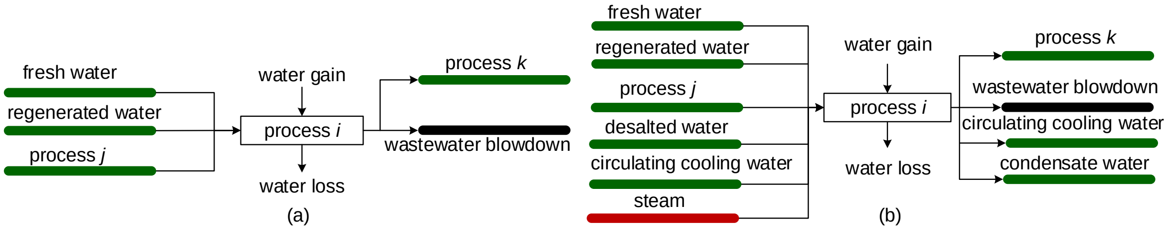

Figure 1: (a) Conventional water-using process. (b) General water-using process.

Besides, the existed water system optimization model can only obtain the minimum fresh water consumption of the extracted or selected water-using processes, but cannot obtain that of the whole water system. For example, the saved desalted water need be converted to the fresh water consumption as some specific ratio (Zheng et al., 2006). The reason is that the relevance existed between different types of water. The reduction of other types of water will influence the minimum fresh water consumption of the whole water system. Fresh water is produced for desalted water through desalted water station. The desalted water could supply for boiler to generate steam. If the water quality of some outlet of process is so high that could be reused as the substitute of desalted water and/or fresh water, the fresh water consumption of the whole water system will decrease accordingly, and the decrease of desalted water also leads to the reduction of fresh water.
To deal with the relevance of all types of water, this paper classified the types of water according to the real plant, proposed a general superstructure containing multiple types of water and developed corresponding mathematical model in which the mass balance relationships between the types of water are integrated.

2. Problem statement

Given a water network of coal-based chemical complex and the original data of water network, shown as Figure 2. It includes water supply units (shown as the main production units in the left dashed box in Figure 2) and water consuming units (shown as the assisted production units in the right dashed box in Figure 2). Water supply units include water supply branch plant which can be divided into fresh water station, desalted water station, circulating water station and wastewater treatment station. The functions of these stations are the treatment of some types of water and production of other types of water. For instance, desalted water station is used for the treatment of fresh water and production of desalted water, as supplement of water-using units.

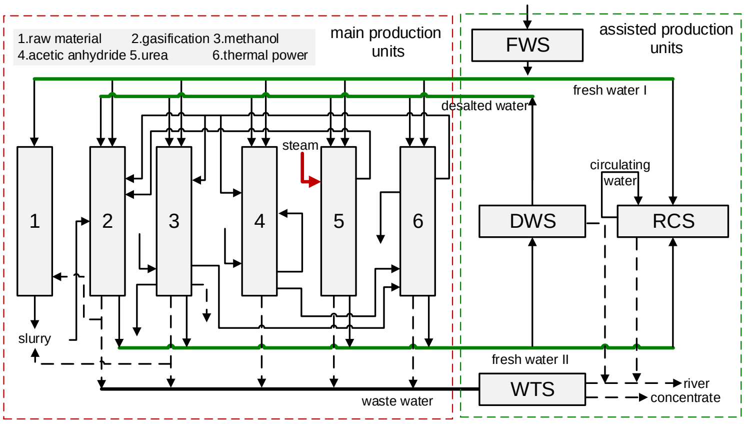

Figure 2: Coal-based chemical complex water system

Water using units include raw material branch plant, gasification branch plant, methanol branch plant, acetic anhydride branch plant, urea branch plant and thermal power branch plant. These branch plants consume different types of water meanwhile accomplishing their duty of production. Main production units utilize water from assisted production units and water reusing from other main production units. Once reusing water from other units, the flowrate of water from assisted production units will be reduced. This paper aims to develop an optimization model of water system in coal-based chemical complex minimizing the fresh water flowrate of the whole system which integrates the mass balance equation about flowrates of different types of water.

3. Mathematical model

In this section, a mathematical model of coal-based chemical complex water system is developed for optimization of minimum water resource consumption of whole system.

