Water Cascade Analysis Technique for Minimum Flowrate Targeting: Tabular and Numerical Approach

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Abstract

This work presents the Water Cascade Analysis (WCA) as a new technique to establish the minimum water and wastewater targets for continuous water-using processes. The WCA is a numerical alternative to the graphical water targeting technique known as the water surplus diagram. The WCA is to the water surplus diagram in water pinch analysis as problem table analysis is to the grand composite curves in heat pinch analysis. By eliminating the tedious iterative steps of the water surplus diagram, the WCA can quickly yield accurate water targets and pinch point locations for a water network, thereby offering a key complimentary role to the water surplus diagram in the design and retrofit of a water recovery network. As in the case of the water surplus diagram, the WCA is not limited to mass transfer based operations and is applicable to a wide range of water using operations.

Keywords:

Water minimisation, minimum water and wastewater targets, pinch analysis, water cascade table, numerical analysis.

Introduction

The current drive towards environmental sustainability and the rising costs of fresh water and effluent treatment have encouraged the process industry to find new ways to reduce freshwater consumption and wastewater generation. Concurrently, the development of systematic techniques for water reduction, reuse and recycling within a process plant has seen extensive progress. The advent of Water Pinch Analysis (WPA) as a tool for the design of optimal water recovery network has been one of the most significant advances in the area of water minimisation over the last ten years. The WPA technique as proposed by Wang and Smith [1] generally considers the potential of using fresh or recycle water as a lean stream to absorb certain contaminants from various process operations, provided there exist a driving force for mass transfer. Maximising water reuse and recycling can minimise freshwater consumption and wastewater generation.

Water-using operations in a process plant can generally be classified into the mass transfer-based and the non mass transfer-based operations. A mass transfer-based water-using operation is characterised by the preferential transfer of species from a rich stream to water, which is being utilised as a lean stream or a mass separating agent (MSA). A typical example of such operation is the cleaning of a process vessel using fresh or recycle water. During cleaning, water is fed into the vessel (as a demand) while wastewater is generated (as a source) as shown in Figure 1(a). Another example of the mass transfer-based water-using operation is the absorption process where water is the MSA used to remove contaminants such as H_2S and SO_2 from a sour gas stream (see Figure 1b).

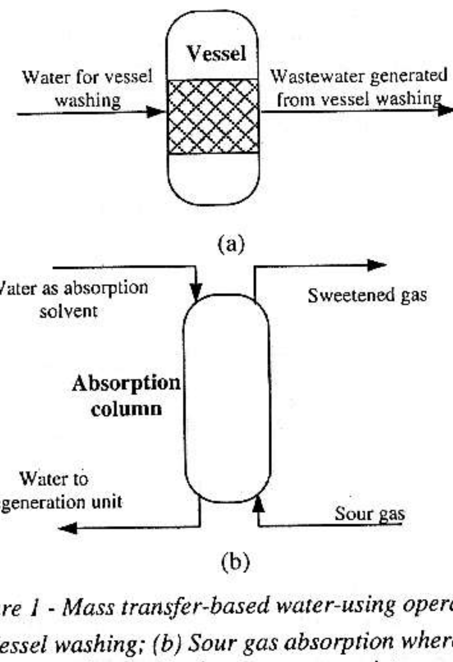

Figure 1 - Mass transfer-based water-using operations: (a) Vessel washing; (b) Sour gas absorption where water demand and water source exist

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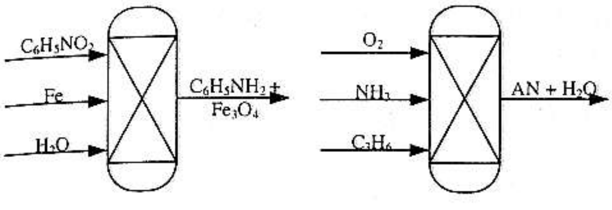

Figure 2 - Non-mass transfer-based water-using operations: (a) a reactor that consumes water in aniline production; (b) a reactor that produces water as a byproduct in acrylonitrile (AN) production [5]

The non-mass transfer-based water-using operation covers functions of water other than as a MSA. A typical example includes water being fed as a raw material, or being withdrawn as a product or a by-product in a chemical reaction (see Figure 2). The non-mass transfer-based operation also covers cases where water is being utilised as heating or cooling media. For such operations, usually, only water demands or water sources exist as shown in Figure 3.

