Eng. Opt., 2000, Vol. 32, pp. 549–584
Reprints available directly from the publisher
Photocopying permitted by license only

OPTIMAL OPERATION OF MULTI-QUALITY WATER SUPPLY SYSTEMS-I: INTRODUCTION AND THE *Q-C* MODEL

DANI COHEN[a], URI SHAMIR[b,*] and GIDEON SINAI[c]

[a]*Command and Control Unit, Mekorot Water Co., Ltd., 9 Lincoln St., Tel Aviv, Israel;* [b]*Faculty of Civil Engineering, Technion, Haifa 32000, Israel;* [c]*Faculty of Agricultural Engineering, Technion, Haifa 32000, Israel*

(Received 7 July 1998; In final form 12 April 1999)

One of three complementary models for optimal operation of multi-quality water supply systems is presented. The other two models are the subject of companion papers. The model, which is known as the *Q-C* (flow-quality) model, includes mass continuity of water and constituents. However, the hydraulic constraints do not appear explicitly. To prevent infeasibilities or unreasonable hydraulic conditions arising from the lack of hydraulic constraints, limits and a cost are associated with the flow in each pipe. The constraints in the model include dilution conditions which depend on flow direction. These dilution conditions are introduced into the model by an exponential function, resulting in a smooth continuous nonlinear programming problem, which is transformed into an equivalent problem and solved by a modified projected gradient method. The method is insensitive to scaling of variables, and the computational complexity depends only slightly on the number of water quality parameters. The method is demonstrated by application to two examples: the solution for a small network is presented in detail, and main results are shown for a larger one. The results of these two applications indicate the method's applicability to real networks.

Keywords: Water supply systems; water quality; optimal operation of water systems; network analysis; hydraulic analysis

*Corresponding author.

INTRODUCTION

Multi-quality water supply systems are networks in which water quality is not uniform in time and/or space. The variable quality may be due to supply coming from sources of varying qualities, changes in treatment plant operation, and mixing and/or chemical reactions as the water flows in the network. While such systems are more common for irrigation and industrial waters, they sometimes also occur in urban supply systems. Interest in the design and operation of multi-quality systems has increased [3, 24] as water of good quality becomes scarcer and more expensive resulting in the incentive to use water of different qualities. Interest in the modelling of multi-quality systems has also arisen from the need to track residual chlorine or other disinfectants in the network.

Models for simulating water quality throughout the network under steady and unsteady conditions have emerged in recent years [2–5, 10, 13, 15–17, 19, 20, 22–26]. Following Sinai *et al.* [25], decomposition is suggested of the solute flow problem (Q-C-H), associated with water flow in multi-quality of water supply system, into two subproblems: the flow-quality (Q-C) problem, and the flow-head (Q-H) problem. These two subproblems are connected by a mutual flow distribution (Q), however, they are somewhat independent. Water quality (C) does not physically affect flow hydraulics, so the flow-head (Q-H) subproblem can be dealt with independently of the flow-quality (Q-C) subproblem. Similarly a flow-quality (Q-C) subproblem can be defined such that it does not depend on the head distribution. This can be achieved by imposing limits on head distribution in pipes. Use of this approach enables decomposition of the complicated solute transport problem (Q-C-H) and the model for optimal operation of multi-quality water supply systems.

In this and two companion papers, optimal operation of multi-quality water supply systems under steady-state conditions is addressed. The three models for optimal operation of multi-quality water supply systems are:

(a) The Q-C Model deals only with continuity of water and the water quality parameters at each node, and not the hydraulics of the system. This model is most applicable when it can be assumed that

the resulting operation will satisfy the required heads at consumer nodes and the other hydraulic constraints. It is a building block for the full (*Q-C-H*) model.

(b) The *Q-H* Model deals only with the hydraulics of the network and disregards the quality aspects. This model can be used for single quality systems. It is the second building block for the full (*Q-C-H*) model.

(c) The *Q-C-H* Model This model includes the full set of hydraulic and water quality constraints and objectives.

This first paper examines the *Q-C* model. Some general tools and methodologies which are used in all three models are also described in the appendices. The purpose of the *Q-C* model is to determine the optimal flows in the network and the treatment at plants.

