

# Cascade Models for Targeting and Synthesis of Total Water Networks

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Success in the race for efficiency means for today's process industries their survival. The most critical resources are energy and water, with the latter being a crisis factor when in shortage. Effective water savings are achieved by reuse, regeneration and recycling. The selection of regeneration technology cannot be addressed separately from targeting reuse, recycle and fresh water flowrates. This work simulates total water networks as cascade systems, represented by transshipment models and uses a the two step iterative procedure to coordinate the targeting of minimum fresh water requirements, the calculation of recycle and treatment flows and the selection of water treatment processes. The procedure offers the advantage of producing optimal solutions ahead of design by using linear mixed integer models. Two examples from literature are used to illustrate the new approach for single contaminant systems, one with fixed mass loads of contaminant and one with fixed flowrates in water using operations.

## 1. Introduction

The stringent legislative framework on discharge limits and the increased public concern on water scarcity force the chemical industry to adopt water management practices with ever increasing costs. The minimization of fresh water consumption and waste treatment costs must be synchronized since the amount of effluents is directly related to fresh water consumption. Additional benefits are brought by the possibility of recycling treated water, while treatment costs depend on the effluent flowrates and the selection of treatment processes. Optimization strategies for the design and synthesis of optimum water networks that enable maximum reuse between operations but also select treatment technologies to regenerate and recycle water have been known to be challenging due to the presence of nonlinearities in the formulation and no guaranty for the optimality of the solutions (Halim et al., 2015). Prior to detailed design it is useful to quantify the target for minimum water consumption together with assessing the maximum potential of a wastewater treatment configuration and calculate minimum wastewater treatment flowrates (Kuo and Smith, 1997). Existing targeting methods for total water regeneration networks developed to target the minimum freshwater, regenerated water, and wastewater flowrates (Parand et al., 2014) are not able to screen treatment technologies. Also graphical targeting methods (Wang and Smith 1994) are unable to screen treatment technologies and target flowrates for multiple treatment units and fresh water, while shortcut models for the selection of treatment processes are absent from literature (Khor et al., 2014).

The method proposed in this paper is an iterative procedure, which links two transshipment models with cascade characteristics and introduces successively increasing recycle flows until convergence to the optimal value based on the total cost criterion. The first model - model (Ia) for fixed mass load or model (Ib) for fixed flowrates - which targets the minimum required flowrate of fresh water, is extended in identifying the flowrates and concentrations of the wastewater streams at the effluent water mains. The second model (II) extends the transshipment model of (Nikolakopoulos et al, 2014), which targets treatment flowrates, in screening alternative treatment technologies. The link between the two models is the wastewater streams resulting from model (I) for which the flowrates and concentrations are allocated at the pinch points.

## 2. Overview of the two step iterative procedure

For the overall system, including the water using operations and the candidate treatment technologies, the objectives are to select the optimal set of treatment technologies, calculate recycle flows and target the minimum treatment flows and clear water consumption. These objectives are competitive since by recycling treated wastewater the consumption of clear water is reduced against an increase of the treatment flows that may in turn also affect the selection of treatment technologies and costs.

Based on the availability of treated and recycled water a first targeting model (Ia) or (Ib), calculates fresh water targets and the flows of the effluent streams. A second model (II) selects treatment processes and calculates minimum treatment flows. An iterative procedure calculates the recycle flow for which the cost of the overall system is minimized.

The methodology consists of the following steps:

Initialization: the value of the recycle flow is set to  $R = 0$ , and the Current Total Cost ( $CTC$ ) to infinity.

Step 1: Calculate minimum fresh water and wastewater flows using model (Ia) for fixed contaminant loads or model (Ib) for fixed flowrates.  $C_1$  is the cost of fresh water requirements.

Step 2: Select treatment technologies and calculate minimum treatment flows by using model (II).  $C_2$  is the sum of the fixed and operating cost for the selected treatment technologies. Set Total Cost  $TC = C_1 + C_2$ .

