Unified Conceptual Approach to Targeting and Design of Water and Hydrogen Networks

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An algorithm is proposed to target the minimum freshwater for fixed flow rate (FF) problems in single-contaminant water networks. The approach is based on an extension of the limiting composite curve concept proposed earlier for fixed contaminant-load (FC) problems. The targeting method is elegant, noniterative, and can be applied to FF problems involving regeneration to minimize waste discharge. To design networks that achieve the minimum freshwater targets set for FF problems, an algorithm is presented based on the principle of nearest neighbors. The principle simply states that the sources to be chosen to satisfy a particular water demand must be the nearest available neighbors in terms of contaminant concentration. A significant advantage of the approach is that the same targeting concepts can be profitably used to determine the minimum makeup utility in hydrogen networks. Furthermore, hydrogen networks may be designed by the unified conceptual approach using the nearest neighbors algorithm. The hydrogen networks may then be evolved to account for the pressure constraints imposed by compressors or improved by regeneration through purification processes such as pressure-swing adsorption. *AIChE J,* 52: 1071–1082, 2006
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Introduction

Stricter environmental protection norms along with rising costs of waste treatment have motivated research to reduce water and hydrogen consumption in refineries and other chemical process industries. This paper presents a unified conceptual approach to water and hydrogen management based on mass integration principles. Mass integration[1-4] is a systems engineering approach that provides a holistic methodology to understand the flow of a species within a process and determines the optimal routing and allocation between sources and demands. Sources can be regenerated by purification techniques to change compositions and allow recycle/reuse to meet demands that would not be possible otherwise.

Wang and Smith[5] proposed a method of targeting and designing water networks that minimized wastewater (or freshwater use) by three ways: reuse, regeneration–reuse, and regeneration–recycle. Their graphical targeting method, based on the limiting composite curve, is elegant and provides minimum freshwater targets before network design. However, the method applies to fixed contaminant-load (FC) operations that are quality controlled[6] and that may be modeled as mass transfer units (such as washing, scrubbing, and extraction). Here, water is used as the only mass separating agent[5,7,8] that picks up a fixed load of contaminant from the process stream. Each operation has the maximum allowable inlet and outlet contaminant concentrations specified based on process constraints. Because the inlet flow rate is identical to the outlet flow rate for each unit operation, the wastewater flow rate for the network equals the targeted freshwater flow rate.

The method as presented by Wang and Smith[5] is not applicable to fixed flow rate (FF) operations that are quantity controlled.[6] For such water-using units such as boilers, cooling towers, and reactors that do not involve any mass transfer, the

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Table 1. Water Data for Example 1

	Contaminant Concentration (ppm)	Flow Rate (t/h)
Demands		
*D*1	20	50
*D*2	50	100
*D*3	100	80
*D*4	200	70
Sources		
*S*1	50	50
*S*2	100	100
*S*3	150	70
*S*4	250	60

main concern is the flow rate[9,10] and not the amount of contaminant picked up. These units have specified inlet and outlet flow rates, which may not necessarily be equal and therefore can account for water losses or gains. Dhole et al.[11] proposed that all the inlet streams be regarded as demands and all the outlet streams as sources. This allows units that have multiple inlet streams and multiple outlet streams to be modeled. Dhole et al.[11] also proposed a targeting method for FF problems. Hallale[10] correctly indicated that the targeting procedure of Dhole et al.[11] does not give absolute targets because it depends on the mixing option chosen. Hallale[10] therefore suggested a procedure based on a water surplus diagram to find the true targets. However, the water surplus diagram method requires transferring of data from one plot to another and is iterative because it needs an initial guess of the freshwater flow rate.

In this work, a targeting approach is proposed for FF problems that is noniterative and gives absolute targets with reduced computation. The limiting composite curve concept, applicable earlier to FC problems only, is extended to FF problems. It is also used to provide targets for regeneration and minimum waste discharge in FF water problems. The targeting approach is further extended to determine the minimum makeup utility in hydrogen networks. Regeneration for hydrogen problems is illustrated through purification processes such as pressure-swing adsorption. Networks that meet the targets are finally designed by an elegant method based on the nearest neighbors principle.

Targeting Approach for Water Networks

The minimum flow rate targeting method based on the limiting composite curve as proposed by Wang and Smith[5] is restricted in its application to FC problems. Consequently, other methods have been proposed[10,12,13] for FF problems. However, these other methods are not suitable to target regeneration problems or multiple water supply sources. The present work overcomes this drawback by using a different approach wherein a FF problem is conceptually recast to an equivalent FC problem. If the FF problem data can yield a limiting composite curve, then the Wang and Smith[5] method is applicable and provides a tested solution.

To illustrate the targeting approach, an example FF problem is considered. The data taken from Polley and Polley[6] for the four demand (inlet) streams and the four source (outlet) streams in Example 1 are given in Table 1. The objective is to rework the data to allow a plot of the limiting composite curve composed of both demands and sources with contaminant concentration on the vertical axis and cumulative contaminant mass load on the horizontal axis. The reciprocal of the slope of this curve is the flow rate because

$$m = F(C_{out} - C_{in}) \tag{1}$$

where m is the mass load of the contaminant, F is the water flow rate, and C_{in} and C_{out} are the inlet and outlet concentrations of contaminant in the water stream.

From Table 1, the flow rate and concentration of each stream are known. Because demands are inlet streams to process units, assume for the moment that the contaminant mass load transferred to them is indefinite and starts from zero. Given that the slope and a point on the concentration vs. mass load plot are known for each stream, the individual demand profiles can be drawn (as shown by the dashed lines in Figure 1). Concentration intervals can be now identified such that a new interval starts when a new demand stream is introduced. Within each interval, the total flow rate can be calculated by adding the individual flow rates that exist in that interval. Then, the mass load in that interval can be calculated using Eq. 1. For instance, the concentrations 50 and 100 ppm define one of the intervals in Figure 1. Within this interval, the demand streams *D1* and *D2* exist and thus the total flow rate is 150 tons/h. Using Eq. 1, the mass load in this interval is found to be 7.5 kg/h. The mass load of each interval can now be used to calculate the cumulative mass load and plot the total demand composite (as shown by the solid line in Figure 1). The composite will always be monotonically increasing in nature because additional demand streams are added as the contaminant concentration increases. This is not yet the limiting composite curve because the source streams have not been taken into consideration.

The aim in FF problems is to satisfy the demands by sources of the same concentration and flow rate. To achieve the minimum freshwater target, Prakash and Shenoy[13] showed that this is a necessary condition below the pinch, whereas the sources can be of lower concentrations above the pinch. If the source flow rate falls short of the demand, then the flow rate is met by a mixture of a source stream of higher concentration and freshwater supply. This provides an insight into the manner in which sources can be incorporated into the demand composite to obtain the limiting composite curve. The sources are introduced at the concentrations at which they are available (as given in Table 1) into the demand composite by simply sub-

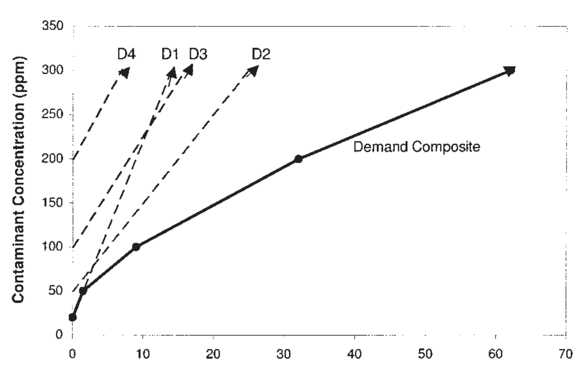


Figure 1. Individual demand profiles and demand composite for Example 1.

