Jurnal Teknologi, 51(F) Dis. 2009: 41–51

OPTIMAL DESIGN OF WATER NETWORKS INVOLVING SINGLE CONTAMINANT

ZAINATUL BAHIYAH HANDANI[1], SHARIFAH RAFIDAH WAN ALWI[2*], HASLENDA HASHIM[3] & ZAINUDDIN ABDUL MANAN[4]

Abstract. This work presents the development of a systematic technique to target freshwater consumption and wastewater generation to achieve the maximum water recovery for systems involving single contaminant. A generic linear programming (LP) model has been developed based on water network superstructure to simultaneously generate the maximum water recovery targets and design minimum water network, for both mass transfer-based and non-mass transfer-based problems (i.e., global water-using operations). The approach is illustrated by using an urban case study involving a mosque and an industrial case study involving an acrylonitrile process. The results show the potential maximum freshwater and wastewater reduction are 43.4% and 49.3% respectively for Sultan Ismail Mosque, and 70.6% and 37.7% for acrylonitrile process, which agree with the previous study performed using water cascade analysis technique.

Keywords: Water minimisation; mathematical modelling; maximum water recovery; optimisation; single contaminant

Abstrak. Kertas kerja ini membentangkan pembangunan teknik sistematik bagi penetapan sasaran penggunaan air bersih dan penghasilan air sisa buangan yang bertujuan mencapai pemulihan air yang maksimum untuk sistem yang melibatkan satu bahan pencemar. Sebuah model umum pengaturcaraan lelurus (LP) telah dibangunkan berdasarkan superstruktur rangkaian air bagi menghasilkan sasaran pemulihan air yang maksimum serta mereka bentuk rangkaian air yang minimum secara serentak bagi masalah yang beroperasi berdasarkan pemindahan jisim dan bukan berdasarkan pemindahan jisim (iaitu operasi penggunaan air secara global). Pendekatan ini dibuktikan melalui satu kajian kes perbandaran yang melibatkan sebuah masjid dan satu kajian kes industri yang melibatkan proses akrilonitril. Pengurangan air yang ketara untuk kedua-dua kajian kes telah tercapai, sekali gus membuktikan keberkesanan teknik yang dicadangkan. Keputusan ini menunjukkan potensi maksimum pengurangan air bersih dan air sisa buangan adalah sebanyak 43.4% dan 49.3% untuk Masjid Sultan Ismail dan 70.6% dan 37.7% untuk proses akrilonitril, di mana ia bertepatan dengan kajian lepas yang menggunakan teknik analisis jepit air.

Kata kunci: Pengurangan air; pemodelan matematik; pemulihan air yang maksimum; pengoptimuman; bahan pencemar

[1,2,3&4]Process Systems Engineering Centre (PROSPECT), Faculty of Chemical and Natural Resources Engineering, Universiti Teknologi Malaysia, 81310 Skudai, Johor, Malaysia
* Corresponding author: Tel.: +607-5535533, Fax: +607-5581463. Email: shasha@fkkksa.utm.my

1.0 INTRODUCTION

As fresh water resources continue to become scarcer and the costs associated with effluent disposal rise, there is growing concern for water conservation. Systems integration through design of maximum water recovery (MWR) networks within urban and industrial sectors has been one of the options which could help reduced water consumption significantly. Two approaches that are mainly used to generate this MWR target and design are the graphical water pinch analysis and the mathematical modeling approaches.

Generally, water-using operations can be classified into two broad categories i.e. mass transfer-based (MTB) and non-mass transfer-based (NMTB). A MTB water-using operation is characterised by the preferential transfer of a species from a rich stream to water, which is being utilised as a lean stream or a mass separating agent (MSA) [1]. A typical example of this type operation is the cleaning of container using fresh or spent water. The cleaning process involves the preferential transfer of species (contaminants) from a "rich stream" (in this case, the container being washed that contains unwanted species) to a lean stream or a MSA (in this case, water). Fresh or spent water is fed into the equipment (as a demand) while wastewater is generated (as a source) during cleaning process. Scrubbing and extraction process also are included in this category. It is important to note that, inlet and outlet flow rates of this operation are assumed to be equal. The MTB operation is also known *as fixed contaminant load problem*.