Step 3: If  $TC < CTC$ , then  $CTC = TC$ . Reserve the recycle flow  $R_{res} = R$ , the selected technologies and the fresh water flow. Increase the recycle flow  $R = R + a$ , and go to Step 2.

If  $TC \geq CTC$ , then STOP. The optimal recycle flow is  $R_{res}$ .

## 3. Cascade models

### 3.1 Cascade model (Ia) - Water targets in systems with fixed contaminant loads

Let us denote by  $I = \{i | i = 1, 2, \dots, No\}$  the index set of the water using operations. Associated with each operation are maximum inlet and outlet concentrations  $C_i^{in,max}$  and  $C_i^{out,max}$  respectively. The mass load of the contaminant transferred to each water-using operation is  $M_i^c$ .  $S = \{s | s = 1, 2\}$  is the set of water sources. The fresh and recycled water sources are represented by  $s = 1$  and  $s = 2$  respectively. The limiting water flow rate, for the water-using operation  $i$  is  $F_i^l = M_i^c / (C_i^{out,max} - C_i^{in,max})$ . The index set of concentration intervals is

$CI = \{k | k = 1, 2, \dots, K\}$ , and  $C_k$  is the inlet concentration of interval  $k$ . Figure 3 shows how the transshipment concept is adapted to the case of the water using system. The water using operations dispose contaminant to water sources through specific concentration intervals, defined by the concentration limits of the contaminant receivers and providers. Contaminant is allowed to be transferred between concentration intervals. This cascade feature enables the reuse of water among operations and debottlenecks the search of the minimum fresh water flowrate. The mass transferred from water-using operation  $i$  through the  $k^{th}$  concentration interval is  $W_{i,k}^p = F_i^l (C_k - C_{k+1})$ , and the residual mass from water using operation  $i$  leaving interval  $k$ , is  $r_{i,k}$ . The mass of contaminant transferred from water-using operation  $i$  to water source  $s$  through interval  $k$  is  $W_{s,i,k}$ . Eqs(1-7) are the model Ia with the objective to minimize  $C_1$ :

$$\min Cost_1 = \sum_{s \in S} c_s L_s \quad (1)$$

$$r_{i,k} - r_{i,k-1} + \sum_{s \in S} W_{s,i,k} = W_{i,k}^p, \quad \forall i, k \quad (2)$$

$$\sum_i W_{s,i,k} = W_{s,k}^w, \quad \forall s, k \quad (3)$$

$$W_{s,k}^w = L_s (C_k - C_{k+1}), \quad \forall s, k \quad (4)$$

$$0 \leq L_s \leq L_s^U, \quad \forall s \quad (5)$$

$$\sum_i r_{i,k} \leq y_k M, \quad \forall k \quad (6)$$

$$r_{i,0} = r_{i,k} = 0, \quad r_{i,k} \geq 0, \quad \forall i \quad \text{and} \quad y_k \in \{0, 1\}, \quad \forall k \quad (7)$$

Since the cost of treatment is calculated by the Transshipment model 3, the recycle flow comes at no cost in this model ( $c_2 = 0$ ). Therefore, although the objective of this model is to minimize the cost of water sources, it actually minimizes at the same time the flow of fresh water  $L_1$ .

Eq(2) is the mass balances around interval  $k$  for every operation  $i$ . If  $\sum_i r_{i,k} \geq 0$ , then  $k$  is one of the pinch points.  $M$  is a sufficiently large number. Then from (Eq(6))  $y_k = 1$ , and  $k$  is a pinch point. Let  $KP = \{k^p \mid k^p = 1, \dots, K^p\}$  be the index set of all pinch points, including the pseudo pinch  $K$ . The pseudo pinch is the point at the total mass of contaminant and the maximum concentration (i.e.  $C_i^{out,max}$ ). The total mass of contaminant is  $MC^{tot} = \sum_i M_i^c$ . The overarching element of the two Transshipment models is the allocation of the pinch points at the upper limit of the concentration intervals where the sum of the residuals of the contaminant obtains positive values, while at any other interval the residuals are vanishing. The flow-rate in the identified water mains is not influenced by the particulars of the water reuse network. Thus, let the mass of contaminant removed between pinch points  $k^p - 1$  and  $k^p$  be  $W_{k^p}$ ;

$$W_{k^p} = \sum_{s \in S} \sum_i \sum_{k=k^p-1}^{k=k^p} W_{s,i,k}, \quad \forall k^p \quad (8)$$

