CHEMICAL ENGINEERING TRANSACTIONS
VOL. 61, 2017
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Guest Editors: Petar SVarbanov, Rongxin Su, Hon Loong Lam, Xia Liu, Jiří J Klemeš

ISBN978-88-95608-51-8; **ISSN** 2283-9216
DOI: 10.3303/CET1761052

Design and Analysis of Water-Using Networks Involving Regeneration

Ai-Hong Li[a], Xiao-Yan Fan[b], Zhi-Yong Liu[b,*]

[a]Department of Chemical Engineering, Chengde Petroleum College, Hebei 067000, China
[b]School of Marine Science and Engineering, Hebei University of Technology, Tianjin 300130, China
liuzhiyong@hebut.edu.cn

With the addition of regeneration units into a water-using network is an efficient way for wastewater minimization. However, it is often difficult to target and design the water networks involving regeneration. Liu et al. (AIChE J, 2009) compared the difference between the water networks involving regeneration and that involving reuse only and obtained an insight that the former network can be formed by adding one or a few additional sources, the regenerated stream(s), into the latter one. Then, the key for design of a water-using network involving regeneration is to determine the flowrate and concentrations of the regenerated stream(s). The above insight can be used to simplify the design procedure of water networks involving regeneration. This paper reviews the applications of the above insight in the design of water/hydrogen networks involving regeneration reuse/recycling and the analysis of the above networks.

1. Introduction

The introduction of regeneration units into a water network can significantly reduce both freshwater consumption and wastewater discharge. If the wastewater produced from a water-using process is regenerated and reused in other processes, it is called regeneration reuse. If the wastewater after regeneration is reused in the process where it is produced, it is called regeneration recycling (Wang and Smith, 1994). The prevailing integration techniques for the water-using networks (WUNs) involving regeneration can be classified into Pinch Analysis method and mathematical programming method.

Wang and Smith (1994) first introduced the Water-Pinch-Analysis method into the integration of water networks. They used Limiting Composite Curves (LCC) to target the minimum flowrates of freshwater and regeneration water. Kuo and Smith (1998) developed an improved procedure, which included pinch identification, operation grouping and operation migration, to overcome the limitations of Wang and Smith (1994). Gomes et al. (2007) presented Water Source Diagram procedure for the synthesis of water mass-exchange networks of single contaminant with a wide variety of process features (including regeneration reuse and regeneration recycling). Parand et al. (2014) developed an Extended Composite Table Algorithm to target the total water regeneration network of single contaminant and a Composite Matrix Algorithm to find the maximum feasible post-regeneration concentration. Fan et al. (2016) considered the situation when the regenerated concentration is higher than the lowest limiting inlet concentration by presenting a modified graphical method based on the work of Kuo and Smith (1998). Liu et al. (2016) proposed a simple and effective method to target the WUNs of single contaminant involving regeneration. Parand et al. (2016) developed an Automated Composite Table Algorithm based on the LCC for achieving Zero Liquid Discharge by means of regeneration recycling.

Mathematical programming method is another effective tool for the integration of WUNs involving regeneration. Alva-Argáez et al. (1998) presented a superstructure, which included reuse, regeneration reuse and regeneration recycling, and solved the MINLP model developed with decomposition strategy. Many other optimization approaches, such as sequential optimization (Feng et al., 2008a), improved genetic algorithms (Iancu et al., 2009), adaptive random search method (Poplewski et al., 2011), were proposed to optimize the WUNs involving regeneration. Khor et al. (2012) considered the membrane separation-based regenerators and obtained the global optimality using GAMS/BARON software. Poplewski (2014) applied superstructure optimization-based algorithmic to the design of flexible water network, in which the variation of regenerated

Please cite this article as: Li A.-H., Fan X.-Y., Liu Z.-Y., 2017, Design and analysis of water-using networks involving regeneration, Chemical Engineering Transactions, 61, 325-330 DOI:10.3303/CET1761052

concentration and periodic downtimes of selected sources and sinks were considered. García-Montoya et al. (2015) put forward optimization formulation for the water networks of residential complexes for recycle, regeneration, and storage of water. Sujak et al. (2015) presented an MINLP model for the synthesis of optimal total water network. Sujak et al. (2017) took all levels of water management hierarchy and cost constraints into account simultaneously.