On the contrary, a NMTB water-using operation covers function of water other than as a mass separating agent. A typical example of this type operation includes water is fed as raw material or being withdrawn as product or byproduct in chemical reaction. This clearly represents a non-mass transfer operation since the operations are not designed to preferentially transfer species (contaminants) between streams. Note that, for non-mass transfer-based water-using operations, water flow rate is more important than the amount of contaminant accumulated. Therefore, the inlet and outlet flow rate for NMTB operation can have different flow rate. The operation in this category may include water-using operation such as boilers, cooling towers and reactors. This operation type is also widely known *as fixed flow rate problem*.

Wang and Smith [2] initiated research on water system integration using a graphical approach for targeting maximum water reuse and manual for design. Since its introduction by Wang and Smith [2], various noteworthy water pinch analysis to obtain maximum water recovery network for global water-using operations have emerged. These include works on processes with MTB and NMTB for single contaminant system [1, 3–7].

Recently, several works have been done to synthesise optimal water networks using mathematical modelling approach. Mathematical programming is a more suitable approach for optimum water networks, for both grassroots and retrofit application. They serve as a good synthesis tool in handling complex systems with different complex constraint. The water recovery network problem illustrated by using superstructure, transformed into mathematical programming and applied for single contaminant systems was first reported by Takama *et al.* [8] for a petroleum refinery problem. Bagajewicz and Savelski [9] have modelled a mathematical programming using linear programming (LP) formulation for fresh water usage targeting to obtain maximum water recovery in industrial plants involving single contaminant and a series of MILP problems to design different network alternatives. According to Savelski and Bagajewicz [10], the outlet concentrations must be equal to their maximum allowable values for an optimal water network. They also identified which processes need to be fed first using fresh water and which processes must receive reuse wastewater by introducing the concept of monotonicity in process-to-process connection. The major claim they made is mathematical programming can produce global optimal solutions and practically important sub-optimal solution when conceptual insights are employed to build the models. However, these works are limited to MTB operations only.

El-Halwagi *et al.* [11] have developed a rigorous graphical approach for identifying rigorous targets for resource conservation involving recycle/reuse problem. The authors have proven the optimality conditions using a dynamic programming formulation and used the results of the mathematical analysis to develop a conceptual graphical representation. Recently, Pillai and Bandyopadhyay [12] proposed targeting algorithm that combines simplicity of pinch analysis with mathematical optimisation technique for resource allocation network involving MTB and NMTB operations. However, there is no specific resource allocation since the problems have multiple allocation networks satisfying the minimum resource requirement.

This work presents the development of a generic LP model based on water network superstructure to achieve the maximum water recovery targets for both mass transfer-based and non-mass transfer-based problems involving single contaminant system. Two case studies are used to demonstrate the application of the methodology. This method is superior since the result can be used directly to obtain a guarantee global solution for the problem and simultaneously generate the maximum water recovery targets and design minimum water network. Note that, the method can also be applied to wide range of buildings including those from urban and industrial sectors.

2.0 METHODOLOGY

In single contaminant case, LP model is used to maximise water recovery through water reuse and recycle. The major claim made is mathematical programming can produce global optimal solutions. LP is a powerful tool, capable of finding the optimal value of a linear objective function subject to linear constraints. In this case, the objective function is to minimise total fresh water flow rate. Maximising water recovery consequently also minimises fresh water consumption and wastewater generation. The minimum water targets establishment consists of the overall fresh water requirement and wastewater generation for a process after looking at the possibility of using the available water sources within a process to meet its water demands. This method consists of four main steps as shown in Figure 1.