Then the flowrate of the wastewater main of pinch point  $k^p$  is

$$F_{k^p} = W_{k^p} / (C_{k^p} - C_{k^p+1}), \quad \forall k^p \quad (9)$$

where  $C_{k^p}$  is the concentration of the effluent stream  $k^p$ . The effluent streams participate at the wastewater treatment optimization configuration to be assessed at the next step of the procedure.

### 3.2 Cascade model (Ib) - Water targets in systems with fixed flowrates

In model Ib instead of mass of contaminant, it is water that falls through cumulative mass load intervals as illustrated in Example 2. The index set of cumulative load intervals is  $Cl_i = \{k \mid k = 1, 2, \dots, K\}$ , and  $Cl_{i,k}$  is the exiting cumulative load of interval  $k$ .

$$\min Fw \quad (10)$$

s.t.

$$Fw + \sum_i Fout_{i,1} = r_1 + \sum_j Fin_{1,j} \quad (11)$$

$$r_{k-1} + \sum_i Fout_{i,1} = r_k + \sum_j Fin_{k,j}, \quad \forall k \in \{2, \dots, K-1\} \quad (12)$$

$$r_{K-1} + \sum_i Fout_{i,K} = r_K + \sum_j Fin_{K,j} \quad (13)$$

Balances of water in the first and last interval are given by Eqs(11) and (13). Eq(12) gives the balance of water in any other interval.  $Fout$  and  $Fin$  are the outlet and inlet flows of water using processes. In each equation the indexes  $i$  and  $j$  belong into pre-calculated sets of processes connected to each interval as described in Example 2.

The algorithm proposed by (Bandyopadhyay et al., 2006) for calculating the total waste flowrate was modified for calculating the pinch points and wastewater flowrates originating from the pinch points. First all distinct concentrations are arranged in descending order:  $C_1 > C_2 > C_3 > \dots > C_n$ . Next, for each  $C_i$ , the net flow  $F_i$  is calculated by taking the algebraic sum of flow rates corresponding to a concentration  $C_i$ . The cumulative flow rates given by  $Q_i = \sum_{j=1}^i F_j$ . The contaminant mass loads are calculated by  $P_i = Q_{i-1} (C_{i-1} - C_i)$ , where  $Q_0 = 0$ .

The cumulative contaminant mass loads are  $\Delta m_i = \sum_{j=1}^i P_j$ . The corresponding wastewater flow rate is

$f_{ww,i} = (\Delta m_T - \Delta m_i) / (C_i - C_{fw})$  where  $C_{fw}$  is the concentration of the freshwater and  $\Delta m_T$  is the total contaminant load of the process. The largest entry in the last column is the minimum wastewater flow-rate target and it corresponds to the pinch point concentration  $C_{pinch1}$ , where  $pinch1 = \arg \max_i \{f_{ww,i}\}$ . Then the

wastewater flowrate from the first pinch will be  $F_{pinch1} = (\Delta m_T - \Delta m_{pinch1}) / C_{pinch1}$  leaving at concentration  $C_{pinch1}$ .

The wastewater flowrate from the second pinch (assuming without of loss of generality that it will be the maximum concentration  $C_{max}$ ) will be  $F_{pinch1} = \Delta m_{pinch1} / (C_{max} - C_{pinch1})$ .