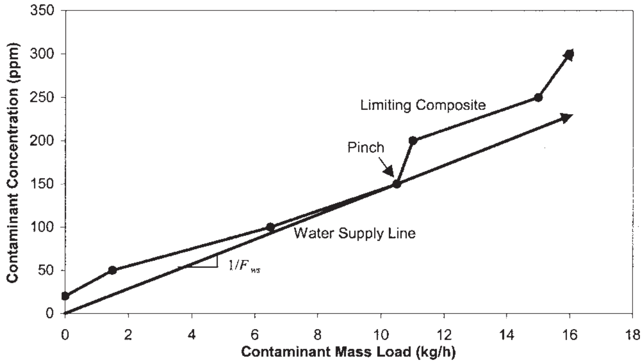


Figure 2. Limiting composite curve and minimum freshwater targeting with water reuse for Example 1.

tracting the source flow rate from the demand composite flow rate at that concentration. Each introduction reduces the flow rate (that is, increases the slope of the line segment) until the final limiting composite curve (Figure 2) is obtained.

The limiting composite takes into consideration all the process streams and provides the net demand of the system. The curve (drawn here for a FF problem) is completely analogous to that obtained by Wang and Smith[5] for a FC problem. Thus, freshwater targeting may be done by rotating the horizontal axis with the origin as pivot until it just touches the limiting composite curve. The reciprocal of the slope of this rotated water supply line gives the minimum freshwater flow rate. For Example 1, the minimum freshwater required is 70 tons/h and the pinch concentration is 150 ppm (Figure 2), which agrees with the results of Polley and Polley.[6] Hallale[10] also obtained the same results, but through trial and error using the water surplus diagram.

The above method at first glance may appear complicated to implement graphically; however, it is easily implemented by taking the sources into consideration while constructing the demand composite itself. The *composite table algorithm* (CTA) for this purpose, where all calculations are done conveniently through a compact table (Table 2 for Example 1), is proposed below. The CTA is analogous to the *problem table algorithm*[14,15] used in energy targeting during heat exchanger network synthesis. It is similar to the *mass problem table* method[16] used in water targeting for FC problems. However, the vertical arrows representing the streams in Table 2 all terminate at the last concentration for FF problems in the CTA, whereas such arrows terminate at different concentrations for FC problems in the mass problem table. The CTA is conceptually similar to, but simpler than, the recently published *water cascade table* technique,[17] which requires the water cascade and the pure water surplus cascade diagrams to be integrated with the interval water balance table. Further, unlike the water cascade table, the CTA directly provides the limiting composite curve representation. The steps for the CTA are given below.

(1) Tabulate all concentrations (of demands and sources together) in increasing order in the first column. Do not repeat a concentration value if the same concentration occurs more than once. Add one more arbitrary concentration (in parentheses) at the bottom of the column such that it is the largest value. The arbitrary concentration (supposed to be infinity) serves to provide only an endpoint and facilitates the plotting of the last segment of the limiting composite, whose slope and initial point are well defined.

(2) Tabulate the net flow rates in the second column. The sum of the flow rates of the sources is subtracted from the sum of the flow rates of the demands present in each concentration interval and entered against the higher concentration limit of the interval. To conveniently determine the stream populations in each interval, the streams may be represented by vertical arrows with flow rates indicated below them as in Table 2. The net flow rate corresponds to the reciprocal of the slope of a segment on the limiting composite curve.

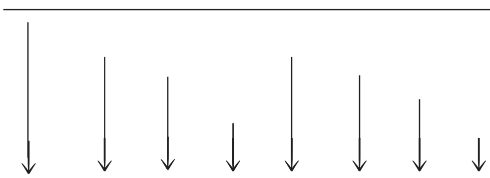
(3) Tabulate the net mass loads in the third column using Eq. 1. Multiply the net flow rate by the concentration difference of the corresponding interval to obtain the net mass load.

(4) Tabulate the cumulative mass load in the fourth column. The concentration column may be plotted against the cumulative mass load column to obtain the limiting composite curve.

(5) Tabulate the possible water supply flow rates in the fifth column. Divide the cumulative mass load by $(C - C_{ws})$ to obtain the possible water supply flow rate. Here, C is the contaminant concentration and C_{ws} is the initial concentration of the water supply. In the case of freshwater, $C_{ws} = 0$. The possible water supply flow rate corresponds to the reciprocal of the slope of a line originating from C_{ws} on the vertical axis to the limiting composite curve.

Because the water supply line can never be above the limiting composite, the maximum value in the last column gives the minimum flow rate target (70 tons/h of freshwater for Example 1 according to Table 2) and the corresponding concentration specifies the pinch (150 ppm corresponding to source *S3*).

Table 2. Implementation of Composite Table Algorithm (CTA) for Example 1



*D*1	*D*2	*D*3	*D*4	*S*1	*S*2	*S*3	*S*4
50	100	80	70	50	100	70	60

Contaminant Concentration, C (ppm)	Net Flow Rate (t/h)	Net Load (kg/h)	Cumulative Load, m_{cum} (kg/h)	$m_{cum}/(C - C_{ws})$ (t/h)
20			0	0
50	50	1.5	1.5	30
100	100	5	6.5	65
150	80	4	10.5	70
200	10	0.5	11	55
250	80	4	15	60
(300)	20	(1)	(16)	(53.33)

In general, mass balances for water and contaminant over the total system give

$$F_{ws} - F_{ww} = \Delta_1 \qquad \text{where } \Delta_1 \equiv \sum F_d - \sum F_s \tag{2}$$

$$F_{ws}C_{ws} - F_{ww}C_{ww} = \Delta_2 \qquad \text{where } \Delta_2 \equiv \sum F_d C_d - \sum F_s C_s \tag{3}$$

where F denotes water flow rate, C denotes contaminant concentration, and subscripts *ws* and *ww* denote water supply and wastewater, respectively. The net system flow rate (Δ_1) and the net system mass load (Δ_2) are obtained by subtracting the sum of all sources (denoted by subscript *s*) from the sum of all demands (denoted by subscript *d*). They are constant for a given problem ($\Delta_1 = 20$ tons/h and $\Delta_2 = -10$ kg/h for Example 1 from Table 1).

It is useful to define[18] such net system quantities (Δ) that are constant for process systems. Because $F_{ws} = 70$ tons/h and $C_{ws} = 0$, Eqs. 2 and 3 give $F_{ww} = 50$ tons/h and $C_{ww} = 200$ ppm. Thus, the minimum targets for freshwater and wastewater are 70 and 50 tons/h, respectively.

Note that when the maximum value in the last column occurs at the bottommost entry (corresponding to the arbitrary concentration in parenthesis), then the minimum freshwater target is given by Δ_1 (which is the limit when the arbitrary concentration tends to infinity). This physically corresponds to zero wastewater discharge (and a threshold or unpinched problem).

It must be emphasized that the above algorithm works with demands and sources; therefore, it can be applied to all FF problems including cases of water gains and losses as well as multiple water streams entering and leaving a single operation. Data for FC problems can also be modeled as demands and sources by assuming the inlet and outlet concentrations to be at their maximum values for targeting purposes.[5]

Design of Water Networks by Nearest Neighbors Algorithm

A network should be ideally designed to have only the inevitable exergy losses according to second-law analysis,[15] and not the practically avoidable losses. Toward minimizing the exergy losses or thermodynamic irreversibilities, the cleanest water sources must be preserved. For this purpose, Prakash and Shenoy[13] recently proposed the principle of nearest neighbors and formally proved its optimality. The principle states that "the source streams to be chosen for satisfying a particular water demand are the nearest available neighbors to the demand in terms of contaminant concentration. " Thus, a source that is just cleaner and a source that is just dirtier than the demand are mixed to meet the demand. A similar but more complicated strategy was used by Savelski and Bagajewicz[19,20] for FC problems to satisfy the requirements of a certain type of process (maximum reuse for wastewater users). The algorithm used below is simpler because targets for minimum freshwater and pinch established a priori are used during the network design. Savelski and Bagajewicz[19,20] used no such targets.