Mathematical Representation of the Network

A water supply system can be described as a graph consisting of n nodes connected by n_e arcs. There are three sub-groups of nodes: N_1 are source nodes: reservoirs which feed the network, wells, and the connection points of the network to other networks; N_2 are consumer nodes and N_3 are intermediate nodes. The arcs represent the pipes between two nodes. In this paper, treatment plants are considered as components located on pipes. The arcs can be categorized into two sub-groups: E_1 are regular pipes, and E_2 are pipes which have treatment plants. Each arc is assigned an arbitrary positive direction.

The topology of the network can be represented by the connectivity matrix, D, with components defined by: $D_{ij} = \pm 1$ if there is an arc between node i and j, $+1$ when the arc is directed from i to j, -1 when from j to i. $D_{ij} = 0$ if there is no arc between nodes i and j. The adjacency between the nodes and the arcs is represented by the adjacency matrix, A, with components defined by: $A_{ij} = 1$ if arc j is connected to node i and its positive direction is out of node i. $A_{ij} = -1$ if arc j is connected to node i and its positive direction is to node i. $A_{ij} = 0$ if arc j is not connected to node i.

The cyclic structure of the network is defined by loops and pseudo-loops, each with a defined positive direction. Pseudo-loops are paths

between nodes at which the heads are fixed and do not depend on the flows in the network; for example the path between two reservoirs or wells. Henceforth "loops" will mean loops plus pseudo-loops. Loops are represented by a cyclic matrix, L, with components defined by: $L_{ij} = \pm 1$ if loop i includes arc j; $+1$ if the positive directions of both coincide; -1 if their positive directions are opposite. $L_{ij} = 0$ if loop i does not include arc j. The connectivity of the treatment plants to the pipes is represented by a matrix B_t of order $n_t \times n_e$ (n_t = number of treatment plants, n_e = number of pipes), whose components are: $(B_t)_{ij} = 1$, if treatment plant i is on pipe j; $(B_t)_{ij} = 0$, otherwise.

Decision Variables

The decision variables are therefore: water flow and water quality distribution, and the removal ratios in the treatment plants. Note that the flow distribution is to be determined as part of the solution process, as follows. An initial flow distribution, which satisfies water continuity at all nodes, is specified. This initial solution is then modified in the solution process, in a way in which continuity is retained. The maintenance of continuity is achieved by considering the circular flows, $\mathbf{q}$, in loops and pseudo-loops as decision variables, since when these flows are modified, continuity at nodes is maintained. As a consequence of this definition, the water flow continuity equations can be omitted, thus reducing the size of the optimization model.

The vector $\mathbf{q}$ is of order n_1, the number of loops, with the ith component of the vector being the flow in the positive direction of loop i. Since the number of loops is considerably smaller than the number of pipes, using the circular flows in the loops rather than the flows in the pipes as the decision variables in this manner, results in an even smaller model.

The relationships between pipe discharges, $\mathbf{q}_a$, and circular discharge vector, $\mathbf{q}$, is given by:

$$\mathbf{q}_a = \mathbf{q}_a^0 + L^T\mathbf{q} \tag{1}$$

where $\mathbf{q}_a^0$ are the initial pipe discharges, which satisfy the water flow continuity equations, and $(\cdot)^T$ denotes the transpose. The relationship between the discharges from the sources, $\mathbf{q}_s$, and the

pipes discharges is:

$$\mathbf{q}_s = \hat{A}\mathbf{q}_a \tag{2}$$

where $\hat{A}$ is a submatrix of A, obtained from the rows of A which are related to source nodes. From Eqs. (1) and (2) $\mathbf{q}_s$ is defined by:

$$\mathbf{q}_s = \hat{A}[\mathbf{q}_a^0 + L^T\mathbf{q}] \tag{3}$$

The relationship between the treatment-plant discharges, $\mathbf{q}_t$, and cyclic discharges is obtained from Eq. (1) and the definition of B_t, *i.e.*,

$$\mathbf{q}_t = B_t[\mathbf{q}_a^0 + L^T\mathbf{q}] \tag{4}$$

Equations (2)–(4) show that the flow values in all network components are related to the circular flows.

Water quality may be described by primary and dependent quality parameters. The distribution of the primary water quality parameters is defined by matrix C. This matrix is three dimensional. One dimension is n_3, which is the number of the primary quality parameters with the other two dimensions both being equal to the number of nodes and therefore symmetric. Cell ijm contains the concentration of quality parameter m in the arc between nodes i and j. The diagonal cells contain the concentration at nodes. The distribution of the dependent quality parameters is denoted by matrix C^d, which has the same structure as C, with its primary dimension being equal to the number of dependent quality parameters.