### 3.3 Cascade model (II) – Screening of of treatment processes

The design of a waste water network can be described with reference to a set of  $S_K$  wastewater mains:  $KP = \{k^p \mid k^p = 1, \dots, K\}$ , and a set of  $S_J$  treatment processes  $J = \{j \mid j = 1, 2, \dots, S_J\}$ . Associated with each wastewater main are the original inlet concentrations  $C_{o,k^p}^{in} = C_{k^p}$ . The outlet concentrations of all treated waste streams are equal to the original discharge concentration limits  $C_{o,k^p}^{out}$ . The mass load  $W_{k^p}$  of the contaminant transferred from main  $k$ , is already calculated. The minimum water flow rate,  $MWF_{k^p}$  for the waste water stream  $k$  in treatment process  $j$  is given by:

$$MWF_{k^p} = W_{k^p} (C_{o,k^p}^{in} - C_{o,k^p}^{out}), \forall k^p. \text{ Let } IN = \{n \mid n = 1, 2, \dots, N\} \text{ be the index set of the concentration intervals. } C_n$$

is defined as the outlet concentration of interval  $n$ . The mass transferred from main  $k^p$  through the  $n^{\text{th}}$  interval is given by:  $M_{n,k^p}^P = MWF_{k^p} (C_{n+1} - C_n)$ . Similarly, the mass transferred to stream  $j$  through the  $n^{\text{th}}$  interval is  $M_{j,n}^W = Ft_j (C_{n+1} - C_n)$ . The solution will select a cost effective set of treatment processes and determine the minimum treatment flowrates  $Ft_j$ . If  $fc_j$  is the fixed cost and  $coef_j$  is the coefficient of the variable cost of the  $j^{\text{th}}$  treatment unit, the problem of selecting treatment processes and minimizing the treatment flowrates is represented by equations (10-16), where  $u_{n,k^p}$  is the residual mass of main  $k^p$  leaving interval  $n$ :

$$\min Cost = \sum_{j \in J} (fc_j x_j + coef_j Ft_j) \quad (14)$$

$$u_{n-1,k^p} - u_{n,k^p} + \sum_j M_{n,j,k^p} = M_{i,k^p}^P, \quad \forall n, k^p \quad (15)$$

$$\sum_k M_{k,j,n} = M_{j,n}^W, \quad \forall j, n \quad (16)$$

$$M_{j,n}^W = Ft_j (C_{n+1} - C_n), \quad \forall n \quad (17)$$

$$0 \leq Ft_j \leq Ft_j^U, \quad \forall j \quad (18)$$

$$x_j M \geq Ft_j, \quad \forall j \quad (19)$$

$$u_{N+1,k^p} = u_{1,k^p} = 0, \quad u_{n,k^p} \geq 0, \quad \forall n, k^p \text{ and } x_j \in \{0, 1\}, \quad \forall j \quad (20)$$

The constraint set (10) is the mass balance of the contaminant around each interval.  $M_{k,j,n}$  is the mass of contaminant transferred from waste stream  $k$  to through interval  $n$  to treatment process  $j$ . For treatment processes with fixed outlet concentration, before the construction of the concentration intervals the concentrations of all waste streams must be shifted by the minimum of the outlet concentration of the treatment units  $C_{\min}^{out} = \min_j \{C_j^{out}\}$ , thus the concentration leaving the treatment processes will have virtually

zero value and can be assigned to the first concentrations interval:  $C_{k^p}^{in} = C_{o,k^p}^{in} - C_{\min}^{out}$  and

$C_{k^p}^{out} = C_{o,k^p}^{out} - C_{\min}^{out}, \forall k^p$ . The same shift applies to the inlet and outlet concentrations of all treatment

processes  $C_{S_j}^{in} = C_j^{in} - C_{\min}^{out}$  and  $C_{S_j}^{out} = C_j^{out} - C_{\min}^{out}, \forall j$ . The intervals are defined by the shifted limiting concentrations.

