A conceptual decomposition of MINLP models for the design of water-using systems

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Abstract: The work presents a systematic methodology for the design of industrial water systems that combines principles of water-pinch (Wang and Smith, 1994a, 1994b) with mathematical programming techniques that enable the imposition of practical constraints and the generalisation of the conceptual tools into multi-contaminant problems. A superstructure model is formulated as an MINLP and solved via decomposition. Layout constraints and flowrates compatible with existing networks can be enforced. Elements of capital and operating cost, including piping are analysed. The solution strategy is based upon a penalty-based search, coupled with an iterative projection procedure. The approach is tested and illustrated on several examples.

Keywords: water networks design; water minimisation; MINLP; MILP.

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1 Introduction

Some of the most toxic pollutants are introduced to water bodies through industrial wastewater and, in some developed countries, freshwater for industrial and domestic use already accounts for as much as 60–86% of total water extraction (Chandak, 2001). The efficient use of freshwater and subsequent reduced discharges of wastewater have become important priorities in the selection of manufacturing processes. A significant amount of work was published in recent years to address design challenges in the area (Bagajewicz, 2000). Takama et al. (1980) addressed the problem of optimal water allocation in a petroleum refinery. In their design approach the water system is modelled as a superstructure with reuse and regeneration options optimised through a two-level strategy. Based on fixed water demands, uneconomic features are removed sequentially.

Wang and Smith (1994b) pioneered the development of Water Pinch, a graphical method for designing a water distribution system featuring maximum water reuse. They considered the possibility of partial treatment before reuse (water regeneration) or recycling. The method was extended to deal with multiple pollutants and with flow rate constraints and multiple water sources. They later (Wang and Smith, 1994a) extended the conceptual method to the design of a distributed effluent treatment system. Kuo (1996) and Kuo and Smith (1997, 1998) addressed the interactions between water-using and water treatment systems with a methodology that could be incorporated in the graphical approach and a design approach illustrated in several industrial cases. El-Halwagi and Manousiouthakis (1989, 1990a, 1990b) and El-Halwagi et al. (1992, 1996) pursued an equally insightful method, applying the concept of mass exchange network synthesis to industrial problems (e.g., dephenolisation of refinery wastewaters). Hallale and Fraser (1998) presented pinch-based capital cost targets for the mass-exchanger network approach. Papalexandri et al. (1994) formulated the mass exchange network problem as an MINLP simultaneous optimisation of a hyperstructure. Galan and Grossman (1998) approached the problem by employing a superstructure approach (non-convex NLP) and introducing linear under-estimators in a solution strategy to locate the global optimum.

Huang et al. (1999) presented the allocation problem as an NLP problem, they included water users and water treatment options and, realising how sensitive are the mathematical programming models to the initial point, they made use of the Water Pinch method (Smith, 2005) to initialise the NLP. Savelski and Bagajewicz (2001) published a series of papers on single contaminant water-using problems identifying necessary conditions on some simplified problems and, later, extending the analysis to multi-component systems (Savelski and Bagajewicz, 2003). Forstmeier et al. (2005) proposed their CROWN strategy as an attempt to alleviate the simplifications made by all mathematical models with respect to water chemistry. They showed that in some cases it is required to perform significant experimentation in parallel with the synthesis method. Ullmer et al. (2005) presented an approach that combines heuristic rules for the sequencing of treatment units and a set of rules to generate a reduced superstructure MINLP model that is solved using a sequence of MILP-NLP subproblems.

None of these previous mathematical programming techniques has made a systematic effort to capitalise on the Water Pinch method. Water Pinch does not provide near-optimal solutions that one could use as starting points. Indeed, such solutions could instead prove as 'bad' initial points in the optimisation. The problem of designing distributed wastewater treatment systems for multi-contaminant effluent streams (Kuo, 1996; Kuo and Smith, 1997, 1998) was based on the merging of various single-contaminant analyses without any guarantees of optimality, the structure of the proposed networks could then determine a topology trap and the local optimum for the non-linear solver, in our experience this initialisation procedure has not been successful. Water Pinch provides knowledge concerning the apparent location of the bottleneck, critical limits in the concentration profile, and information to simplify the larger problem into its major components. Gunaratnam et al. (2005) first exploited the potential of Water Pinch in a systematic projection scheme to automate design decisions.

The paper makes use of the Water Pinch projection scheme for the development of a conceptual decomposition approach that uses an augmented formulation and a penalty barrier method. The decomposition is termed conceptual because it is based on the concept of Water Pinch. The augmented terms include the objective function and the constraints, whereas a dynamic deployment scheme is applied for the penalty used at each iteration. The penalties enable an outer search for the optimum and lead to a robust solution strategy presented, alongside a sensitivity analysis, in several case studies.

2 Problem statement

Given in the problem are

- freshwater sources of known availability quality and cost; the water quality is expressed with respect to the concentrations of its key pollutants
- water and wastewater treatment plants of given maximum capacity and efficiency expressed in the form of removal capacity for the key pollutants and the water losses occurring at each case

- water-using operations with given specifications and demands
- wastewater discharge points where environmental regulations (maximum concentrations of key contaminants) apply.

The design objective is to determine the:

- most economic supply of water as available from different locations and different qualities
- maximum reuse opportunities for water and optimal schemes for regeneration and recycling
- efficient integration between the treatment and water-using systems
- a flowsheet capable of complying with environmental objectives.

The design is assessed with respect to the:

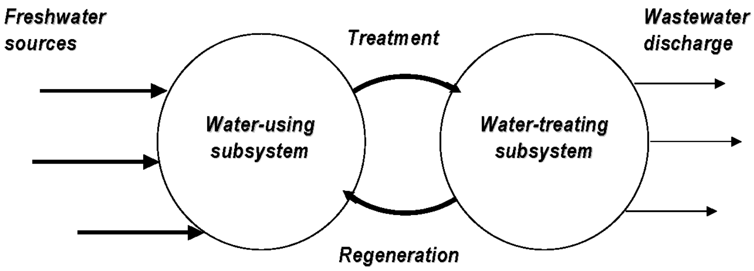
- capital investment costs associated with the effluent treatment operations
- piping costs of the network
- water quality considerations and quantity requirements for each individual user
- operating costs and availability constraints associated with each source of freshwater
- capital costs associated with degradation of mass transfer driving forces (when mass exchangers are involved in the water network)
- integration aspects between water-using and effluent treatment operations and among treatment plants and users.

Following the practical approach of Wang and Smith (1994a, 1994b), water-using operations are described by limiting water profiles, allowing a user with low quality requirements to satisfy its demand with a low quality source (untreated or partially treated wastewater).

3 Design representation

Figure 1 illustrates the input-output structure of the water using and wastewater treatment operations of the problem. Inputs are freshwater streams; the output comprises contaminated water discharged to the environment. The first subsystem accounts for process operations that demand water; the second subsystem accounts for treatment units available to clean the contaminated water. Links are possible between processes (water re-use), treatment units, processes to treatment units and treatment to process units (recycle, regeneration). The problem is to define the optimal water paths from inputs to outputs through all the process and the wastewater systems available.

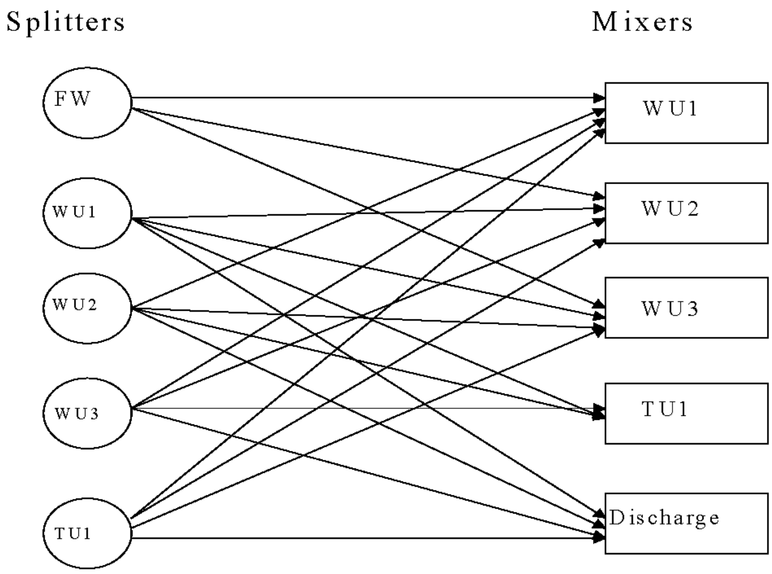
Figure 1 Total water system design



In order to explore the full range of opportunities for water reuse and effluent treatment, the model should be general enough to allow all options.

A superstructure representation of the design problem is developed where all the integration options are considered. Figure 2 shows a schematic of the superstructure model for three water-using operations and a single treatment unit.

Figure 2 Superstructure representation



The superstructure is constructed according to the following steps:

- each freshwater stream entering the network is split towards all operations
- all the effluent streams generated from each operation are mixed in a final discharge point, where the environmental limitations must hold
- prior to each operation, a mixer is considered where the flows from the freshwater splitters and re-use flows from all other operations are merged into a flow towards the operation
- after each operation, a splitter is considered from which potential flows are driven towards the final mixer and the other operations in the system.