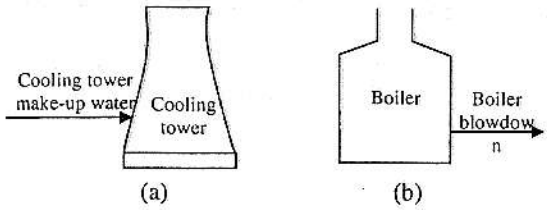

Figure 3 - Two other common types of the non-mass transfer-based water-using operations: (a) cooling tower make up; (b) boiler blow-down

Note that, for the non-mass transfer-based water-using operations, the water flowrate is more important than the amount of contaminant accumulated. Though the conventional water network studies have focused on the mass transfer-based model [1, 2], recent studies have shown that the non-mass transfer-based water-using operations are also important to consider [3, 4]. Figure 4 shows a reactor with several input and output streams at different concentrations [4]. Clearly, such system cannot be modelled using the mass transfer-based techniques proposed [1, 2].

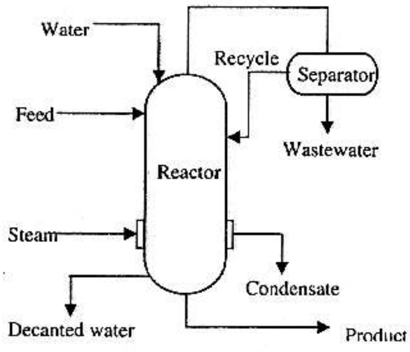

Figure 4 - A reactor system that cannot be modelled purely as mass transfer operation

Previous work on water targeting

In targeting the minimum utility requirements and in locating the pinch points, the graphical technique such as the composite curves and the numerical technique such as the problem table have both been used in the heat [6], mass [5] and water recovery problems [7] that are based on pinch analysis. Why then are both techniques usually used together even though they apparently yield the same information? The answer lies in the complimentary roles they play in pinch analysis. The graphical tool like the composite curves is vital in terms of providing an understanding of the overall heat and mass transfer potentials in a process. On the other hand, the numerical targeting tools like the problem table in heat integration [6] or the composition interval table (CIT) in mass integration [8] are advantageous from the point of view of accuracy and speed, and therefore, are more amenable to computer programming. Note that the majority of researchers have extended the use of composite curves and problem table analysis established for heat recovery based on pinch analysis to the mass recovery, and later, to the water recovery problems.

Wang and Smith [1] introduced the plot of composition versus contaminant mass load, or the water composite curves, for which they termed as the limiting water profile, for graphical water targeting. They also made use of the composition interval table from mass integration to pinpoint the pinch location and generate the exact minimum water targets prior to network design. The limiting water profile represents a major stride in establishing the baseline water requirement and wastewater generation for a process. However, its applicability is only limited to mass transfer-based operations. Water as cooling and heating media in cooling towers and boilers, and as a reactant may not be appropriately represented as mass transfer operations. To overcome this limitation, Dhole *et al.* [3] introduced the water source and demand composite curves. They also suggested process changes like mixing and bypassing to further reduce the fresh water consumption. However, Polley and Polley [9] later pointed out that, unless the correct stream mixing system was identified, the apparent targets generated by Dhole's technique [3] could be substantially higher than the true minimum fresh water and wastewater targets.

Sorin and Bédard [10] developed the Evolutionary Table to numerically determine the fresh water and wastewater targets. They pointed out that the targeting technique introduced by Dhole *et al.* [3] could result in a number of "local" pinch points, which might not necessarily be the actual or the "global" pinch points. However, Hallale [4] recently showed that, when more than one global pinch points occurred in water-using processes, the Evolutionary Table failed to locate them correctly.

Hallale [4] presented an alternative graphical method called the water surplus diagram (Figure 5) to target the minimum

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fresh water and wastewater. The method, which was adapted from the hydrogen pinch analysis [11], had a similar representation to the water source and demand composite curves proposed by Dhole *et al.* [3] thereby was not limited to the mass transfer-based operations. The new representation by Hallale [4] could handle all mixing possibilities and yet resulted in the true pinch point and reuse target.

