

# Targeting the Minimum Water Flow Rate Using Water Cascade Analysis Technique

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*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 (WPA) as problem table analysis (PTA) 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 minimum water targets, pinch point locations, and water allocation targets for a maximum water recovery (MWR) network, thereby offering a key complementary role to the water surplus diagram in the synthesis of water 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. © 2004 American Institute of Chemical Engineers AIChE J, 50: 3169–3183, 2004*

**Keywords:** water minimization, minimum water and wastewater targets, water allocation targets, pinch analysis, Water Cascade Table

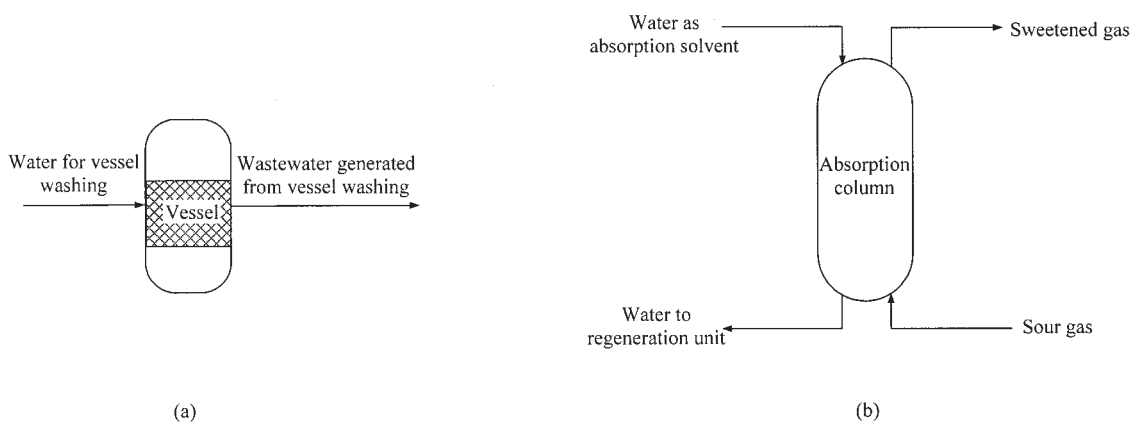
## Introduction

The current drive toward 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 minimization over the last 10 years. The WPA technique, as proposed by Wang and Smith,<sup>1</sup> generally considers the potential of using fresh or recycle water as a lean stream to absorb certain contaminants from various process operations, provided

there is a driving force for mass transfer. Maximizing water reuse and recycling can minimize freshwater consumption and wastewater generation.

Water-using operations in a process plant can generally be classified into mass-transfer-based and non-mass-transfer-based operations. A mass-transfer-based water-using operation is characterized by the preferential transfer of species from a rich stream to water, which is being used 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 recycled water. Cleaning involves the preferential transfer of species (contaminant) from a “rich stream” (in this case, the vessel) to a lean stream or an MSA (in this case, water). During cleaning, water is fed into the vessel (as a demand) while wastewater is generated (as a source) as shown in Figure 1a. Another example of a mass-transfer-based water-using operation is the absorption process where water is the MSA used to remove contaminants such as H<sub>2</sub>S and SO<sub>2</sub> from a sour gas stream (see Figure 1b). Note that the input

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**Figure 1. Mass transfer-based water-using operations.**

(a) Vessel washing; (b) sour gas absorption where water demand and water source exist.

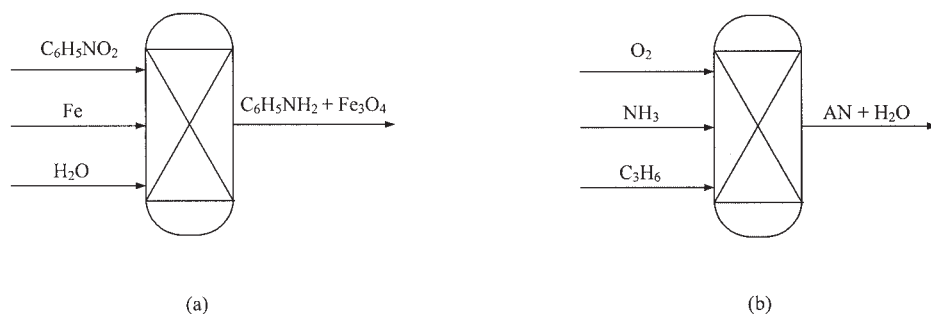
and output flow rates of a mass-transfer process are assumed to be equal.

The non-mass-transfer-based water-using operation covers functions of water other than as a mass separating agent. 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 used as heating or cooling media. Water, as a raw material fed into a reactor or as heating or cooling medium, is clearly typical of non-mass-transfer operations because these operations are not designed to preferentially transfer species (contaminant) between streams. For such operations, sometimes, only water demands or water sources exist as shown in Figure 3. Note that, for non-mass-transfer-based water-using operations, the water flow rate is more important than the amount of contaminant accumulated. Thus, a non-mass-transfer-based process can have different inlet and outlet flow rates. Although the conventional water network studies have focused on the mass-transfer-based model,<sup>1-4</sup> recent studies have shown that the non-mass-transfer-based water-using operations are also important to consider.<sup>5-8</sup> Figure 4 shows a reactor with several input and output streams at different concentrations.<sup>8</sup> Clearly, such a system cannot be modeled using the mass-transfer-based techniques such as those proposed by Wang and Smith.<sup>1</sup>

### Previous Work on Water Targeting

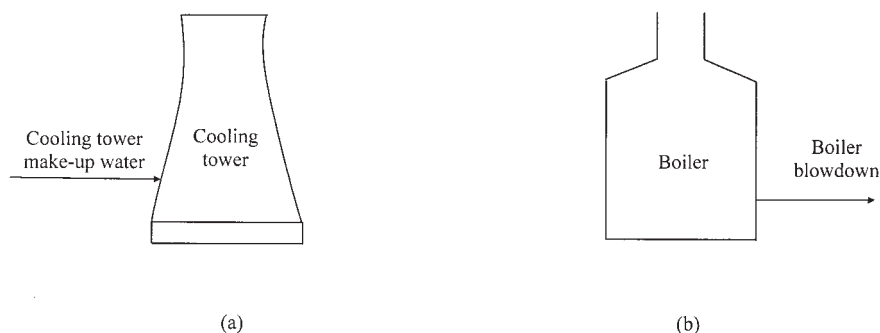
In targeting the minimum utility requirements and in locating the pinch points, the graphical technique such as the composite curves and the numerical technique such as the problem table have both been used in the heat,<sup>9</sup> mass,<sup>10,11</sup> and water recovery problems<sup>4,12</sup> that 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 complementary roles they play in pinch analysis. Graphical tools such as composite curves are 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 such as the *problem table analysis* (PTA) in heat integration<sup>9</sup> or the *composition interval table* (CIT) in mass integration<sup>10,11</sup> are advantageous from the perspective of accuracy and speed and are thus 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<sup>1</sup> introduced the plot of composition vs. contaminant mass load, or the water composite curves, which they termed as the limiting water profile, for graphical water targeting. They made use of the limiting water profile to



**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 by-product in acrylonitrile (AN) production.



**Figure 3. Two other common types of the non-mass-transfer-based water-using operations.**

(a) Cooling tower make up; (b) boiler blow-down.

pinpoint the pinch location and generate the exact minimum water targets before network design. Various options for water reuse, regeneration–reuse, and regeneration–recycling were also explored. The limiting water profile represents a major stride in establishing the baseline water requirement and wastewater generation for a process. However, its applicability is limited to only mass-transfer–based operations. Water used 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.<sup>5</sup> introduced the water source and demand composite curves. They also suggested process changes such as mixing and bypassing to further reduce the fresh water consumption. However, Polley and Polley<sup>7</sup> later indicated that, unless the correct stream mixing system was identified, the apparent targets generated by Dhole’s technique<sup>5</sup> could be substantially higher than the true minimum fresh water and wastewater targets.

Sorin and Bédard<sup>6</sup> 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.<sup>5</sup> could result in a number of “local” pinch points, which might not necessarily be the actual or the “global” pinch points. However, Hallale<sup>8</sup> recently showed that, when more than one global pinch points occurred in water-using processes, the evolutionary table failed to locate them correctly.