The superstructure enables the exploration of trade-offs between minimum water demand, effluent treatment, network cost and environmental performance.

Figure 2 illustrates the combinatorial nature of the interactions between water-using operations and effluent treatment. Wang and Smith (1994a, 1994b) explained that treatment units could be used either for regeneration or for effluent treatment. However, once the two problems are combined in a simultaneous approach the distinction between treatment and regeneration becomes irrelevant. A given water re-use scheme defines a specific effluent treatment problem. The introduction of a regeneration unit reduces the water demand and the effluent. One should distinguish between reuse and recycling. While recycling between operations is sometimes allowed, there are cases where this is discouraged so to avoid the build-up of contaminants not removed by the regeneration/treatment processes.

The superstructure of Figure 2 is quite general, but there exist major complications in eliminating recycles, as the identity of water streams is lost as they pass through the network mixers. When dealing with the total water system design, the development of these complex loops in the network becomes a major consideration. Following Kuo (1996) and Kuo and Smith (1997, 1998), a grouping strategy is developed to control recycles in the network. The main idea is to separate the operations in two groups:

- *Group 1* consists of those units feeding a given treatment operation
- *Group 2* of those units fed by that same treatment operation.

The grouping needs to be performed with respect to every treatment unit available. Eliminating the possibility of reusing water from Group 2 into Group 1 eliminates recycles in the network.

4 Mathematical formulation

The design model is described with respect to a set of constraints formulated on the basis of continuous and integer variables. First, the following sets are defined:

Sets

$I = \{i \mid i \text{ is an operation involved in the water system}\}, \quad i = 1, 2, \ldots, N_{OP}$

$I_{OP} = \{i \mid i \text{ is a water user}\}, \quad i = 1, 2, \ldots, N_{WU}$

$I_{TR} = \{i \mid i \text{ is a water treatment operation}\}, \quad i = N_{WU} + 1, \ldots, N_{OP}.$

$I_{ME} = \{i \mid i \text{ is a water user and a mass exchanger}\} \subseteq I_{OP}, \quad i = 1, 2, \ldots, N_{ME}$

$C = \{c \mid c \text{ is a contaminant in the analysis}\}, \quad c = 1, 2, \ldots, N_C$

$J = \{j \mid j \text{ is a freshwater source}\}, \quad j = 1, 2, \ldots, N_S$

Problem variables and parameters

Decision variables include continuous and binary variables. The continuous variables are associated with flowrates,

$F_{j,i}^{Fw}$ freshwater stream from source j to operation $i \in I$

$F_{i,i'}^{IP}$ stream from operation i to operation i', i, $i' \in I$

F_{i}^{OUT} stream discharged from operation $i \in I$

F_{i}^{Tot} total flow through operation $i \in I$.

Cross-sectional areas of the pipes associated to different connections,

$A_{j,i}^{Fw}$ between freshwater source $j \in J$ and operation $i \in I$

$A_{i,i'}^{IP}$ between operation $i \in I$ and operation $i' \in I$

A_{i}^{OUT} from operation $i \in I$ to discharge.

Mass load and contaminant concentrations,

$M_{c,i}^{\text{in}}$ inlet load in operation $i \in I$,

$M_{c,i}^{\text{out}}$ outlet load in operation $i \in I$,

$C_{c,i}^{\text{out}}$ contaminant concentration from $i \in I$, $c \in C$.

Cost terms associated with the,

$\text{Cost}_{j}^{\text{sup}}$ freshwater supply $j \in J$

Cost_{i}^{T} water treatment $i \in I_{TR}$

$\text{Cost}_{j,i}^{Fw,\text{pipe}}$ piping from source $j \in J$ to operation $i \in I$

$\text{Cost}_{i,i'}^{IP,\text{pipe}}$ piping from operation $i \in I$ to operation $i' \in I$

$\text{Cost}_{i}^{\text{OUT,pipe}}$ piping for discharge from operation $i \in I$

Cost_{i}^{ME} mass exchanger $i \in I_{ME}$

Cost^{TAC} total annualised cost.

Binary variables are introduced to account for the,

$Y_{j,i}^{Fw}$ stream from freshwater source $j \in J$ to operation $i \in I$

$Y_{i,i'}^{IP}$ stream from operation $i \in I$ to operation $i' \in I$

Y_{i}^{OUT} stream discharged from operation $i \in I$

$Y_{i,\hat{i}}^{G1}$ operation $i \in I$ belongs to Group 1 with respect to treatment $\hat{i} \in I_{TR}$

$Y_{i,\hat{i}}^{G2}$ operation $i \in I$ belongs to Group 2 with respect to treatment $\hat{i} \in I_{TR}$.

The parameters required to formulate the design problem include bounds on the,

$C_{c,i}^{\mathrm{in,max}}$ inlet concentration of operation $i \in I$, contaminant $c \in C$ (upper)

$C_{c,i}^{\mathrm{out,max}}$ outlet concentration of operation $i \in I$, contaminant $c \in C$ (upper)

$F_i^{\mathrm{Tot},L}$ total flow through operation $i \in I$ (lower)

$F_i^{\mathrm{Tot},U}$ total flow through operation $i \in I$ (upper)

$W_j^{\mathrm{sup},U}$ withdrawal from freshwater source $j \in J$ (upper)

$F_{j,i}^{Fw,U}$ flow from source $j \in J$ to $i \in I$ (upper)

$F_{j,i}^{Fw,L}$ flow from source $j \in J$ to $i \in I$ (lower).

Distances between sources and sinks of water,

$d_{j,i}^{Fw}$ from freshwater $j \in J$ to operation $i \in I$

$d_{i,i'}^{IP}$ from operation $i \in I$ to operation $i' \in I$

d_i^{OUT} from operation $i \in I$ to discharge.

Flow velocities in the connections,

$v_{j,i}^{Fw}$ from freshwater $j \in J$ to operation $i \in I$

$v_{i,i'}^{IP}$ from operation $i \in I$ to operation $i' \in I$

v_i^{OUT} from operation $i \in I$ to discharge.

Regression parameters for the fixed charge for piping costs from,

$b_{j,i}^{Fw,\mathrm{pipe}}$ freshwater $j \in J$ to operation $i \in I$

$b_{i,i'}^{IP,\mathrm{pipe}}$ operation $i \in I$ to operation $i' \in I$

$b_i^{\mathrm{OUT,pipe}}$ operation $i \in I$ to discharge

and the variable charge for piping costs, from

$a_{j,i}^{Fw,\mathrm{pipe}}$ from freshwater $j \in J$ to operation $i \in I$

$a_{i,i'}^{IP,\mathrm{pipe}}$ from operation $i \in I$ to operation $i' \in \mathrm{I}$

$a_i^{\mathrm{OUT,pipe}}$ from operation $i \in I$ to discharge.

Other parameters include the,

$m^L_{c,i}$ mass load of contaminant $c \in C$ from user $i \in I_{OP}$

$RR_{c,i}$ removal ratio of contaminant c in treatment $i \in I_{TR}[0 \le RR_{c,i} < 1]$

$cw^{\text{in}}_{c,j}$ concentration of contaminant $c \in C$ in freshwater source $j \in J$

Ce_c environmental limit on contaminant $c \in C$

R^L_c minimum load of contaminant c to be removed

α_j cost of freshwater source j per unit volume

F^{loss}_i flow rate loss at the inlet of $i \in I$.

The limiting flow rate is related to the mass load of contaminants by:

$$F^L_i = \max_c \frac{m^L_{c,i}}{C^{\text{out},\max}_{c,i} - C^{\text{in},\max}_{c,i}}. \tag{1}$$

Design constraints

The model (Problem P) has a non-linear objective function and linear and non-linear constraints. It consists of mass balances around the operations, mixers and splitters of the superstructure. Availability and capacity constraints, design equations, cost calculations and logical statements complete the formulation.

4.1 Balances around units, mixers and splitters

Mass loads at the inlet/outlet of each operation

$$\sum_{i' \in I}(F^{IP}_{i',i} \cdot C^{\text{out}}_{c,i'}) + \sum_{j \in J}(F^{Fw}_{j,i} \cdot cw^{\text{in}}_{c,j}) - M^{\text{in}}_{c,i} = 0 \quad \forall c \in C, \quad i \in I \tag{2}$$

$$C^{\text{out}}_{c,i} \cdot \left[\sum_{j \in J} F^{Fw}_{j,i} + \sum_{i' \in I} F^{IP}_{i',i} - F^{\text{loss}}_i\right] - M^{\text{out}}_{c,i} = 0 \quad \forall c \in C, \quad i \in I. \tag{3}$$

Mass balances around each water-using and treatment operation

$$M^{\text{in}}_{c,i} - M^{\text{out}}_{c,i} + m^L_{c,i} = 0 \quad \forall i \in I_{OP}, \tag{4}$$

$$(1 - RR_{c,i}) \cdot M^{\text{in}}_{c,i} - M^{\text{out}}_{c,i} = 0 \quad \forall i \in I_{TR}. \tag{5}$$

Overall balances around the water system

$$\sum_{j \in J}\sum_{i \in I} F^{Fw}_{j,i} - \sum_{i \in I} F^{\text{out}}_i = \sum_{i \in I} F^{\text{loss}}_i \tag{6}$$

$$\sum_{i' \in I} F^{IP}_{i',i} + \sum_{j \in J} F^{Fw}_{j,i} - \sum_{i' \in I} F^{IP}_{i,i'} - F^{\text{out}}_i = F^{\text{loss}}_i \quad \forall i \in I. \tag{7}$$

Constraints (2) and (3) define the contaminant mass loads at the inlet and outlet of each operation. Constraints (4) represent the mass balances for the water-using operations where the mass pick-up of the contaminants is assumed fixed. For treatment operations however, Constraint (5) the mass removal is variable and depends on the removal ratio. Constraints (6) and (7) ensure that the water balances are satisfied around every operation, as well as around the entire system.