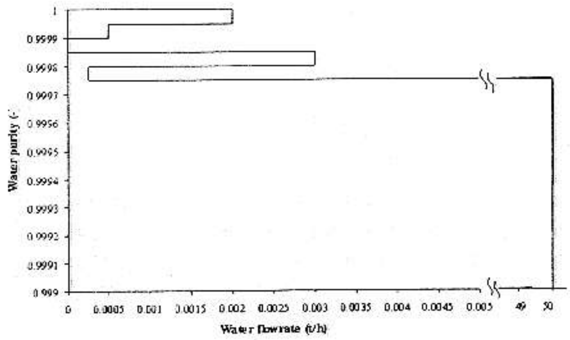

Figure 5 - Water surplus diagram

However, the water surplus diagram has the same drawbacks like the composite curves. It is tedious and time consuming to draw as it involves trial an error to find the pinch points and water targets. Besides, it has limitations in terms of generating highly accurate targets due to its graphical nature. The tedious iterative procedure to construct the water surplus diagram is shown in Figure 6. In order to eliminate the trial an error steps and compliment the graphical method, there is a need for a numerical equivalent of the water surplus diagram similar to the composition interval table in mass integration. This is the subject of this paper.

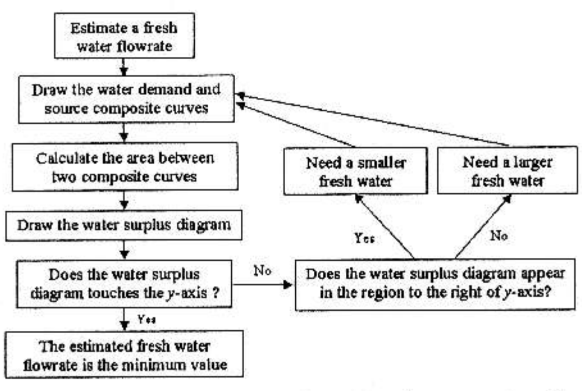

Figure 6 - The tedious iterative steps of constructing the water surplus diagram

This work presents the *water cascade analysis* (WCA), a new numerical technique to establish the minimum water and wastewater targets in a water recovery network. The WCA technique eliminates any tedious iterative step to quickly yield the exact utility targets and the pinch location(s). As in the case of the water surplus diagram, the WCA is not limited to mass transfer-based operations and is therefore applicable to a wide range of water using operations.

Two approaches may be employed in WCA, i.e. the tabular as well as the numerical approach. The former enables us to identify the minimum water targets via hand or a simple spreadsheet calculation, while the latter is a more powerful tool for complex problems (e.g. problems with multiple water-using operations), as it can be easily translated into any computer language for ease of calculation and software development. We will first demonstrate how the tubular approach is employed to identify the minimum water targets using a literature case study [12]. Next, the tabular approach is automated using linear programming (LP). In this section, a multiple-stream literature case study [13] will be used to demonstrate the usefulness of the approach.

Case study 1 – Organic chemical production case study

Figure 7 shows the process flowsheet of an organic chemical production case study from Hall (12). The limiting data for the water demands and sources of this case study are summarised in Table 1.

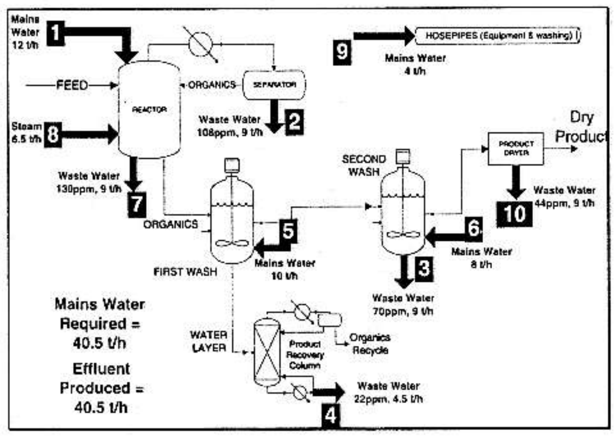

Figure 7 - Organic chemical production plant

Table 1 - Limiting water data for AN production

Water demands, D_j		Flowrate	Concentration
j	Stream	F_j (t/h)	C_j (ppm)
1	Reactor inlet	12	63
5	First wash	10	140
6	Second wash	8	63
8	Steam to reactor	6.5	46

