CHEMICAL ENGINEERING TRANSACTIONS

VOL. 52, 2016

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Petar Sabev Varbanov, Peng-Yen Liew, Jun-Yow Yong, Jiří Jaromír Klemeš, Hon Loong Lam

ISBN 978-88-95608-42-6; **ISSN** 2283-9216

DOI: 10.3303/CET1652193

Design of Water Networks with Multiple Contaminants by Concentration Potential Concepts

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It is often difficult to design water networks with multiple contaminants with literature methods. This paper provides a review about the concepts of Concentration Potential and their applications in design of water using networks with multiple contaminants. The values of Concentration Potential of Demands (CPDs) can be used to identify the precedence order of the processes to be performed. The values of Concentration Potential of Sources (CPSs) can be used to determine the reuse order of the source streams. The concepts of Concentration Potential have been successfully applied in design of different types of water using networks with multiple contaminants. It shows that the concepts of Concentration Potential are powerful tools in design of water using networks with multiple contaminants.

1. Introduction

As an important technique to reduce the consumption of freshwater, water integration has received more and more attention.

Water-using processes can be divided into two types (Prakash and Shenoy, 2005), Fixed Contaminant Load (FC) operations and Fixed Flowrate (FF) ones. FC operations are known as mass transfer ones, which are used to remove a certain amount of contaminants. The contaminant load (M) can be calculated with Eq(1):

$$M = F \times (C^{lim,out} - C^{lim,in}) \tag{1}$$

FF operations are known as non-mass transfer ones, which have specified inlet and outlet flowrates and they may not be equal. The water losses or gains can be brought to FF operations. The outlet concentrations of FF operations are also specified, which are independent on the inlet concentration (Teles et al., 2009).

Two main techniques have been developed for water integration, pinch analysis methods and mathematical programming methods. The pinch analysis methods proposed in the literature include Limiting Composite Curve (Wang and Smith, 1994), Material Recovery Pinch Diagram (El-Halwagi et al., 2003), Water Cascade Analysis (WCA, (Manan et al., 2006), Surplus Composite Curve (Saw et al., 2011), and Composite Table Algorithm (CTA, (Parand et al., 2014). Recently, the pinch analysis methods were improved and applied to solve the complex problems. Parand et al., (2013) combined the Water Cascade Analysis and material recovery pinch diagram to target the wastewater minimization. The “threshold problems” with zero discharge was solved. Then Parand et al., (2015) solved the same problem in regeneration-recycle networks by the improved CTA. Zhu et al., (2015) modified the graphical method to obtain the targets of the water networks involving regeneration. The pinch of freshwater and regeneration were obtained separately by the different parts of the Limiting Composite Curve. Kralj (2015) analyzed the wastewater re-use by impact of contaminants. The pinch was obtained by Mass Composite Curve (MCC), which was analogy with Limiting Composite Curve.

The pinch analysis method is visible, simple and easy to understand, but only can be applied to the single contaminant water networks. The mathematical programming methods are more efficient for targeting and design of the water networks with multiple contaminants. The mathematical programming methods, including Nonlinear Programming (Khor et al., 2012), Mixed Integer Nonlinear Programming (Jimenez-Gutierrez et al., 2014), Mixed Integer Linear Programming (Poplewski, 2015), Mixed Integer Linear Programming (Ong et al., 2015), and Linear Programming (Zhao et al., 2016), can be used to solve the models developed based on the superstructure of the networks. Ong et al. (2015) focused on reducing the complexity of the water networks. The piping length and piping connections were considered based on freshwater minimization. The results were evaluated by annual cost. Mughees and Al-Ahmad (2015) combined pinch technique and mathematical programming to target the maximum reuse/recycle and minimum waste discharge. Rubio-Castro et al. (2016) optimized the water networks in agriculture, which included both operation and allocation. The targets for the economic, environmental and social benefits were obtained simultaneously.

The target and design for water networks with multiple contaminants can be obtained by mathematical programming method rapidly. However, it is often complex to build a superstructure and to solve the models developed. In addition, the model of mathematical programming is often "black box" one, which is lack of engineering meaning. To overcome these drawbacks, the concepts of Concentration Potential were presented. The concepts and applications will be shown as follows.

2. Concepts of Concentration Potential

To target and design a water network with single contaminant, the demand (inlet) streams and source (outlet) streams can be arranged in ascending order of their concentrations (Liu et al., 2004), respectively. The demand streams can be satisfied by the source streams in the above order. Then, very good design can be obtained. The above methodology might be used to design the networks of multiple contaminants as well. However, for a water network with multiple contaminants, it is difficult to identify the concentration order of the streams. For example, let us consider stream 1 (20, 100, 90) ppm, and stream 2 (50, 80, 200) ppm. It is difficult to judge the concentration order of the two streams. To solve this problem, Liu et al. (2009) presented the concepts of Concentration Potential, which were used to identify the relative concentration order of the water streams with multiple contaminants in FC systems.