Consider a problem with n sources (*S1* to *Sn*) and m demands (*D1* to *Dm*) serially numbered in order of increasing contaminant concentration. Because the freshwater supply is a source, it is accordingly numbered *S0*. To fulfill the demand *Dp* in accordance with the principle of nearest neighbors, two sources [Sk and $S(k+1)$] are chosen, where Sk has contaminant concentration just less than the concentration of Dp and $S(k+1)$ has contaminant concentration just more than that of Dp. The flow rates of the two neighbor sources required to meet the demand are determined by simultaneously solving the overall material balance and the contaminant material balance equations given as

$$F_{Sk,Dp} + F_{S(k+1),Dp} = F_{Dp} \tag{4}$$

$$F_{Sk,Dp}C_{Sk} + F_{S(k+1),Dp}C_{S(k+1)} = F_{Dp}C_{Dp} \tag{5}$$

If the flow rates $F_{Sk,Dp}$ and $F_{S(k+1),Dp}$ obtained by solving the two equations are less than the available flow rates of the two sources, then the demand can be met by these sources using the calculated flow rates. If the required flow rate is not available for a source, then whatever is available of that source is entirely used and the next neighbor source is considered to satisfy the demand. In other words, if a clean (dirty) neighbor source to the demand is insufficient in quantity, then a source is considered that is just cleaner (dirtier) than the neighbor source used thus far.

In general, if *Ss* is the cleanest source to be used and *St* is the dirtiest source to be used, then the required flow rates of *Ss* and *St* for the demand *Dp* are given by

$$F_{Ss,Dp} + F_{St,Dp} = F_{Dp} - \sum F_{Si,Dp} \tag{6}$$

$$F_{Ss,Dp}C_{Ss} + F_{St,Dp}C_{St} = F_{Dp}C_{Dp} - \sum F_{Si,Dp}C_{Si} \tag{7}$$

The summation for the last terms in Eqs. 6 and 7 goes from $i = s + 1$ to $i = t - 1$.

For the special case where a source *Sk* exists that has a contaminant concentration exactly equal to that of a demand *Dp*, the demand *Dp* is met by it if the source *Sk* is available in sufficient amount. If not, then the available amount of source *Sk* is entirely exhausted and the two adjacent sources, that is, $S(k-1)$ and $S(k+1)$, are considered to meet the remaining demand.

The *nearest neighbors algorithm* (NNA) essentially involves applying the principle of nearest neighbors to the remaining problem (on eliminating the demands and sources already matched) at each stage. It is illustrated below by designing a network (Figure 3a) for Example 1. Because the pinch concentration is 150 ppm (from Table 2), it is observed from Table 1 that sources *S1* and *S2* are below the pinch, source *S3* is at the pinch, and source *S4* is above the pinch. On the other hand, *D1*, *D2*, and *D3* are the demands below the pinch and *D4* is the only demand above the pinch. In fact, of the total 70 tons/h of source *S3*, 10 tons/h is below the pinch and the remaining 60 tons/h is above the pinch. The amount of source *S3* below the pinch (10 tons/h) is obtained by subtracting the freshwater target (70 tons/h) from the net flow rate (80 tons/h) at the pinch concentration (150 ppm) according to Table 2.

Analogous to heat exchanger networks,[15,21] the amount of water transferred across the pinch from sources to demands gives the freshwater penalty. As a consequence, the wastewater also increases by the same amount as dictated by Eq. 2. Thus, to achieve the minimum freshwater target, there should be no cross-pinch water transfer, which may be ensured by designing separately above and below the pinch.

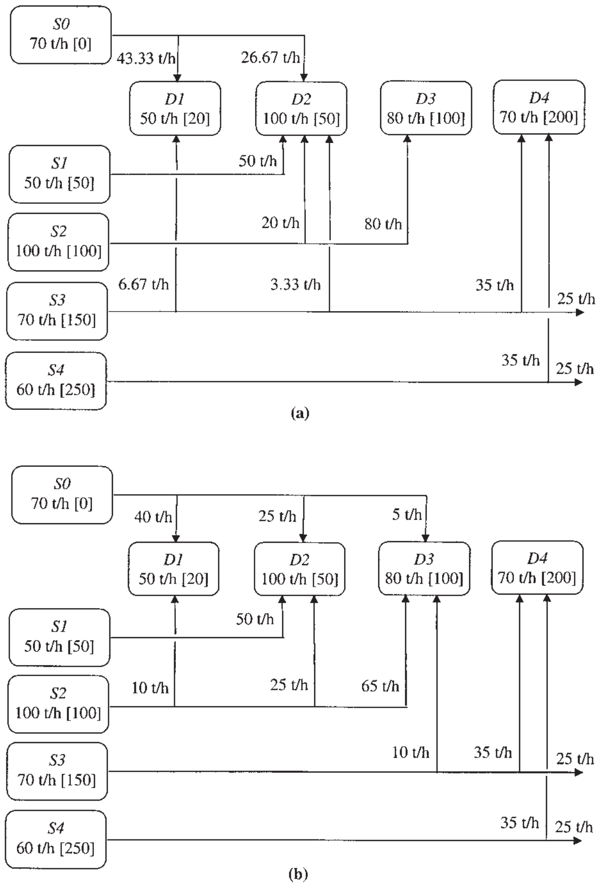


Figure 3. Minimum freshwater networks for Example 1 by NNA for water reuse.

Labels show contaminant concentrations (ppm) and flow rates (tons/h).

Consider the above-pinch design starting with demand *D4*, which has a contaminant concentration of 200 ppm. The nearest neighbor sources *Sk* and *S*($k + 1$) are *S3* and *S4*. Equations 4 and 5 give $F_{S3,D4} + F_{S4,D4} = 70$ and $F_{S3,D4}$ (150) + $F_{S4,D4}$ (250) = 70 (200), which may be solved to obtain $F_{S3,D4} = F_{S4,D4} = 35$ tons/h. Both these flow rates are less than the available amounts (70 and 60 tons/h, respectively), and thus the entire demand for *D4* is fulfilled by sources *S3* and *S4*. The flow rates now available for *S3* and *S4* are 35 and 25 tons/h.

Consider next the below-pinch design starting with demand *D3*, whose contaminant concentration is 100 ppm. Because source *S2* has the same contaminant concentration, the demand for 80 tons/h can be completely satisfied with *S2*. The flow rate now available for source *S2* is 20 tons/h.

Now, demand *D2* has a contaminant concentration of 50 ppm, which is equal to that of source *S1*. The demand is for 100 tons/h; however, only 50 tons/h of *S1* are available and so source *S1* is completely used (that is, $F_{S1,D2} = 50$ tons/h). For the remaining 50 tons/h, the nearest neighbor sources are therefore *S0* (freshwater) and *S2*. Equations 6 and 7 give $F_{S0,D2} + F_{S2,D2} = 100 - 50$ and $F_{S0,D2}$ (0) + $F_{S2,D2}$ (100) = 100 (50) − 50 (50), which may be solved to obtain $F_{S0,D2} = F_{S2,D2} = 25$ tons/h. Because only 20 tons/h of *S2* are available, source *S2* is totally used (that is, $F_{S2,D2} = 20$ tons/h). The nearest neighbor sources are now *S0* and *S3*. Equations 6 and 7 give $F_{S0,D2} + F_{S3,D2} = 100 - 50 - 20$ and $F_{S0,D2}$ (0) + $F_{S3,D2}$ (150) = 100 (50) − 50 (50) − 20 (100), which are solved to obtain $F_{S0,D2} = 26.67$ tons/h and $F_{S3,D2} = 3.33$ tons/h. Both these values are less than the available flow rates (70 and 35 tons/h, respectively), and thus demand *D2* is satisfied.

At this stage, the remaining problem is composed of demand *D1* and sources *S0* (43.33 tons/h), *S3* (31.67 tons/h), and *S4* (25 tons/h). The nearest neighbor sources for demand *D1* (20 ppm) are therefore *S0* and *S3*. Equations 4 and 5 give $F_{S0,D1} + F_{S3,D1} = 50$ and $F_{S0,D1}$ (0) + $F_{S3,D1}$ (150) = 50 (20), which yield $F_{S0,D1} = 43.33$ tons/h and $F_{S3,D1} = 6.67$ tons/h.

The final network in Figure 3a with the matches between sources and demands shows that 25 tons/h of source *S3* (150 ppm) and 25 tons/h of source *S4* (250 ppm) give a total of 50 tons/h of wastewater with a contaminant concentration of 200 ppm. Thus, the network meets the minimum targets of 70 tons/h (for freshwater) and 50 tons/h (for wastewater).