4.2 Availability and capacity constraints

Capacity constraints on water flow rates for each operation

$$\sum_{j\in J} F_{j,i}^{Fw} + \sum_{i'\in I} F_{i',i}^{IP} - F_i^{\text{loss}} \geq F_i^{\text{Tot},L} \quad \forall i \in I \tag{8}$$

$$\sum_{j\in J} F_{j,i}^{Fw} + \sum_{i'\in I} F_{i',i}^{IP} - F_i^{\text{loss}} \leq F_i^{\text{Tot},U} \quad \forall i \in I. \tag{9}$$

Water availability and quality constraints

$$\sum_{i\in I} F_{j,i}^{Fw} \leq W_j^{\text{sup},U} \quad \forall j \in J \tag{10}$$

$$M_{c,i}^{\text{in}} \leq C_{c,i}^{\text{in,max}} \cdot F_i^{\text{Tot}} \quad \forall c \in C \text{ and } i \in I \tag{11}$$

where

$$F_i^{\text{Tot}} - \left[\sum_{j\in J} F_{j,i}^{Fw} + \sum_{i'\in I} F_{i',i}^{IP} - F_i^{\text{loss}}\right] = 0. \tag{12}$$

Limits on the load and concentration at the final discharge

$$\sum_{i\in I} (C_{c,i}^{\text{out}} \cdot F_i^{\text{OUT}}) \leq Ce_c \cdot \sum_{i\in I} F_i^{\text{out}} \quad \forall c \in C \tag{13}$$

$$\sum_{i\in I_{TR}} (RR_{c,i} \cdot M_{c,i}^{\text{in}}) \geq R_c^L. \tag{14}$$

The water losses, F_i^{loss}, are assumed constant. The implicit assumption is that these losses occur at the inlet of the operation. Constraints (10) bound the availability of water. Constraints (11) enforce quality specifications for each user and equation (13) ensure regulatory limits on the discharge.

For a worst case scenario where water is used once through, a lower bound can be calculated for the mass load of a contaminant *c* to be removed from the system. The total load of contaminant is assumed to be a known quantity. Thus, the amount that needs to be removed depends only on the amount of water in the system. The parameter R_c^L is useful in the solution of the optimisation problem and is given by

$$R_c^L = \sum_{i\in I_{OP}} \{F_i^{\text{in},OT} (C_{c,i}^{\text{out},OT} - Ce_c)\}.$$

The parameter $F_i^{\text{in},OT}$ represents the water demand of operation *i if only freshwater* is used in a once-through policy. The parameter can be calculated in advance along with the corresponding outlet concentrations $C_{c,i}^{\text{out},OT}$. The demand of a once-through scenario is an upper bound on the total water demand.

Constraints (14) restraint contaminant loads removed from the system by R_c^L.

4.3 Costing constraints

The cost of freshwater supply $j \in J$ is expressed as

$$\text{Cost}_j^{\text{Sup}} = \sum_{i \in I} \alpha_j F_{j,i}^{Fw}. \tag{15}$$

The piping costs are functions of the water volume in the pipe with the flow velocity assumed fixed (typically 1–2 m/s). The cross sectional area is calculated by:

$$F_{j,i}^{Fw} = A_{j,i}^{Fw} \cdot v_{j,i}^{Fw} \tag{16}$$

and varies for different connections. Similar sets of constraints can be generated for the remaining connections of the network. The piping costs are given by,

$$\text{Cost}_{j,i}^{Fw,\text{pipe}} = \lfloor (a_{j,i}^{Fw,\text{pipe}} \cdot A_{j,i}^{Fw}) + (b_{j,i}^{Fw,\text{pipe}} \cdot Y_{j,i}^{Fw}) \rfloor \cdot d_{j,i}^{Fw} \tag{17}$$

$a_{j,i}^{Fw,\text{pipe}}$ and $b_{j,i}^{Fw,\text{pipe}}$ depend on the materials of construction for each connection.

Water and wastewater treatment operations can be costed using a similar form as the freshwater costs, expressed as:

$$\text{Cost}_i^T = \alpha_i F_i^{\text{Tot},\beta_i}, \quad \forall i \in I_{TR}. \tag{18}$$

These Cost_i^T do not account for the removal accomplished by the treatment process.

The cost of mass exchangers can generally be expressed as a function of the number of equilibrium stages required to achieve the desired separation.

$$\text{Cost}_i^{ME} = f(N_i) \quad \forall i \in I_{ME}. \tag{19}$$

4.4 Logical constraints

Upper and lower bounds on the flows

$$F_{j,i}^{Fw} - Y_{j,i}^{Fw} \cdot U_{j,i}^{Fw} \leq 0 \tag{20}$$

$$F_{j,i}^{Fw} - t_{j,i} \cdot Y_{j,i}^{Fw} \geq 0. \tag{21}$$

Maximum number of sources to feed each operation

$$\sum_{i' \in I} Y_{i',i}^{IP} + \sum_{j \in J} Y_{j,i}^{Fw} \leq M_i^{NS}. \tag{22}$$

Elimination of direct and indirect recycling

$$Y_{i,i'}^{IP} + Y_{i',i}^{IP} \leq 1 \tag{23}$$

$$Y_{i,\hat{i}}^{IP} - Y_{i,\hat{i}}^{G1} \leq 0 \quad i \in I \quad \hat{i} \in I_{TR} \tag{24}$$

$$Y^{IP}_{\hat{i},i} - Y^{G2}_{i,\hat{i}} \leq 0 \quad i \in I \quad \hat{i} \in I_{TR} \tag{25}$$

$$Y^{G2}_{i,\hat{i}} = 1 - Y^{G1}_{i,\hat{i}} \quad i \in I \quad \hat{i} \in I_{TR} \tag{26}$$

$$2 - (Y^{G2}_{i,\hat{i}} + Y^{G1}_{i',\hat{i}}) \geq Y^{IP}_{i,i'} \quad i,i' \in I \quad \hat{i} \in I_{TR} \tag{27}$$

$$\sum_i Y^{G1}_{i,\hat{i}} + \sum_i Y^{G2}_{i,\hat{i}} = N_{OP} - 1. \tag{28}$$

Constraints (20) and (21) are introduced to relate the binary variables to the continuous variables. Both upper and lower bounds can be considered for an emerging superstructure stream. $U^{Fw}_{j,i}$ is a suitable upper bound on the flow between freshwater source j and operation i, $t_{j,i}$ is a scalar defining the minimum allowable flow in the connection. The parameter M^{NS}_i in constraints (22) represents the maximum number of sources (both freshwater and re-used water) that can feed operation i. This can be used as an indirect control of the complexity of the network.

A set of constraints is emulating work produced by Kuo (1996) and Kuo and Smith (1998) who decomposed the regeneration problem noting the two actual sources of water: freshwater and regenerated. Their approach had a single regeneration unit with water users accordingly divided in two sub-groups: one using freshwater and the other using regenerated water. Starting with an initial grouping based on Water Pinch, they proposed a migration procedure that yielded an optimal grouping. This procedure used rules on conceptual reasoning that at times required complete enumeration. The model proposed in this paper uses a set of constraints that emulates this migration strategy, enabling the elimination of recycles in cases contaminants are built-up in the problem. The set of constraints (23) is introduced to eliminate *direct* recycles between i and $i' \in I$. The elimination of indirect recycles is more difficult as the identity of a water stream is lost through mixing and splitting points. Based on the grouping strategy discussed above, the set of constraints (24) assigns to Group 1 any operation that is feeding treatment operation $\hat{i} \in I_{TR}$; the set (25) assigns to Group 2 any operation that is receiving regenerated water from treatment operation $\hat{i} \in I_{TR}$. The set (26) ensures that every operation either belongs to Group 1 or to Group 2, but not both. The set (27) is eliminating all re-use connections from the operations in Group 2 into operations in Group 1, thus eliminating the recycles. The final constraint (28) is making explicit the fact all units must necessarily be assigned to either Group 1 or Group 2.

4.5 Objective function

The objective function is expressed to account for the annual cost of the network and includes terms for:

- water and wastewater treatment
- piping network that supports links between sources and sinks of water
- capital cost for the mass exchange operations and for water treatment units.

