CHEMICAL ENGINEERING TRANSACTIONS Volume 21, 2010
Editor J. J. Klemeš, H. L. Lam, P. S. Varbanov

DOI: 10.3303/CET102100149

Optimisation of Water Networks Using Ranking as Pre-processing Step to Get Driving Force Equipartition

Petrica Iancu*, Vasile Lavric, Valentin Pleşu
Centre for Technology Transfer in the Process Industries, University Politehnica of Bucharest, UPB-CTTIP, 1 Polizu Street, 011061 Bucharest, Romania
cttip@chim.upb.ro

Some ordering criteria are proposed in this paper, as pre-processing step for process design and optimisation of water networks, leading to equipartition of driving forces for mass transfer along of the associated system. The water network is abstracted as an oriented graph, the water using units being ranked based upon maximum of load, fresh water need, inlet or outlet constraints. This way, the local recycling is avoided and the driving force of the mass transfer could be more or less constant for the cascaded units. Optimal solution for a water network using as ranking criterion a properly chosen design variable is presented.

1. Introduction

Wastewater minimisation for a water using network is an efficient process integration methodology for process design that considers abatement of technological utilities (supply water flowrate) and diminution of the environmental impact (wastewater flowrate) using an optimisation based framework. Water network is considered as a whole system, the quantity and quality of water is allocated to each water-using unit such as to maximise water-reusing and minimise wastewater discharge. In the end, a complex water network is described by a NLP mathematical model to be solved with an optimisation tool able to tackle problems involving high number of variables. Different simplifications (LP, MILP, MINLP – depending on model complexity) were proposed, considering reuse/recycling and/or regeneration strategies, or including treatment units in the water network. The general approach is to consider water network as superstructure taking into account all possible connections between units, sources and treatment units. For simple water networks, the mathematical models are easily solved using different methods: graphical or mathematical optimisation. But, for complex water networks (like oil refinery and petrochemical water network) with large number of variables, well known solving methods can fail. Sauar *et al.*, 1996, used the driving force equipartition principle for heat, mass, and charge using irreversible thermodynamics combined with optimization procedures as a new tool for process design and optimisation. The principle says that the best trade-off between energy dissipation and transfer area is achieved when the thermodynamic driving forces are uniformly distributed over the transfer area. They claimed that process design should be

Please cite this article as: Iancu P., Lavric V. and Pleşu V., (2010), Optimisation of water networks using ranking as pre-processing step to get equipartition driving force, Chemical Engineering Transactions, 21, 289-294 DOI: 10.3303/CET1021049

optimized by the equal distribution of the driving forces throughout the process by assuming that the rates of entropy production are proportional to the square of the driving forces. Rosen (2009), use this analysis to define predictive indicators for the environmental impact of waste emissions, and chose exergy which can be viewed as a measure of the potential of the substance to change or impact the environment.
In this paper, the authors propose for design of water network an optimisation method based on equipartition of driving forces principles applied to contaminants mass transfer. The water network is abstracted as an oriented graph using as ranking criteria a design variables analysis.

2. Abstraction of Water Network

In Figure 1, a schematic representation for water using unit handling more contaminants is presented. This unit is characterised by the following variables: mass load of each contaminant transferred between process streams and water streams, m_i (i=1,2…N), limiting concentrations at input $C_{k,i}^{in,\max}$ (k=1,2,…K, i=1,2…,i-1,i+1,…N) and output $C_{k,i}^{out,\max}$ (k=1,2,…K, i=1,2…,i-1,i+1,…N) of each water using unit, water source flowrates, F_i (i=1,2,…,N) and wastewater flowrates W_i (i=1,2…N).

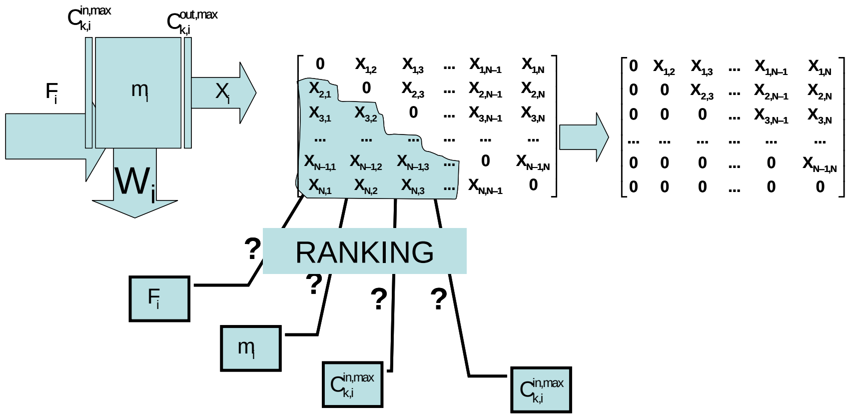

Figure 1: Optimisation of water network using ranking for equipartition of driving force