(1) Fresh water station

Water resource is extracted from rivers and lakes, goes through fresh water station and then supplies fresh water I for the whole complex.

$$f_{\text{FWS,in}}^{\text{resource}} = f_{\text{FWS,out}}^{\text{fresh I}} \tag{1}$$

(2) Desalted water station

Desalted water station is utilized to produce desalted water from fresh water II for the whole complex.

$$f_{\text{DWS,in}}^{\text{fresh II}} = f_{\text{DWS,out}}^{\text{desalt}} + f_{\text{DWS,out}}^{\text{waste}} \tag{2}$$

(3) Circulating water station

Circulating water station receives fresh water I and II as supplement of circulating water system, resulting evaporation loss during the process.

$$f_{\text{RCS,in}}^{\text{fresh I}} + f_{\text{RCS,in}}^{\text{recy}} + f_{\text{RCS,in}}^{\text{fresh II}} = f_{\text{RCS,out}}^{\text{recy}} + f_{\text{RCS,out}}^{\text{vapor}} + f_{\text{RCS,out}}^{\text{loss}} \tag{3}$$

(4) Water treatment station

Water treatment station is the treatment of sewage from production units and then sends them to the river for draining, with other concentrate sent for evaporation crystallization.

$$f_{\text{WTS,in}}^{\text{waste}} = f_{\text{WTS,out}}^{\text{blowdown}} + f_{\text{WTS,out}}^{\text{concentrate}} \tag{4}$$

Equation (1)-(4) describe the balance relevance of water supply units.

(5) Raw material branch plant

Raw material branch plant receives fresh water I and part of wastewater from gasification and methanol branch plant, without drain except water into slurry.

$$f_{\text{raw,in}}^{\text{fresh I}} + f_{\text{raw,in}}^{\text{reuse}} = f_{\text{raw,out}}^{\text{reuse}} \tag{5}$$

(6) Gasification branch plant

Fresh water I is needed as cooling water of cooling tower, desalted water is utilized for deaerator, etc. units, reuse water and hydrolysate are used for gasification process. The effluent includes fresh water II for production of desalted water, as well as reuse water to mill and wastewater to wastewater treatment station.

$$f_{\text{gasify,in}}^{\text{fresh I}} + f_{\text{gasify,in}}^{\text{desalt}} + f_{\text{gasify,in}}^{\text{reuse}} = f_{\text{gasify,out}}^{\text{fresh II}} + f_{\text{gasify,out}}^{\text{reuse}} + f_{\text{gasify,out}}^{\text{waste}} \tag{6}$$

(7) Methanol branch plant

Methanol branch plant consumes fresh water, desalted water, chemical reaction water, boiler water from thermal power branch plant for these systems. There exists steam loss during the processes. The fresh water II is for production of desalted water, reuse water is reused to mill and wastewater discharge to north trench and wastewater treatment plant.

$$f_{\text{methanol,in}}^{\text{fresh I}} + f_{\text{methanol,in}}^{\text{desalt}} + f_{\text{methanol,in}}^{\text{reuse}} + f_{\text{methanol,in}}^{\text{other}} = f_{\text{methanol,out}}^{\text{fresh II}} + f_{\text{methanol,out}}^{\text{waste}} + f_{\text{methanol,out}}^{\text{reuse}} + f_{\text{methanol,out}}^{\text{loss}} \tag{7}$$

(8) Urea plant

Urea plant consumes fresh water I as cooling water of air compressor, desalted water for urea process, chemical reaction water and steams of reuse. Fresh water II is delivered to desalted water station, reuse water is reused to methanol branch plant and wastewater discharges to wastewater treatment station.

$$f_{\text{urea,in}}^{\text{fresh I}} + f_{\text{urea,in}}^{\text{desalt}} + f_{\text{urea,in}}^{\text{steam}} + f_{\text{urea,in}}^{\text{other}} = f_{\text{urea,out}}^{\text{fresh II}} + f_{\text{urea,out}}^{\text{waste}} + f_{\text{urea,out}}^{\text{reuse}} \tag{8}$$

(9) Acetic anhydride branch plant

Acetic anhydride branch plant uses fresh water as supplement of circulating water, desalted water as water block of torch, and reuse water from boiler water and other water. There exists steam loss during process, the steam condensate is supplied to thermal power plant, other drain is sent to wastewater treatment station.