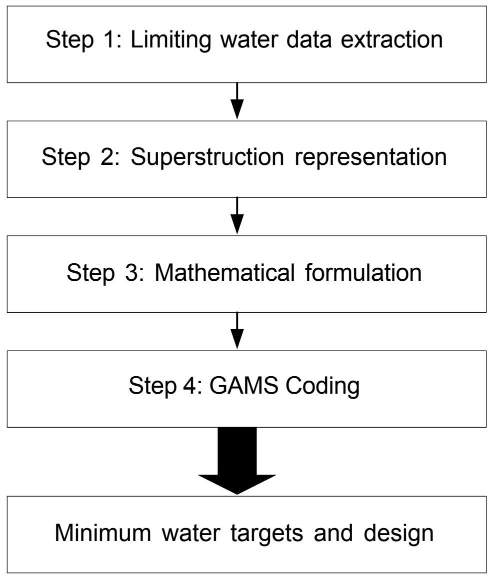

Figure 1 The step-wise of minimum water targets through maximum water recovery network

2.1 Step 1: Limiting Water Data Extraction

The first step is to identify water sources and water demands having potential for integration. This involved line-tracing, establishing process material balances and isolating the appropriate water sources and water demands that having potential for reuse and recycle. Water sources are water available for possible recycling/reuse while water demands reflect the actual requirements for various water-using operations. The limiting water data consists of water sources and demands and were listed in terms of quality (flow rate) and quantity (contaminant concentration). Assume that the contaminant concentration of each demand and source is fixed to it maximum values, hence leading to LP.

2.2 Step 2: Superstructure Representation

The second step is to generate superstructure. Similar to any other optimisation study in a process synthesis, it is necessary to build a superstructure in which all possible flow configurations are embedded. For each water-using operation, the inlet stream can be freshwater, used water from same or different processes while at the outlet stream, the generated wastewater may be directly discharged to the end of pipe treatment or reused in the same or different processes. The superstructure represents all possible connections between water sources and demands as well as and wastewater discharges. The following notation is adopted throughout the paper: S_i, D_j, FW and WW which represents water flow rate of source i, demand j, freshwater and wastewater respectively. The superstructure framework features a number of feasible networks developed based on given limiting water data. Figure 2 shows the general water network superstructure.

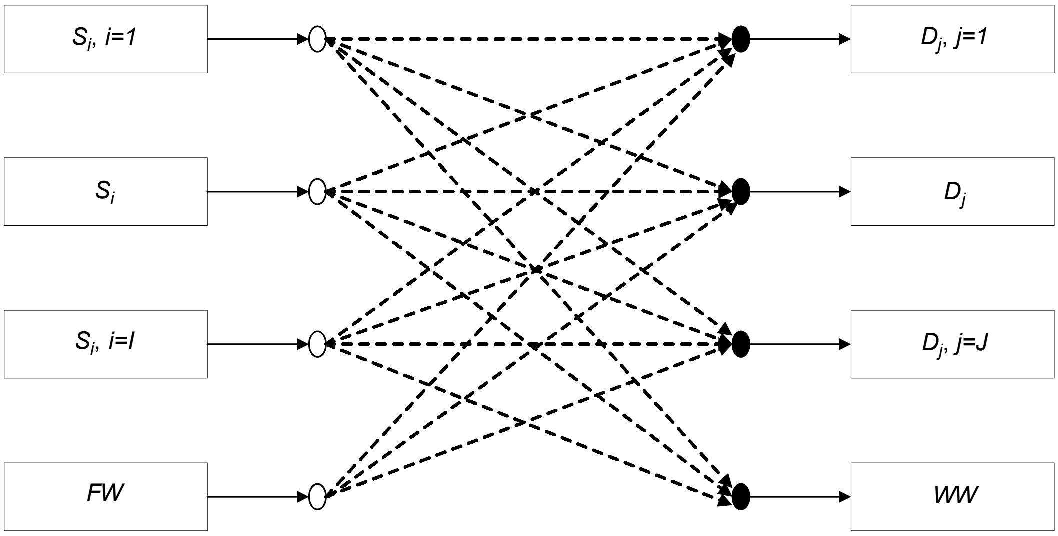

Figure 2 General superstructure for maximum water recovery network

2.3 Step 3: Mathematical Formulation

The third step is to develop a mathematical model based on the superstructure in Figure 2. The objective of this model is to determine the minimum fresh water target which leads to the minimum wastewater generation and the maximum total water reused/recycled in the system. S_i and D_j are the water flow rate of source i and demand j with a given maximum contaminant concentration, Cs_i and Cd_j, respectively. Let $F_{i,j}$ denotes the flow transferred from source i to demand j. Similarly, FW_j represents the flow transferred from freshwater to demand j, with a quality Cw. WW_i refers the flow transferred from source i to waste without any maximum quality limit. For a better understanding of the network superstructure, refer to Figure 3.