For process design and optimisation is needed to define a superstructure of water network or a kind of representation to obtain the best solution. In literature almost all work are oriented on getting the best superstructure. Lavric *et al.* (2005) and Iancu *et al.* (2009), proposed the representation of water network as a graph, where water using units are nodes and water streams are arches. In agreement with the approaches of Wang and Smith (1994), who introduced the concept of *Limiting Water Profile*, each water-using unit is defined by maximum inlet/outlet concentration and the mass load of the contaminants to be transferred. The flowrate from supply water source is determined from consistency and feasibility conditions for multiple contaminants. A matrix can be the formal representation of encoded water network internal flowrates. The complexity of the matrix increases with the number of water using units and internal flows.

A method to reduce the number of elements of matrix is proposed in two steps:

a) The graph can be oriented: the arch's arrow indicates either the direction of the flow of property (mass, energy, momentum, information, etc) or a cause-effect relationship (Himmelblau and Bischoff, 1968). The water network is an oriented graph starting from water-using units with inlet contaminant-free constraints, which are supplied with fresh water only.

b) According to the principle of driving force equipartition (Sauar et al., 1996;) across the water using units (Figure 2), these units can be ranked using some criterion, recycling water streams being avoided "*ab initio*". The internal streams become more and more contaminated from the entrance to the exit. This approach demonstrate necessary conditions of optimality as special cases of the principle of the driving force equipartition along a process, which ensures minimum entropy generation for given operating conditions, as a measure of the process irreversibility.

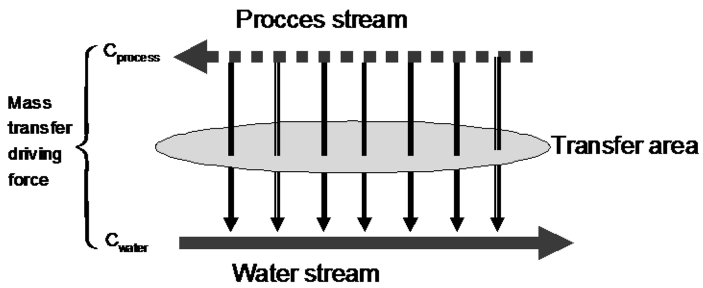

Figure 2: Parallel transport paths from process stream to water stream

As a consequence of oriented nature of the graph in ascending order, ranking of water using units can be performed based on one of following criteria:

a) water source flowrate (driving force is a ratio between mass load of contaminant k which gives maximum source flowrate F_{ik}):

$$\Delta C_i = \frac{m_{ik}\big|_{\max(F_{ik})}}{\max(F_{ik})} \tag{1}$$

b) mass load of contaminants (driving force is a ratio between mass load of contaminant k and source flowrate F_{ik} of contaminant with maximum mass load):

$$\Delta C_i = \frac{\max(m_{i,k})}{F_{ik}\big|_{\max(m_{ik})}} \tag{2}$$

c) limiting inlet contaminant concentrations imposed as limiting data by different constrains: physical, technological, economical, mechanical, etc (driving force is a ratio between mass load of contaminant k with maximum inlet concentration and source flowrate F_{ik} of this contaminant):

$$\Delta C_i = \frac{m_{i,k}\Big|_{\max\left(C_{ik}^{in}\right)}}{F_{ik}\Big|_{\max\left(C_{ik}^{in}\right)}} \tag{3}$$

d) limiting outlet contaminant concentrations (driving force is a ratio between mass load of contaminant k with maximum outlet concentration and source flowrate F_{ik} of this contaminant):

$$\Delta C_i = \frac{m_{i,k}\Big|_{\max\left(C_{ik}^{out}\right)}}{F_{ik}\Big|_{\max\left(C_{ik}^{out}\right)}} \tag{4}$$