Either with Pinch Analysis method or mathematical programming method, it is complex to target and design the WUNs involving regeneration, compared with that involving reuse only. Liu et al. (2009a) compared the difference between the WUNs involving regeneration and that involving reuse only and obtained an insight to simplify the design of the WUNs involving regeneration. This paper will give a review of the above insight and its applications in the design and analysis of water/hydrogen networks.

2. The insight of Liu et al. (2009a) for the design of the WUNs involving regeneration

For the WUNs involving regeneration, Liu et al. (2009a) pointed out that it includes one or a few additional sources, the regenerated stream(s) (S_{reg}), compared with the WUNs involving reuse only. A WUN involving regeneration can be formed by adding the regenerated stream(s) into the WUN involving reuse only. If the concentrations and flowrate of the regenerated stream(s) can be obtained, a WUN involving regeneration can be designed with the methods proposed for the WUN involving reuse only. In this way, the complex task of designing a WUN involving regeneration is converted into a simple task of obtaining the concentrations (C_{reg}) and flowrate (F_{reg}) of the regenerated stream(s).

The regeneration units can be classified into two types: fixed regenerated concentration model and fixed Removal Ratio (RR) model (Wang and Smith, 1994). For the regeneration unit of fixed regenerated concentration model, C_{reg} is given. For the regeneration unit of fixed-RR model, when the inlet flowrate and outlet flowrate are assumed to be equal, the regenerated concentration of contaminant *i* ($C_{reg,i}$) is:

$$C_{reg,i} = C_{in,i}\,(1\text{-RR}_i) \quad (1)$$

It can be inferred that the task of obtaining the regenerated concentrations and flowrate for a fixed-RR regeneration unit focuses on identifying which sources should be regenerated.

3. Applying the insight to the design of the WUNs involving regeneration

3.1 Designing the WUNs involving regeneration reuse

For the design of the WUNs involving regeneration reuse, Liu et al. (2009a) divided the whole network into two subnetworks, the one before regeneration and that after regeneration, depending on the concentration features of inlet and outlet streams. By designing the subnetwork before regeneration, the flowrate and concentration(s) of the streams to be regenerated can be identified. Then, the values of C_{reg} can be obtained from the before-regeneration concentrations and the RR values with Eq(1). Including the S_{reg} with known F_{reg} and C_{reg} in the sources of WUN involving reuse only, the design of WUNs involving regeneration reuse can be obtained by using the method of Liu et al. (2009b) which was proposed for the WUNs involving reuse only. The comparison of the results for two examples obtained by Liu et al. (2009a) and that obtained with the methods in the literature is shown in Table 1.

Table 1: Comparison of the results for the WUNs involving regeneration reuse obtained by Liu et al. (2009a) and those obtained with the methods in the literature

		Results in the literature			Results of Liu et al. (2009a)		
NC	Model	F_{fresh} ($t \cdot h^{-1}$)	F_{reg} ($t \cdot h^{-1}$)	C_{reg} (ppm)	F_{fresh} ($t \cdot h^{-1}$)	F_{reg} ($t \cdot h^{-1}$)	C_{reg} (ppm)
1	Fixed RR	44 Kuo and Smith (1998)	40	17.5	43.5	40	17.5
3	Fixed RR	59.7 Kuo and Smith (1998)	55.6	----	59.7	55.5	85.6, 8.31, 116.9

NC is the number of contaminants, the same below

3.2 Designing the WUNs involving regeneration recycling

Pan et al. (2012) presented an iterative method for the design of regeneration recycling WUNs of multiple contaminants based on the insight of Liu et al. (2009a) and the concepts of concentration potential proposed by Liu et al. (2009b). The concepts of concentration potential, which include the Concentration Potential of Demands (CPD) and the Concentration Potential of sources (CPS), are presented to rank the water streams of multiple contaminants by concentration order. For the networks of fixed regenerated concentration model, the final design can be obtained without iteration. For the networks of fixed-RR model, the initial regenerated concentrations in the first iteration need to be evaluated based on the appropriate source streams, which can be determined by the values of CPS and RR. In the design procedure, the performing order of water-using processes is identified with CPD values. The final design for the fixed-RR model WUNs can be obtained in a few iterations. With the method of Pan et al. (2012), the freshwater consumption, regenerated stream flowrate, and the before-regeneration concentrations can be obtained simultaneously. The comparison of the results for three examples obtained by Pan et al. (2012) and that obtained with the methods in the literature is shown in Table 2.