Objective function:
The objective function is to minimise the total amount of freshwater demand, FW_j.

$$Min\sum_j FW_j \tag{1}$$

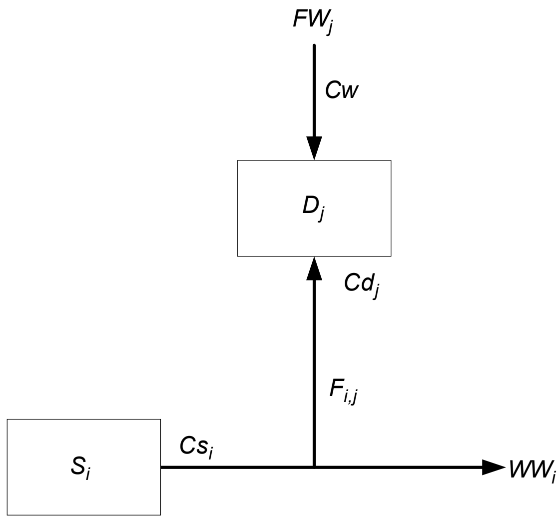

Figure 3 A water network superstructure for maximum water recovery network

The minimisation of the objective function represented by equations (1) is subjected to the following constraints:

(1) Water balance for each source:
For each source i, the generated wastewater, WW_i and reused/recycled water from source i to demand j, $F_{i,j}$ must be equal to available water source, S_i. The water balance for each source i is given by:

$$WW_i + \sum_j F_{i,j} = S_i \qquad \forall i \in I \tag{2}$$

(2) Water balance for each demand:
For each demand j, the water supply from fresh water, FW_j or/and potential reused/recycle water, $F_{i,j}$ must be equal to the desired water demand, D_j. The water balance for each demand j is given by:

$$FW_j + \sum_i F_{i,j} = D_j \qquad \forall j \in J \tag{3}$$

(3) Demand contaminant load satisfaction:
Contaminant mass load for demand j is supplied from a mixed of contaminant mass load from different sources (e.g fresh water, FW_jCw or/and potential reused/recycle water, $F_{i,j}CS_i$). Thus, the contaminant load from all sources must satisfy the contaminant load for demand j. Note that,

$$FW_jCw + \sum_i F_{i,j}Cs_i \le D_jCd_j \qquad \forall j \in J \tag{4}$$

(4) Non-negativity constraints:
The fresh water supply, wastewater generation and reused/recycled water flow rate must be greater than zero, therefore the fresh water supply, wastewater generation and reuse/recycle water flow rate is defined as positive/non-negativity variables.

$$FW_j, \quad WW_i, \quad F_{i,j} \geq 0 \qquad\qquad \forall i \in I, \quad \forall j \in J \tag{5}$$

2.4 Step 4: GAMS Coding

The problem is formulated as LP and implemented in General Algebraic Modeling System (GAMS) to determine the minimum freshwater and wastewater targets. Through the commercial mathematical optimisation software package GAMS, the optimal water network can be found.

3.0 CASE STUDIES

The approach was applied to an urban case study involving a mosque and an industrial case study involving an acrylonitrile process to demonstrate the applicability of the proposed model. For both cases, the model takes on the form of a linear program. The commercial software, GAMS is employed here to solve LP problem using the CPLEX solver.

3.1 Example 1: Urban Case Study – Sultan Ismail Mosque (SIM), UTM

Considering the example data of a mosque used by Wan Alwi *et al.* [13], the initial water demand and source data of the mosque is as shown in Table 1. For this example, the biological oxygen demand (BOD) was the most significant water quality factor chosen for water quality analysis. The limiting water-using operation data for SIM is presented in Table 1. In this example, there are eight water demands and five water sources. Water sources are water available for possible recycle/reuse while water demands reveal the actual requirements for various water-using operations. Water from toilet flushing and toilet pipes which are known as "blackwater" are not considered as water source since it highly contaminated with urine and faeces while water from irrigation is assumed to be completed absorbed by the soil.