$$f_{\text{acetic,in}}^{\text{fresh I}}+f_{\text{acetic,in}}^{\text{recy}}+f_{\text{acetic,in}}^{\text{reuse}}+f_{\text{acetic,in}}^{\text{other}}=f_{\text{acetic,out}}^{\text{recy}}+f_{\text{acetic,out}}^{\text{cond}}+f_{\text{acetic,out}}^{\text{waste}}+f_{\text{acetic,out}}^{\text{loss}} \tag{9}$$

(10) Thermal power branch plant

Thermoelectricity factory utilizes fresh water and desalted water as cooling water of fun, and steam loss exists during production process. The fresh water II is delivered for production of desalted water, the reuse water is allocated to gasification branch plant. And other wastewater is treated in wastewater treatment station.

$$f_{\text{thermo,in}}^{\text{fresh I}}+f_{\text{thermo,in}}^{\text{desalt}}+f_{\text{thermo,in}}^{\text{cond}}+f_{\text{thermo,in}}^{\text{reuse}}=f_{\text{thermo,out}}^{\text{fresh II}}+f_{\text{thermo,out}}^{\text{waste}}+f_{\text{thermo,out}}^{\text{reuse}}+f_{\text{thermo,out}}^{\text{loss}} \tag{10}$$

(11) Water balance of fresh water I

Fresh water I from outlet of fresh water station is sent to raw material, gasification, methanol, urea, acetic anhydride and thermal power branch factory.

$$f_{\text{FWS,out}}^{\text{fresh I}}=f_{\text{raw,in}}^{\text{fresh I}}+f_{\text{gasify,in}}^{\text{fresh I}}+f_{\text{methanol,in}}^{\text{fresh I}}+f_{\text{urea,in}}^{\text{fresh I}}+f_{\text{acetic,in}}^{\text{fresh I}}+f_{\text{thermo,in}}^{\text{fresh I}} \tag{11}$$

(12) Water balance of fresh water II

Fresh water II from outlets of gasification, methanol, urea and thermoelectricity factory are delivered to desalted water station for producing desalted water and supplementing circulating cooling water station.

$$f_{\text{gasify,out}}^{\text{fresh II}}+f_{\text{methanol,out}}^{\text{fresh II}}+f_{\text{urea,out}}^{\text{fresh II}}+f_{\text{thermo,out}}^{\text{fresh II}}=f_{\text{DWS,in}}^{\text{fresh II}}+f_{\text{RCS,in}}^{\text{fresh II}} \tag{12}$$

(13) Water balance of desalted water

Desalted water from outlet of desalted water station is assigned to gasification, methanol, urea and thermal power branch plant.

$$f_{\text{DWS,out}}^{\text{desalt}}=f_{\text{gasify,in}}^{\text{desalt}}+f_{\text{methanol,in}}^{\text{desalt}}+f_{\text{urea,in}}^{\text{desalt}}+f_{\text{thermo,in}}^{\text{desalt}} \tag{13}$$

(14) Water balance of waste water

Waste water to the inlet of wastewater treatment station equals the sum of waste water from gasification, methanol, acetic hydride, urea and thermal power branch plant.

$$f_{\text{WTS,in}}^{\text{waste}}=f_{\text{gasify,out}}^{\text{waste}}+f_{\text{methanol,out}}^{\text{waste}}+f_{\text{acetic,out}}^{\text{waste}}+f_{\text{urea,out}}^{\text{waste}}+f_{\text{thermo,out}}^{\text{waste}} \tag{14}$$

Equations (11)-(14) describes the mass balance of fresh water I & II, desalted water and waste water.

(15) Conventional water using process

For conventional water-using process *i*, its inlet water plus generated water quantity equals to the sum of the effluent plus water loss of the process. The water balance is shown as equation (15). However, the conventional water using process only includes fresh water, regenerated water and other effluent of water using process *j*. Its effluent can either be reused to other water using process *k*, or to discharge.

$$f_{i,\text{in}}+f_i^{\text{gain}}=f_{i,\text{out}}+f_i^{\text{loss}} \tag{15}$$

(16) General water using process

The general water-using process model considers more detailed types of water, besides traditional fresh water and regenerated water, and desalted water, circulating cooling water and steam. It is more general comparing with conventional water using process model. The water balance relationship is shown as equation (16)

$$\sum^{\text{TypeIn}} f_{i,\text{in}}^{\text{TypeIn}}+f_i^{\text{gain}}=\sum^{\text{TypeOut}} f_{i,\text{out}}^{\text{TypeOut}}+f_i^{\text{loss}} \tag{16}$$

It's worth noting that the difference between equation (16) and (1)-(10) is that they describe separately water-using process *i* and production unit *p*. All water balance of process *i* in unit *p* can be described as equation (16). Summing them and it will get water balance of water quantity of unit *p*, shown as equation (1) - (10).