## 4. Examples

### 4.1 Example 1 – System with fixed loads of contaminant at water using operations

The system of the first example consists of five water using operations and three candidate treatment technologies with fixed outlet concentration (Smith, 2005). Table 1 contains the data for Example 1.

The first iteration of model (Ia) results in three pinch points leading to three wastewater streams; STI with a flow of 20 t/h at 200 ppm, STII with a flow of 20 t/h at 400 ppm, and STIII with a flow of 40 t/h at 600 ppm. The minimum fresh water flow is 80 t/h.

Solving with model (II) for process selection, the results show that 80 t/h will have to be processed by process I και 50.91 t/h by process IIb. Treatment processes I and IIb are selected, at a cost of 2.08 M€. If the flowrate of the ST III was 53 t/h then TP IIa would have been selected instead of TP IIb, with a treatment flowrate of 49.45 t/h. At the optimal solution the fresh water flowrate is 40 t/h, the recycle flowrate is 47.06 t/h, and the fresh water cost is 800 k€.

Table 1: Example with five water using processes and three waste treatment processes

Water using operations				
Operation No	Cont. Mass load (kg/h)	$C_{in}$ (ppm)	$C_{out}$ (ppm)	Limiting flowrate (t/h)
1	8	0	200	40
2	5	100	200	50
3	9	100	400	30
4	6	300	400	60
5	8	400	600	40
Wastewater treatment processes				
Process No	$C_{in}$ (ppm)	$C_{out}$ (ppm)	Fixed cost K€	Variable cost coefficient K€/t/h
I	200	5	200	15
IIa	1,000	50	50	10
IIb	1,000	50	150	8
Environmental discharge limit:				$C_e = 30$ ppm

#### 4.2 Example 2 – System with fixed water flowrates at water using operations

Table 2 contains the flowrates and concentrations of inlet and outlet streams of four water using processes (Polley and Polley, 2000). The environmental discharge limit is 50 ppm. Two are the candidate treatment processes, one with an outlet concentration of 30 ppm, fixed cost 700 k€ and variable cost 6 k€/t/h, and another one with 25 ppm outlet concentration fixed cost 860 k€ and variable cost 5 k€/t/h.

Table 2: Data for fixed flowrate operations in Example 2

Inlet	Concentration (ppm)	Flowrate (t/h)	Outlet	Concentration (ppm)	Flowrate (t/h)
In1	20	50	Out1	50	50
In2	50	100	Out2	100	100
In3	100	80	Out3	150	70
In4	200	70	Out4	250	60

Demands and sources are arranged in increasing order of contaminant concentration. Figure 1(a), contains the cascade of water flows and Figure 1(b) presents the contaminant load intervals. From left to right water is transferred from outlets to inlets, from the top fresh water enters the cascade and the residual of the last interval is the wastewater flow. The fresh water target calculated by model (Ib) is 70 t/h, and the total wastewater flowrate is 50 t/h. By applying the iterative methodology involving models (Ib) and (II), the fresh water target is calculated at 20 t/h. The final pinch wastewater flowrates are 10.24 t/h at 100 ppm and 60 t/h at 250 ppm. The wastewater is treated only at the first treatment process with a flowrate of 70.24 t/h which is fully recycled and the treatment cost is 1.12 M€. There is no discharge since all the fresh water is used inside the system.

## 5. Conclusions

The paper tackles water integration in process industry for systems that include a set of water using operations and a set of candidate treatment technologies. The objective is to identify targets for water use and select treatment technologies exploiting the possibility of recycles in systems with fixed loads or fixed flowrates. The total cost consisting of the clear water and treatment costs. The proposed methodology produces ahead of design optimal targets for clear water use, recycle flows and treatment flowrates, while at the same time it selects the best configuration for regeneration technologies. Future research may expand the models for treatment processes characterized by removal ratios instead of fixed outlet concentrations.