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9	Hosepipes	4	130
Water sources, S_i		**Flowrate**	**Concentration**
i	**Stream**	F_i **(t/h)**	C_i **(ppm)**
2	Reactor overhead	9	108
3	Second wash	9	70
4	Distillate bottom	4.5	22
7	Reactor outlet	9	130
10	Dryer outlet	9	44

As shown in Table 1, none of these water-using operations can be modelled as a mass transfer process [1]. Utilising the water source and demand composite curves [3], Hall [12] located the water targets for this system to be 13 t/h for both fresh water and wastewater flowrate. However, as will be shown in the next section of this paper, this targeting tool is actually a sub-optimal solution where no fresh water is actually needed in this process.

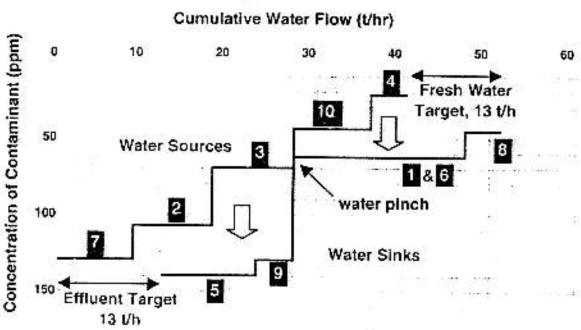

Figure 8 - Water source and demand composite curves for organic chemical production case study

Water Cascade Analysis technique – tubular approach

The main objective of the Water Cascade Analysis (WCA) is to establish the minimum water targets, i.e. 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. To achieve this objective, one has to establish the net water flowrate as well as the water surplus and deficit at the different water purity levels within the process under study. The *interval water balance table* has been introduced for this purpose. The AN production case study described in the previous section is used to illustrate the WCA water targeting technique is presented next.

The first step in the WCA is to set up the *interval water balance table* (Table 2) to determine the net water source or water demand at each purity level. The first column of Table 2 contains the contaminant concentration levels (C) arranged in ascending order. Each concentration level is expressed in terms of the water purity (P) in the second column. With the concentration of pure water set at one million ppm, the fraction of pure water in a contaminated stream, or the *water purity*, can be expressed as [4]:

$$\text{Purity, } P = \frac{1000000 - C}{1000000} \qquad (1)$$

where:

C = contaminant concentration in ppm.

The number of purity intervals (n) equals the number of water demands (N_D) and the number of water sources (N_S) minus any duplicate purity (N_{DP}):

$$n = N_D + N_S - N_{DP} \qquad (2)$$

Table 2 - The interval water balance table for Case Study 1

Column	1	2	3	4	5	6	7
Interval, n	**Conc. C_n(ppm)**	**Purity, P_n**	ΔP	$\Sigma F_{D,j}$ **(t/h)**	$\Sigma F_{S,i}$ **(t/h)**	$\Sigma F_{D,j}+\Sigma F_{S,i}$ **(t/h)**	**Net water source / demand**
1	0	1.000000	0.000022			0	
2	22	0.999978	0.000022		4.5	4.5	Source
3	44	0.999956	0.000002		9	9	Source
4	46	0.999954	0.000017	-6.5		-6.5	Demand
5	63	0.999937	0.000007	-20		-20	Demand
6	70	0.999930	0.000038		9	9	Source
7	108	0.999892	0.000022		9	9	Source
8	130	0.999870	0.000010	-4	9	5	Source
9	140	0.999860	0.999860	-10		-10	Demand
10		0					

Column 3 of Table 2 contains the water purity difference (ΔP), calculated as follows:

$$\Delta P = P_n - P_{n+1} \qquad (3)$$

Columns 4 and 5 contain the flowrates for the water demands ($\sum_j F_{D,j}$) and water sources ($\sum_i F_{S,i}$) at their corresponding purity levels. The flowrate of water demand is fixed as negative, and the water source positive. These flowrates are summed up at each purity level to give the *net* *interval* water flowrate, ($\sum_j F_{D,j} + \sum_i F_{S,i}$, column 6); (+) representing *net water source*, (-) *net water demand* (column 7).

