ASSESSING OPTIONS FOR PROCESS CHANGES VIA WATER CASCADE ANALYSIS

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ABSTRACT

Water Cascade Analysis (WCA) is a newly developed technique to establish the minimum water and wastewater targets for water-using processes. The WCA is a numerical alternative to the graphical water targeting technique known as the water surplus diagram. 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. In this work, WCA is utilised to assess options for process changes in a water network. A case study on water minimisation involving acrylonitrile production (El-Halwagi, 1997) is used to illustrate the developed procedure.

Keywords: Water minimisation; Water Cascade Analysis; process changes; water regeneration; equipment modifications

1.0 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 (1994) 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.

Wang and Smith (1994) 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.* (1996) 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 (2000) later pointed out that, unless the correct stream mixing system was identified, the apparent targets generated by Dhole's technique could be substantially higher than the true minimum fresh water and wastewater targets.

Sorin and Bédard (1999) 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.* (1996) could result in a number of "local" pinch points, which might not necessarily be the actual or the "global" pinch

points. However, Hallale (2002) recently showed that, when more than one global pinch points occurred in water-using processes, the Evolutionary Table failed to locate them correctly.
Hallale (2002) presented an alternative graphical method called the water surplus diagram to target the minimum fresh water and wastewater. The method has a similar representation to the water source and demand composite curves proposed by Dhole *et al.* (1996), thereby was not limited to the mass transfer-based operations. The new representation by Hallale (2002) 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 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.

Manan and Foo (2003) recently presented 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. In this work, we will utilise the newly developed WCA technique in systematically identifying process changes opportunities in a water recovery network.

2.0 PROCESS CHANGES

Making appropriate changes to a process has been widely accepted as an effective measure to further reduce utility targets in heat and mass Pinch Analysis (Linnhoff *et al.*, 1982; El-Halwagi, 1997). The same principle applies to Water Pinch Analysis. Two possible scopes for process changes to further reduce the water targets, and hence, 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 either be reused in other water-using processes or recycled to the same process to further reduce water consumption and wastewater generation. To increase water availability, Hallale (2002) 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 while 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 Water Cascade Table (WCT) that is very amenable to computer programming.

3.0 CASE STUDY

Acrylonitrile (AN) is produced via the vapour-phase ammoxidation of propylene that takes place in a fluidised-bed reactor at 450ºC and 2 atm, according to Equation 1.

$$C_3H_6 + NH_3 + 1.5O_2 \xrightarrow{catalyst} C_3H_3N + 3H_2O \tag{1}$$

This is a single-pass reaction with almost complete conversion of propylene. Products from the reactor is cooled and partially condensed. The reactor off-gas is sent to a scrubber that uses 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. **Figure 1** shows the process flow diagram for AN production along with the pertinent material balance data.

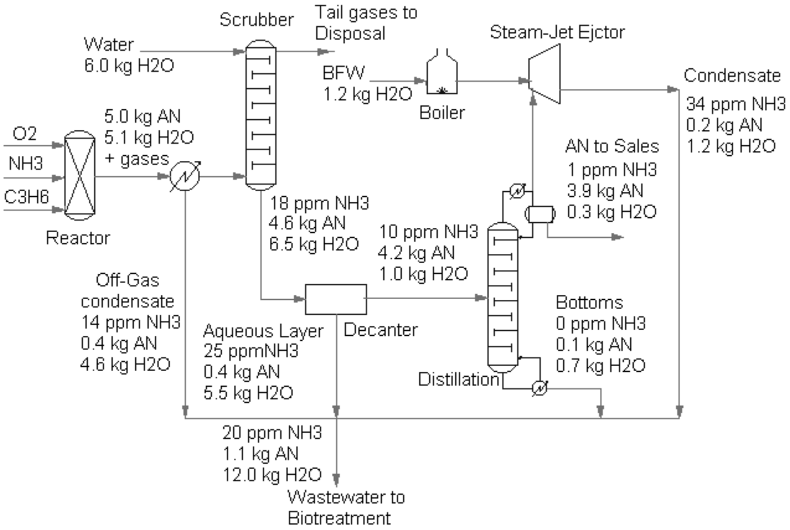


Figure 1. The flowsheet for AN production

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 (NH_3) is the main contaminant in this process. Here, the water sources are regarded as wastewater and sent to a bio-treatment facility operated at full capacity. The limiting data for the water demands and sources are summarised in **Table 1**.