The Concentration Potential of Demand streams (CPDs) are defined as:

$$CPD(D_j) = \sum_{i=1}^{NS} R_{i,j} = \sum_{i=1}^{NS} \min_{k=1,2,\cdots,NC} \left[\frac{C_{Dj,k}^{lim}}{C_{Si,k}} \right] \qquad (i \neq j) \tag{2}$$

where $C_{Dj,k}^{lim}$ is the limiting inlet concentration of contaminant k in demand stream D_j, $C_{Si,k}$ is the concentration of contaminant k in source stream S_i, NS is the number of the source streams, NC is the number of the contaminants, and $R_{i,j}$ is the maximum quasi-allocation amount of S_i for 1 ton of D_j.

The Concentration Potential of Source streams (CPSs) are defined as:

$$CPS(S_i) = \frac{1}{\sum_{j=1}^{ND} R_{i,j}} = \frac{1}{\sum_{j=1}^{ND} \min_{k=1,2,\cdots,NC} \left[\frac{C_{Dj,k}^{lim}}{C_{Si,k}} \right]} \qquad (i \neq j) \tag{3}$$

where ND is the number of the demand streams.

The CPD value of D_j reflects the overall possibility of demand D_j to reuse the source streams. The bigger the value of CPD (D_j) is, the larger the overall possibility for demand D_j to reuse the source streams. The value of CPS(S_i) reflects the overall possibility for source S_i to be reused by the demand streams. The higher the value of CPS(S_i) is, the lower the possibility for source S_i to be reused by the demand streams. The restrictive conditions ($i \neq j$) indicate that recycling is not permitted in the systems. Because recycling cannot reduce the consumption of freshwater for FC systems, which has been proved by Fan et al. (2012).

With the concepts of Concentration Potential, the design procedure for the water networks with single contaminant can be applied to that of the multiple contaminants (Liu et al., 2009). The CPD values can be used to identify the precedence order of the processes: the lower the CPD value is, the earlier the demand is satisfied. The design for FC systems can be obtained. The designs obtained with the method proposed are comparable to that obtained with mathematical programming methods (Liu et al., 2009).

3. Appling the concepts of Concentration Potential to FF systems

Recycling is a necessary measure in FF systems to meet flow rate constraint. Fan et al., (2012) omitted the restriction ($i \neq j$) of Eq(2) and (3), which made the concepts of Concentration Potential be applied to FF systems.

In the design procedure, the values of Concentration Potential of Demands (CPDs) are used to identify the precedence order of the demand streams to be satisfied as well. The values of Concentration Potential of Sources (CPSs) can be used to determine the reuse order of the source streams. The design procedure is similar as that of FC systems (Liu et al., 2009).

4. Appling the concepts of Concentration Potential to the water networks with internal water mains

The internal water main is considered as a reservoir (Feng and Seider, 2001), which receives outlet water streams from upstream processes and provides water for downstream processes. In a conventional water network, the processes are connected directly. When a little change in quality or quantity of the upstream process(es) occurs, the operation of the downstream process(es) will be affected. Therefore, it is difficult to operate or control a conventional water network. With the adding of internal water mains into a water network, the connections between the processes are simplified. The operational flexibility of the system can be increased. However, more freshwater will be consumed by the water networks with internal water mains compared to that of corresponding conventional network. It is a tradeoff between the number of mains and freshwater consumption (Feng and Seider, 2001).

Su et al. (2012) applied the concepts of Concentration Potential to design the water networks with single internal water main. A conventional network without internal water main was obtained first. The initial structure of the single internal water main was identified based on the conventional network, which was obtained with the CPD method of Liu et al. (2009). The final design could be obtained based on the initial structure in a few iterations by adjusting the amount of the internal water main, based on the CPD and CPS values. The impact factor was presented to reduce the times of adjusting.

Zhao et al. (2014) applied the concepts of Concentration Potential to design the water networks with two internal water mains. The design procedure was similar as that of the single internal water main of Su et al. (2012), except the structure was divided into three parts.

5. Developing computer software based on the concepts of Concentration Potential

Wang et al. (2012) developed a computer software to design the water networks with multiple contaminants. The mathematical model was built based on the mass balance and the constraints of process concentration. A Linear Programming (LP) method was used to solve this model. To design the water network, the precedence order was identified by the CPD values of the demand streams. The usage of source streams were determined with weighting factors of source streams, which were calculated based on the CPS values to reflect the qualities of the source streams. The computer software developed could reduce the computation effort significantly. Another advantage of the software is that initial values were not needed.