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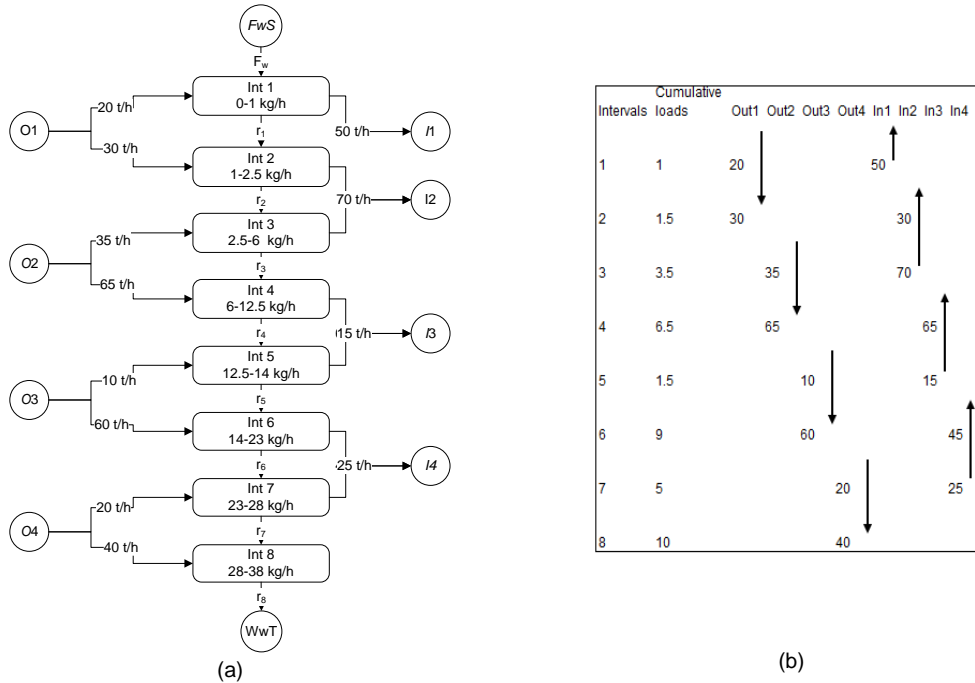


Figure 1: The water cascade (a), and the concentration intervals (b) for model Ib

## Reference

- Alva-Argáez A., Vallianatos A., Kokossis A., 1999, A multi-contaminant transshipment model for mass exchange networks and wastewater minimisation problems, *Comp. Chem. Eng.*, 23(10), 1439-1453.
- Bandyopadhyay S., Ghanekar, M.D., Pillai, H.K., 2006, Process water management, *Ind. Eng. Chem. Res.*, 45(15), 5287-5297.
- Halim I., Adhitya A., Srinivasan R., 2015, A novel application of genetic algorithm for synthesizing optimal water reuse network with multiple objectives, *Chem. Eng. Res. Des.* 100, 39–56.
- Khor C.S., Chachuat B., Shah N., 2014, Optimization of water network synthesis: Milestones, challenges, and future directions, *Ind. Eng. Chem. Res.*, 53(25), 10257-10275.
- Kuo W.-C.J., Smith R., 1997, Effluent treatment system design, *Chem. Eng. Sci.*, 52(23), 4273–90.
- Nikolakopoulos A., Thomaidis, L., Kokossis, A., 2014, Mathematical programming shortcut screening models for the design of integrated waste treatment systems, *Comp. Aid. Chem. Eng.*, 34, 381-386.
- Parand R., Yao H.M., Pareek V., Tade M.O., 2014, Use of pinch concept to optimize the total water regeneration network, *Ind. Eng. Chem. Res.*, 53(8), 3222-3235.
- Polley G.T., Polley, H.L., 2000. Design better water networks, *Chem. Eng. Prog.*, 96, 47–52.
- Smith R., 2005, *Chemical process: design and integration*. John Wiley & Sons, Chichester, England
- Wang Y.P., Smith R., 1994, Wastewater minimisation, *Chem. Eng. Sci.*, 49(7), 981–1006.