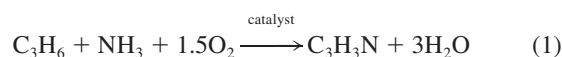
Hallale<sup>8</sup> presented an alternative graphical method called the

*water surplus diagram* (Figure 5) to target the minimum fresh water and wastewater. The method, which was adapted from the hydrogen pinch analysis,<sup>13</sup> had a similar representation to the water source and demand composite curves proposed by Dhole et al.,<sup>5</sup> and is thereby not limited to mass-transfer–based operations. The new representation by Hallale<sup>8</sup> could handle all mixing possibilities and yet resulted in the true pinch point and reuse target. However, the water surplus diagram has the same drawbacks as those of the composite curves. It is tedious and time consuming to draw because it involves trial-and-error solution to find the pinch points and water targets. Besides, it has limitations in terms of generating highly accurate targets because of its graphical nature. The tedious iterative procedure to construct the water surplus diagram is shown in Figure 6. To eliminate the trial-and-error steps and complement the graphical method, there is a need for a numerical equivalent of the water surplus diagram similar to the PTA in heat integration or the CIT in mass integration, which constitutes the subject of this article.

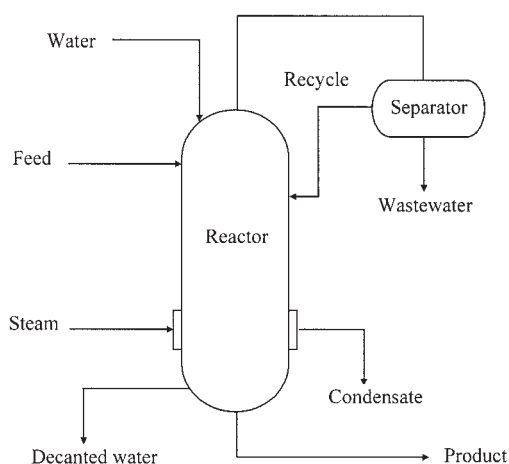
This work presents the *Water Cascade Analysis* (WCA), a new numerical technique to establish the minimum water and wastewater targets in a maximum water recovery (MWR) network. The WCA eliminates any tedious iterative step to quickly yield the exact utility targets and the pinch location(s). As in the 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. A case study on water minimization involving acrylonitrile production from El-Halwagi<sup>11</sup> is used to illustrate the procedure for water and wastewater targeting using the WCA.

### Acrylonitrile Case Study

Figure 7 shows the process flow diagram for acrylonitrile (AN) production. AN is produced by the vapor-phase ammoxidation of propylene that takes place in a fluidized-bed reactor at 450°C and 2 atm, according to the following equation



This is a single-pass reaction with almost complete conversion of propylene. Products from the reactor are cooled and partially condensed. The reactor off-gas is sent to a scrubber that uses



**Figure 4. A reactor system that cannot be modeled purely as a mass-transfer-based operation.<sup>8</sup>**

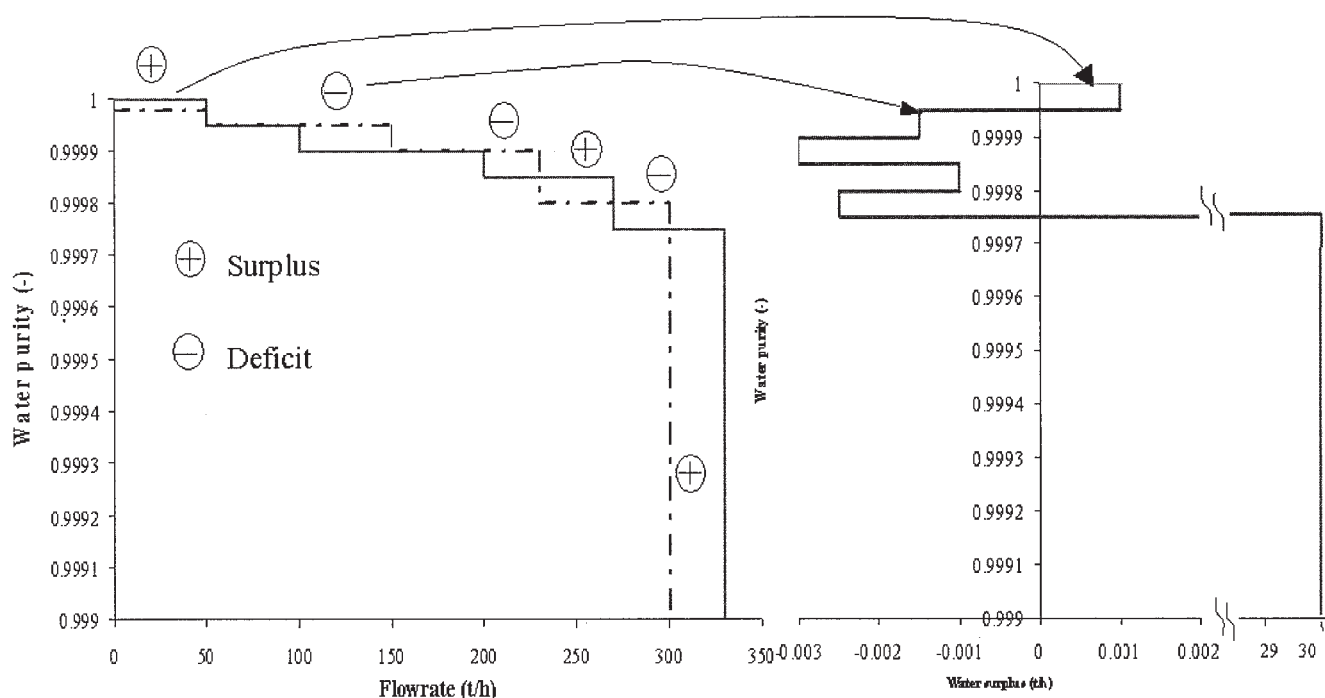


Figure 5. Water surplus diagram by Hallale.<sup>8</sup>

fresh water as the scrubbing agent. The bottom product from the scrubber is separated into the aqueous layer and an organic layer in a decanter. The organic layer is later fractionated in a slightly vacuumed distillation column that is induced by a steam-jet ejector. Material balance data for the case study are shown in Figure 7.

There are two water demands for this process: the boiler feed water (BFW) and the water feed stream to the scrubber. There are four water sources that include the off-gas condensate, the aqueous layer from the decanter, the distillation column bottoms product, and the condensate from the steam-jet ejector. Ammonia ( $\text{NH}_3$ ) is the main contaminant in this process. Here, the water sources are regarded as wastewater and sent to a biotreatment facility operated at full capacity.

One way to debottleneck the overall process is by water reuse and recycling. However, any proposed solution must

comply with the flow rate and concentration constraints imposed on the water demands and sources, as listed below.

- (1) Scrubber
  - $5.8 \leq \text{flow rate of wash feed (kg/s)} \leq 6.2$
  - $0.0 \leq \text{NH}_3 \text{ content of wash feed (ppm)} \leq 10.0$
- (2) BFW
  - $\text{NH}_3 \text{ content} = 0.0 \text{ ppm}$
  - $\text{AN content} = 0.0 \text{ ppm}$
- (3) Decanter
  - $10.6 \leq \text{feed flow rate (kg/s)} \leq 11.1$
- (4) Distillation column
  - $5.2 \leq \text{feed flow rate (kg/s)} \leq 5.7$
  - $0.0 \leq \text{NH}_3 \text{ content of feed (ppm)} \leq 30.0$
  - $80.0 \leq \text{AN content of feed (wt\%)} \leq 100.0$

The first step in establishing the minimum water target is to identify the limiting water data for the process, subject to the constraints listed above. Note that, of the four listed constraints, only the first two (that is, scrubber and BFW), which involve the streams selected for water reuse analysis, are considered. The first constraint requires the flow rate and the concentration of  $\text{NH}_3$  in the scrubber wash feed to be bounded within the given range. Thus, to maximize water reuse, one should maximize the  $\text{NH}_3$  concentration while keeping the flow rate of this water demand to a minimum. The second constraint means that only pure water should be used as the BFW. The limiting data for the water demands and sources are summarized in Table 1. Note from Figure 7 and Table 1 that none of these operations can be modeled as a mass-transfer process. Also note that the limiting flow rate of each water demand and source in Table 1 is based on the total stream mass flow rate that includes all components present in the streams (that is, water,  $\text{NH}_3$ , and acrylonitrile), which is inconsistent with the original limiting data used in El-Halwagi.<sup>11</sup>

El-Halwagi<sup>11</sup> proposed a targeting technique for the limiting

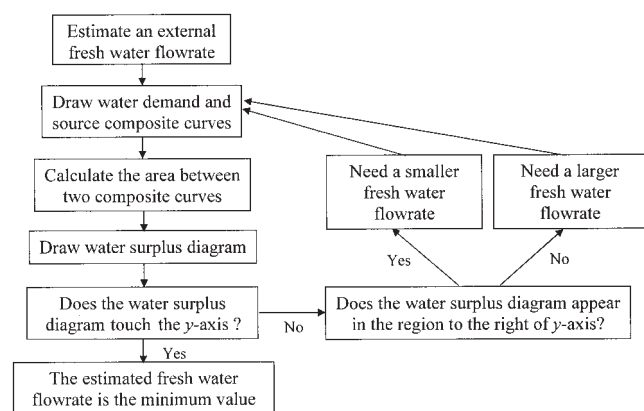


Figure 6. Tedious iterative steps of constructing the water surplus diagram.