The next key step in the WCA is to establish the fresh water and wastewater targets for the process. In doing so, it is important to consider *both* the water flowrate balance and the concentration driving force (water purity) so that the *true minimum* water targets can be obtained. The water flowrate balance involves using the water cascade diagram shown in Figure 9 to get the *cumulative* net water source/demand (F_C) for a process.

For the water cascade diagram in Figure 9(a), a fresh water flowrate (F_{FW}) of 0 kg/s is assumed. Here, the net water demand of 4.5 t/h at the second purity level (no water source and demand is found in the first purity interval) is cascaded to the third purity level to meet another water source of 9.0 t/h, giving a cumulative net of 13.5 t/h (source). This cumulative source meets the net water demand (6.5 t/h) down the fourth purity level to yield a cumulative water source of 7.0 t/h. The water cascade operation is then carried out until the lowest purity level (140 ppm) and locates a wastewater flowrate (F_{WW}) of 0 t/h.

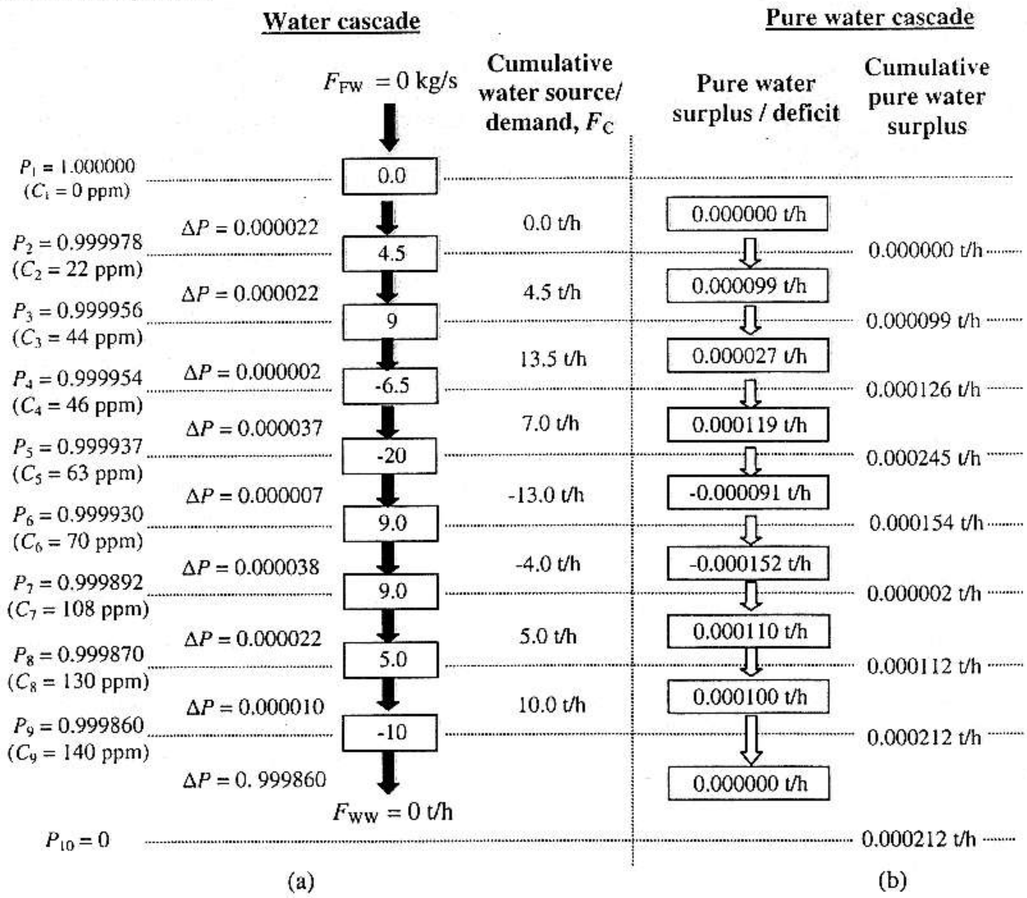

Figure 9 - (a) Water cascade diagram with an assumed fresh water flowrate of 0 kg/s; (b)Pure water cascade is used to check the feasibility of the water cascade

The *cumulative* net water source/demand for the process (F_C) at each purity interval forms the net interval water cascade diagram. The water cascade diagram is similar to the *interval heat balance table* for the problem table algorithm in heat integration [6] and the table of exchangeable loads for mass exchange cascade diagram in mass integration [5]. A conceptual illustration of how water cascading can minimise fresh water needs and wastewater generation is represented by Figure 10. By making use of 9 t/h of the net water source at the third purity level of 0.999956 (44 ppm) to satisfy the water demand of 6.5 t/h at the fourth purity level of 0.999954 (46 ppm), it is possible to avoid sending part of the net water source directly to effluent. Doing so will reduce both the wastewater generation and the fresh water consumption.