The network in Figure 3a was obtained by applying the NNA starting with demand *D4* (above pinch) and then satisfying demands *D3*, *D2*, and *D1* (below pinch) in that order. In general, many different water networks may be generated by the NNA, depending on the order in which the demands are satisfied, all of which meet the freshwater target. For instance, a different network (Figure 3b) may be obtained by applying the NNA to satisfy demands *D2*, *D1*, and *D3* in that order below the pinch. Although there is only one above-pinch design, three more alternative networks may be obtained corresponding to three different below-pinch designs by satisfying the demands in the following order: (1) *D1*, *D2*, *D3*; (2) *D2*, *D3*, *D1*; and (3) *D1*, *D3*, *D2* and *D3*, *D1*, *D2*, which yield the same design. The first of these three designs was reported by Prakash and Shenoy,[13] who generated only one network using the NNA by starting with the demand *D1* of the lowest contaminant concentration level and proceeding in order to demands (*D2*, *D3*, and so on) of higher contaminant concentration. No such restriction on the order is necessary. In fact, using the NNA with different permutations of the demands, ensuring that there is no cross-pinch water transfer, generates many different networks that meet the freshwater target. Simpler networks with fewer matches may be obtained by first matching all demands with sources of exactly the same concentration. Any network may be chosen by the designer and evaluated further for practical implementation considering cost, layout, controllability, flexibility, operability, and other intangibles.

Water Regeneration Networks

The advantage of the approach presented thus far is that it can be also used in regeneration networks for FF problems. Because the resulting limiting curve in Figure 2 is analogous to that obtained by Wang and Smith[5] for FC problems, their targeting method for regeneration–reuse and regeneration–recycle can be extended here too.

For the case of regeneration–reuse, Figure 4 shows the limiting composite along with a (dashed) water supply line matched against it. Freshwater is taken to the pinch concentration C_p and then enters a regeneration process, which reduces the contaminant concentration to C_o. The remaining contaminant is picked up by regenerated water. Although the dashed water supply line appears infeasible below the pinch because it

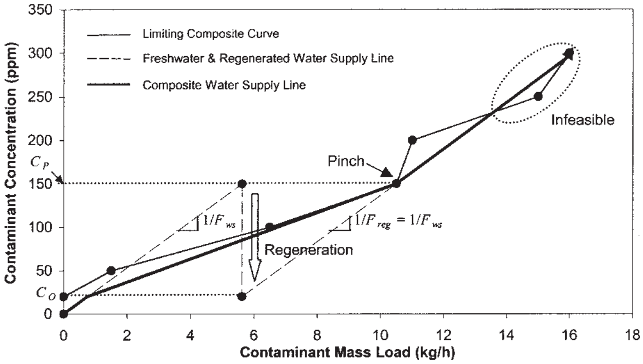


Figure 4. Targeting for Example 1 with total regeneration, where $F_{reg} = F_{ws}$.

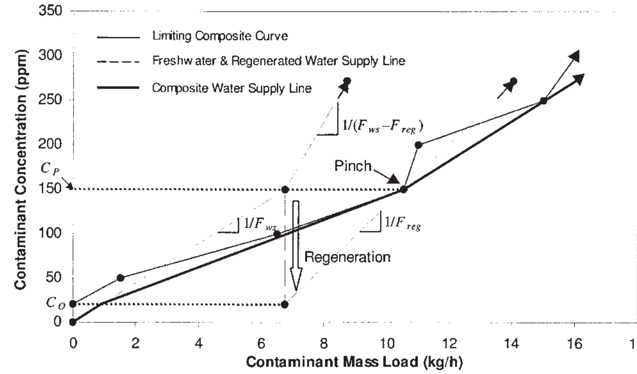


Figure 5. Targeting for Example 1 with partial regeneration, where $F_{reg} < F_{ws}$.

crosses the limiting composite, the composite water supply line (solid line in Figure 4 obtained by combining the dashed lines before and after regeneration) shows that regeneration at the pinch concentration is just feasible below the pinch. Wang and Smith[5] proved that allowing the freshwater supply line to achieve the pinch concentration before regeneration actually achieves both the targets of minimum water flow rate and minimum concentration reduction during regeneration.

For a regeneration process starting at or above the pinch concentration C_p and achieving an outlet concentration of C_o, a mass balance over the below-pinch region yields

$$m_p = F_{ws}(C_p - C_{ws}) + F_{reg}(C_p - C_o) \tag{8}$$

where m_p is the cumulative mass load of the pinch point on the limiting composite, F_{ws} is the water supply flow rate before regeneration, and F_{reg} is the regeneration flow rate. Also, Eq. 3 is modified (on considering the stream entering the regeneration process at C_{in} as a demand and the stream leaving at C_o as a source) to yield

$$F_{ws}C_{ws} - F_{ww}C_{ww} = \Delta_2 + F_{reg}(C_{in} - C_o) \tag{9}$$

Because the system constitutes three equations (2, 8, 9) in five unknowns (F_{ws}, F_{ww}, F_{reg}, C_{ww}, and C_{in}), there are two degrees of freedom. So, two variables may be specified and then the equations used to determine the targets as illustrated below for three cases: total regeneration ($F_{reg} = F_{ws}$ and $C_{in} = C_p$); partial regeneration ($F_{reg} < F_{ws}$ with F_{reg} specified by the limiting composite and $C_{in} = C_p$); and zero discharge ($F_{ww} = 0$ and $C_{ww} = 0$).

Consider Example 1 allowing total regeneration (first case) with a regeneration unit that can deliver an outlet concentration C_o of 20 ppm. From Table 2, the pinch is at $C_p = 150$ ppm and $m_p = 10.5$ kg/h. If the flow rates of water before and after regeneration are the same, then Eq. 8 gives the freshwater ($C_{ws} = 0$) and regeneration targets as $F_{ws} = F_{reg} = m_p/(2C_p - C_{ws} - C_o) = 37.5$ tons/h. Then, Eq. 2 gives $F_{ww} = 17.5$ tons/h and Eq. 9 with $C_{in} = C_p = 150$ ppm gives $C_{ww} = 292.86$ ppm. However, these total regeneration targets are impossible to achieve in a network design in practice for this example, as is evident in Figure 4, where the composite water supply line crosses the last portion of the limiting composite above the pinch. Such infeasibilities have been identified by Wang and Smith[5] and Castro et al.,[16] who suggested increasing the freshwater requirement and doing partial regeneration.

For partial regeneration (second case), the freshwater flow rate is increased such that the composite water supply line just touches the limiting composite [above the pinch at (15 kg/h, 250 ppm) as in Figure 5]. The new freshwater target dictated by the shape of the limiting composite is $F_{ws} = (15 - 10.5) \times 10^3/(250 - 150) = 45$ tons/h. Substituting this value for F_{ws} in Eq. 8, the partial regeneration target is $F_{reg} = 28.846$ tons/h. Then, Eq. 2 gives $F_{ww} = 25$ tons/h and Eq. 9 with $C_{in} = C_p = 150$ ppm gives $C_{ww} = 250$ ppm. Figure 5 shows the water supply lines for partial regeneration where $F_{reg} < F_{ws}$.