The objective function is the minimisation of the sum of freshwater costs, piping costs, treatment costs and mass exchanger costs, i.e.,

$$\begin{aligned}\text{Cost}^{\text{TAC}} = {} & \left(\sum_{j\in J}\text{Cost}_j^{\text{sup}}\right) + \left(\sum_{j\in J}\sum_{i\in I}\text{Cost}_{j,i}^{Fw,\text{pipe}} + \sum_{i\in I}\sum_{i'\in I}\text{Cost}_{i,i'}^{IP,\text{pipe}} + \sum_{i\in I}\text{Cost}_i^{\text{OUT,pipe}}\right) \\ & + \left(\sum_{i\in I_{TR}}\text{Cost}_i^{T}\right) + \left(\sum_{i\in I_{ME}}\text{Cost}_i^{ME}\right).\end{aligned} \tag{29}$$

Problem (P) defines the optimisation model comprised by equations (2)–(28) and optimised against the objective (29). The problem involves binary variables related to structural decisions as well as non-linear terms in equations (2)–(3), (13) and (19). The MINLP model is solved with a novel decomposition approach that is discussed next.

5 Solution strategy

A decomposition scheme is presented that exploits concepts from Water Pinch analysis. The first piece of knowledge used is that at least one of the contaminants will be at its maximum value ($C^{\text{out,max}}$) in an optimal solution of (P). In the case of treatment units the assumption involves starting the procedure at perfect treatment performance. The initial assumption of perfect treatment performance defines an infeasible point for the original problem (P), as no treatment unit can have $RR_{c,i} = 1$. To account for the infeasibilties, a penalty function is introduced in the objective function of (P_1), which drives the distance from the feasible region to zero.

The decomposition presented here applies successive projections on the concentration space and an augmented objective function with penalty terms to enforce feasibility of the relaxed constraints following Palacios-Gomez et al. (1982), Viswanathan and Grossman (1990) and Zhang et al. (1985). The procedure converges to a feasible solution that initialises a (fixed structure) formulation in the form of an NLP problem. In the natural decomposition described in this work the outlet concentrations for all contaminants are projected iteratively so that a sequence of MILP-LP problems is solved before embarking on an NLP stage.

The initial choice of concentrations leads to an infeasible setting for problem (P). The assumption that contaminants reach their maximum values for total system design will not hold in the general case. However, the main trade-offs can be captured by the procedure. The decomposition problems and the iterative procedure are explained in the following discussion.

Primal problem (P_1)

The problem involves the design constraints of the formulation in problem (P) with constraints (4)–(5), (13)–(14) relaxed in the form

$$M_{c,i}^{\text{in}} - M_{c,i}^{\text{out}} + M_{c,i}^{L} + s_{c,i}^{1} = 0 \quad \forall i \in I_{OP}, \tag{4'}$$

$$(1 - RR_{c,i}) \cdot M_{c,i}^{\text{in}} - M_{c,i}^{\text{out}} + s_{c,i}^{1} - s_{c,i}^{2} = 0 \quad \forall i \in I_{TR}, \tag{5'}$$

$$\sum_{i\in I}(C_{c,i}^{\text{out},k} \cdot F_i^{\text{OUT}}) - s_c^3 \le Ce_c \cdot \sum_{i\in I} F_i^{\text{out}} \quad \forall c \in C \tag{13'}$$

$$\sum_{i \in I_{TR}} (RR_{c,i} \cdot M_{c,i}^{\text{in}}) + s_c^4 \geq R_c^L \quad \forall c \in C \tag{14'}$$

and constraints (2) and (3) projected on the concentration space of outlet concentrations $C_{c,i}^{\text{out}}$:

$$\sum_{i' \in I} (F_{i',i}^{IP} \cdot C_{c,i'}^{\text{out},k}) + \sum_{j \in J} (F_{j,i}^{Fw} \cdot cw_{c,j}^{\text{in}}) - M_{c,i}^{\text{in}} = 0 \quad \forall c \in C, \quad i \in I \tag{2'}$$

$$C_{c,i}^{\text{out},k} \cdot \left[\sum_{j \in J} F_{j,i}^{Fw} + \sum_{i' \in I} F_{i',i}^{IP} - F_i^{\text{loss}} \right] - M_{c,i}^{\text{out}} = 0 \quad \forall c \in C, \quad i \in I \tag{3'}$$

where

$C_{c,i}^{\text{out},k}$ fixed concentration of c leaving operation i, $c \in C$, $i \in I$, iteration k.

Note that relaxed constraints (13') are similarly projected onto the concentration space. In summary, problem (P_1) consists of

(a) constraints (6)–(12), and (15)–(28) from (P)

(b) constraints (2')–(3'), (13')–(14') as described above.

(i) The slack and surplus variables in equations (4') and (5') account for the mass load in operations and, for treatment units, these can take positive values depending on whether the removal ratio is adequate to achieve the projected outlet concentration.

(ii) Variables s_c^3 and s_c^4 allow violations in the environmental regulations on the discharge.

(iii) Problem (P_1) is solved against an objective that minimises slacks and costs and assumes the form:

$$\min z_1 = \left[\begin{array}{l} \sum_{j \in J} \text{Cost}_j^{\text{sup}} + \sum_{i \in I_{TR}} \text{Cost}_i^T + \sum_{j \in J} \sum_{i \in I} \text{Cost}_{j,i}^{Fw,\text{pipe}} + \sum_i \sum_{i'} \text{Cost}_{i,i'}^{IP,\text{pipe}} \\ + \sum_i \text{Cost}_i^{\text{OUT,pipe}} + \sum_{i \in I_{ME}} \text{Cost}_i^{ME} \end{array} \right] + p^k \chi^{\text{inf}} \tag{29'}$$

where the term χ^{inf} is defined as:

$$\chi^{\text{inf}} = \sum_c \sum_i s_{c,i}^1 + \sum_c \sum_i s_{c,i}^2 + \sum_c s_c^3 + \sum_c s_c^4 \tag{30}$$

and p^k is a weight attached to the χ^{inf} term. The solution of (P_1) provides a flow pattern and the inclusion of s_c^3 and s_c^4 in χ^{inf} drives the solution towards achieving the environmental constraints.

Primal problem (P_2)

The problem includes the relaxed mass balances around treatment operations (constraints (5.3') and (5.4')) and constraints (5.1) and (5.2) projected on the space $[F_{j,i}^{Fw}, F_{i,i'}^{IP}, F_i^{OUT}]$.

$$\sum_{i' \in I}(F_{i',i}^{IP,k} \cdot C_{c,i'}^{\text{out}}) + \sum_{j \in J}(F_{j,i}^{Fw,k} \cdot cw_{c,j}^{\text{in}}) - M_{c,i}^{\text{in}} = 0 \quad \forall c \in C, \quad i \in I \tag{2''}$$

$$C_{c,i}^{\text{out}} \cdot \left[\sum_{j \in J} F_{j,i}^{Fw,k} + \sum_{i' \in I} F_{i',i}^{IP,k} - F_i^{\text{loss}}\right] - M_{c,i}^{\text{out}} = 0 \quad \forall c \in C, \quad i \in I \tag{3''}$$

Problem (P_2) thus consists of

(a) constraints (4') and (5')

(b) constraints (2'') and (3'') as described above.

(i) The outlet concentrations $C_{c,i}^{\text{out}}$ are the only variables of (P_2).

(ii) The inlet concentrations are calculated from $C_{c,i}^{\text{out}*}$,

(iii) Problem (P_2) is solved against an objective that minimises slacks and assumes the form:

$$\min z_2^k = \sum_c \sum_i s_{c,i}^1 + \sum_c \sum_i s_{c,i}^2. \tag{31}$$

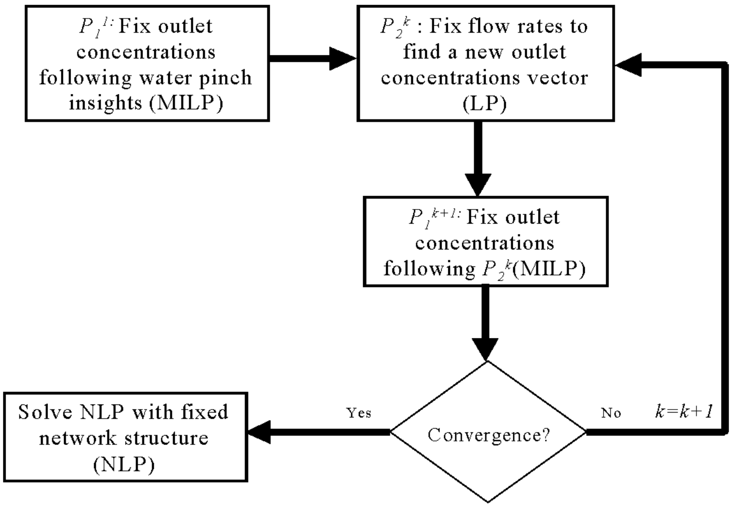
Outline of the solution procedure

An iterative scheme is devised where the projection of equations (2)–(3) and (13) in (P_1) is available from the preceding iterations; the projection of equations (2) and (3) in (P_2) is available from the solution of (P_1). Let $(P_1)^k$ and $(P_2)^k$ be the formulation of (P_1) and (P_2) at iteration *k*, the algorithm involves the following steps.