The comparison of the results obtained with concepts Concentration Potential and those obtained with literature methods are listed in Table 1. It can be seen that the designs obtained with concepts Concentration Potential are comparable to or better than that obtained with literature methods.

6. Conclusion

This paper provides a review to illustrate the concepts of Concentration Potential and their applications in design of water using networks with multiple contaminants. The precedence order of the processes can be identified by the values of Concentration Potential of Demands (CPDs), and the reusing order of the source streams can be identified by the values of Concentration Potential of Sources (CPSs). The concepts of Concentration Potential have been applied in design of the multiple contaminants water networks involving reuse, recycling and internal water mains. A computer software has been developed based on the concepts of Concentration Potential as well. It shows that the concepts of Concentration Potential are powerful tools in design of the water networks with multiple contaminants.

Table 1: The comparable results of application of concepts Concentration Potential

	No. of contaminants	No. of processes	Results in literature		Results by concepts of Concentration Potential	
			Fresh water consumption	Connections	Fresh water consumption	Connections
FC network	3	8	177.1 t/h (Wang et al., 2003)	20	174.95 t/h (Liu et al., 2009)	20
	3	7	1,053.4 t/h (Alva-Argáez et al., 2007)	20	1,057.24 t/h (Liu et al., 2009)	17
	3	3	105.65 t/h (Doyle and Smith, 1997)	8	106.7 t/h (Liu et al., 2009)	8
FF network	3	4	86.83 t/h (Teles et al., 2008)	9	86.83 t/h (Fan et al., 2012)	9
	2	7	197.69 t/h (Teles et al., 2008)	20	200.47 t/h (Fan et al., 2012)	19
	6	7	323.51 t/h (Teles et al., 2009)	21	330.43 t/h (Fan et al., 2012)	18
Network with single internal water main	3	7	156.85 t/h (Feng et al., 2008)	16	156.76 t/h (Su et al., 2012)	17
	3	8	198.4 t/h (Wang et al., 2003)	22	183.33 t/h (Su et al., 2012)	20
Network with two internal water mains	3	7	144.6 t/h (He et al., 2010)	20	144.6 t/h (Zhao et al., 2014)	20
	3	8	183.33 t/h (Ma et al., 2007)	20	178.66 t/h (Zhao et al., 2014)	21
Computer software	3	7	143.53 t/h (Zheng et al., 2006)	20	140.93 t/h (Wang et al., 2012)	17
	3	4	81.22 t/h (Doyle and Smith, 1997)		81.22 t/h (Wang et al., 2012)	12
	3	3	106.7 t/h (Wang et al., 2003)	9	105.6 t/h (Wang et al., 2012)	9

Notation

C	concentration of contaminant (g/t)
CPD	concentration potential of demand
CPS	concentration potential of source
D	demand stream
F	flowrate (t/h)
FC	fixed contaminant load operation
FF	fixed flowrate operation
M	mass load (kg/h)
NC	number of contaminants
ND	number of demands
NS	number of sources
$R_{i,j}$	maximum quasi-allocation amount of S_i for 1 ton of D_j
S	source stream

Superscript

in	inlet
lim	limiting
out	outlet

Subscript

i,j	process unit
k	contaminant

Reference

Alva-Argáez A., Kokossis A., Smith R., 2007, The design of water-using system in petroleum refining using a water-pinch decomposition, Chemical Engineering Journal, 128, 33-46.

Doyle S.J., Smith R., 1997, Targeting Water Reuse with Multiple Contaminants, Process Safety & Environmental Protection, 75, 181-189.

El-Halwagi M.M., Gabriel F., Harell D., 2003, Rigorous graphical targeting for resource conservation via material recycle/reuse networks, Industrial & Engineering Chemistry Research, 42, 4319-4328.

Fan X.Y., Li Y.P., Liu Z.Y., Pan C.H., 2012, A new design method for water-using networks of multiple contaminants with the concentration potential concepts, Chemical Engineering Science, 73, 345-353.

Feng X., Liu Y.Z., Shen R.J., Wang L., 2008, Water system integration Optimization, Chemical Industry Press, Beijing (China), 137, 129-135.

Feng X., Seider W.D., 2001, New Structure and Design Methodology for Water Networks, Industrial & Engineering Chemistry Research, 40, 6140-6146.

He H.N., Wan L.Z., Liu Z.Y., 2010, A simple design method for water network with multi-contaminant internal water mains, Chinese Journal of Chemical Engineering, 61, 1176-1182.

Jimenez-Gutierrez A., Lona-Ramirez J., Ponce-Ortega J.M., El-Halwagi M., 2014, An MINLP model for the simultaneous integration of energy, mass and properties in water networks, Comput Chem Eng, 71, 52-66.