3. Case Study

In Table 1, limiting data for a complex water network with 6 contaminants and 15 water using units, with one source available on the site (freshwater) are presented. The maximum amount of freshwater needed to satisfy this network is 1198.8 t/h, 326 t/h is lost, due to evaporation in units U1-U4 and 872.8 t/h is wastewater. An optimal solution is requested by site management team to reduce water consumption considering optimization design approach based on equipartition of mass transfer driving forces. Based on different ranking criteria, the following optimization scenarios are studied to determine minimum flowrate of supply water source: F-CRT (freshwater flowrate), L-CRT (mass load of contaminant), CIN-CRT (limiting inlet contaminant concentrations),

Table 1 Data for case study (C1-C6 are contaminants; U1-U15 are water using units)

		U1	**U2**	**U3**	**U4**	**U5**	**U6**	**U7**	**U8**	**U9**	**U10**	**U11**	**U12**	**U13**	**U14**	**U15**
Cin, ppm	C1	300	130	150	150	150	140	130	130	130	130	120	130	120	120	130
	C2	120	110	120	120	120	85	85	85	110	85	80	80	80	80	85
	C3	32	30	35	40	100	40	40	35	60	30	30	30	30	30	30
	C4	300	270	300	300	240	220	220	210	220	220	215	215	215	215	215
	C5	20	15	25	15	22	22	23	20	22	22	22	22	22	22	22
	C6	0	0	0	0	100	2	5	1	1	1	100	20	20	20	25
Cout,ppm	C1	600	150	250	350	300	200	200	150	150	150	130	150	130	130	150
	C2	250	140	250	200	200	100	100	100	150	100	90	90	90	90	100
	C3	40	35	60	200	320	100	100	74	200	50	40	40	40	40	50
	C4	435	310	435	450	400	300	300	250	300	300	250	250	250	250	250
	C5	40	30	40	34	30	30	30	30	30	30	30	30	30	30	30
	C6	10	10	10	10	200	5	10	10	10	10	400	150	200	100	200
Flowrate t/h	C1	3.8	1.1	36.4	7.5	23.4	14.0	2.0	2.6	2.0	4.0	1.2	1.0	0.3	0.1	0.2
	C2	29.4	2.3	47.6	6.0	23.4	7.0	1.0	2.6	3.6	4.0	1.7	0.6	0.4	0.1	0.2
	C3	12.3	1.1	35.0	28.8	35.3	24.5	3.5	7.7	17.0	8.0	3.8	1.3	1.0	0.3	0.4
	C4	14.0	49.0	36.2	4.8	18.5	10.5	1.5	2.1	6.0	6.0	2.4	0.8	0.6	0.2	0.2
	C5	36.8	5.3	35.0	8.5	13.0	11.7	1.7	1.7	6.7	6.7	0.0	1.7	1.3	0.3	0.3
	C6	0.0	0.0	0.7	0.0	39.0	5.0	0.2	0.3	0.2	0.2	15.0	5.0	4.0	1.0	1.0

COUT-CRT (limiting outlet contaminant concentrations).

4. Results and Discussion

Ranking this water network, the following results are obtained. Water using units U1 till U4 are placed at the top of oriented graph because these units are inlet-free of contaminants. The other units are ranked using different ranking criteria as follows:

- F-CRT: U2, U3, U4, U1, U14, U15, U7, U13, U1, U8, U10, U11, U9, U6, U5
- L-CRT: U2, U3, U1, U4, U14, U15, U7, U8, U12, U13, U10, U6, U9, U11, U5
- C_{IN}-CRT: U4, U1, U3, U2, U4, U11, U12, U13, U14, U15, U6, U7, U9, U10, U5
- C_{OUT}-CRT: U1, U4, U3, U2, U8, U12, U13, U14, U15, U6, U7, U9, U10, U5, U11

Using Eqs 1-4, mass transfer driving forces for each water using is calculated different scenarios. Some results are presented in Figures 3 and 4. For scenario F-CRT, mass transfer driving force is uniform in domain 20-200 ppm (Figure 3). For next criterion (L-CRT), the concentration difference domain is larger, 100-700 ppm, water using units U2 and U11 are not considered into this interval (Figure 4). Where water units are ranked by CIN-CRT and COUT-CRT criteria, this domain is constant over the water network.