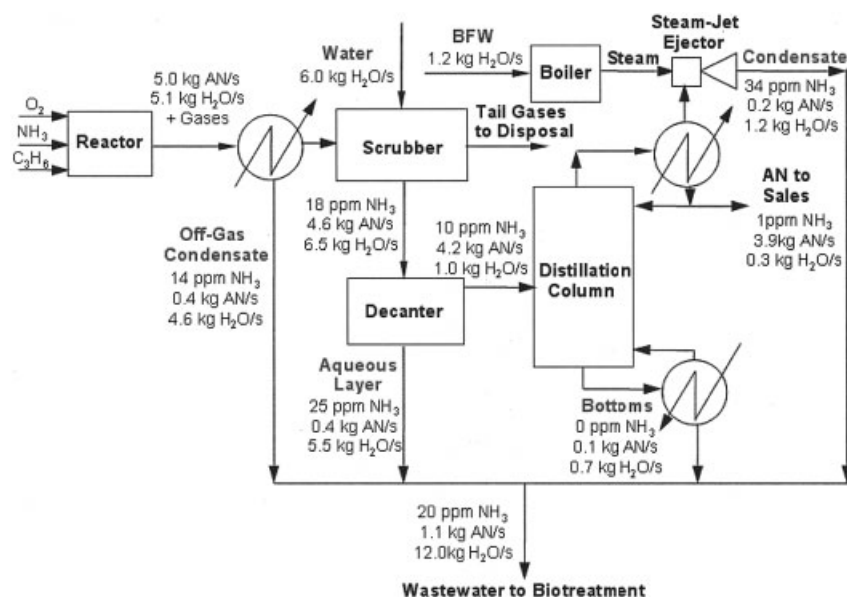


Figure 7. Flowsheet for AN production.<sup>11</sup>

data in Figure 8. However, his simplified technique considers only the overall water flow rate balance and ignores the driving force for water reuse. Clearly, without considering the thermodynamic constraint (the concentration driving force), one could easily overlook the true minimum target. Based on this simplified technique, El-Halwagi<sup>11</sup> reported that no fresh water was needed for this operation while the wastewater flow rate was targeted at 4.8 kg/s. As will be shown later, the target predicted by El-Halwagi<sup>11</sup> is valid only after various approaches have been taken to reduce the inherent water requirement of the process. This includes water reuse, regeneration, and implementation of process changes (that is, by substituting steam-jet ejector with a vacuum pump). Note that there was no mention of the minimum water target for the base case process, that is, before regeneration and process changes take place.

In the same work, El-Halwagi<sup>11</sup> also proposed a systematic method to design the water reuse network for the process by means of the source-sink mapping diagram. However, without the knowledge of the *true minimum* target ahead of design, there will always be questions as to whether further improvements on the network are still possible. Clearly, it is essential to have a good targeting tool to determine the true minimum target. As a guideline, a good tool should satisfy three basic requirements as follows:

- (1) It should be capable of handling both mass-transfer-based and non-mass-transfer-based water operations.
- (2) It should consider the flow rate and the concentration driving force for water reuse.
- (3) It should be noniterative, and thus can quickly yield the exact targets.

In the next section, we demonstrate the use of WCA as a new tool for water targeting that fulfills all the basic requirements outlined.

### The Water Cascade Analysis Technique

The main objective of the *Water Cascade Analysis* (WCA) is to establish the minimum water targets, that is, 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

Table 1. Limiting Water Data for AN Production

Water Demands, $D_j$		Flow Rate, $F_j$ (kg/s)	Concentration, $C_j$ (ppm)
$j$	Stream		
1	BFW	1.2	0
2	Scrubber	5.8	10
Water Sources, $S_i$		Flow Rate, $F_i$ (kg/s)	Concentration, $C_i$ (ppm)
$i$	Stream		
1	Distillation bottoms	0.8	0
2	Off-gas condensate	5	14
3	Aqueous layer	5.9	25
4	Ejector condensate	1.4	34

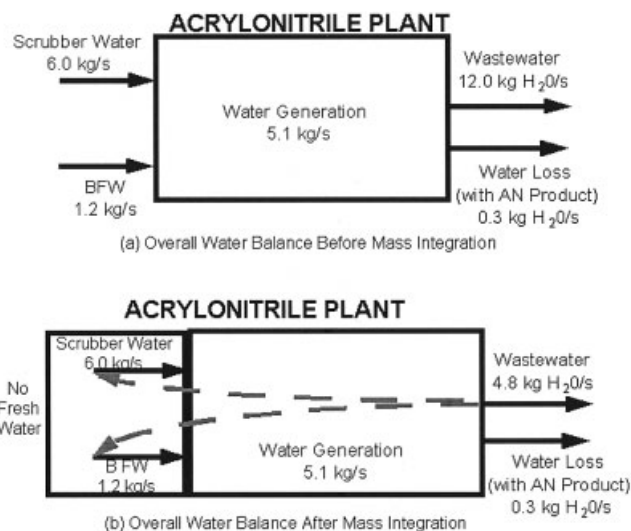


Figure 8. Targeting model by El-Halwagi.<sup>11</sup>



**Table 2. Interval Water Balance Table for AN Production Case Study**

Level, $k$	Column Number						Net Water Source/ Demand
	1 Concentration, $C_k$ (ppm)	2 Purity, $P_k$	3 $\Delta P$	4 $\sum_j F_{D,j}$ (kg/s)	5 $\sum_i F_{S,i}$ (kg/s)	6 $\sum_j F_{D,j} + \sum_i F_{S,i}$ (kg/s)	
1	0	1.000000		-1.2	0.8	-0.4	Demand
2	10	0.999990	0.000010	-5.8		-5.8	Demand
3	14	0.999986	0.000004		5.0	5.0	Source
4	25	0.999975	0.000011		5.9	5.9	Source
5	34	0.999966	0.000009		1.4	1.4	Source
6	1,000,000	0	0.999966				

this objective, one has to establish the net water flow rate 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.

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<sup>8</sup>

$$P = \frac{1,000,000 - C}{1,000,000} \quad (2)$$

where  $C$  is the contaminant concentration in ppm.