By applying the data to the formulated model, the minimum freshwater and wastewater flowrate targets of this water system are 16.46 t/day and 12.99 t/day respectively. This gives reduction of 43.4% for freshwater consumption and 49.3% for wastewater generation. The results matched with those proposed by Wan Alwi *et al.* [11] using water cascade analysis technique. Figure 4 gives the corresponding optimal design of water network.

Table 1 Limiting water data for Sultan Ismail Mosque

Stream	Demands Descrip -tion	Flow rate (t/day)	BOD Concen -tration (ppm)	Stream	Sources Descrip -tion	Flow rate (t/day)	BOD Concen -tration (ppm)
D1	Kitchen	0.03	0	S1	Ablution	25.03	23
D2	Ablution	25.03	10	S2	Wash basin	0.14	23
D3	Wash basin	0.14	10	S3	Showering	0.14	216
D4	Showering	0.14	10	S4	Mosque cleaning	0.29	472
D5	Mosque cleaning	0.29	10	S5	Kitchen	0.03	536
D6	Irrigation	1.46	10				
D7	Toilet pipes	0.44	10				
D8	Flushing toilet	1.57	10				

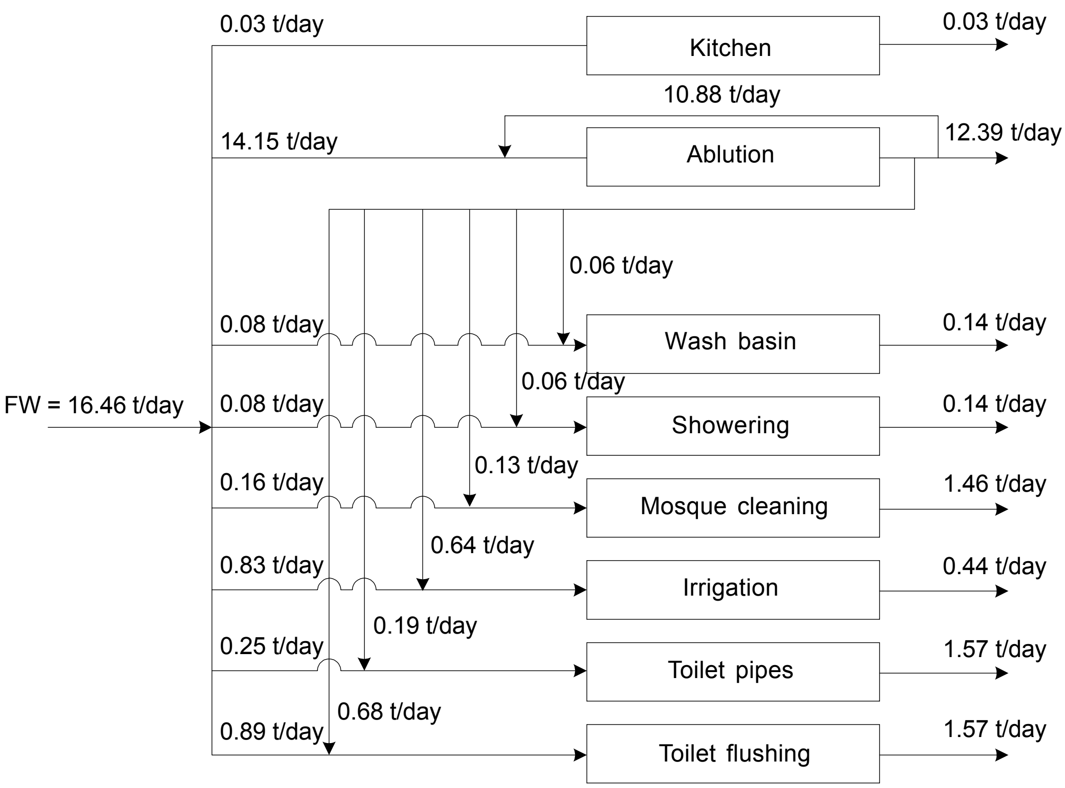

Figure 4 Optimal design of water network for Sultan Ismail Mosque

3.2 Example 2: Industrial Case Study – Acrylonitrile Process

The acrylonitrile process data by El-Halwagi [14] consists of two water demands and four water sources. Table 2 shows the limiting water data for each water demand and source involves in this process. Contaminant in concern for water minimisation study in this process is ammonia (NH_3).