Khor C.S., Shah N., Mahadzir S., Elkamel A., 2012, Optimisation of petroleum refinery water network systems retrofit incorporating reuse, regeneration and recycle strategies, Can J Chem Eng, 90, 137-143.

Kralj A.K., 2015, The re-usages of wastewater within industry: the positive impact of contaminants, Journal of Cleaner Production, 95, 124-130.

Liu Z.Y., Yang Y., Wan L.Z., Wang X., Hou K.H., 2009, A heuristic design procedure for water-using networks with multiple contaminants, AIChE Journal, 55, 374-382.

Liu Z.Y., Zhang Z.J., N. H.L., Wu Z.L., 2004, Wastewater Minimisation Using a Heuristic Procedure, International Journal of Chemical Reactor Engineering, 2: A25.

Ma H., Feng X., Cao K., 2007, A rule-based design methodology for water networks with internal water mains, Chem Eng Res Des, 85, 431-444.

Manan Z.A., Wan Alwi S.R., Ujang Z., 2006, Water pinch analysis for an urban system: a case study on the Sultan Ismail Mosque at the Universiti Teknologi Malaysia (UTM), Desalination, 194, 52-68.

Mughees W., Al-Ahmad M., 2015, Application of water pinch technology in minimization of water consumption at a refinery, Comput Chem Eng, 73, 34-42.

Ong B.H.Y., Pang Y.S., Wan J.Y., Yap A.K.S., Ng W.P.Q., Foo D.C.Y., 2015, Water network optimisation with consideration of network complexity, Chemical Engineering Transactions, 45, 13-18.

Parand R., Yao H.M., Foo D.C.Y., Tade M.O., 2015, Improved Composite Table Algorithm for Targeting Regeneration-Recycle Water Network, Chemical Engineering Transactions, 45, 55-60.
Parand R., Yao H.M., Pareek V., Tade M.O., 2014, Use of Pinch Concept To Optimize the Total Water Regeneration Network, Industrial & Engineering Chemistry Research, 53, 3222-3235.
Parand R., Yao H.M., Tade M.O., Pareek V., 2013, Targeting water utilities for the threshold problem without waste discharge, Chem Eng Res Des, 91, 2569-2578.
Poplewski G., 2015, A new methodology for the synthesis of an optimum flexible water networks, Process Saf Environ Protect, 95, 172-183.
Prakash R., Shenoy U.V., 2005, Targeting and design of water networks for fixed flowrate and fixed contaminant load operations, Chemical Engineering Science, 60, 255-268.
Rubio-Castro E. et al., 2016, Optimal design of integrated agricultural water networks, Comput Chem Eng, 84, 63-82.
Saw S.Y., Lee L., Lim M.H., Foo D.C.Y., Chew I.M.L., Tan R.R., Klemes J.J., 2011, An extended graphical targeting technique for direct reuse/recycle in concentration and property-based resource conservation networks, Clean Technol Environ Policy, 13, 347-357.
Su W.-N., Li Q.-H., Liu Z.-Y., Pan C.-H., 2012, A new design method for water-using network of multiple contaminants with single internal water main, Journal of Cleaner Production, 29-30, 38-45.
Teles J., Castro P.M., Novais A.Q., 2008, LP-based solution strategies for the optimal design of industrial water networks with multiple contaminants, Chemical Engineering Science, 63, 376-394.
Teles J.P., Castro P.M., Novais A.Q., 2009, MILP-based initialization strategies for the optimal design of water-using networks, Chemical Engineering Science, 64, 3736-3752.
Wang B., Feng X., Zhang Z., 2003, A design methodology for multiple-contaminant water networks with single internal water main, Comput Chem Eng, 27, 903-911.
Wang Y.P., Smith R., 1994, Wastewater minimisation, Chemical Engineering Science, 49, 981-1006.
Wang Z.-F., Zhao H.-P., Liu Z.-Y., 2012, Design of water-using networks by combining the concentration potential concepts with an LP approach, Chemical Engineering Science, 69, 565-570.
Zhao H.-P., Su W.-N., Liu Z.-Y., 2014, Design of water-using networks of multiple contaminants with two internal water mains, Journal of Cleaner Production, 67, 37-44.
Zhao H.P., Wang Z.F., Chan T.C., Liu Z.Y., 2016, Design of regeneration recycling water networks by means of concentration potentials and a linear programming method, Journal of Cleaner Production, 112, 4667-4673.
Zheng X.S., Feng X., Shen R.J., Seider W.D., 2006, Design of optimal water-using networks with internal water mains, Industrial & Engineering Chemistry Research, 45, 8413-8420.
Zhu J.F., Xu D.L., Liu Z.Y., 2015, A Modified Graphical Method to Target the Regeneration Stream Flow Rate for Water-Using Networks, Chemical Engineering Transactions, 45, 229-234.