- Set $k = 1$. Solve problem $(P_1)^k$ with $C_{c,i}^{\text{out},k} = 0$ (treatment), $C_{c,i}^{\text{out},k} = C_{c,i}^{\text{out},\max}$ (water users) to obtain z_1^{k*} and the optimal values of the flow rates in the network, $F_{j,i}^{Fw*}$, $F_i^{\text{OUT}*}$ and $F_{i,i'}^{IP*}$. Let $F_{j,i}^{Fw,k} = F_{j,i}^{Fw*}$, $F_i^{\text{OUT},k} = F_i^{\text{OUT}*}$ and $F_{i,i'}^{IP,k} = F_{i,i'}^{IP*}$.
- Solve problem $(P_2)^k$ for a new vector of outlet concentrations, $C_{c,i}^{\text{out},*}$. Set $C_{c,i}^{\text{out},k+1} = C_{c,i}^{\text{out},*}$.
- Set $k = k + 1$, update p^{k+1} and solve problem $(P_1)^{k+1}$ to obtain new values for the flow rates. Let z_1^{k+1} be the new optimal value for the objective.
- If $\chi^{\inf,k} \le \varepsilon_2$ or $|(z_1^k - z_1^{k+1})/z_1^k| \le \varepsilon_1$, stop. Otherwise, go to Step 2.
- Solve the NLP that results from problem (P) with all structural features fixed according to the solution from Step 4.

The uncoupling of the bilinear terms (flow times concentration) with the introduction of the mass flows and the relaxation-projection strategy allows the search to be performed in the space defined by the convex feasible region of problem $(P_1)^k$. The projection scheme follows Gunaratnam et al. (2005) and the solution strategy is based on the penalty barrier parameters of Step 3. The value of the weight p^k is such that the search does not get too far into the infeasible region and premature termination in a feasible but far from optimal solution is avoided. In order to ensure termination with a feasible solution, the value of p is increased at each iteration. In the computer implementation p is increased by an order of magnitude from iteration k to iteration $k + 1$ to enforce feasibility. Figure 3 illustrates the main steps of the decomposition.

Figure 3 Iterative procedure to find a feasible solution



6 Example 1

The method is illustrated with an industrial water system from a petroleum refinery (Kuo, 1996; Kuo and Smith, 1997). Table 1 presents the operating data for the water-using system that involves five major water users and the three contaminants of interest. The performance of the treatment units is given as recovery ratios for the different contaminants and is shown in Table 2. The capital and operating costs of the steam-stripping column (T1) are given by:

$$\text{Cost}_{T1}^{T}(\$) = 16{,}800 \cdot F_i^T (t/h)^{0.7},$$
$$\text{Cost}_{T1}^{T,op}(\$/h) = F_i^T (t/h).$$

For the biological treatment unit (T2):

$$\text{Cost}_{T2}^{T}(\$) = 12{,}600 \cdot F_i^T (t/h)^{0.7},$$
$$\text{Cost}_{T2}^{T,op}(\$/h) = 0.0067 \cdot F_i^T (t/h)$$

and for the API separator (T3):

$$\text{Cost}_{T3}^{T}(\$) = 4{,}800 \cdot F_i^T (t/h)^{0.7}.$$

Table 1 Water-using operations for example 1

Operation (*i*)	*Contaminant* (*c*)	$C_i^{\text{in,max}}$ (ppm)	$C_{c,i}^{\text{out,max}}$ (ppm)	$m_{c,i}^L$ (g/h)
O1	HC	0	15	750
	H_2S	0	400	20,000
	SS	0	35	1,750
O2	HC	20	120	3,400
	H_2S	300	12,500	414,800
	SS	45	180	4,590
O3	HC	120	220	5,600
	H_2S	20	45	1,400
	SS	200	9,500	520,800
O4	HC	0	20	160
	H_2S	0	60	480
	SS	0	20	160
O5	HC	50	150	800
	H_2S	400	8,000	60,800
	SS	60	120	480

Identification of the water users

Operation	*Description*
O1	Steam stripping
O2	HDS-1
O3	Desalter
O4	VDU
O5	HDS-2

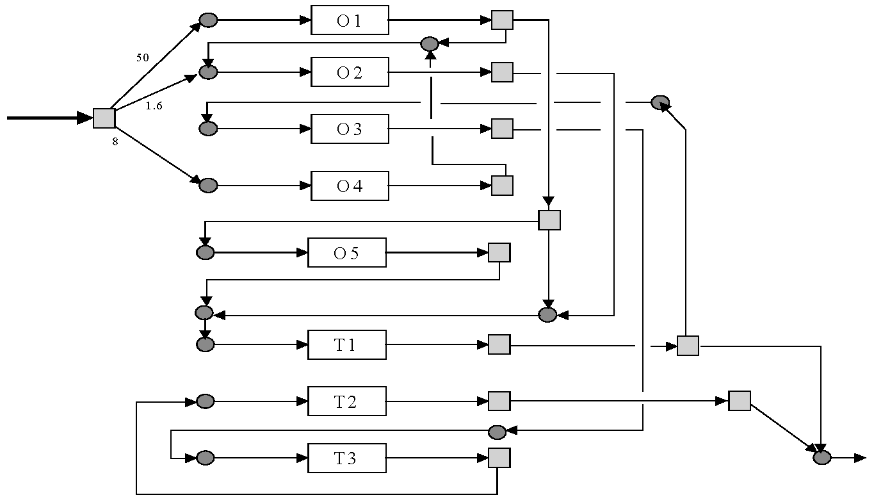
Table 2 Performance data for treatment operations. Example 1

	Removal ratio (%)		
Operation	*HC*	H_2S	*SS*
T1	0	99.9	0
T2	70	90	98
T3	95	0	50

The environmental limits for HC, H_2S and SS are set to 20 ppm, 5 ppm and 100 ppm respectively. The annual interest rate is 10% and the freshwater costs for S_1 is \$0.2/*t*. The operating year is assumed as 8,600 hr/y.

Base case. The water system design by Kuo and Smith (1998) is illustrated in Figure 4. The design is obtained with a sequential procedure. Once the water target for regeneration re-use is identified at 59.7 t/h, grouping and migration rules follow to determine the number of treatment units required. The worst-case single-contaminant design is chosen as the final solution. T1 has been relocated from the effluent system to a regeneration duty on the basis of an overall reduction of freshwater and wastewater without increasing the number of treatment units. As explained later, the case illustrates that the number of units is not a reliable indication of the total treatment cost.

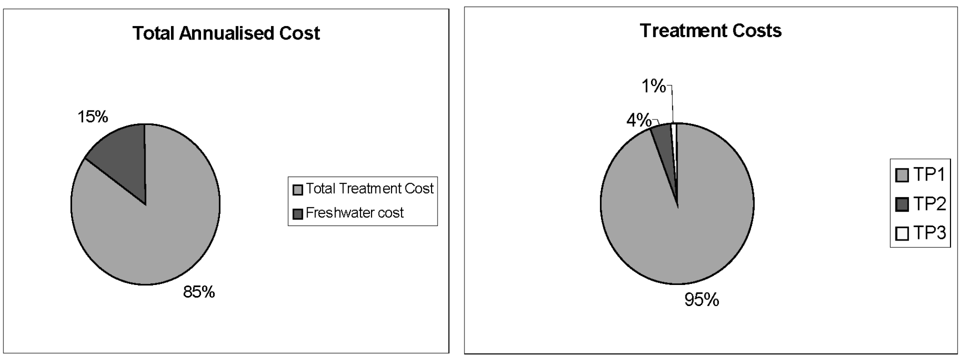
Figure 4 Design for example 1



Source: Proposed by Kuo and Smith (1997)

In the approach by Kuo and Smith, once the water-using system design is produced, the effluent streams can then be identified and the treatment system can be targeted and designed. The concept of wastewater degradation is unable to guide the design and the annualised cost of the process is \$677,710. Figure 5 shows the breakdown of the costs in the design of Figure 4. The treatment costs are dominant and treatment operation T1 accounts for over 90% of the total treatment cost.

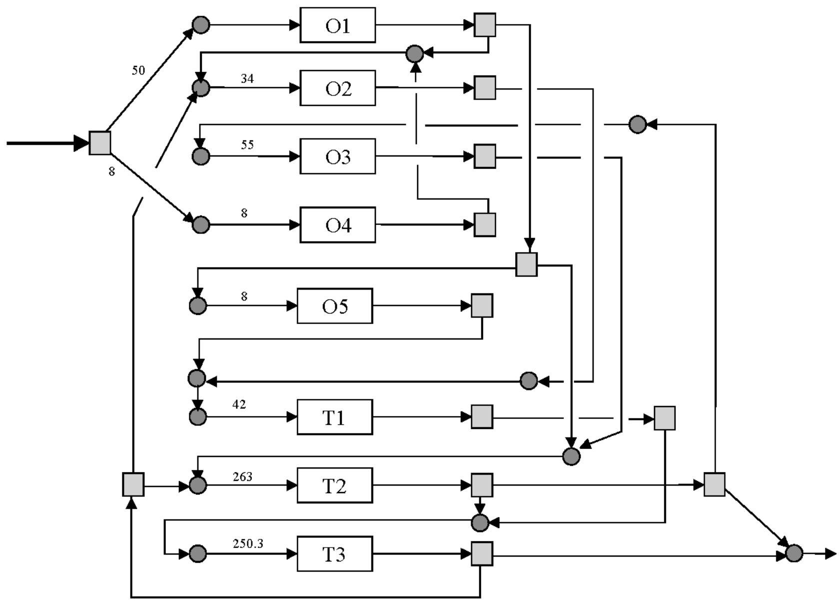
Figure 5 Costs associated with the design from pinch analysis



Source: Kuo and Smith (1998)

Case A. The objective function is the total annualised cost (excluding pipework). The problem is solved allowing recycling. Consequently constraints (23)–(28) are not included. The approach converged in five iterations (40.6 CPU sec overall). Problem $(P_1)^k$ had 622 continuous and 75 binary variables whereas $(P_2)^k$ had 142 continuous variables. The procedure terminated in a design with a small violation to the environmental limit for H_2S (2 ppm above). The solution forwarded to the NLP has a cost of $672,721/yr and is improved after the NLP optimisation to the design of Figure 6.