Table 2: Comparison of the results for the WUNs involving regeneration recycling obtained by Pan et al. (2012) and those obtained with the methods in the literature

		Results in the literature			Results of Pan et al. (2012)		
NC	Model	F_{fresh} $(t \cdot h^{-1})$	F_{reg} $(t \cdot h^{-1})$	C_{reg} (ppm)	F_{fresh} $(t \cdot h^{-1})$	F_{reg} $(t \cdot h^{-1})$	C_{reg} (ppm)
3	Fixed RR	59.7	55.6	----	58	56.08	89.16, 8.39, 121.09
		Kuo and Smith (1998)					
3	Fixed RR	27.10	24.75	37.61, 59.69, 42.27	25.55	20.86	31.48, 7.01, 13.33
		Xu (2004)					
3	Fixed C_{reg}	30	223.36	10, 30, 40	30	223.36	10, 30, 40
		Feng et al. (2008a)					

3.3 Designing the regeneration recycling WUNs with internal water mains

Zhao et al. (2013) proposed an iterative method for the regeneration recycling WUNs of multiple contaminants with internal water mains, also based on the insight of Liu et al. (2009a) and the concentration potential concepts of Liu et al.(2009b). The design procedure includes: (1) estimate the concentrations of the initial regenerated stream and add the regenerated stream into the other sources; (2) divide the water-using processes into three parts based on the values of CPD and flowrates of the streams; (3) form the internal water mains by the values of CPS and construct an initial network. The final design can be obtained in a few iterations according to adjusting the initial network. The freshwater consumption for an example obtained by Zhao et al. (2013) is the same as that obtained by Feng et al. (2008b), but the flowrate of regenerated stream obtained by Zhao et al. (2013) is lower.

3.4 Designing the hydrogen networks involving purification (regeneration) reuse

The purification reuse of hydrogen is one of the most economical approaches to relieve the significant increase of hydrogen resource. Yang et al. (2013) extended the iterative strategy of Pan et al. (2012) to the design of hydrogen networks with single contaminant. The hydrogen network structure was designed by using the method of Liu et al. (2009c). The model of hydrogen purification unit is different from that of water regeneration unit because there is a residual stream in the former one. Even for a hydrogen network with fixed purified concentration model, iteration is required. For the hydrogen networks with fixed recovery (R) ratio, the purified concentration and flowrate need to be estimated based on the maximum concentration of residual stream deduced. The comparison of the results for two examples obtained by Yang et al. (2013) and that obtained with the methods in the literature is shown in Table 3.

Table 3: Comparison of the results for the hydrogen networks involving purification reuse obtained by Yang et al. (2013) and those obtained with the methods in the literature

	Results in the literature			Results obtained by Yang et al. (2013)		
Model	F_{fresh} $(t \cdot h^{-1})$	F_{reg} $(t \cdot h^{-1})$	C_{reg} (ppm)	F_{fresh} $(t \cdot h^{-1})$	F_{reg} $(t \cdot h^{-1})$	C_{reg} (ppm)
Fixed C_{reg}	196.77	----	2	196.76	64.33	2
	Liao et al. (2011)					
Fixed C_{reg}	158.31	34.37	5	158.31	34.37	5
	Agrawal and Shenoy (2006)					
Fixed R	No literature			158.05	31.38	Fixed R of 90%

4. Designing the WUNs by combing the insight with mathematical programming method

The WUNs involving regeneration reuse are generally formulated as MINLP problems. To simplify the solving procedure, Li and Guan (2016) adopted a similar strategy of Liu et al. (2009a): dividing the whole network into the subnetwork before regeneration and that after regeneration by using four heuristic rules proposed. With this strategy, an MINLP problem for the WUNs involving regeneration reuse was converted into an NLP problem for the WUNs involving direct reuse. To reduce freshwater consumption further, the regeneration recycling network with the minimum recycle flowrate was developed based on the regeneration reuse structure.