Table 1. Limiting water data for AN production

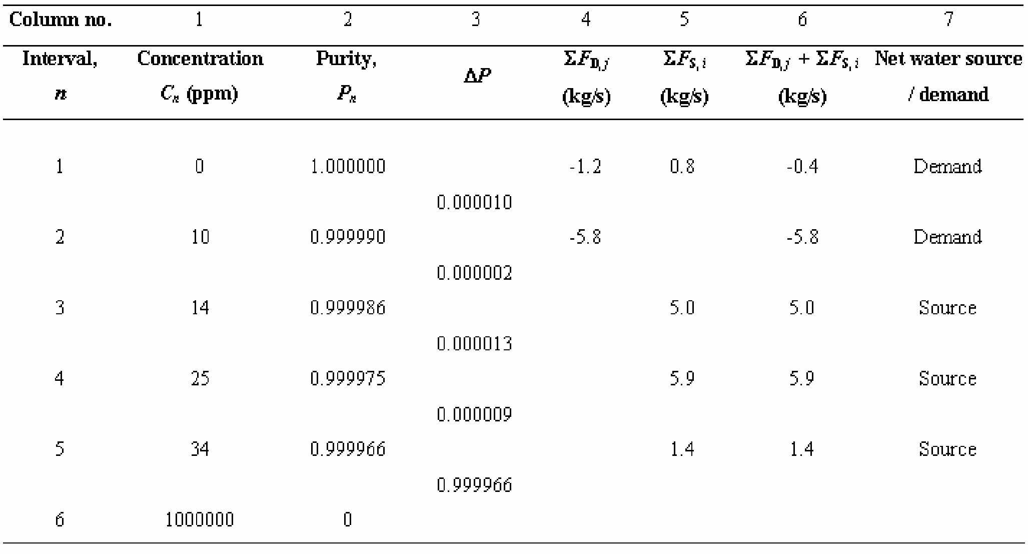
Water demands, D_j		**Flowrate**	**Concentration**
j	Stream	F_j (kg/s)	C_j (ppm)
1	BFW	1.2	0
2	Scrubber	5.8	10

Water sources, S_i		**Flowrate**	**Concentration**
i	Stream	F_i (kg/s)	C_i (ppm)
1	Distillation bottoms	0.8	0
2	Off-gas condensate	5	14
3	Aqueous layer	5.9	25
4	Ejector condensate	1.4	34

4.0 WATER CASCADE ANALYSIS

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 (**Table 2**).

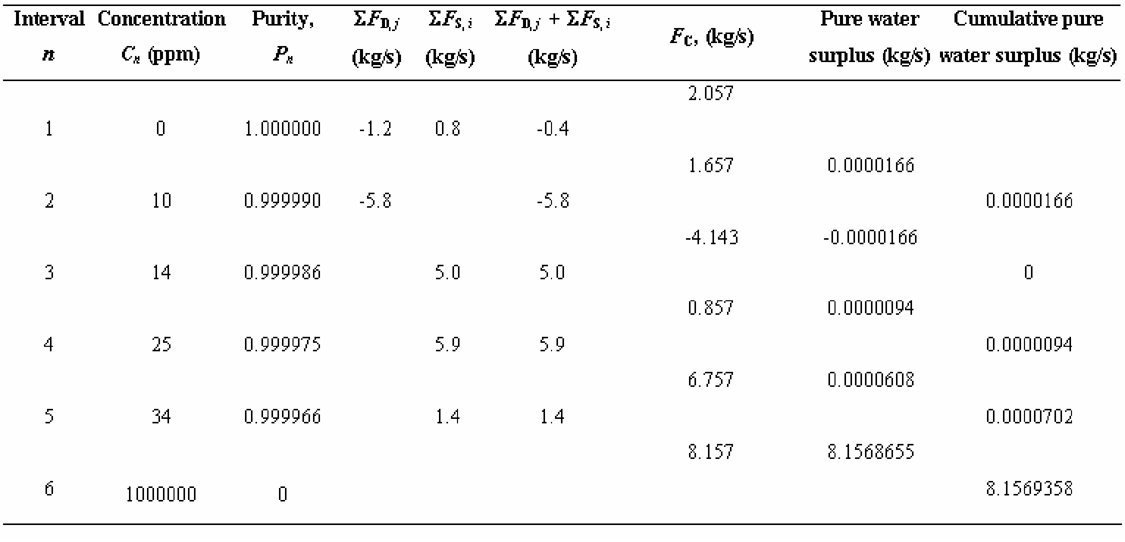
Table 2. The interval water balance table for AN production case study