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

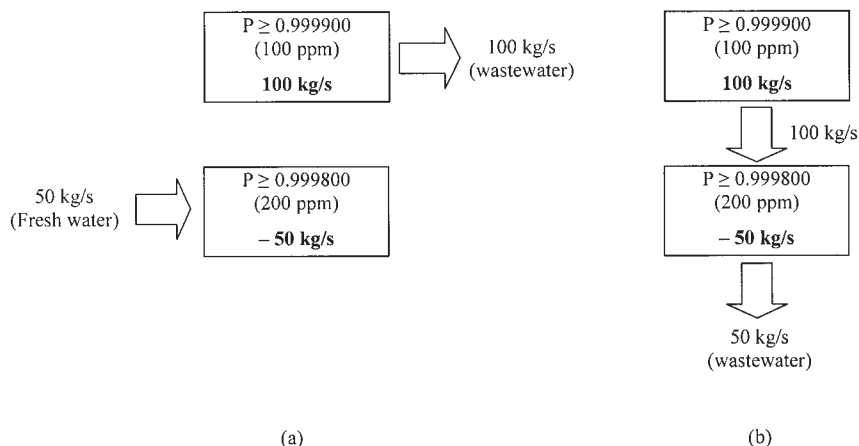
$$n = N_D + N_S - N_{DP} \quad (3)$$

Application of Eq. 3 to the AN case study yields six purity levels. Next, the water purity difference ( $\Delta P$ ) in column 3 of Table 2 is calculated as the difference between purity level at intervals  $k$  and  $k + 1$ , as follows

$$\Delta P = P_n - P_{n+1} \quad (4)$$

Columns 4 and 5 contain the total flow rates for the water demands ( $\sum_j F_{D,j}$ ) and water sources ( $\sum_i F_{S,i}$ ) at their corresponding purity levels. The flow rate of water demand is fixed as negative, and the water source positive. These flow rates are summed up at each purity level to give the *net interval* water flow rate ( $\sum_j F_{D,j} + \sum_i F_{S,i}$ , column 6), where (+) represents *net water source* and (-) is *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 flow rate balance and the concentration driving force (water purity) so that the true minimum water targets can be obtained. The water flow rate balance involves using the *water cascade diagram* (Figure 10) to obtain the *cumulative* net water source/demand for a process ( $F_C$ ). A conceptual illustration of how water cascading can minimize fresh water needs and wastewater generation is represented by Figure 9. In Figure 9a, 100 kg/s of wastewater is produced by a water source at the purity level of 0.999900 (100



**Figure 9. Principle of water cascading.**

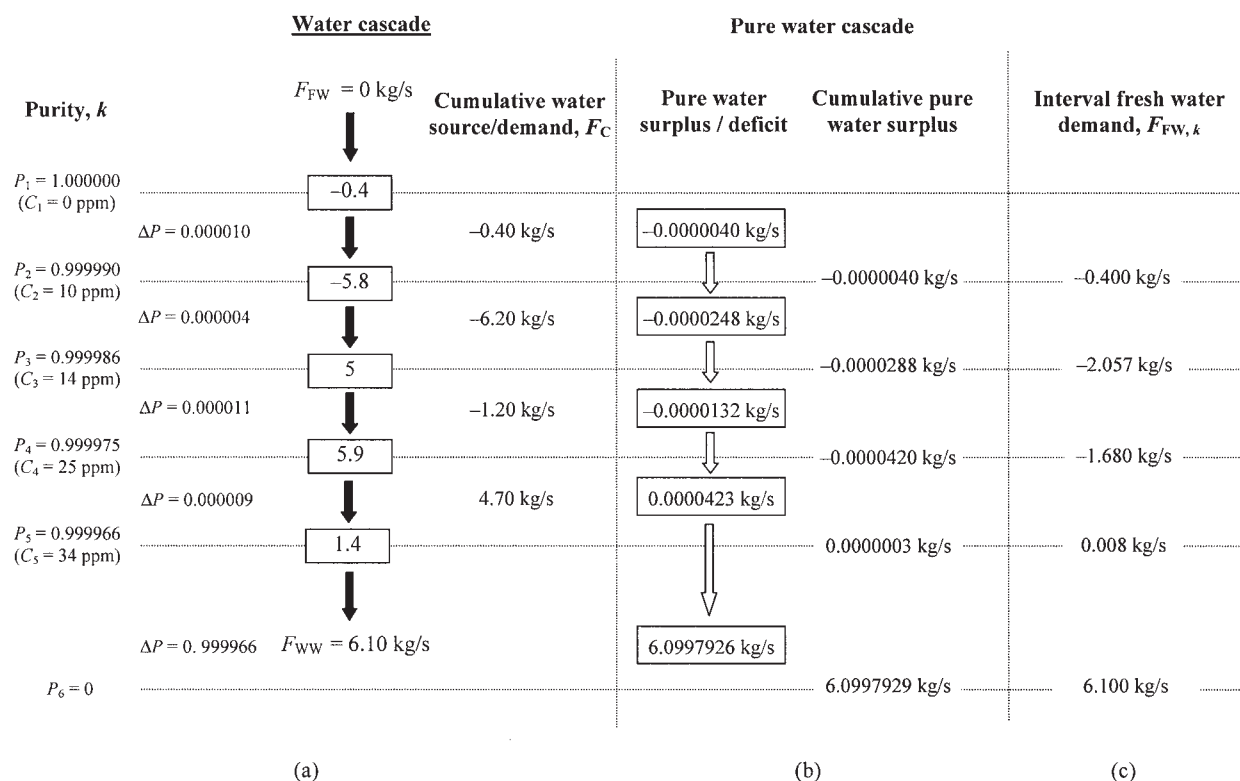


Figure 10. (a) Water cascade diagram with an assumed fresh water flow rate of 0 kg/s; (b) pure water cascade is used to check the feasibility of the water cascade; (c) interval fresh water demand to determine the fresh water amount needed in each purity interval.

ppm) and 50 kg/s of water is needed by a water demand at the purity level of 0.999800 (200 ppm). Without considering water reuse, 100 kg/s of wastewater would be generated, whereas 50

kg/s of fresh water would be required. However, as shown in Figure 9b, by making use of 100 kg/s of the water source at the purity level of 0.999900 (100 ppm), to satisfy the water de-

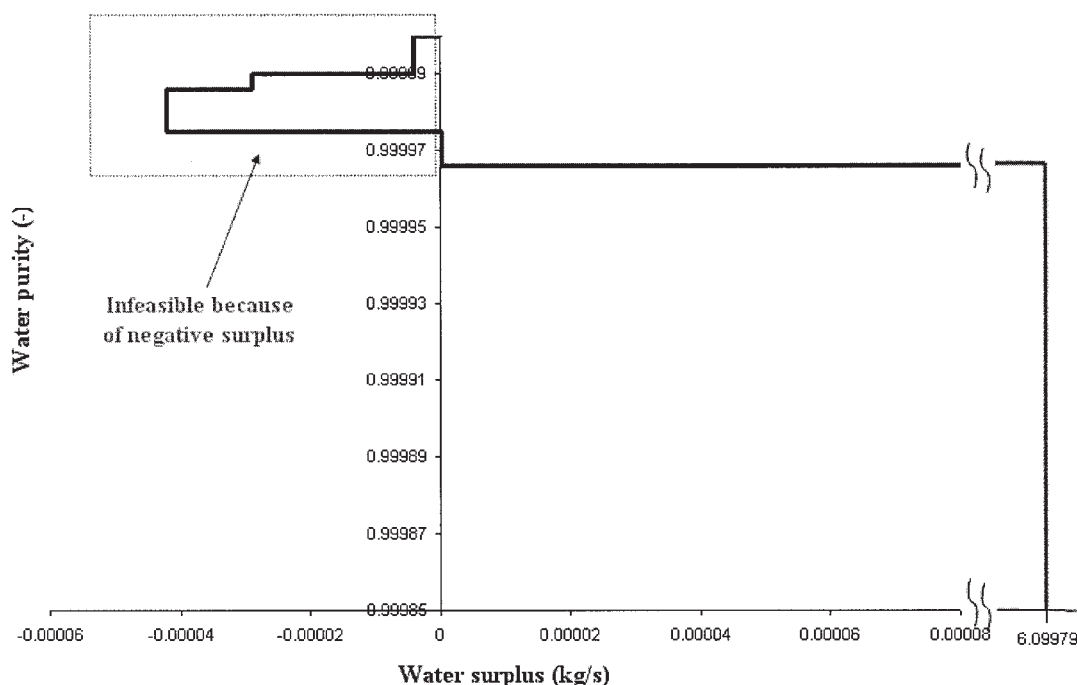


Figure 11. An infeasible water surplus diagram<sup>8</sup> for AN case study with assumed zero fresh water flow rate.