The water cascade diagram depicting the preliminary water balance (i.e., with F_{FW} = 0 kg/s) is essential as a basis to generate a feasible water cascade, and ultimately, the true minimum water targets. Note again that, in addition to considering the water flowrate balance, the true

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minimum targets can only be realised by also taking into account the pure water surplus or deficit, which is a product of the cumulative net water source/demand (F_C) and the purity difference (ΔP) across two purity levels (Figure 9b). A pure water surplus (+) means that water is available with purity higher than what is required in this region. On the other hand, a pure water deficit (-) means that water of higher purity than those available is required [4]. Cascading the pure water surplus/deficit down the purity intervals yields the pure water cascade that represents the cumulative amount of pure water surplus/deficit (Figure 9b). The cumulative pure water surplus/deficit at each purity level is a numerical representation of the water surplus diagram introduced by Hallale [4] (Figure 5).

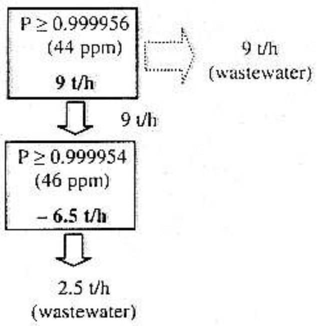

Figure 10 - The principle of water cascading

Notice that in this case study, none of the purity levels of the pure water cascade in Figure 9(b) consist of cumulative pure water deficits. The deficits on the pure water cascade, which quite often occur in other case studies [14], correspond to the negative region of Hallale's water surplus diagram (Figure 11) [4], indicate that the pure water cascade is "infeasible". These deficits means that there is insufficient fresh water in the network and are the result of assuming zero fresh water flowrate (F_{FW}) during water cascading. Thus, additional fresh water should be supplied to remove all pure water deficits and yield a feasible pure water cascade.

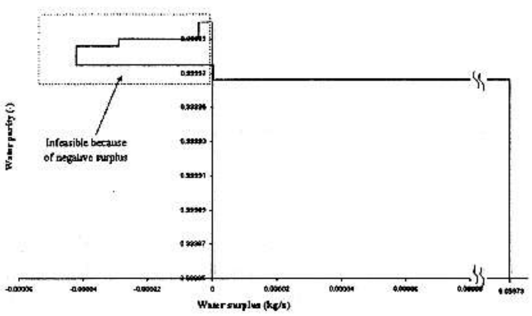

Figure 11 - A negative water surplus in the water surplus diagram indicate an infeasible water network

In order to remove the pure water deficits, we need to have the *cumulative fresh water flowrate* ($F_{FW,cum}$) for each purity level. This value is obtained by dividing the cumulative pure water surplus/deficit by the contaminant concentration, $1 - P$ as follows,

$$F_{FW,cum} = \frac{\text{cumulative pure water surplus/deficit}}{1 - P} \quad (4)$$

A negative $F_{FW,cum}$ means that there is insufficient fresh water whereas a positive $F_{FW,cum}$ means that there is excess fresh water at the given purity level. In order to ensure that there is sufficient fresh water at all points in the network, a fresh water flowrate (F_{FW}) of exactly the same magnitude as the absolute value of the largest negative $F_{FW,cum}$ should be supplied at the highest purity level of a *feasible water cascade*. A feasible water cascade is the one that results in positive, or at least, zero cumulative pure water surplus value in the pure water cascade. A case study utilising the feasible water cascade in locating the *true minimum* fresh water and wastewater flowrate targets is presented in another paper by the authors [15].

In this organic chemical case study, since there is no pure water deficit in the pure water cascade, we conclude that the 0 t/h of fresh water and wastewater flowrate to be the minimum utility targets for the process. It should also be noted that, since there is neither fresh water needed nor wastewater generated from the process, this is a special kind of threshold problem in water network analysis. All the wastewater generated by the water sources is fully reused by the water demands. This eventually leads to a fully "zero-emission" process.