Figure 6 Design for case A. Example 1



The total cost is $584,397/yr and is consistent with the target presented in Gunaratnam et al. (2005). In this network, some re-use opportunities arise without water regeneration. As the water becomes more contaminated, regeneration is needed. The sequence of treatments T1–T3 functions as a regeneration 'unit' since it is after both treatments that the effluent is recycled back to O2. Recycling can be found in the circuits O2–T1–T3–O2 and T2–T3–T2. As mentioned earlier, these may not be desirable due to concerns on contaminants building up to unacceptable levels.

Case B. The objective function is the annualised total cost (excluding pipework) but recycling is not allowed. Therefore, constraints (23)–(28) are included in the formulation. The procedure converged in four iterations consuming 69.1 CPU sec overall. Problems $(P_1)^k$ had 670 continuous variables and 107 binary variables. The design from the MILP-LP decomposition costs $714,865 (5.4% higher than the base case) and is used to initialise the NLP formulation to yield the design shown in Figure 7. The total annual cost of this design is $662,755/yr (3% lower than the base case) and consistent with the target presented in Gunaratnam et al. (2005). The grouping of operations is shown in Table 3. T1 operates both as a regenerator and effluent treatment unit, while T2 and T3 deal with the wastewater discharge. Operation 3 is classified as Group 2 (G2) to ensure the effluent from O3 will not enter any Group 1 operation (with respect to T1).

Figure 7 Design for case B. Example 1

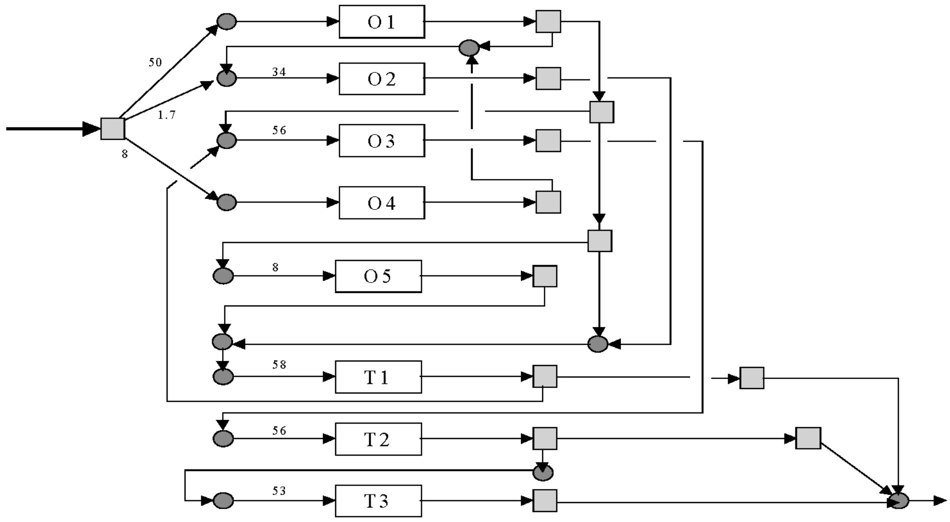


Table 3 Grouping of operations to eliminate recycling

Operation	*T1*	*T2*	*T3*
O1	G1	G1	G1
O2	G1	G1	G1
O3	G2	G1	G1
O4	G1	G1	G1
O5	G1	G1	G1
T1	n.a	G1	G1
T2	G2	n.a	G1
T3	G2	G2	n.a

Source: Kuo and Smith (1998)

Table 4 presents a comparison of the results. The table explains there are savings of $78,359/yr in case that recycling is allowed. An interesting point is that Case B and the base case consume the same amount of freshwater. The difference is found in the distribution of the effluent from O3: the new design accomplishes a reduction in the flow through T3 by operating the pair T2–T3 in a series arrangement (in that sequence) with a bypass to the discharge from T2. Similarly, the effluent from O1 to T1 is reduced.

Table 4 Comparison of results

Cost ($/y)	*Base case*	*Case A*	*Case B*
Freshwater	102,684	99,760	102,684
T1	542,830	384,192	527,987
T2	24,190	77,524	24,324
T3	7,995	22,920	7,760
TAC	*677,697*	*584,397*	*662,755*

Case C. The objective function is the total annualised cost including pipework. No recycling is allowed and the data for the distances are shown in Table 5. The flow velocity is 1 m/s and carbon steel is used as the material of construction for all pipes. The parameters for the piping costs are IChemE (1988):

$$a_{j,i}^{Fw,\text{pipe}} = a_{i,i}^{IP,\text{pipe}} = a_{j}^{\text{OUT},\text{pipe}} = 3,603.4 \text{ and}$$
$$b_{j,i}^{Fw,\text{pipe}} = b_{i,i}^{IP,\text{pipe}} = b_{j}^{\text{OUT},\text{pipe}} = 124.6.$$

The CE plant index (December 1997) is 389.1.

Table 5 Distance matrix (in m) for example 1

	O1	*O2*	*O3*	*O4*	*O5*	*T1*	*T2*	*T3*	*Discharge*
S1	30	25	70	50	90	200	500	600	2000
O1	0	30	80	150	400	90	150	200	1200
O2	30	0	60	100	165	100	150	150	1000
O3	80	60	0	50	75	120	90	350	800
O4	150	100	50	0	150	250	170	400	650
O5	400	165	75	150	0	300	120	200	300
T1	90	100	120	250	300	0	125	80	250
T2	150	150	90	170	120	125	0	35	100
T3	200	150	350	400	200	80	35	0	100

The procedure converged in six iterations consuming 105.6 CPU sec overall. (P_1) has 670 continuous variables and 96 binary variables. The design converged from the MILP-LP stage costs (piping cost subtracted) \$970,590 and is used to initialise the NLP model that results in the network shown in Figure 8. Considering freshwater and treatment cost alone the total cost is \$654,245/yr. This is \$30,000 less than the solution reported in Gunaratnam et al. (2005) but this is probably due to the introduction of constraints for the maximum number of sources to the mixers in the other approach. Although the network consumes the same freshwater (59.7 t/h) with Case B, a different structure is found that minimises the piping costs. The effluent treatment sequence is T2–T3 (in that order). The connection between T1 and the discharge point is removed since the distance is relatively large. As a result, the flow rate through T2 is slightly increased.

Table 6 presents a final comparison of the cases studied so far. There are three different designs corresponding to regeneration re-use. These three designs consume the same amount of freshwater (same freshwater costs). The effluent treatment system in each one of them is capable of achieving the environmental discharge regulations on the final wastewater. However, the design obtained with the simultaneous approach minimises the total annual cost of the system.

Figure 8 Design for case C. Example 1

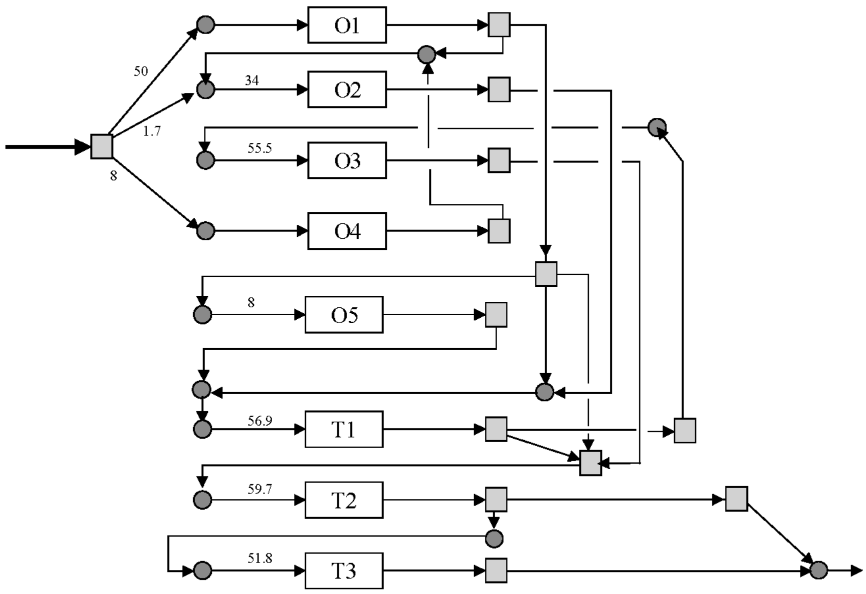


Table 6 Comparison of results for example 1

Case	*Freshwater* ($/y)	*Treatment* ($/y)	*Piping* ($/y)	*TAC* ($/y)
Base case	102,684	575,013	36,069	713,767
Case A	99,760	484,637	32,426	616,824
Case B	102,684	560,071	34,932	697,687
Case C	102,684	551,560	32,249	686,494

7 Example 2

The limiting data for the water users is presented in Table 7. A single contaminant, A, is analysed.