Table 2 Limiting water data for acrylonitrile process

Stream	Demands Description	Flow rate (kg/s)	Concentration (ppm)	Stream	Sources Description	Flow rate (kg/s)	Concentration, (ppm)
D1	Boiler feed water	1.2	0	S1	Distillation bottoms	0.8	0
D2	Scrubber	5.8	10	S2	Off-gas condensate	5.0	14
				S3	Aqueous layer	5.9	25
				S4	Injector condensate	1.4	34

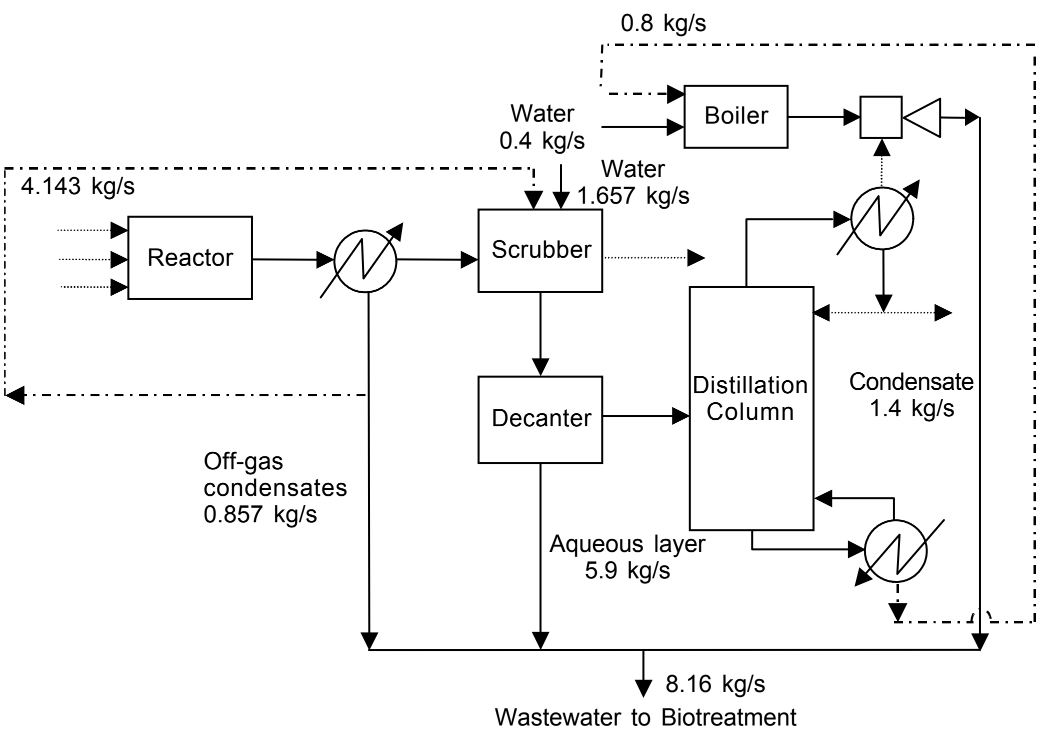

Figure 5 Optimal design of water network for acrylonitrile process

Using the developed LP model, the minimum freshwater and wastewater flow rate targets are at 2.057 kg/s and 8.157 kg/s respectively. This agrees with the result obtained by Manan *et al*. [1] using water cascade analysis. Targeting the maximum water recovery through reuse and recycle model resulted in savings of up to 70.6% freshwater and 37.7% wastewater for acrylonitrile process. The final water distribution network after integration is shown in Figure 5.