Case Study 2 – Multiple stream problem

Savelski and Bagajewicz [13] presented an algometric procedure in handling the multiple stream problem. They claimed that even without going through the utility targeting step, the algometric procedure is able to design a minimum utility water network. However, this claim is not always true. As will be demonstrated in this case study, omitting the targeting step will always lead to a higher utility network.

Limiting data for this twenty-stream case study is shown in Table 3. Savelski and Bagajewicz [13] reported the fresh water flowrate for this case study to be at 299.35873 t/h. Though the authors reported a 36.6% of water reduction compared to the process without water reuse, this does not guarantee that the minimum utility solution is reached. As will be shown in the following section, more water recovery is actually possible.

Table 3 - Limiting water data for Case Study 2

Water demand			Water source		
D_j	F_j	C_j	S_i	F_i	C_i
1	12.5	0	1	12.5	80
2	20	0	2	20	100
3	16.6667	0	3	16.6667	120
4	25	25	4	25	80
5	32	25	5	32	90
6	16.6667	40	6	16.6667	90
7	30	50	7	30	100
8	33.3333	75	8	33.3333	120
9	20	25	9	20	200
10	66.6667	75	10	66.6667	150
11	40	120	11	40	200
12	6	200	12	6	300
13	66.6667	75	13	66.6667	300
14	21.6667	150	14	21.6667	300
15	3.3333	200	15	3.3333	60
16	37.5	50	16	37.5	800
17	6.25	400	17	6.25	800
18	14	400	18	14	500
19	3	600	19	3	850
20	0.63158	800	20	0.63158	950

Water Cascade Analysis technique – LP approach

This section will highlight the use of linear programming (LP) approach in automating the WCA procedure. Firstly, we need to generalise the interval water balance table (Table 2) in the numerical way. The entire purity range of the table is divided into n purity level, with the highest purity level being donated to n = 1. The number of n is given by Equation 2.

At each individual purity level, the net interval water flowrate ($F_{\text{sum},\ n}$) is given by the different between the individual total water source and demand flowrate, i. e.

$$F_{\text{sum},n} = \sum_i F_{\text{S},i} - \sum_j F_{\text{D},j} \qquad (5)$$

Then, the minimum utility targeting problem can be formulated as follows:

$$\min F_{\text{FW}} \qquad (6)$$

subject to

$\delta_{n-1} + F_{\text{sum},\,n} = \delta_n\ ,\ n \geq 1$

$\delta_n \times \Delta P_n = \varepsilon_{n+1}\ ,\ n \geq 1$

$\delta_0 = F_{\text{FW}}$

$\varepsilon_n \geq 0\ ,\ n \geq 1$

where ΔP_n is the difference between two subsequent purity level, i. e. $P_n - P_{n+1}$; while ε_n represents the value of the cumulative pure water surplus in the pure water cascade.

The above formulation is a LP problem which can be easily solved using any mathematical modelling software. The location of the pinch point between two consecutive purity level, n and n +1 is indicated when the cumulative pure water surplus ε_n vanishes.

Applying this formulation to the multiple stream problem of Case Study 2 will yield a minimum fresh water flowrate (F_{FW}) of 198.2556 t/h. This is an additional 34% reduction of utility consumption compared to the solution proposed by Savelski and Bagajewicz [13], or a total amount of 70% reduction compared to the original solution with water reuse. As can be seen, the targeting tool plays an important role in locating the right target in the water minimisation problem.

Conclusions

A new method to establish the minimum water and wastewater targets for continuous water-using processes, known as the Water Cascade Analysis (WCA), has been developed. WCA is a numerical technique that can quickly yield accurate water targets and pinch point locations for a water network. By eliminating the tedious iterative steps of the water surplus diagram, WCA offers a key complimentary role to the water surplus diagram in the design and retrofit of water recovery network. Various options involving process changes, including water regeneration and equipment modifications can be systematically assessed using the WCA. Problems involving multiple-streams can now be handled more efficiently, accurately and with much less effort. All the key features and the systematic nature of the WCA make it easy for the technique to be automated and translated into any computer language for software development.

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