Table 7 Limiting water profiles. Example 2

Operation (*i*)	$C_{c,i}^{\text{in,max}}$ (ppm)	$C_{c,i}^{\text{out,max}}$ (ppm)	$m_{c,i}^{L}$ (g/h)
O1	0	200	8,000
O2	100	200	5,000
O3	100	400	9,000
O4	300	400	6,000
O5	400	600	8,000

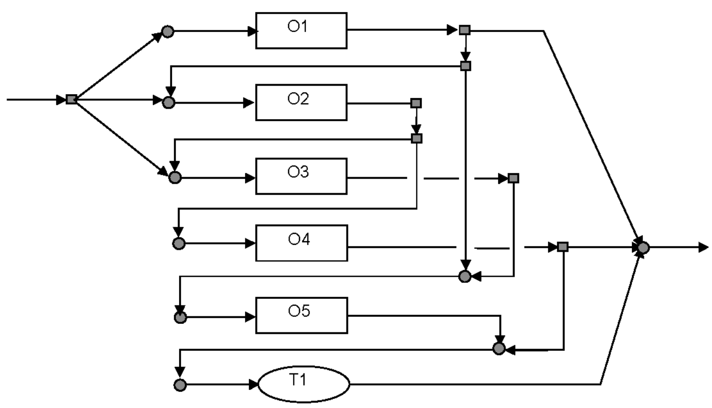
The limiting flow rate for each operation, F_i^L, can be calculated from the table data using equation (1):

Operation	*Limiting flow rate* (t/h)
O1	40
O2	50
O3	30
O4	60
O5	40

There is a single treatment unit, its performance defined with a removal ratio at 95%; no inlet concentration restrictions exist for this unit. The environmental limit on the concentration of A is 100 ppm. A clean freshwater cost of £1/t, and an operating year for the network is 8,600 hr/y.

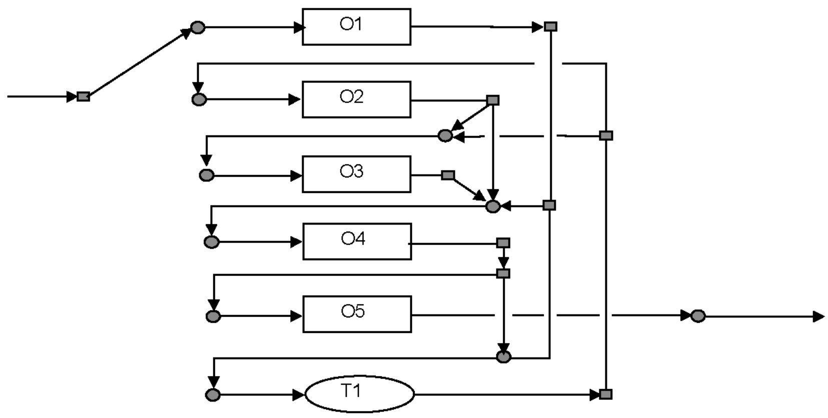
Case A. The objective function is selected to minimise freshwater cost. This first scenario is generated following a sequential approach. First the water-using system is designed considering re-use only. The treatment system is designed last to achieve the environmental restriction of 100 ppm maximum. In the first stage, the approach converged in a single iteration (2.2 CPU sec). Problem (P_1) had 314 continuous and 42 binary variables whereas (P_2) had 36 continuous variables. The effluent treatment system is designed minimising the flow of effluent to be treated leading to a freshwater annual cost of £688,000/yr; NLP optimisation is not required. The design is illustrated in Figure 9. In this network, some re-use opportunities arise without water regeneration. The flow of effluent treated by T1 amounts to 60.4 t/h; there are bypass streams from O1 and O4.

Figure 9 Design for case A. Example 2



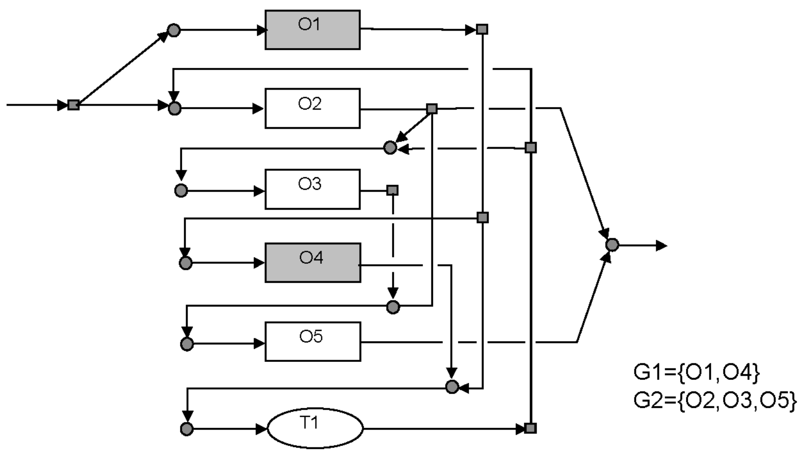
Case B. The objective is selected to be the freshwater cost. The treatment unit is included as a regeneration unit and recycling is allowed. The iterative approach converged in six iterations (11.4 CPU sec overall). Problem (P_1) had 314 continuous and 42 binary variables whereas (P_2) had 36 continuous variables. The solution after NLP optimisation is illustrated in Figure 10. In this network, the freshwater demand is reduced to its minimum of 40 t/h. However, the network features extensive recycling. The freshwater cost is of £344,000/yr. The flow of effluent through T1 is 65 t/h. Since the treatment unit is operating as a regenerator only, the final effluent discharged does not comply with the environmental regulations.

Figure 10 Design for case B. Example 2



Case C. The objective is selected to be the freshwater costs disallowing recycles. The procedure converged in five iterations (43.5 CPU sec overall). Problem (P_1) had 314 continuous and 48 binary variables whereas (P_2) had 36 continuous variables. The solution after NLP optimisation is illustrated in Figure 11. In this network, freshwater demand is of 43.5 t/h and no recycling appears in the network. The grouping of operations with respect to T1 has O1 and O4 in Group 1 (i.e., no regenerated water enters these operations). The freshwater cost is £374,100/yr. The flow of effluent through T1 is 65.5 t/h. The treatment unit is operating as a regenerator only and the final effluent discharged does not comply with the environmental regulations. An additional treatment unit is required.

Figure 11 Design for case C. Example 2



Case D: The objective function remains unchanged; as in Case C no recycling is allowed. The environmental constraint is enforced and the procedure was developed as in Case C. The solution after the NLP optimisation is illustrated in Figure 12. T1 operates both as a regenerator and treatment unit such that the final discharge complies with the environmental limit. The freshwater demand is increased to 65.5 t/h for an annual cost of £563,300/yr. The grouping of the operations is different from Case C and here only O2 belongs to Group 2 (i.e., only O2 uses regenerated water). Table 8 presents a summary of results for Example 2.

Figure 12 Design for case D. Example 2

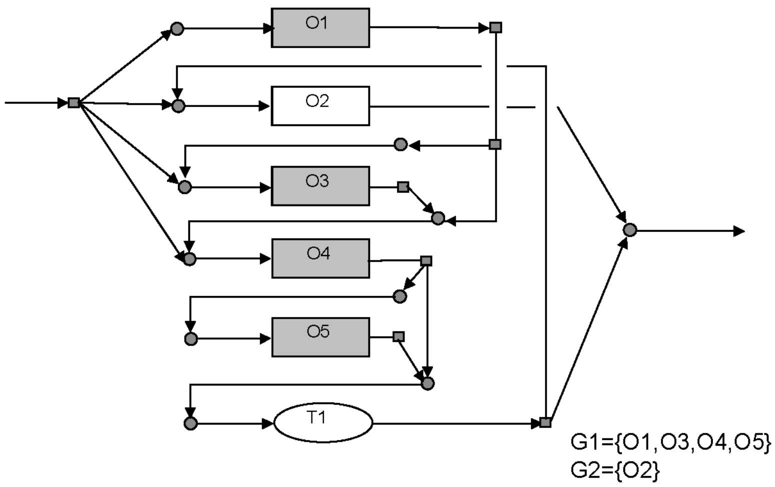
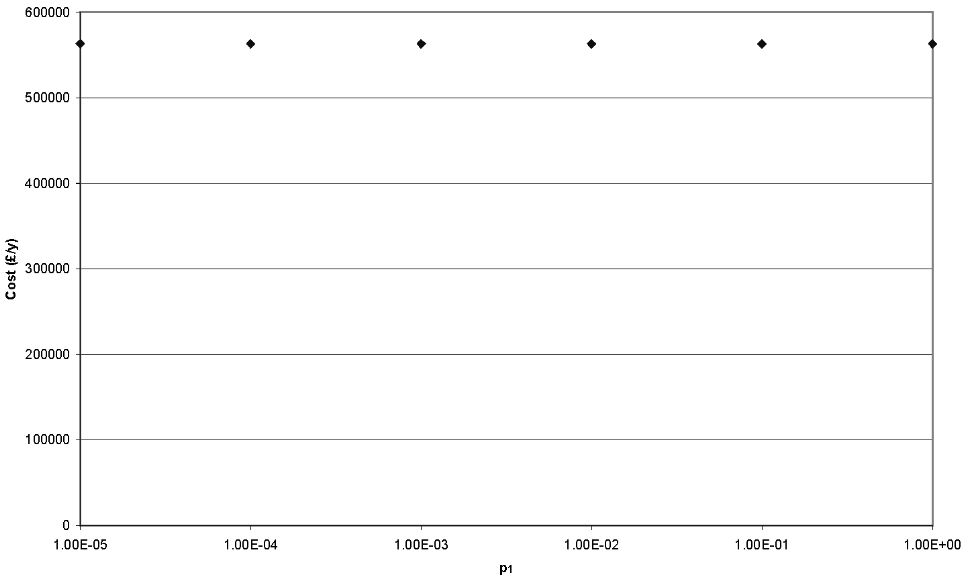