Zhao et al. (2016) extended the method of Wang et al. (2012), which was proposed for the design of the WUNs of multiple contaminants involving reuse only, to regeneration recycling water networks based on the insight of Liu et al. (2009a). The precedence order of water-using processes is determined by the values of CPD and the allocations of sources to demands are obtained with LP approaches. The method proposed by Zhao et al. (2016) has the advantages of needing no initial values and reducing calculation effort significantly. It has been developed into computing software, which is applicable to the large and complex systems. Table 4 shows that the results obtained by combining the insight with mathematical programming approaches are comparable to or even better than those obtained with the methods in the literature.

Table 4: Comparison of the results obtained by combining the insight with mathematical programming methods and those obtained with the methods in the literature

		Results in the literature			Results obtained by combining the insight with mathematical programming methods		
NC	Model	F_{fresh} ($t \cdot h^{-1}$)	F_{reg} ($t \cdot h^{-1}$)	C_{reg} (ppm)	F_{fresh} ($t \cdot h^{-1}$)	F_{reg} ($t \cdot h^{-1}$)	C_{reg} (ppm)
3	Fixed RR	44	40	17.5	43.5	40	17.5
		Kuo and Smith (1998)			Li and Guan (2016)		
3	Fixed RR	59.7	55.6	----	59.7	54.04	----
		Kuo and Smith (1998)			Li and Guan (2016)		
3	Fixed RR	58	56.08	89.16, 8.39, 121.09	58	55.63	88.82, 8.35, 120.57
		Pan et al. (2012)			Zhao et al. (2016)		
3	Fixed RR	27.10	24.75	37.61, 59.69, 42.27	25.55	20.83	31.21, 6.85, 13.15
		Xu (2004)			Zhao et al. (2016)		

5. Applying the insight to the analysis of WUNs involving regeneration recycling

The insight mentioned above can also be used to predict the relationships between the regeneration targets and the regenerated concentrations for the WUNs of single contaminant, and identify the contaminant which has the most influence on the regeneration targets for the WUNs of multiple contaminants.

5.1 Predicting the regeneration targets for the systems of single contaminant

For a WUN of single containment involving regeneration recycling, when the regenerated stream is considered as an added source, the demands can be satisfied by the sources in the ascending order of containment concentration, as shown in Figure 1. Based on the balances of mass and flowrate below the Regeneration Pinch in Figure 1, Xu et al. (2013) developed a few relationships between regeneration targets and the regenerated concentration. By the relationships developed, the regeneration targets at different regenerated concentrations can be predicted easily if the Regeneration Pinch does not change. When the regenerated concentrations change, the Regeneration Pinch might change correspondingly. Xu et al. (2013) deduced a few relationships to identify the critical regenerated concentration, at which the Regeneration Pinch changes, for both normal and abnormal networks. An abnormal network is characterized by a Pseudo-Pinch Point, at which a minor variation of the regenerated concentration will cause the change of Regeneration Pinch.

5.2 Predicting the regeneration targets for the systems of multiple contaminants

Li et al. (2015) investigated the influences of the regenerated concentrations on the regeneration targets for the WUNs of multiple contaminants involving regeneration recycling. For convenience, Li et al. (2015) classified the above networks into simple ones and complex ones, and defined the contaminant which has the most influence on the regeneration targets as key contaminant. A simple network is similar to a single contaminant one, in which only one contaminant (key contaminant) determines the usage of regenerated water. The regeneration targets of a simple network can be predicted easily, similar to the work of Xu et al. (2013) when the regenerated concentration of the key contaminant changes. Other contaminants, which might influence the regeneration targets as well, should be removed by regeneration unit to the maximum allowable values deduced. For a complex network, based on the partial differential equations of mass balances of the contaminants, the influence of regenerated concentrations on regeneration targets is analysed, and the key contaminant is identified.