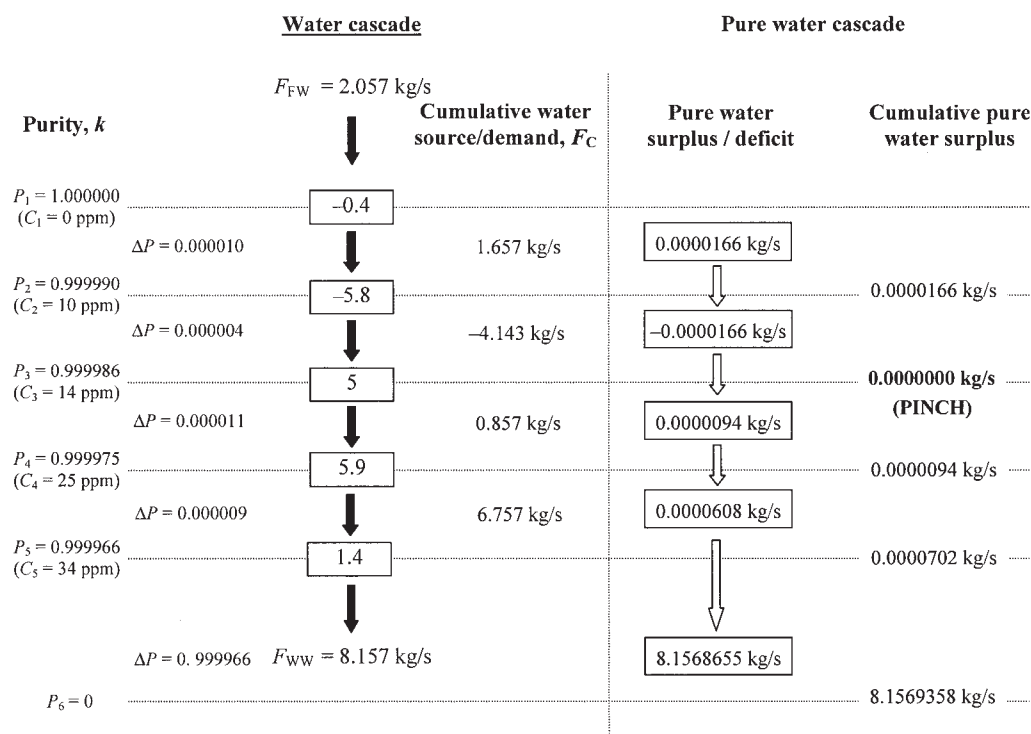


Figure 12. A feasible water cascade for the AN case study.

mand of 50 kg/s at the purity level of 0.999800 (200 ppm), it is possible to avoid sending part of the water source directly to effluent (at  $P = 0.999900$ ). Doing so not only reduces the wastewater generation but also the fresh water consumption, in both cases, by 50 kg/s.

For the water cascade diagram in Figure 10a, a fresh water flow rate ( $F_{FW}$ ) of 0 kg/s is assumed. Here, the net water demand of 0.4 kg/s at the first purity level is cascaded to the second purity level to meet another water demand of 5.8 kg/s, giving a cumulative net of  $-6.20$  kg/s (demand). This cumulative demand meets only net water sources down the next three purity levels to yield a cumulative water source, or wastewater flow rate ( $F_{WW}$ ), of 6.10 kg/s at the lowest purity level of the water cascade diagram. 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

PTA in heat integration<sup>9</sup> and the table of exchangeable loads for CIT in mass integration.<sup>11</sup>

The water cascade diagram depicting the preliminary water balance (that is, 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 flow rate balance, the true minimum targets can be realized only 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 ( $\Delta P$ ) across two purity levels (Figure 10b). 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 that available is required.<sup>8</sup> 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

Table 3. Water Cascade Table (WCT) for AN Production Case Study

Level, $k$	Concentration, $C_k$ (ppm)	Purity, $P_k$	$\sum_j F_{D,j}$ (kg/s)	$\sum_i F_{S,i}$ (kg/s)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (kg/s)	$F_C$ (kg/s)	Pure Water Surplus (kg/s)	Cumulative Pure Water Surplus (kg/s)
						$F_{FW} = 2.06$		
1	0	1.000000	−1.2	0.8	−0.4	1.66	0.0000166	
2	10	0.999990	−5.8		−5.8	−4.14	−0.0000166	0.0000166
3	14	0.999986		5.0	5.0	0.86	0.0000094	<b>0</b>
4	25	0.999975		5.9	5.9	6.76	0.0000608	0.0000094
5	34	0.999966		1.4	1.4	$F_{WW} = 8.16$	8.1568655	0.0000702
6	1,000,000	0						8.1569358



**Table 4. WCT for Process Involving Partial Regeneration of Off-Gas Condensate**

Level, $k$	Concentration, $C_k$ (ppm)	Purity, $P_k$	$\sum_j F_{D,j}$ (kg/s)	$\sum_i F_{S,i}$ (kg/s)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (kg/s)	$F_C$ (kg/s)	Pure Water Surplus (kg/s)	Cumulative Pure Water Surplus (kg/s)
						$F_{FW} = 1.2$		
1	0	1.0000000	-1.2	0.8	-0.4	0.8	0.0000080	
2	10.0	0.9999900	-5.8		-5.8	-5.0	-0.0000080	0.0000080
3	11.6	0.9999884		5.0	5.0	0	0.0000000	0
4	25.0	0.9999750		5.9	5.9	5.9	0.0000531	<b>0</b>
5	34.0	0.9999660		1.4	1.4			0.0000531
						$F_{WW} = 7.3$	7.2997518	
6	1,000,000	0						7.2998049

10b). The cumulative pure water surplus/deficit at each purity level is a numerical representation of the water surplus diagram introduced by Hallale<sup>8</sup> (Figure 5).

Notice that for the *pure water cascade* in Figure 10b, cumulative pure water deficits are observed from second to fourth purity levels ( $P_2$ ,  $P_3$ , and  $P_4$ ). The deficits on the pure water cascade, which correspond to the negative region of Hallale's water surplus diagram (Figure 11),<sup>8</sup> indicate that the pure water cascade is "infeasible." These deficits mean that there is insufficient fresh water in the network and are the result of assuming zero fresh water flow rate ( $F_{FW}$ ) during water cascading. Thus, additional fresh water should be supplied to remove all pure water deficits and yield a feasible pure water cascade.

Fresh (or pure) water is to be supplied at the highest purity level. To minimize fresh water, it is necessary to determine the minimum flow rate of fresh water, or, the *interval fresh water demand* that will satisfy the total water requirement at each purity level. The interval fresh water demand will restore a feasible pure water cascade throughout the entire water network. Figure 10c shows that the *interval fresh water demand* ( $F_{FW,k}$ ) for each purity level  $k$  is obtained by dividing the cumulative pure water surplus/deficit by the purity difference between the fresh water supply ( $P_{FW}$ ) and purity level ( $P_k$ ) of interest, as follows

$$F_{FW,k} = \frac{\text{cumulative pure water surplus/deficit}}{P_{FW} - P_k} \quad (5)$$

Referring to Figure 10c, a negative value for  $F_{FW,k}$  means that there is insufficient fresh water, whereas a positive  $F_{FW,k}$  means that there is excess fresh water at the purity level  $k$ . To

ensure that there is sufficient fresh water at all points in the network, a fresh water flow rate of exactly the same magnitude as the absolute value of the largest negative  $F_{FW,k}$  should be supplied at the highest purity level of a feasible water cascade (Figure 12).  $F_{FW,3}$  value of -2.057 kg/s, found at the third purity level ( $P_3$ ) in Figure 10c, has the largest negative value. This quantity of fresh water is added at the highest purity level of the feasible water cascade in Figure 12. Note that 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. The feasible water cascade yields the true minimum fresh water ( $F_{FW}$ ) and wastewater flow rate ( $F_{WW}$ ) targets of 2.057 and 8.157 kg/s, respectively, for the AN case study.

At the third purity level ( $P_3 = 0.999986$ ;  $C_3 = 14$  ppm) of Figure 12, where there is zero cumulative pure water surplus, is the pinch for the AN problem. The *pinch* is the most constrained part of the network that results in maximum water recovery. The detailed network design proposed by El-Halwagi<sup>11</sup> confirmed the utility targets for this case study. Note that, through the WCA, we have obtained the utility targets ahead of design and are able to verify whether the proposed initial design<sup>11</sup> has achieved the MWR objective for the plant. The water cascade and the pure water surplus cascade diagrams can be integrated with the interval water balance table to form the *Water Cascade Table* (WCT) in Table 3.