(17) Objective function

This objective is to determine the minimum fresh water quantity, shown as equation (17).

$$obj = \min f_{\mathrm{FWS,in}}^{\mathrm{resource}} \tag{17}$$

4. Case study

The case is obtained from water-using network of coal producing methanol and coal producing urea processes of a fertilizer plant in the literature (Zhou, 2013). This section will illustrate the application of water system optimization of coal chemical industry. The whole system mainly includes seven branch plants, namely raw material, water supply, gasification, methanol, acetic anhydride, urea and thermal power branch plant. In the original water network, the fresh water consumption is 1,511 t/h, and the flowrates of each type of water described in the above equations are listed in Table 1. For the model developed in this paper, the linear programming model has been solved using commercial software GAMS (General Algebraic Modeling System) by CPLEX solver (the PC information: Intel Core i5-3550 CPU@3.0 GHZ, x64 Windows 10 OS). It is worth noting that the optimization of the model is on the premise that the contaminant concentration meets the water-using processes' limitations on TSS (total suspended solid) and TOC (total organic carbon), which are the selected key contaminants for the case. Only water sources with concentrations that fulfil the inlet concentration limitation of water-using processes can be reused or recycled. The factor of contaminant concentration is taken into consideration for the optimization in this way.
The fresh water of RCS and branch plant 6 and desalted water of branch plant 2, 3 and 6 are altered with other altered types of water. The flowrate of desalted water is reduced, then the water of inlet of desalted water station is cut down and the flowrate of fresh water of the whole system is decreased accordingly. After optimization, the fresh water consumption is reduced from 1,511 t/h to 1,346 t/h.

Table 1: Inlet flowrates comparison of production units before and after optimization

		Current data (t/h)						After optimization (t/h)			
Items	Resource	Fresh I	Fresh II	Desalted	Waste	Items	Resource	Fresh I	Fresh II	Desalted	Waste
FWS	1,511	0	0	0	0	FWS	1,346	0	0	0	0
RCS	0	447	566	0	0	RCS	0	314.5	650.5	0	0
WTS	0	0	0	0	208	WTS	0	0	0	0	120.25
DWS	0	0	440	0	0	DWS	0	0	355.5	0	0
1	0	1	0	0	0	1	0	1	0	0	0
2	0	50	0	60	0	2	0	50	0	40	0
3	0	748	0	165	0	3	0	748	0	133	0
4	0	35	0	0	0	4	0	35	0	0	0
5	0	180	0	22	0	5	0	180	0	22	0
6	0	50	0	180	0	6	0	17.5	0	147.5	0

5. Conclusion

This paper proposed a general water-using process model considering more types of water. Combining with actual coal-based chemical complex case, a general superstructure of water system and corresponding linear programming mathematical model is developed. The model is integrated with material balance equations reflecting the relevance of flowrates of different types of water. In this case, the water resource consumption is optimized from 1,511 t/h to 1,346 t/h in one step. And the reduction ratio of water resource reaches 10.9 %.

Notation

Variables

f	flowrate	*i, j, k*	*i, j, k*th process	*p*	*p*th production unit

Superscript

blowdown	Water for blowdown	concentrate	concentrate after treatment	cond	condensate water
desalt	desalted water	fresh I	I type fresh water	fresh II	II type fresh water
gain	water for gain	loss	water for loss	other	other water
recy	circulating water	resource	water resource from outside	reuse	water for reuse

steam	steam from water	TypeIn	water type of inlet	TypeOut	water type of outlet
vapor	water for vaporization	waste	waste water		
Subscript					
acetic	acetic anhydride branch plant	DWS	desalted water station	FWS	fresh water station
gasify	gasification branch plant	methanol	methanol branch plant	raw	raw material branch plant
RCS	recycling cooling water station	thermo	thermal power branch plant	urea	urea branch plant
WTS	waste water treatment station				

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