Table 8 Summary for example 2

Case	*Freshwater cost* (£/y)	*Number of treatment units*
Case A	688,000	1
Case B	344,000	2
Case C	374,100	2
Case D	563,300	1

The presentation of results does not suggest a particular solution but explains that the method allows a transparent study of different alternatives. The choice depends on whether recycling is allowed as well as on the costs of treatment units. Considering the difficulty to calculate costs for the recycles (the actual factors are combinations of dynamic and steady-state aspects), a set of simple runs were employed to justify network complexity and its impact on cost: penalties were introduced to the objective for the recycles and the effect of the penalty terms is illustrated in Figure 13. The figure concludes that penalising recycles has a negligible impact and simpler designs could be developed at a small expense.

Figure 13 Effect of the weight on the final solution



Alternative designs can be generated with integer cuts. Figures 14–16 illustrate six alternative networks all of which feature similar freshwater consumption and achieving environmental constraints.

Figure 14 Alternative solutions for example 2

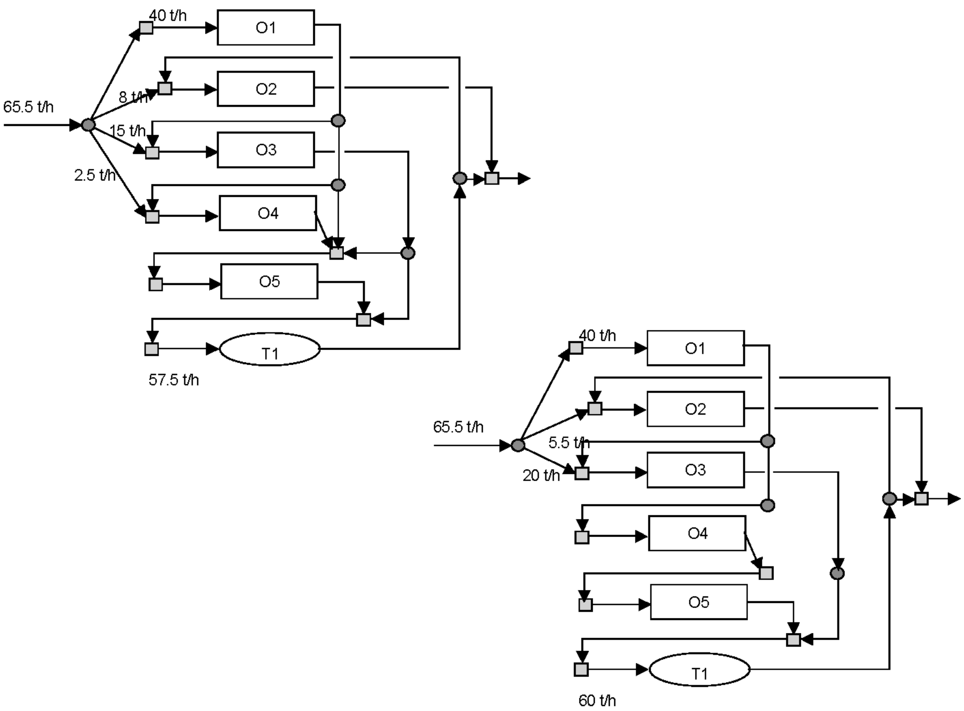


Figure 15 Alternative solutions for example 2

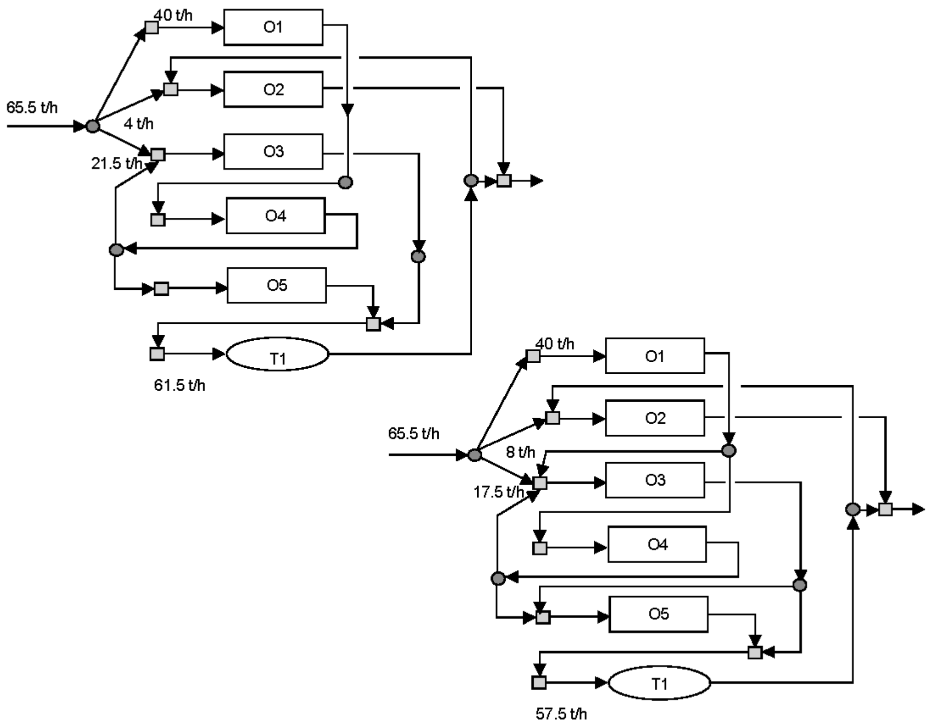
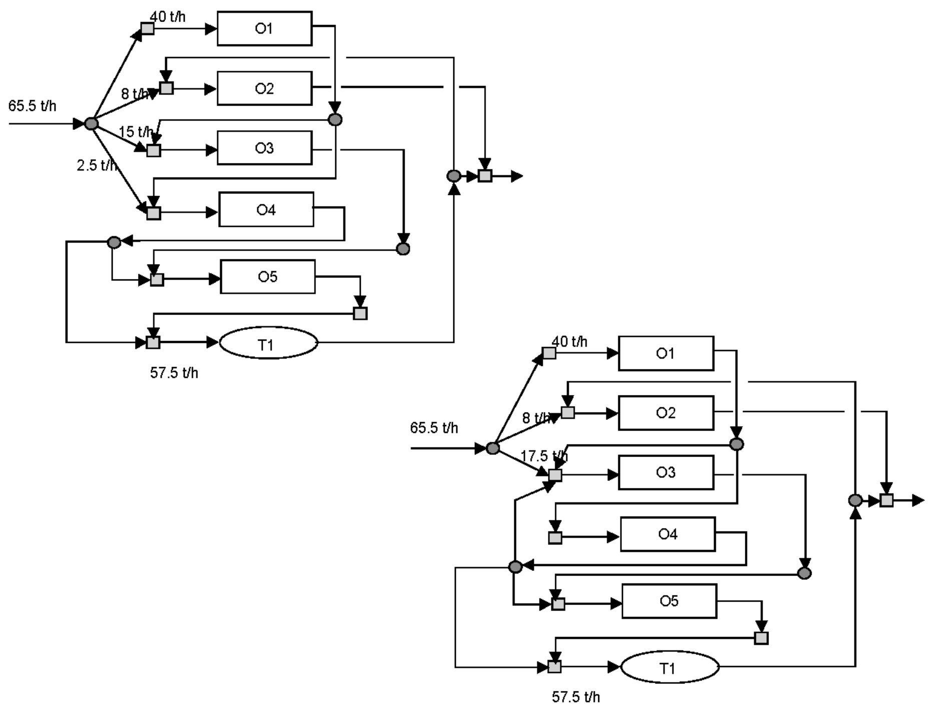


Figure 16 Alternative solutions for example 2



8 Conclusions

A systematic method has been developed that capitalises fully on Water Pinch and extends the conceptual approach to a general and powerful formulation that addresses cost and operational issues. The work is based upon a decomposition scheme that searches for solutions in the spirit of barrier and penalty based methods. The resemblance to the barrier methods relates to the optimal search following an infeasible track of intermediate points and an iterative search that converges to a final feasible solution. As in penalty and barrier methods, penalties are manipulated progressively until convergence is achieved. The method has been particularly successful to water using design, handling practical constraints and industrial sized problems. Applied to the total system design, the performance appears in need for further research, as the progression of penalties at each iteration should take into account the more general considerations of the integration between re-use and wastewater treatment.

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