Through WCT, the WCA technique offers two other key advantages over the water surplus diagram in realizing the minimum water targets, apart from its power to eliminate tedious iterative steps of water surplus diagram to quickly yield the exact utility targets and the pinch location(s). The first key advantage is that the WCT clearly displays both the minimum

**Table 5. WCT for Stream Regeneration and Process Changes**

Level, $k$	Concentration, $C_k$ (ppm)	Purity, $P_k$	$\sum_j F_{D,j}$ (kg/s)	$\sum_i F_{S,i}$ (kg/s)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (kg/s)	$F_C$ (kg/s)	Pure Water Surplus (kg/s)	Cumulative Pure Water Surplus (kg/s)
						$F_{FW} = 0$		
1	0	1.0000000	0	0.8	-0.8	0.8	0.0000080	
2	10.0	0.9999900	-5.8		-5.8	-5.0	-0.0000080	0.0000080
3	11.6	0.9999884		5.0	5.0	0	0.0000000	0
4	25.0	0.9999750		5.9	5.9			<b>0</b>
						$F_{WW} = 5.9$	5.8998525	
5	1,000,000	0						5.8998525

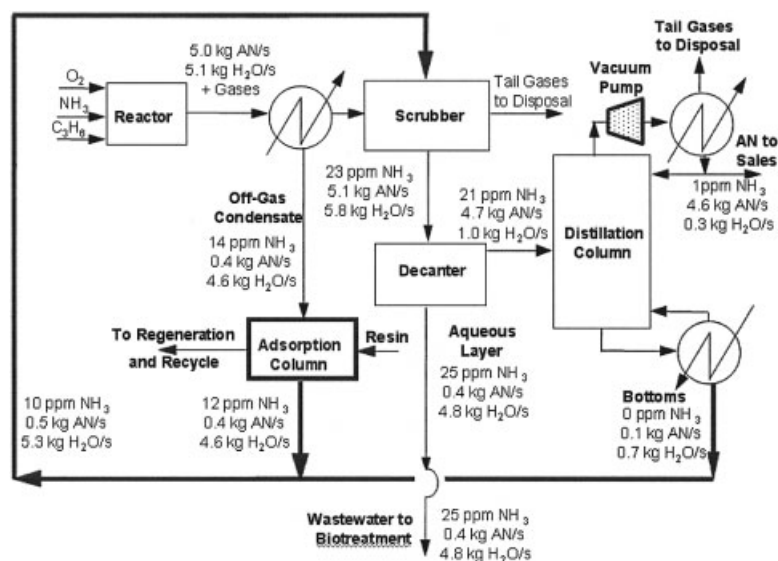


Figure 13. Final solution to the AN case study with water reuse and process changes by El-Halwagi.<sup>11</sup>

fresh water ( $F_{FW}$ ) and wastewater flow rate ( $F_{WW}$ ) targets in the cumulative net water source/demand ( $F_C$ ) column (see, for example, Table 3). Note that, in the case of the water surplus diagram, only the minimum fresh water target is known (obtained from the trial-and-error procedure outlined in Figure 6). However, the value of the minimum wastewater flow rate target is not available from the diagram.

The second key advantage of using WCT is that it enables a designer to clearly identify the pinch-causing stream and the exact water allocation for the regions above and below pinch to achieve the minimum water targets during network design. Hallale<sup>8</sup> reported that a pinch will always occur at the purity of a source, and is the point where the source switches from being below a demand (that is, deficit) to being above a demand (that is, surplus). Referring to Table 3, a zero cumulative pure water surplus at the purity level of 0.999986 ( $P_3$ ) represents the pinch point. Note that the pinch-causing stream(s), which exists at this purity level, is the water source ( $\sum_i F_{S,i}$ ) with a total flow rate of 5.0 kg/s. Referring to Table 1, this stream is a single water source, that is, the off-gas condensate ( $S_2$ ).

To realize the pinch point and to achieve the MWR objective, a portion of the pinch-causing source stream (in this case, the off-gas condensate) has to be allocated to a region above the pinch, whereas the rest is allocated to a region below the pinch during network design. The exact water allocation is available from the WCT. Referring to cumulative net water source ( $F_C$ ) column of Table 3, out of 5.0 kg/s water source from off-gas condensate, 4.14 kg/s of water (found at the

interval between  $P_2$  and  $P_3$ ) must be sent to the region above the pinch (the negative sign indicates sending water across the driving force). On the other hand, 0.86 kg/s of water (found at the interval between  $P_3$  and  $P_4$ ) must be sent to the region below the pinch. The exact water allocation flow rates can be readily verified with any detailed network design techniques for non-mass-transfer-based water-using processes, such as source-sink mapping diagram<sup>11,14,15</sup> or sink-source allocation.<sup>8,16</sup>

Such important insights on pinch-causing stream and water allocation are evident from the WCT but not available from the graphical technique of the water surplus diagram. With the water surplus diagram, it is necessary to construct the *balanced composite curve* to obtain the exact water allocation targets.<sup>8</sup>

### Assessing Options for Process Changes by the WCA

Making appropriate changes to a process has been widely accepted as an effective measure to further reduce utility targets in heat and mass integration.<sup>9,11</sup> The same principle applies to WPA. Two possible scopes for process changes to further reduce the water targets, and thus water consumption, include water regeneration and equipment (hardware) modifications. Water regeneration involves the partial or total upgrading of water purity using purification techniques such as adsorption, ion exchange, membrane separation, or steam stripping. The regenerated water can be either reused in other water-using

Table 6. Limiting Water Data for Case Study 2

Water Demand, $D_j$	Flow Rate, $F_j$ (ton/h)	Concentration, $C_j$ (ppm)	Water Source, $S_i$	Flow Rate, $F_i$ (ton/h)	Concentration, $C_i$ (ppm)
1	120	0	1	120	100
2	80	50	2	80	140
3	80	50	3	—	—
4	140	140	4	140	180
5	80	170	5	80	230
6	195	240	6	195	250

Table 7. WCT for Case Study 2

Level, $k$	Concentration, $C_k$ (ppm)	Purity, $P_k$	$\sum_j F_{D,j}$ (ton/h)	$\sum_i F_{S,i}$ (ton/h)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (ton/h)	$F_C$ (ton/h)	Pure Water Surplus (ton/h)	Cumulative Pure Water Surplus (ton/h)
<b><math>F_{FW} = 200</math></b>								
1	0	1.000000	-120		-120			
2	50	0.999950	-160		-160	80	0.00400	0.00400
3	100	0.999900		120	120	-80	-0.00400	<b>0</b>
4	140	0.999860	-140	80	-60	40	0.00160	0.00160
5	170	0.999830	-80		-80	-20	-0.00060	0.00100
6	180	0.999820		140	140	-100	-0.00100	<b>0</b>
7	230	0.999770		80	80	40	0.00200	0.00200
8	240	0.999760	-195		-195	120	0.00120	0.00320
9	250	0.999750		195	195	-75	-0.00075	0.00245
<b><math>F_{FW} = 120</math></b>								
10	1,000,000	0					119.97000	119.97245

processes or recycled to the same process to further reduce water consumption and wastewater generation. To increase water availability, Hallale<sup>8</sup> proposed the use of water composite curves and the pinch purity to guide the regeneration of water sources as follows:

(1) *Regeneration above the pinch*: Water source(s) in the region above the pinch are partially treated to upgrade its purity.

(2) *Regeneration across the pinch*: Water source(s) in the region below the pinch are partially treated to achieve purity higher than the pinch purity.

(3) *Regeneration below the pinch*: Water source(s) in the region below the pinch are partially treated to upgrade its purity. However, the resulting water source is still maintained below the pinch.

Note that regeneration above and across the pinch will reduce the fresh water consumption and wastewater generation, whereas regeneration below the pinch will only reduce wastewater generation.

The main problem of dealing with process changes is that assessment of the impact of changes involves repetitive calculations to revise the utility targets and relocate the pinch. Such tasks can be quite cumbersome in the absence of an efficient targeting tool. The WCA has managed to overcome this problem through the introduction of the WCT that is very amenable to computer programming.

Table 3 shows the pinch concentration for the AN process located at 14 ppm. One possible option of regenerating the water source is to purify the off-gas condensate ( $S_2$ ). El-Halwagi<sup>11</sup> proposed regeneration using resin to reduce the

composition of ammonia in the off-gas condensate to 11.6 ppm. The WCT in Table 4 shows the new pinch purity at 0.999975 (25 ppm), and the fresh water and wastewater flow rates reduced to 1.20 and 7.30 kg/s, respectively. The network design by El-Halwagi<sup>11</sup> confirmed these targets.