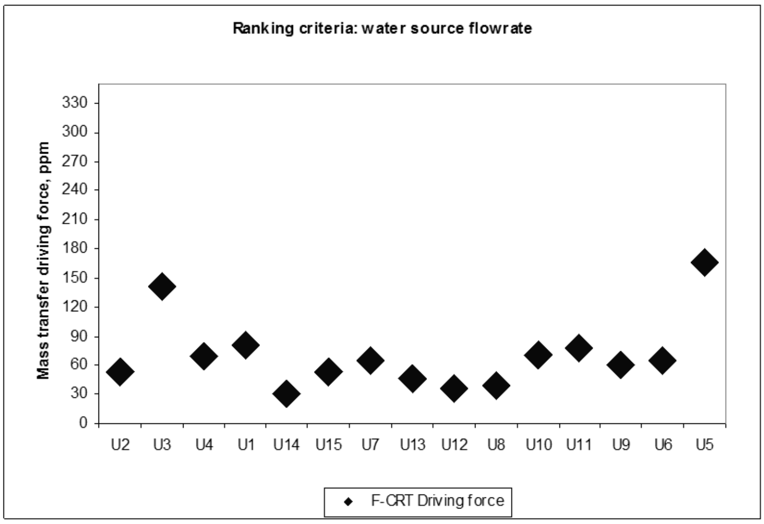

Figure 3: Mass transfer driving force for water network for F-CRT criterion

Based on different strategies of ranking water-using units, different optimization scenarios are studied to determine minimum flowrate of supply water for the large industrial site. If reused water is allowed, when the water network is fed by one water source, the minimum supply water flowrate for the network has different values for each criterion (F-CRT - 442.1 t/h, L-CRT - 452.8 t/h).

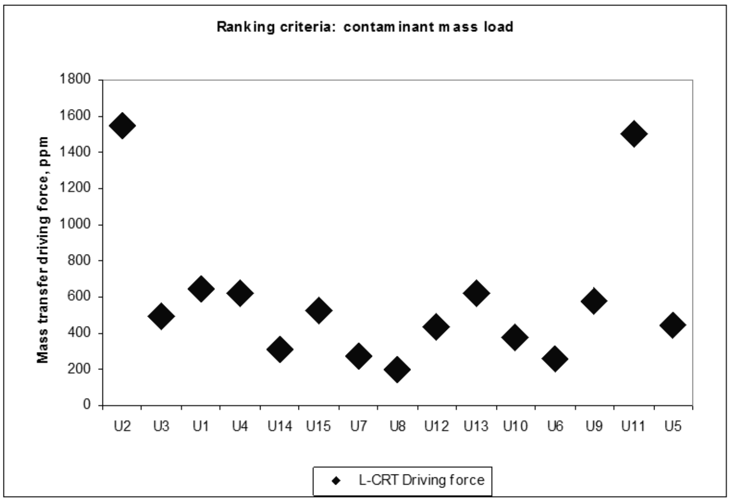

Figure 4: Mass transfer driving force for water network for L-CRT criterion

5. Conclusions

Consequently, 62-63 % savings are obtained compared to the existing topology for optimization of a complex water network using ranking as pre-processing step to get equipartition mass transfer driving force. For this approach, different ranking criteria were proposed for optimal water source consumption, keeping in mind uniform equipartition of mass transfer driving force along units. Ranking of units by water source flowrate assures a good optimality of water network.

Acknowledgements

The authors gratefully acknowledge the financial support provided by Romanian National Programme PNII grants no. 663/IDEI.

References

Sauar, E., Ratkje, S. K. and Lien, K. M., 1996, Equipartition of Forces: A New Principle for Process Design and Optimization, Ind. Eng. Chem. Res. 35, 4147-4153.

Lavric, V., Iancu, P. and Plesu V., 2005, Genetic algorithm optimisation of water consumption and wastewater network topology, J. Clean. Prod. 13(15), 1405-1415

Iancu, P., Plesu V., Lavric, V., 2009, Regeneration of internal streams as an effective tool for wastewater network optimisation, Comp. and Chem. Eng. 33(3), 731-742.

Marc, A. and Rosen, M. A., 2009, Indicators For The Environmental Impact Of Waste Emissions: Comparison Of Exergy And Other Indicators, Trans. Can. Soc. Mech. Eng. 33(1), 145-160

Himmelblau, D. M. and Bischoff K. B., 1968, Process analysis and simulation, John Wiley and Sons, Inc., New York.