The NNA may be now applied to design a possible network (Figure 6) for Example 1 with partial regeneration that meets the targets of 45 tons/h (for freshwater), 25 tons/h (for wastewater), and 28.846 tons/h (for regeneration). The regenerated water provides an additional source *SR* of 28.846 tons/h at 20 ppm, which is entirely used to satisfy the demand *D1* (also at

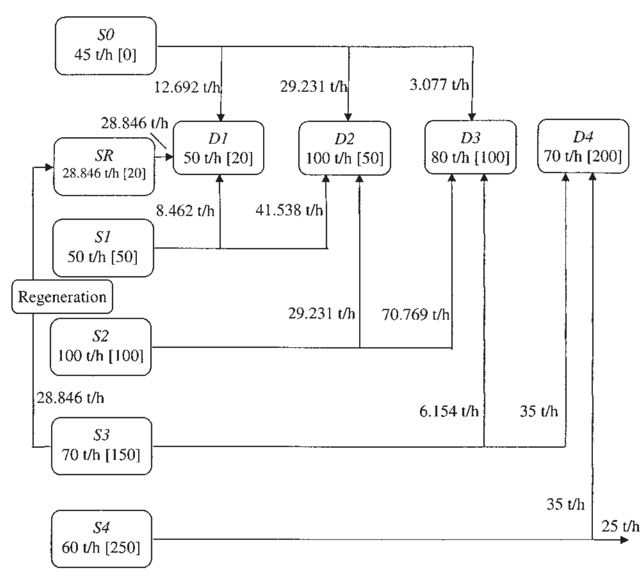


Figure 6. Network for Example 1 by NNA for partial regeneration.

Labels show contaminant concentrations (ppm) and flow rates (tons/h).

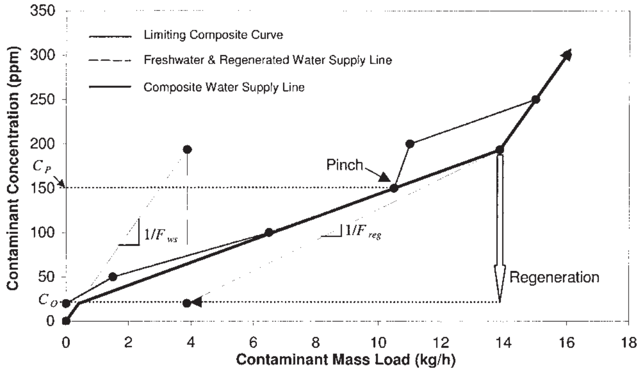


Figure 7. Targeting for Example 1 for zero waste discharge.

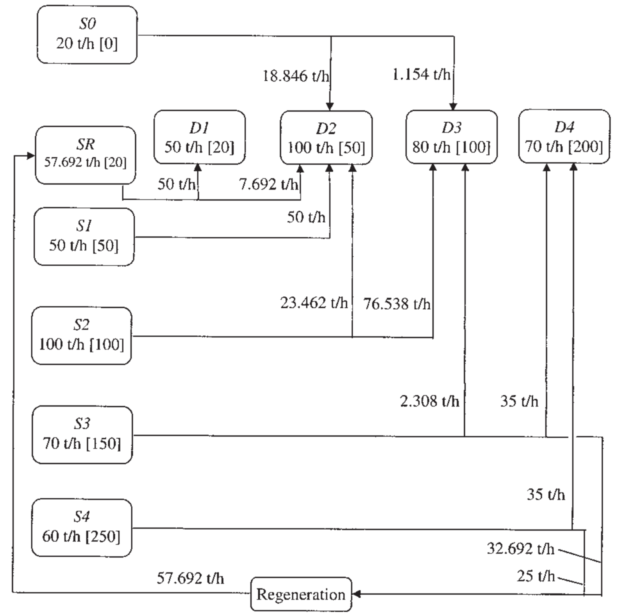


Figure 8. Network for Example 1 by NNA for zero waste discharge.

Labels show contaminant concentrations (ppm) and flow rates (tons/h).

20 ppm). The source SR is itself obtained by regenerating water from source S3 at the pinch concentration of 150 ppm. The rest of the matches between sources and demands are obtained by a straightforward application of the NNA (starting with demand *D1* and then satisfying demands *D2*, *D3*, and *D4* in that order).

The freshwater requirement for Example 1 of 70 tons/h (for reuse without regeneration) was reduced to 45 tons/h through regeneration–reuse. It can be further reduced to the absolute minimum (through regeneration with recycle according to Wang and Smith[5]) as illustrated next. The slope of the limiting composite below C_o sets the minimum freshwater flow rate. For Example 1, the limiting composite starts at C_o (20 ppm) and therefore its slope below C_o is infinite. The water flow rate required would therefore be zero if Example 1 were a FC problem [$F_{ws} = F_{ww} = 0$ according to Eq. 2 because $\Delta_1 = 0$]. However, Example 1 is a FF problem with $\Delta_1 = 20$ tons/h, and Eq. 2 gives the absolute minimum water requirement as $F_{ww} = 0$ and $F_{ws} = 20$ tons/h. Substituting this value for F_{ws} in Eq. 8, the regeneration–recycle target is $F_{reg} = 57.692$ tons/h. Then, Eq. 9 gives $C_{in} = 193.33$ ppm. Figure 7 shows the water supply lines for zero waste discharge (third case).

The NNA is now applied to design a zero discharge network (Figure 8) for Example 1 that meets the targets of zero wastewater, 20 tons/h (for freshwater), and 57.692 tons/h (for regeneration). The regenerated water is considered an additional source *SR* of 57.692 tons/h at 20 ppm. It is obtained by regenerating what could otherwise have been wastewater. Note that if the regeneration outlet concentration is less than or equal to the lowest inlet demand concentration, then the regeneration network will have zero waste discharge (for a FF problem with $\Delta_1 \geq 0$), or require no freshwater (for a FF problem with $\Delta_1 \leq 0$), or have zero waste discharge and require no freshwater (for a FC problem where Δ_1 is always zero).

Targeting Approach for Hydrogen Networks

The targeting approach outlined earlier is not limited to water networks only. It can be used in any problem involving matching of sources and demands with load (quantity) and level (quality) as the parameters. Recently, Singhvi and Shenoy[22] and Singhvi et al.[23] applied it to aggregate production planning in supply chain management. Here, it is shown how it may be profitably used in (refinery) hydrogen networks to target the minimum makeup hydrogen.

Graphical approaches to hydrogen targeting use the concept of the *surplus diagram*.[24,25] However, like the water surplus diagram,[10] the method based on the hydrogen surplus diagram is iterative in nature and requires an initial assumption of the hydrogen target. A noniterative method has been recently proposed by El-Halwagi et al.[12] The approach presented here also provides the target without any trial and error. In addition, it is suitable to target regeneration problems and multiple hydrogen sources.

To illustrate the methodology, consider the example used by Alves,[24] Hallale and Liu,[26] and Hallale et al.[27] The existing system, composed of two hydrogen consumers (Reactor 1 and Reactor 2) in Example 2, is shown in Figure 9. Each consumer has a makeup, recycle, and purge.

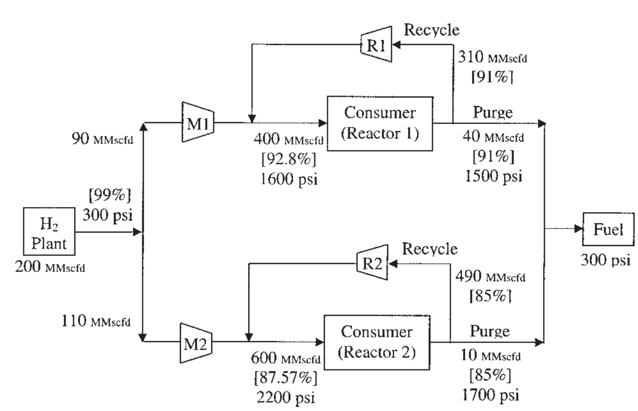


Figure 9. Existing flow sheet showing hydrogen consumers for Example 2.

Table 3. Hydrogen Data for Example 2

	Purity, y (Fraction)	Flow Rate, F (MMscfd)
Sinks (Demands)		
$D1$	0.928	400
$D2$	0.875667	600
Sources		
$S1$	0.91	350
$S2$	0.85	500

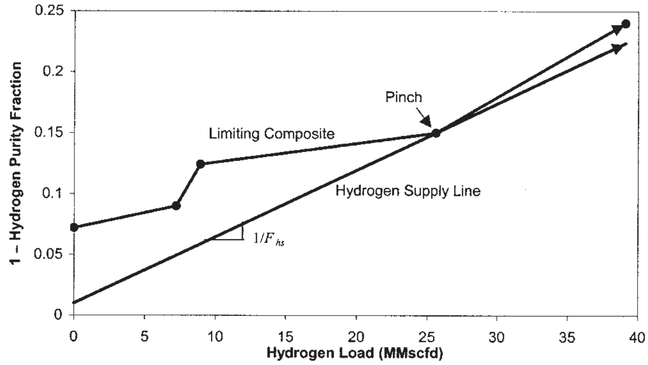


Figure 10. Limiting composite curve and minimum hydrogen utility targeting for Example 2.