The second option for process change to further reduce water consumption involves the change of water-using process equipment. Referring back to the AN case study, it is possible to replace the steam-jet ejector by a vacuum pump to eliminate the bulk of fresh water demand in the vacuum distillation unit.<sup>11</sup> Using the WCA technique, the new water targets are quickly and accurately identified. With the process change mentioned, the fresh water flow rate is reduced to zero, whereas the wastewater flow rate is reduced to 5.9 kg/s (see Table 5). These utility targets were also predicted by the simplified targeting technique in Figure 8,<sup>11</sup> and confirmed by the detailed network design for the case study, found in Figure 13.<sup>11</sup>

## Problems with Multiple Pinch Points

The correct identification of the true pinch purity is crucial in water network analysis, especially with problems involving multiple pinch points and near pinches. Hallale<sup>8</sup> shows that the wrong pinch point will result in missed opportunities during network debottlenecking. This is another area where quick and accurate determinations of the true pinch point and water targets are crucial in water network analysis. Here, once again, WCA has an important role to play. We will now use a case study involving multiple pinch points from Sorin and Bédard,<sup>6</sup>

Table 8. Limiting Water Data for Case Study 3

Water Demand, $D_j$	Flow Rate, $F_j$ (ton/h)	Concentration, $C_j$ (ppm)	Water Source, $S_i$	Flow Rate, $F_i$ (ton/h)	Concentration, $C_i$ (ppm)
1	20	0	1	20	100
2	100	50	2	100	100
3	40	50	3	40	800
4	10	400	4	10	800

Table 9. WCA for Case Study 3

Level, $k$	Concentration, $C_k$ (ppm)	Purity, $P_k$	$\sum_j F_{D,j}$ (ton/h)	$\sum_i F_{S,i}$ (ton/h)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (ton/h)	$F_C$ (ton/h)	Pure Water Surplus (ton/h)	Cumulative Pure Water Surplus (ton/h)
$F_{FW} = 90$								
1	0	1.0000000	-20		-20	70	0.0035	
2	50	0.999950	-140		-140	-70	-0.0035	0.0035
3	100	0.999900		120	120	50	0.0150	0
4	400	0.999600	-10		-10	40	0.0160	0.0150
5	800	0.999200		50	50			0.0310
$F_{WW} = 90$								
6	1,000,000	0					89.9280	89.9590

to highlight the problems of determining the true pinch points. The limiting water data for the case study are shown in Table 6.

Table 7 shows the WCT for this problem. The minimum fresh water and wastewater targets calculated using the WCA are 200 and 120 ton/h, respectively, as previously predicted both by Sorin and Bédard<sup>6</sup> and by Hallale.<sup>8</sup> Table 7 also shows that two pinch points exist in this problem, consistent with the results obtained using the water surplus diagram.<sup>8</sup> Sorin and Bédard,<sup>6</sup> however, managed to identify only a single pinch point at the purity of 0.99982 using the evolutionary table, a numerical technique based on Dhole's composites plot.<sup>5</sup>

Hallale<sup>8</sup> further reported that the pinch point at the higher purity of 0.999900 was the limiting pinch point, that is, the one that influenced the utility targets when any process changes were made. Note that the pinch point identified by Sorin and Bédard<sup>6</sup> was not the limiting pinch point. Hallale<sup>8</sup> demonstrated that beneficial changes to a process may be overlooked without knowledge of the limiting pinch purity.

In problems involving multiple pinches, more than two thermodynamic regions exist with respect to the pinch location. For case study 2, three distinct thermodynamic regions exist because of the occurrence of a limiting pinch ( $P_3 = 0.999900$ ) and a secondary pinch ( $P_6 = 0.999820$ ). These include the region above the limiting pinch, the region between two pinches, and the region below the secondary pinch. Using the WCT, one can easily identify the pinch-causing source streams and the exact water allocation for the water sources in each of the thermodynamic regions. Thus, the WCT provides very useful guidelines in designing the MWR network.

Referring to the limiting data in Table 6 and the WCT (Table 7),  $S_1$  was identified as the pinch-causing water source that exists at the limiting pinch point of  $P_3 = 0.999900$ . From the column of cumulative net water source ( $F_C$ ) in Table 7, 80 ton/h of  $S_1$  (interval between  $P_2$  and  $P_3$ ) must be fed to the region above the limiting pinch, whereas the remaining 40

ton/h of  $S_1$  (interval between  $P_3$  and  $P_4$ ) must be fed to the region between two pinches. Similarly,  $S_4$  was identified as the pinch-causing stream that exists at the secondary pinch point ( $P_4 = 0.999820$ ). Thus, 100 ton/h water must be fed from  $S_4$  to the region between the two pinches, whereas 40 ton/h water must be fed from  $S_4$  to the purity level below the secondary pinch. These water allocation targets can be verified through a detailed water network design.

### WCA Application for Mass-Transfer-Based Processes

It has been demonstrated that the WCA technique enables quick and accurate determination of the utility targets, pinch purities, and water allocation targets. In addition, it has been shown that the WCA technique can provide insights for beneficial process changes and eliminate uncertainties in handling problems with multiple pinches. These have so far been accomplished using case studies that primarily involve non-mass-transfer-based processes. It is important to note, however, that the WCA technique is equally applicable to mass-transfer-based processes. In this section, we demonstrate the versatility of the WCA technique in solving problems involving a number of classical literature case studies that are classified as mass-transfer-based water-using processes.

#### Case study 3<sup>1</sup>

Table 8 details the limiting water data for case study 3, taken from Wang and Smith.<sup>1</sup> This case study consists of four mass-transfer-based water-using operations. For this case study, the minimum fresh water and wastewater targets, computed using the WCA technique, were both 90 ton/h as shown in the WCT (Table 9). The utility targets and pinch concentration (100 ppm) agree precisely with the values reported by Wang and Smith.<sup>1</sup> From the cumulative net water source ( $F_C$ ) column

Table 10. Limiting Water Data for Case Study 4

Water Demand, $D_j$	Flow Rate, $F_j$ (ton/h)	Concentration, $C_j$ (ppm)	Water Source, $S_i$	Flow Rate, $F_i$ (ton/h)	Concentration, $C_i$ (ppm)
1	36.3636	25	1	36.3636	80
2	66.6667	25	2	66.6667	100
3	22.8571	25	3	22.8571	200
4	100	50	4	100	100
5	40	50	5	40	800
6	10	400	6	10	800

Table 11. WCT for Case Study 4

Level, $k$	Concentration, $C_k$ (ppm)	Purity, $P_k$	$\sum_j F_{D,j}$ (ton/h)	$\sum_i F_{S,i}$ (ton/h)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (ton/h)	$F_C$ (ton/h)	Pure Water Surplus (ton/h)	Cumulative Pure Water Surplus (ton/h)
<b><math>F_{FW} = 157.143</math></b>								
1	0	1.000000				157.1428	0.0039	
2	25	0.999975	-125.8874		-125.8874	31.25543	0.0008	0.003929
3	50	0.999950	-140		-140	-108.745	-0.0033	0.004710
4	80	0.999920		36.3636	36.3636	-72.381	-0.0014	0.001448
5	100	0.999900		166.6667	166.6667	94.286	0.0094	<b>0</b>
6	200	0.999800		22.8571	22.8571	117.143	0.0234	0.009429
7	400	0.999600	-10		-10	107.143	0.0429	0.032857
8	800	0.999200		50	50			0.075714
<b><math>F_{WW} = 157.143</math></b>								
9	1,000,000	0					157.0171	157.092830

(Table 9), the WCT also enabled a user to identify  $S_1$  and  $S_2$  as the pinch-causing streams. To achieve the MWR objective, 70 ton/h of water from either  $S_1$  or  $S_2$  should be fed to the region above the pinch, whereas another 50 ton/h should be fed to the region below the pinch. Note that such insights are missing from the established graphical targeting tools such as limiting water profile,<sup>1</sup> source and demand composite curves,<sup>7</sup> and water surplus diagram.<sup>8</sup>

#### Case study 4<sup>3</sup>

Table 10 presents the limiting water data for case study 4, taken from Olesen and Polley.<sup>3</sup> This case study consists of six mass-transfer-based water-using operations. The WCA technique computed the minimum fresh water and wastewater targets to be both 157.14 ton/h and the pinch point at the purity level of 0.999900 (100 ppm) according to the values reported by Olesen and Polley<sup>3</sup> (see the WCT, Table 11). Water sources  $S_2$  and  $S_4$  were identified as the pinch-causing streams in this case.