4.0 CONCLUSION

A mathematical modelling approach to target freshwater consumption and wastewater generation to achieve the maximum water recovery for systems involving single contaminant has been presented. A generic LP model has been developed based on water network superstructure to achieve the maximum water recovery targets, for both mass transfer-based and non-mass transfer-based problems (i.e., global water-using operations). The proposed model has been successfully implemented in an urban (Sultan Ismail Mosque at UTM) and industrial (acrylonitrile process) case studies. The results show the potential maximum freshwater and wastewater reduction are 43.4% and 49.3% respectively for Sultan Ismail Mosque and 70.6% and 37.7% for acrylonitrile process, which agree with the previous study performed using water cascade analysis technique.

ACKNOWLEDGEMENTS

The authors would like to thank Malaysia Ministry of Science, Technology and Innovation (MOSTI) and National Science Fellowship (NSF) scholarship for the financial support.

NOMENCLATURE

Cs_i	-	Concentration of contaminant in water stream from source i
Cd_j	-	Concentration limit of contaminant in water demand j
Cw	-	Concentration of contaminant k in freshwater
D_j	-	Flow rate of water demand j
F_{ij}	-	Flow rate variable for link from source i to demand j
FW_j	-	Freshwater supplied to demand j
S_i	-	Flow rate of water source i
Min	-	Minimum
WW_i	-	Unused portion of water source i (waste)

REFERENCES

[1] Manan, Z. A, Y. L. Tan and D. Y. C., Foo. 2004. Targeting the Minimum Water Flowrate Using Water Cascade Analysis Technique. *AIChE Journal*. 50(12): 3169–3183.

[2] Wang, Y. P. and R. Smith. 1994. Wastewater Minimization. *Chemical Engineering Science.* 49: 981–1006.

[3] Dhole, V. R., N. Ramchandani, R. A. Tainsh and M. Wasilewski. 1996. Make your Process Water Pay for Itself. *Chemical Engineering.* 103: 100–103.

[4] Sorin, M. and S. Bédard. 1999. The Global Pinch Point in Water Reuse Networks. *Transactions of the Institute of Chemical Engineers Part B.* 77: 305–308.

[5] Hallale, N. 2002. A New Graphical Targeting Method for Water Minimization. *Advances in Environmental Research.* 6(3): 377–390.

[6] Aly, S., S. Abeer and M. Awad. 2005. A New Systematic Approach for Water Network Design. *Clean Technologies and Environmental Policy*. 7(3): 154–161.

[7] Prakash, R. and U. V. Shenoy. 2005. Targeting and Design of Water Networks for Fixed Flowrate and Fixed Contaminant Load Operations. *Chemical Engineering Science*. 60(1): 255–268.

[8] Takama, N., T. Kuriyama, K. Shikoko and T. Umeda. 1980. Optimal Water Allocation in Petroleum Refinery. *Computers and Chemical Engineering*. 4: 251–258.

[9] Bagajewicz, M. J. and M. J. Savelski. 2001. On the Use of Linear Models for the Design of Water Utilisation Systems in Process Plants with a Single Contaminant. *Transactions of the Institute of Chemical Engineers, Part A*. 79: 600–610.

[10] Savelski, M. J. and M. J. Bagajewicz. 2000. On the Optimality Conditions of Water Utilization System in Process Plants with Single Contaminant. *Chemical Engineering Science*. 55: 5035–5048.

[11] El-Halwagi, M. M., F. Gabriel and D. Harell. 2003. Rigorous Graphical Targeting for Resource Conservation via Material Recycle/reuse Networks. *Industrial and Engineering Chemistry Research.* 42: 4319–4328.

[12] Pillai, H. K. and S. Bandyopadhyay. 2007. A Rigorous Targeting Algorithm for Resource Allocation Networks. *Chemical Engineering Science.* 62: 6212–6221.

[13] Wan Alwi, S. R., Z. A. Manan, M. H. Samingin and N. Misran. 2008. A Holistic Framework for Design of Cost-effective Minimum Water Utilization Network. *Journal of Environmental Management*. 88(2): 219–252.

[14] El-Halwagi, M. M. 1997. *Pollution Prevention through Process Integration: Systematic Design Tools*. San Diego, CA: Academic Press.