A few differences between water and hydrogen networks may be noted. The demands in water networks are also referred to as *sinks* in hydrogen networks. Water flow rates are typically in tons/h, whereas flow rates in hydrogen networks are in MMscfd (million standard cubic feet per day) or Nm^3/h (normal cubic meters per hour). The analog of contaminant concentration in water is purity of hydrogen. If and when required, percentage hydrogen purity (y) may be treated in terms of equivalent contaminant concentration (C) using $C \equiv 1 - y$. An important difference to be observed is that the water supply is often freshwater with 0 ppm contaminant concentration (that is, $C_{ws} = 0$), whereas the makeup hydrogen supply will not be available at 100% purity (that is, $C_{hs} = 1 - y_{hs} \neq 0$). The makeup hydrogen supply obtained from a hydrogen plant or import is usually termed a *utility*. The purge streams (analogous to wastewater sent to effluent treatment) are often sent to the fuel system where they are burned for their heating value or flared.

Table 3 shows the data extracted from the existing hydrogen flow sheet (Figure 9) and represented in a format similar to the water data in Table 1. The hydrogen sinks (demands) consist of the makeup and recycle, whereas the hydrogen sources constitute the purge and recycle taken together.

Given that the overall data representation in the FF water problem and the hydrogen problem is similar in terms of demands and sources, the methodologies developed earlier for water networks should apply to hydrogen networks with some adaptations. The CTA may be implemented on the data in Table 3 to obtain Table 4. In the case of hydrogen, the purities are tabulated in decreasing order and therefore the arbitrary addition at the bottom will be the lowest purity. Figure 10 shows the limiting composite obtained by plotting $(1 - y)$ vs. cumulative load from Table 4. A hydrogen supply line originating from 0.01 (corresponding to 99% purity) on the vertical axis is rotated until it just touches the limiting composite. The reciprocal of the slope of this rotated line gives the hydrogen target. For Example 2, the minimum makeup hydrogen is 182.86 MMscfd (from Figure 10 and Table 4), which agrees with the result obtained by Alves[24] and Hallale and Liu[26] using the surplus diagram.

The analogs of Eqs. 2 and 3 are

$$F_{hs} - F_{fuel} = \Delta_1 \qquad \text{where } \Delta_1 \equiv \sum F_d - \sum F_s \tag{10}$$

$$F_{hs}y_{hs} - F_{fuel}y_{fuel} = \Delta_2 \qquad \text{where } \Delta_2 \equiv \sum F_d y_d - \sum F_s y_s \tag{11}$$

where F denotes the stream flow rate, y denotes hydrogen purity, and subscripts *hs* and *fuel* denote hydrogen supply and fuel, respectively. As before, the net system flow rate (Δ_1) and the net system load (Δ_2) obtained by subtracting the sum of all sources from the sum of all demands are constant for a given problem ($\Delta_1 = 150$ MMscfd and $\Delta_2 = 153.1$ MMscfd for Example 2 from Table 3). Because $F_{hs} = 182.86$ MMscfd and $y_{hs} = 0.99$, Eqs. 10 and 11 give $F_{fuel} = 32.86$ MMscfd and $y_{fuel} = 0.85$.

Design of Hydrogen Networks by Nearest Neighbors Algorithm

The *nearest neighbors algorithm* (NNA) may be applied to design hydrogen networks. Equations 4 through 7 are applicable with contaminant concentration C simply replaced by hydrogen purity y (given that $C = 1 - y$).

Two possible hydrogen networks for Example 2 designed by the NNA are shown in Figure 11a (starting with demand *D1* and then satisfying demand *D2*) and Figure 11b (starting with demand *D2* and then satisfying demand *D1*). Both networks meet the minimum targets of 182.86 MMscfd (for makeup hydrogen utility) and 32.86 MMscfd (for hydrogen to fuel).

For Figure 11a, consider first demand *D1*, which requires a

Table 4. Implementation of Composite Table Algorithm (CTA) for Example 2

Purity, y (Fraction)	Net Flow Rate (MMscfd)	Net Load (MMscfd)	Cumulative Load, m_{cum} (MMscfd)	$m_{cum}/(y_{hs} - y)$ (MMscfd)
0.928			0	0
0.91	400	7.2	7.2	90
0.875667	50	1.71667	8.91667	77.9883
0.85	650	16.6833	25.6	182.857
(0.76)	150	(13.5)	(39.1)	(170)

$D1$	$D2$	$S1$	$S2$
400	600	350	500

purity of 92.8%. The nearest neighbor sources are *S0* (makeup from hydrogen plant) and *S1*. Equations 4 and 5 give $F_{S0,D1} + F_{S1,D1} = 400$ and $F_{S0,D1}$ (0.99) + $F_{S1,D1}$ (0.91) = 400 (0.928), which may be simultaneously solved to obtain $F_{S0,D1}$ = 90 MMscfd and $F_{S1,D1}$ = 310 MMscfd. Both these flow rates are less than the available amounts (182.86 and 350 MMscfd, respectively), and thus the entire demand for *D1* is fulfilled by sources *S0* and *S1*. The flow rates now available for *S0* and *S1* are 92.86 and 40 MMscfd, respectively.

Because demand *D2* needs a purity of 87.56%, the nearest neighbor sources are *S1* (91%) and *S2* (85%). Equations 4 and 5 give $F_{S1,D2} + F_{S2,D2} = 600$ and $F_{S1,D2}$ (0.91) + $F_{S2,D2}$ (0.85) = 600 (0.8757), which may be simultaneously solved to obtain $F_{S1,D2}$ = 256.67 MMscfd and $F_{S2,D2}$ = 343.33 MMscfd. However, only 40 MMscfd of *S1* are available and so source *S1* is completely used (that is, $F_{S1,D2}$ = 40 MMscfd). The nearest neighbor sources now are therefore *S0* and *S2*. Equations 6 and 7 give $F_{S0,D2} + F_{S2,D2} = 600 - 40$ and $F_{S0,D2}$ (0.99) + $F_{S2,D2}$ (0.85) = 600 (0.8757) − 40 (0.91), which may be solved to obtain $F_{S0,D2}$ = 92.86 MMscfd and $F_{S2,D2}$ = 467.14 MMscfd. The remainder of source *S2* is 32.86 MMscfd and goes to the fuel system.

Figure 11 shows the final networks with the matches between sources and demands without accounting for pressure constraints, which are considered next. When the network in Figure 11a is redrawn as a conventional hydrogen flow sheet in Figure 12, it is observed to be very similar to the existing flow sheet (Figure 9) with the essential difference being the match

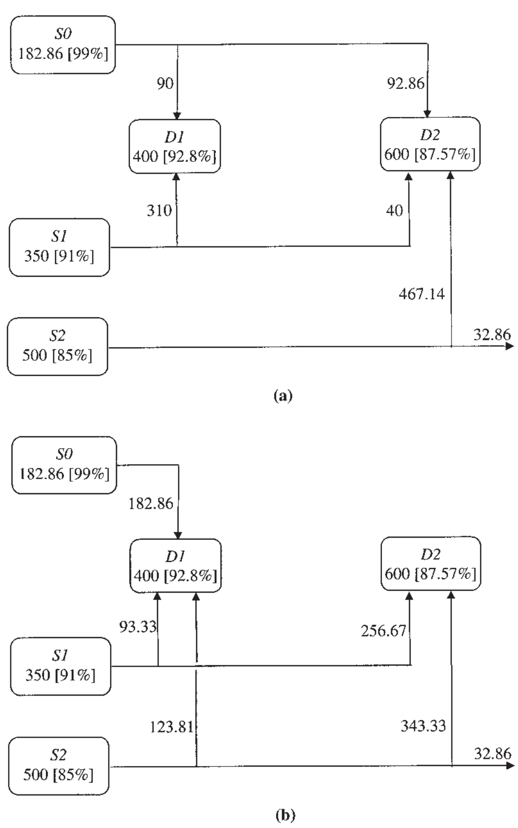


Figure 11. Minimum hydrogen utility networks for Example 2 by NNA.