#### Case study 5<sup>7</sup>

Table 12 shows the limiting water data for case study 5, taken from Polley and Polley.<sup>7</sup> This case study consists of a combination of mass-transfer-based and non-mass-transfer-based water-using operations.  $D_1$ ,  $S_1$  and  $D_2$ ,  $S_2$  are part of processes 1 and 2 that are classified as mass-transfer processes. On the other hand,  $D_3$ ,  $S_3$  and  $D_4$ ,  $S_4$  are part of processes 3 and 4 that are essentially non-mass-transfer-based processes. The WCT for case study 5 (Table 13) shows the minimum fresh water flow rate of 70 ton/h, wastewater flow rate of 50 ton/h,

and the pinch purity at 0.999850 (150 ppm), matching the published results of Polley and Polley.<sup>7</sup> In addition, the WCA technique also enabled  $S_3$  to be identified as the pinch-causing stream.

#### Case study 6<sup>17</sup>

Table 14 presents the limiting water data for case study 6, taken from Wang and Smith.<sup>17</sup> This is a special chemical production case study that consists of a combination of mass-transfer-based and non-mass-transfer-based water-using operations.  $D_1$  and  $S_1$  are part of process 1, which is a reaction process that consumes a portion of feed water and produces a lower flow rate of effluent.  $D_3$  and  $S_3$  are part of process 3, which is a filtration process that receives fresh water for cake wash apart from aqueous slurry feed, and produces wastewater.  $D_4$  and  $S_4$  are part of process 4, which is a steam system that receives make-up water to supplement condensate loss and boiler blowdown.  $D_5$  and  $S_5$  are part of process 5, which is a water-cooling system that receives make-up water and discharges wastewater through continuous blowdown. The nature of operations of processes 1, 3, 4, and 5 clearly indicates that these are non-mass-transfer-based water-using operations.

On the other hand,  $D_2$  and  $S_2$  are part of process 2, which is a cyclone separation that receives water for product washing. Process 2 is a mass-transfer-based process because it involves interphase transfer of contaminants and equal inlet and outlet stream flow rates. The WCT for this case study (Table 15) shows the minimum fresh water flow rate of 90.64 ton/h, wastewater flow rate of 50.64 ton/h, and the pinch purity at 0.999300 (700 ppm), matching the published results of Wang

Table 12. Limiting Water Data for Case Study 5

Water Demand, $D_j$	Flow Rate, $F_j$ (ton/h)	Concentration, $C_j$ (ppm)	Water Source, $S_i$	Flow Rate, $F_i$ (ton/h)	Concentration, $C_i$ (ppm)
1	50	20	1	50	50
2	100	50	2	100	100
3	80	100	3	70	150
4	70	200	4	60	250



Table 13. WCT for Case Study 5

Level, <i>k</i>	Concentration, <i>C<sub>k</sub></i> (ppm)	Purity, <i>P<sub>k</sub></i>	$\sum_j F_{D,j}$ (ton/h)	$\sum_i F_{S,i}$ (ton/h)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (ton/h)	<i>F<sub>C</sub></i> (ton/h)	Pure Water Surplus (ton/h)	Cumulative Pure Water Surplus (ton/h)
<b><i>F<sub>FW</sub> = 70</i></b>								
1	0	1.000000				70	0.0014	
2	20	0.999980	−50		−50	20	0.0006	0.0014
3	50	0.999950	−100	50	−50	−30	−0.0015	0.0020
4	100	0.999900	−80	100	20	−10	−0.0005	0.0005
5	150	0.999850		70	70	60	0.0030	<b>0</b>
6	200	0.999800	−70		−70	−10	−0.0005	0.0030
7	250	0.999750		60	60			0.0025
8	1,000,000	0.000000				<b><i>F<sub>WW</sub> = 50</i></b>	49.9875	49.9900

and Smith.<sup>17</sup> The WCA technique also enabled *S*<sub>2</sub> to be identified as the pinch-causing stream.

Results from all the case studies presented prove that the WCA technique is applicable in solving problems for both mass-transfer-based and non-mass-transfer-based water-using processes. Note that the targets generated can be readily verified using various established network design techniques. For mass-transfer-based water-using processes, network design techniques such as water grid diagram,<sup>1</sup> load table,<sup>3</sup> and water

main method<sup>18</sup> should be used. On the other hand, for cases involving non-mass-transfer-based processes (such as for case studies 5 and 6), network design should be conducted using the source–sink mapping diagram<sup>11,14,15</sup> or sink–source allocation.<sup>8,16</sup>

## Conclusion

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 targets for a maximum water recovery (MWR) network. Apart from the determination of utility targets and the pinch location, it has also been demonstrated that the WCA technique can provide additional insights in identifying the pinch-causing streams. This is beyond those obtainable by some well-established graphical targeting techniques, such as the limiting composite curves,<sup>1</sup> source and sink composite curves,<sup>5</sup> and water surplus diagram.<sup>8</sup>

By eliminating the tedious iterative steps of the water surplus diagram, WCA offers a key complementary role to the water surplus diagram in the design and retrofit of the MWR network. WCA can handle both mass-transfer-based and non-mass-transfer-based operations and is applicable to a wide range of water-using operations. Various options involving process

Table 14. Limiting Water Data for Case Study 6

Water Demands, <i>D<sub>j</sub></i>		Flow Rate, <i>F<sub>j</sub></i> (ton/h)	Concentration, <i>C<sub>j</sub></i> (ppm)
<i>j</i>	Stream		
1	Reactor	80	100
2	Cyclone	50	200
3	Filtration	10	0
4	Steam system	10	0
5	Cooling system	15	10

Water Sources, <i>S<sub>i</sub></i>		Flow Rate, <i>F<sub>i</sub></i> (ton/h)	Concentration, <i>C<sub>i</sub></i> (ppm)
<i>i</i>	Stream		
1	Reactor	20	1000
2	Cyclone	50	700
3	Filtration	40	100
4	Steam system	10	10
5	Cooling system	5	100

Table 15. WCT for Case Study 6

Level, <i>k</i>	Concentration, <i>C<sub>k</sub></i> (ppm)	Purity, <i>P<sub>k</sub></i>	$\sum_j F_{D,j}$ (ton/h)	$\sum_i F_{S,i}$ (ton/h)	$\sum_j F_{D,j} + \sum_i F_{S,i}$ (ton/h)	<i>F<sub>C</sub></i> (ton/h)	Pure Water Surplus (ton/h)	Cumulative Pure Water Surplus (ton/h)
<b><i>F<sub>FW</sub> = 90.64</i></b>								
1	0	1.000000	−20		−20	70.64	0.0007	
2	10	0.999990	−15	10	−5	65.64	0.0059	0.000706
3	100	0.999900	−80	45	−35	30.64	0.0031	0.006614
4	200	0.999800	−50		−50	−19.36	−0.0097	0.009679
5	700	0.999300		50	50	30.64	0.0092	<b>0</b>
6	1000	0.999000		20	20			0.009193
7	1,000,000	0.000000				<b><i>F<sub>WW</sub> = 50.64</i></b>	50.5922	50.601407



changes, including water regeneration and equipment modifications, can be systematically assessed using the WCA. Problems involving multiple pinches 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. As our experience has shown, the WCA has simplified the task of incorporating the water surplus diagram in a computer software by eliminating the tedious iterative steps involved during the construction of water surplus diagram. The WCA feature has been incorporated in *Heat-MATRIX*, a new software for energy and water reduction developed by the Process Synthesis and Design Group, Department of Chemical Engineering, Universiti Teknologi Malaysia.<sup>19</sup>

## Notation

$C$  = contaminant concentration, ppm  
 $F$  = flow rate of water demand or source, kg/s or t/hr  
 $n$  = number of purity intervals  
 $N$  = number of water demands or sources  
 $P$  = purity  
 $\Delta$  = difference  
 $\Sigma$  = summation

## Subscripts

$C$  = cumulative  
 $D$  = water demands  
 $DP$  = duplicate purities  
 $FW$  = fresh water  
 $i$  = sources  
 $j$  = demands  
 $S$  = water sources  
 $WW$  = wastewater

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