Column no.	1	2	3	4	5	6	7
Interval, n	Concentration C_n (ppm)	Purity, P_n	ΔP	$\Sigma F_{D,j}$ (kg/s)	$\Sigma F_{S,i}$ (kg/s)	$\Sigma F_{D,j} + \Sigma F_{S,i}$ (kg/s)	Net water source / demand
1	0	1.000000		-1.2	0.8	-0.4	Demand
			0.000010				
2	10	0.999990		-5.8		-5.8	Demand
			0.000002				
3	14	0.999986			5.0	5.0	Source
			0.000013				
4	25	0.999975			5.9	5.9	Source
			0.000009				
5	34	0.999966			1.4	1.4	Source
			0.999966				
6	1000000	0					

The interval water balance table is then used to form the *water cascade table* (WCT) in **Table 3**. Detailed procedure for constructing this table is illustrated in our previous publication (Manan and Foo, 2003). From WCA, fresh water and wastewater flowrate targets are targeted at 2.057 kg/s and 8.157 kg/s respectively for the AN case study. The third purity level (P = 0.999986) with zero cumulative pure water surplus is identified as the pinch purity 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 (1997) confirmed the utility targets for this case study.

Table 3 Water Cascade Table (WCT) for AN production case study

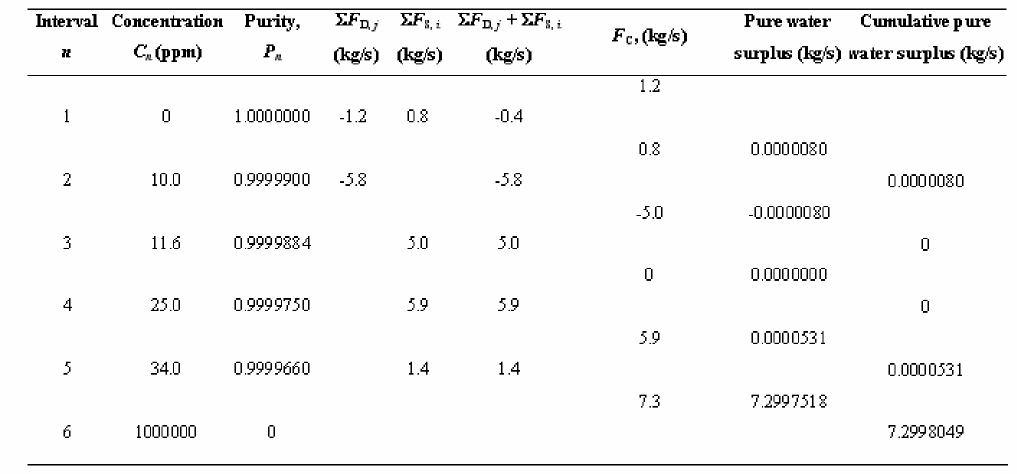


Interval n	Concentration C_n (ppm)	Purity, P_n	$\Sigma F_{D,j}$ (kg/s)	$\Sigma F_{S,i}$ (kg/s)	$\Sigma F_{D,j} + \Sigma F_{S,i}$ (kg/s)	F_C, (kg/s)	Pure water surplus (kg/s)	Cumulative pure water surplus (kg/s)
						2.057		
1	0	1.000000	-1.2	0.8	-0.4			
						1.657	0.0000166	
2	10	0.999990	-5.8		-5.8			0.0000166
						-4.143	-0.0000166	
3	14	0.999986		5.0	5.0			0
						0.857	0.0000094	
4	25	0.999975		5.9	5.9			0.0000094
						6.757	0.0000608	
5	34	0.999966		1.4	1.4			0.0000702
						8.157	8.1568655	
6	1000000	0						8.1569358

5.0 ASSESSING OPTIONS FOR PROCESS CHANGES

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 (1997) proposed regeneration using resin to raise the composition of ammonia in the off-gas condensate to 11.6 ppm. **Table 4** from the WCA shows the new pinch purity at 0.999975 (25 ppm), and the fresh water and wastewater flowrates reduced to 1.20 kg/s and 7.30 kg/s respectively. The network design proposed by El-Halwagi (1997) confirmed these targets.