Labels show flow rates in MMscfd.

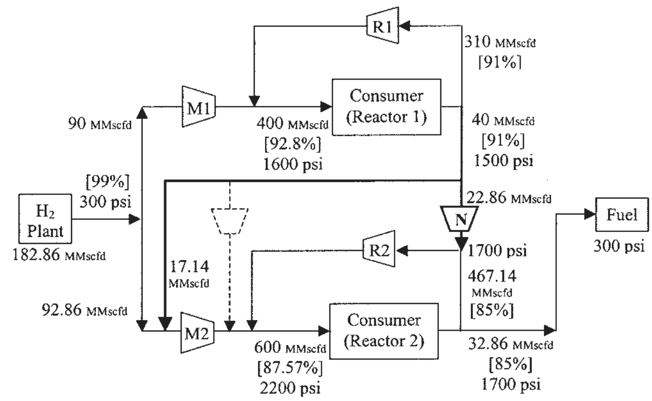


Figure 12. Minimum hydrogen utility flow sheet for Example 2.

between source *S1* and demand *D2* of 40 MMscfd. Considering the pressures at different points in the flow sheet, the hydrogen purge from the outlet of reactor 1 (at 1500 psi) can be introduced to enter reactor 2 in three ways:

(1) at the inlet to the makeup compressor M2 (300 psi)

(2) at the inlet to the recycle compressor R2 (1700 psi) using a new compressor with a pressure ratio of 1.133 (that is, 1700/1500)

(3) at the inlet to reactor 2 directly (2200 psi) using a new compressor with a pressure ratio of 1.467 (that is, 2200/1500)

The first option (shown by the bold line in Figure 12) is the best of the three because it does not require a new compressor; however, only 17.14 MMscfd out of the total of 40 MMscfd of hydrogen can enter the makeup compressor M2 if the maximum flow rate constraint on the existing compressor is 110 MMscfd. The remaining hydrogen (22.86 MMscfd) uses the second option of going through a new compressor N (shown bold in Figure 12) and then entering recycle compressor R2. The last option (shown by the dashed line in Figure 12) requires a new compressor with a higher pressure ratio and is therefore not used.

Importantly, the bottleneck in the above design in Figure 12 is the capacity of the makeup compressor M2. If the compressor M2 has spare capacity, that is, a flow rate margin fraction f over and above its design flow rate (of 110 MMscfd), then $(17.14 + 110f)$ MMscfd out of the total of 40 MMscfd can enter compressor M2 and the remainder of $(22.86 - 110f)$ MMscfd can go through the new compressor N. For instance, if compressor M2 has 5% spare capacity ($f = 0.05$), then 22.64 MMscfd can enter M2 and 17.36 MMscfd can go through the new compressor N. These values agree with the results of Hallale and Liu,[26] who obtained them by solving a mixed-integer nonlinear program (MINLP) for 5% spare capacity on existing compressors.

If no new compressor is to be installed, then compressor M2 must have a spare capacity of 20.78% (that is, f = 22.86/110). If compressor M2 does not have this spare capacity, then the other option (to avoid installing a new compressor) is to use more makeup from the hydrogen plant. The hydrogen penalty may be calculated from the flow rate and hydrogen balances at the inlet to reactor 2 in Figure 12. Thus, $F_{S0,D2} + F_{S1,M2} + F_{S1,N} + F_{S2,D2} = 600$ and $F_{S0,D2}$ (0.99) + $F_{S1,M2}$ (0.91) + $F_{S1,N}$ (0.91) + $F_{S2,D2}$ (0.85) = 600 (0.8757). Now, $F_{S1,N}$ = 0 (no

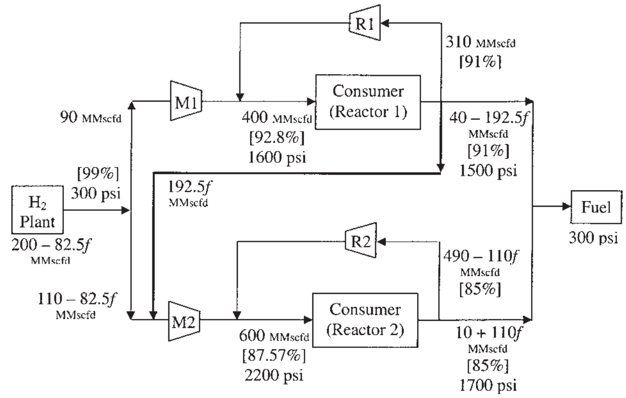


Figure 13. Evolved hydrogen flow sheet for Example 2 with no new compressors shows a utility penalty.

Here, f denotes the flow rate margin fraction of compressor M2.

new compressor N) and $F_{S0,D2} + F_{S1,M2} = 110\ (1 + f)$ (capacity constraint on compressor M2). These equations may be solved to obtain $F_{S2,D2} = 490 - 110f$, $F_{S1,M2} = 192.5f$, and $F_{S0,D2} = 110 - 82.5f$. The minimum makeup hydrogen utility target is given by $F_{S0,D2} + 90 = 200 - 82.5f$. It decreases linearly from 200 to 182.86 MMscfd when the maximum capacity of makeup compressor M2 increases from 110 MMscfd ($f = 0$) to 132.86 MMscfd ($f = 0.2078$). This observation is consistent with that obtained by Hallale and Liu,[26] who performed a sensitivity analysis to determine the minimum utility over a range of different compressor capacities by solving a nonlinear program (NLP). The result is obtained here analytically by a simple calculation. The hydrogen flow sheet for this case using the existing compressors is shown in Figure 13. Note that the minimum hydrogen utility flow sheet in Figure 12 corresponds in a sense to a maximum energy recovery (MER) network in heat exchanger network synthesis[15,21] that meets the utility targets. Just as the MER network can be evolved by reducing the number of heat exchangers and incurring an energy penalty (or a minimum freshwater network can be evolved[28] by reducing the number of matches and incurring a utility penalty), the hydrogen flow sheet in Figure 12 has been evolved to the one in Figure 13 by decreasing the number of compressors and incurring a hydrogen utility penalty.

Hydrogen Regeneration Networks

The approach used for water regeneration networks is extended here to hydrogen regeneration networks. The regeneration in hydrogen networks is achieved through purifiers such as pressure-swing adsorption (PSA) and membrane units. These interception units upgrade the hydrogen purity of sources and allow the minimum utility target established by the method in Figure 10 to be further lowered.

The purifier may be modeled[26] as a demand (the inlet feed stream of flow rate F_{in} and hydrogen purity y_{in}) and two sources (the product stream of flow rate F_{reg} and purity y_{reg}, along with the residue stream of flow rate F_r and purity y_r). Note that the residue is typically of low purity and is sent to the fuel system. The flow rate balance for the purifier is simply given by

$$F_{in} = F_{reg} + F_r \tag{12}$$

For the purifier, the product purity y_{reg} and the hydrogen recovery R, as defined below, are usually specified:

$$R = F_{reg}y_{reg}/(F_{in}y_{in}) \tag{13}$$

Because $C = 1 - y$, the analog of Eq. 8 for hydrogen regeneration networks is

$$m_p = F_{hs}(y_{hs} - y_p) + F_{reg}(y_{reg} - y_p) \tag{14}$$

Equation 11 is modified analogous to Eq. 9 as

$$F_{hs}y_{hs} - F_{fuel}y_{fuel} = \Delta_2 + F_{in}y_{in} - F_{reg}y_{reg} - F_r y_r \tag{15}$$

Because the system constitutes six equations (10–15) in eight unknowns (F_{hs}, F_{fuel}, F_{in}, F_{reg}, F_r, y_{fuel}, y_{in}, and y_r), there are two degrees of freedom. So, two variables may be specified and then the equations solved simultaneously to determine the targets as illustrated in the example below.