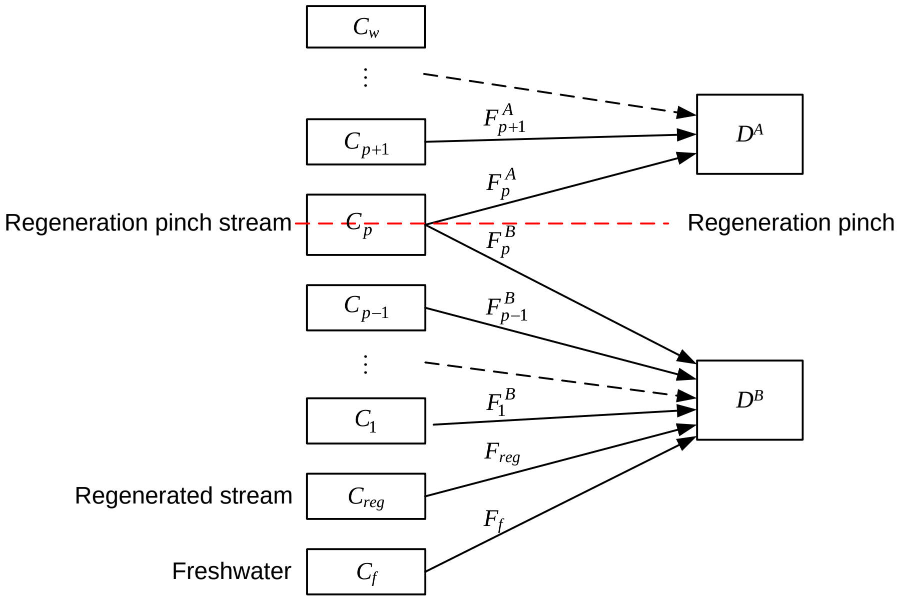

Figure 1: Allocation of sources to demands for the regeneration recycling WUNs of single contaminant.

The relationships developed by Xu et al. (2013) for the WUNs with single contaminant and Li et al. (2015) for the WUNs with multiple contaminants not only simplified the calculation of the regeneration targets significantly, but also provided clear engineering insights for the WUNs involving regeneration recycling.

6. Conclusions

This paper provides a review of the insight proposed by Liu et al. (2009a) for the design of WUNs involving regeneration reuse/recycling. The regenerated stream(s) is considered as additional source(s) of the WUNs involving reuse only. If the flowrate and concentrations of the regenerated stream(s) are determined, the WUNs involving regeneration can be designed with the methods proposed for that involving reuse only. The insight simplifies the design procedure of water/hydrogen networks involving regeneration reuse/recycling. In addition, it has been applied to the analysis of regeneration recycling WUNs, which not only further simplified the calculation of regeneration targets, but provided clear engineering insights for the WUNs involving regeneration.

Acknowledgments

This work is supported by the Natural Science Foundation of Hebei Province, Hebei, China (Grant No. B2017202073) and the Foundation of Educational Commission of Hebei Province, Hebei, China (Z2017032).

References

Agrawal V., Shenoy U.V., 2006, Unified conceptual approach to targeting and design of water and hydrogen networks, AIChE Journal, 52, 1071–1082.

Alva-Argáez A., Kokossis A.C., Smith R., 1998, Wastewater minimisation of industrial systems using an integrated approach, Computers & Chemical Engineering, 22, S741–S744.

Fan X.Y., Xu D.L., Zhu J.F., Liu Z.Y., 2016, Targeting of water-using networks involving regeneration with a graphical approach, Clean Technologies and Environmental Policy, 18, 1–8.

Feng X., Bai J., Wang H.M., Zheng X.S., 2008a, Grass-roots design of regeneration recycling water networks, Computers & Chemical Engineering, 32, 1892–1907.

Feng, X., Shen, R.J., Yu, X.J., 2008b. Optimization of regeneration recycling water networks with internal water mains. Journal of Chemical Industry and Engineering (China), 59, 2046–2051.

García-Montoya M., Ponce-Ortega J.M., Nápoles-Rivera F., Serna-González M., El-Halwagi M.M., 2015, Optimal design of reusing water systems in a housing complex, Clean Technologies and Environmental Policy, 17, 343–357.