Table 4. WCT for process involving partial regeneration of off-gas condensate

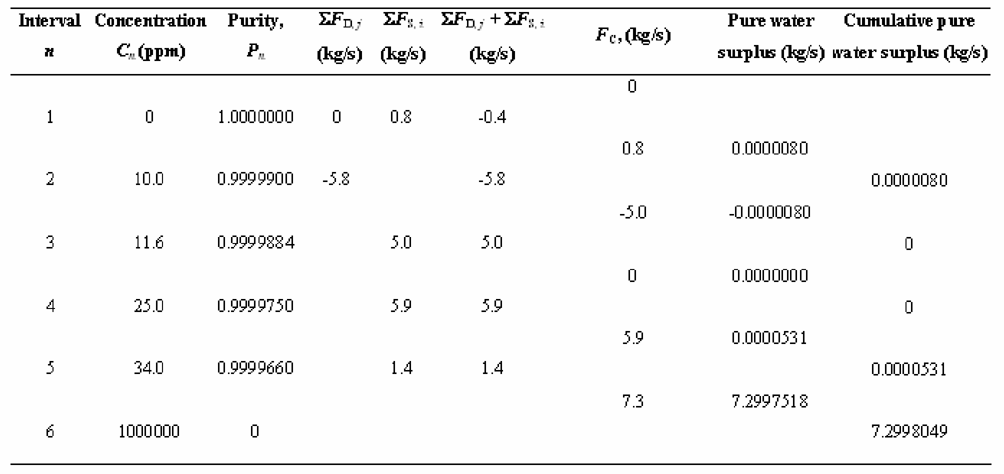


Interval n	Concentration C_n (ppm)	Purity, P_n	$\Sigma F_{D,j}$ (kg/s)	$\Sigma F_{S,i}$ (kg/s)	$\Sigma F_{D,j} + \Sigma F_{S,i}$ (kg/s)	F_C, (kg/s)	Pure water surplus (kg/s)	Cumulative pure water surplus (kg/s)
						1.2		
1	0	1.0000000	-1.2	0.8	-0.4			
						0.8	0.0000080	
2	10.0	0.9999900	-5.8		-5.8			0.0000080
						-5.0	-0.0000080	
3	11.6	0.9999884		5.0	5.0			0
						0	0.0000000	
4	25.0	0.9999750		5.9	5.9			0
						5.9	0.0000531	
5	34.0	0.9999660		1.4	1.4			0.0000531
						7.3	7.2997518	
6	1000000	0						7.2998049

The second option for process change to further reduce water consumption involves changing 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 (El-Halwagi, 1997).

Using the WCA technique, the new water targets are quickly and accurately identified. With the process change mentioned, the fresh water flowrate is reduced to zero while the wastewater flowrate is maintained at 7.30 kg/s (see **Table 5**). These utility targets were also predicted by the simplified targeting technique by El-Halwagi (1997), and confirmed via the detailed network design for the case study (El-Halwagi, 1997).

Table 5. WCT for stream regeneration and process changes



Interval n	Concentration C_n (ppm)	Purity, P_n	$\Sigma F_{D,j}$ (kg/s)	$\Sigma F_{S,i}$ (kg/s)	$\Sigma F_{D,j} + \Sigma F_{S,i}$ (kg/s)	F_C, (kg/s)	Pure water surplus (kg/s)	Cumulative pure water surplus (kg/s)
						0		
1	0	1.0000000	0	0.8	-0.4			
						0.8	0.0000080	
2	10.0	0.9999900	-5.8		-5.8			0.0000080
						-5.0	-0.0000080	
3	11.6	0.9999884		5.0	5.0			0
						0	0.0000000	
4	25.0	0.9999750		5.9	5.9			0
						5.9	0.0000531	
5	34.0	0.9999660		1.4	1.4			0.0000531
						7.3	7.2997518	
6	1000000	0						7.2998049

6.0 CONCLUSION

Water Cascade Analysis (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. 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 Systems Engineering Group, Dept. of Chemical Engineering, Universiti Teknologi Malaysia (Manan *et al.*, 2003).

7.0 ACKNOWLEDGEMENT

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