Consider Example 2 allowing one new PSA unit whose residue must be sent to the fuel system. If only the residue is sent to the fuel system (that is, $F_{fuel} = F_r$ and $y_{fuel} = y_r$), then Eqs. 13–15 yield

$$F_{hs} = [\Delta_2(1 - y_p/y_{reg}) + m_p(1/R - 1)]/[y_{hs}(1/R - y_p/y_{reg}) - y_p(1/R - 1)] \tag{16}$$

The PSA product purity y_{reg} is specified as 95% and the recovery R as 90%. The pressure drop in the PSA unit may be taken as 1 bar. From Table 4, the pinch is at $y_p = 0.85$ and $m_p = 25.6$ MMscfd. Substituting values in Eq. 16 gives $F_{hs} = 158.31$ MMscfd. Equations 10 and 14 then yield $F_{fuel} = F_r = 8.31$ MMscfd and $F_{reg} = 34.37$ MMscfd. Finally, Eqs. 11–13 give $y_{fuel} = y_r = 0.4365$, $F_{in} = 42.68$ MMscfd, and $y_{in} = 0.85$. Note that the regeneration starts at the pinch purity (that is, $y_{in} = y_p$). Figure 14 shows the hydrogen supply lines for this regeneration.

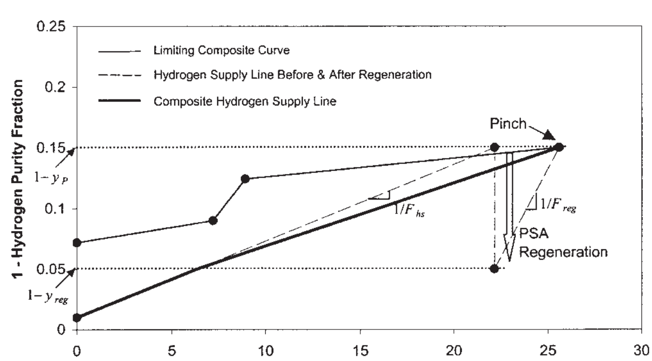


Figure 14. Targeting for Example 2 with regeneration by PSA unit.

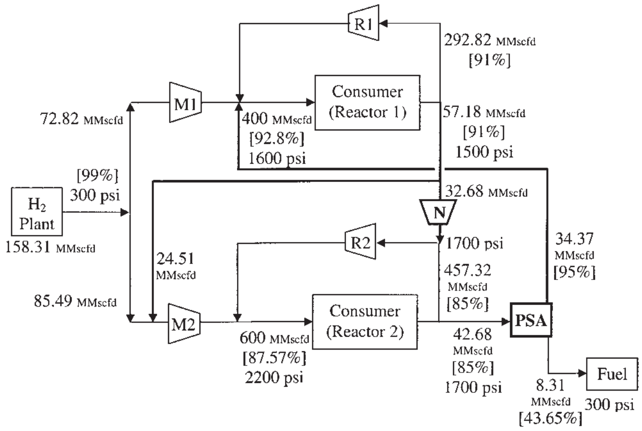


Figure 15. Minimum hydrogen utility flow sheet for Example 2 with regeneration by PSA unit.

The NNA is now applied to design a network (shown as a flow sheet in Figure 15) for Example 2 with regeneration that meets the targets of 158.31 MMscfd (for makeup hydrogen from the plant) and 34.37 MMscfd (for regeneration from the PSA unit). The regenerated hydrogen product stream from the PSA unit is considered an additional source of 34.37 MMscfd at 95% purity. It is obtained by regenerating an input stream of 42.68 MMscfd of 0.85% hydrogen purity, which could otherwise have been sent to the fuel system. The bottleneck continues to be the capacity of the makeup compressor M2. The design in Figure 15 uses one new compressor in addition to the PSA unit. If no new compressor is to be installed, then compressor M2 must have a spare capacity of 29.71% (that is, $f = 32.68/110$). The other option (to avoid installing a new compressor) is to use more makeup from the hydrogen plant. From the flow rate and hydrogen balances at the inlet to reactor 2 in Figure 15 (as done earlier in Figure 12), it is found that $F_{S2,D2} = 490 - 110f$, $F_{S1,M2} = 192.5f$, and $F_{S0,D2} = 110 - 82.5f$. The minimum makeup hydrogen utility target is given by $F_{S0,D2} + 72.82 = 182.82 - 82.5f$. It decreases linearly from 182.82 to 158.31 MMscfd when the maximum capacity of makeup compressor M2 increases from 110 MMscfd ($f = 0$) to 142.68 MMscfd ($f = 0.2971$).

Conclusion

A methodology has been presented here for targeting the minimum freshwater in FF problems based on the graphical method of the limiting composite originally proposed by Wang and Smith[5] for FC problems. It provides several advantages over the approaches of Dhole et al.[11] and Hallale.[10] First, it is noniterative and does not require any initial guesses. Second, it is computationally very easy to implement in the form of the composite table algorithm (CTA), which is very similar to the problem table algorithm[14,15] used in targeting of heat exchanger networks. It does not require any complicated plots or transferring of data from one plot to another. Third, it can be used to target hybrid problems involving both FF and FC units. It can thus deal with water losses and gains, with units having multiple water streams, as well as with units having fixed contaminant loads. Finally, the approach is universal in that it can be applied to reuse, regeneration–reuse, regeneration–recycle problems for water networks, and reuse and regeneration problems for hydrogen networks.

The targeting approach in its generalized form makes use of three phenomena: the constancy of the net system flow rate (Eq. 2 or Eq. 10), the mass balance over the below-pinch region (Eq. 8 or Eq. 14), and the constancy of the net system load (Eq. 9 or Eq. 15). The regeneration process may be modeled using a simple flow rate balance (such as Eq. 12) and its performance may be specified using either of two possible criteria: outlet concentration or removal ratio/recovery as in Eq. 13. These equations may be solved to obtain the fresh/makeup supply flow rate, the waste/purge flow rate and concentration, and the regeneration flow rate and concentration at both the inlet and the outlet.

To summarize, it may be noted that methods for targeting and design of water networks for single contaminant have been developed that apply to both types of units (fixed contaminant load and fixed flow rate) as well as all types of networks (water reuse, regeneration–reuse, and regeneration–recycle). The same targeting and network design methods have been shown to also apply to utility minimization in (refinery) hydrogen networks.

An algorithm based on the principle of nearest neighbors has been used to design minimum utility networks that meet the targets. For hydrogen networks, the minimum utility networks have been evolved for pressure constraints imposed by compressors. Because pressure constraints are often as significant as concentration constraints in hydrogen networks, improved methods may be devised in the future to account for pressure at the targeting and network design stages.

Current work is directed toward extending the methods to cost-optimal networks and water networks with multiple contaminants.

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Notation

- C = contaminant concentration in water stream, ppm
- CTA = composite table algorithm
- D = demand stream for water or hydrogen
- f = flow rate margin fraction for compressor
- F = water flow rate, tons/h or hydrogen flow rate, MMscfd
- FC = fixed contaminant load
- FF = fixed flow rate
- k = index denoting source stream number
- m = mass load of contaminant, kg/h or load of hydrogen, MMscfd; also, total number of demand streams
- NNA = nearest neighbors algorithm
- n = total number of source streams
- p = index denoting demand stream number
- R = recovery or removal ratio
- S = source stream for water or hydrogen
- s = index denoting cleanest source
- t = index denoting dirtiest source
- y = hydrogen purity fraction
- Δ_1 = net system flow rate of water, tons/h or hydrogen, MMscfd

Δ_2 = net system load of contaminant in water, kg/h or hydrogen, MMscfd

Subscripts

d = demand
$fuel$ = to fuel system
hs = hydrogen supply
i, j = from source i to demand j
in = inlet
max = maximum value
o = outlet (concentration after regeneration)
out = outlet
p = pinch
reg = regeneration
s = source
ws = water supply
ww = wastewater

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