Gomes J.F.S., Queiroz E.M., Pessoa F.L.P., 2007, Design procedure for water/wastewater minimization: single contaminant, Journal of Cleaner Production, 15, 474–485.

Iancu P., Plesu V., Lavric V., 2009, Regeneration of internal streams as an effective tool for wastewater network optimisation, Computers & Chemical Engineering, 33, 731–742.
Khor C.S., Chachuat B., Shah N., 2012, Optimal water network synthesis with detailed membrane-based regenerator models, Computer Aided Chemical Engineering, 31, 1457–1461.
Kuo W.C.J., Smith R., 1998, Design of water-using systems involving regeneration, Trans. IChemE, 76(B), 94–114.
Li A.H., Yang Y.Z., Liu Z.Y., 2015, Analysis of water-using networks with multiple contaminants involving regeneration recycling, Chemical Engineering Science, 134, 44–56.
Li Y., Guan J., 2016, A stepwise optimal design of water network, Chinese Journal of Chemical Engineering, 24, 787–794.
Liao Z.W., Rong G., Wang J.D., Yang Y.R., 2011, Rigorous algorithmic targeting methods for hydrogen networks—Part II: Systems with one hydrogen purification unit, Chemical Engineering Science, 66, 821–833.
Liu J.H., Li A.H., Liu Z.Y., 2016, An effective method for targeting water-using networks of single contaminant involving regeneration reuse/recycling, Chemical Engineering Transactions, 52, 829–834.
Liu Z.Y., Li Y.M., Liu Z.H., Wang Y.J., 2009a, A simple method for design of water-using networks with multiple contaminants involving regeneration reuse, AIChE Journal, 55, 1628–1633.
Liu Z.Y., Li Y.M., Zhang G.L., Yang Y.Z., 2009c. Simultaneously designing and targeting for networks with multiple resources of different qualities, Chinese Journal of Chemical Engineering,17, 445–453.
Liu Z.Y., Yang Y., Wan L.Z., Wang X., Hou K.H., 2009b, A heuristic design procedure for water-using networks with multiple contaminants, AIChE Journal, 55, 374–382.
Pan C.H., Shi J., Liu Z.Y., 2012, An iterative method for design of water-using networks with regeneration recycling, AIChE Journal, 58, 456–465.
Parand R., Yao H.M., Foo D.C.Y., Tadé M.O., 2016, An automated composite table algorithm considering zero liquid discharge possibility in water regeneration–recycle network, Clean Technologies and Environmental Policy, 18, 2095–2105.
Parand R., Yao H.M., Pareek V., Tadé M.O., 2014, Use of pinch concept to optimize the total water regeneration network, Industrial & Engineering Chemistry Research, 53, 3222–3235.
Poplewski G., 2014, Design method of optimal and flexible water networks with regeneration processes. Chemical Engineering Transactions, 39, 73–78.
Poplewski G., Jeżowski J.M., Jeżowska A., 2011, Water network design with stochastic optimization approach, Chemical Engineering Research and Design, 89, 2085–2101.
Sujak S., Handani Z.B., Wan Alwi S.R., Manan Z.A., Hashim H., Lim Jeng S., 2017, A holistic approach for design of Cost-Optimal Water Networks, Journal of Cleaner Production, 146, 194–207.
Sujak S., Lim J.S., Wan Alwi S.R., Manan Z.A., 2015, A Model for the Design of Optimal Total Water Network (OTWN), Chemical Engineering Transactions, 45, 697–702.
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.
Xu D.L., Yang Y., Liu Z.Y., 2013, Predicting target values of the water-using networks involving regeneration recycling, Chemical Engineering Science, 104, 525–539.
Xu DM. Study on the optimization design of water-using network. PhD thesis, Ocean University of China, Shandong, China, 2004.
Yang Y., Xu D.L., Liu Z.Y., 2013, An iterative method for designing hydrogen networks with regeneration unit, International Journal of Hydrogen Energy, 38, 12241–12252.
Zhao H.P., Fan X.Y., Liu Z.Y., 2013, Design of regeneration recycling water networks with internal water mains by using concentration potential concepts, Chemical Engineering Science, 91, 162–172.
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.