The removal ratios in the treatment plants are given by the matrix R. Once again, one dimension of the matrix is equal to the number of the primary quality parameters with the other two dimensions being equal to the number of nodes adjacent to the treatment plants; cell ijm contains the removal ratio of quality parameter m in the treatment plant which is located on the arc between the nodes i and j.

Objective Function

The objective of the optimization is to minimize the total cost of operation over the planning horizon t. This total cost is made of several components.

Water Supply Cost

This is the cost of water supplied from the sources. At wells this cost represents the cost of pumping. At other types of sources, such as a transfer from another network, this cost represents the cost of purchasing water from that source. In general, the specific cost (per unit volume) of such water is a function of discharge rather than a constant. Thus, the specific cost of water at sources will be given by a vector of functions, denoted by $\mathbf{w}_s(\mathbf{q}_s)$, the dimension of which is equal the number of sources. Where the unit cost at a source is fixed, the corresponding value in the vector is a constant. The total supply cost from the sources, ϕ_s, for the entire period t, can be described by

$$\phi_s = t\,\mathbf{w}_s(\mathbf{q}_s)^T\mathbf{q}_s \tag{5}$$

Treatment Cost

The specific cost (cost per unit discharge) of treatment is a function of the removal ratio. Because many types of treatment processes can be chosen it is impossible to describe this cost by a single function. It can, however, be assumed that all removal cost functions can be described by a quadratic or at most cubic polynomial, the coefficients of which can be determined through regression analysis of cost data. These functions are included in a cost function vector, denoted by $\mathbf{w}_t(\mathbf{r})$, whose dimension is equal to the number of treatment plants.

The total treatment cost, ϕ_t, is described by

$$\phi_t = t\,\mathbf{w}_t(\mathbf{r})^T\mathbf{q}_t \tag{6}$$

Transportation Cost

The transportation cost in a pipe is related to its hydraulic properties. Schwartz *et al.* [21] and Sinai *et al.* [25] expressed the transportation cost by a linear function of the discharge. The model described in this paper allows a non-linear relationship between transportation cost and pipe flow. Since the flow direction is not known in advance and is included among the decision variables, the cost must be expressed as a function of the absolute value of the discharge. The transportation

cost function is therefore not smooth, and its derivative is not defined at zero flow. To overcome this difficulty, an exponential smoothing procedure which is described in detail in the Appendix is used to define the absolute value of the discharge:

$$\bar{q}_a^j = \frac{q_a^j \exp\{\varpi(q_a^j)\} - q_a^j \exp\{-\varpi(q_a^j)\}}{\exp\{\varpi(q_a^j)\} + \exp\{-\varpi(q_a^j)\}} \tag{7}$$

where

$\varpi(.)$ is the normalized direction function defined by

$$\varpi(x) = k_p \frac{x}{\sqrt{x^2 + \varepsilon}} \tag{8}$$

k_p is a gain coefficient, and ε is a small arbitrary number to prevent division by zero.

The specific transportation cost in a pipe is $w_p(q_a)q_a$, which is continuous and smooth. The total transportation cost over all pipes ϕ_p is therefore given by

$$\phi_p = t\mathbf{w}_p(\mathbf{q}_a)^T\mathbf{q}_a \tag{9}$$

As mentioned in the introduction, it is important to note at this time that the *Q-C* problem is assumed to have a wide hydraulic feasibility domain. However, in order to prevent infeasibilities or unreasonable hydraulic conditions, limits and costs are associated with the flow in each pipe.

Yield Reduction Cost

Consumers are categorized into 3 types:

1. Agricultural consumers, who have a relative yield function which depends on water quality. Mass and Hoffman [12] and Finerman and Yaron [6] examined the salt tolerance of a wide range of crops and proposed either a bi-linear or quadratic function to describe crop yield reduction due to increased salinity. The quadratic form, is used as follows: denote the relative yield function vector by $\mathbf{y}$, the yield achieved under ideal conditions by $\mathbf{y}_0$ and the income matrix by B_0. The B_0 matrix is diagonal. The total loss due to

yield reduction, ϕ_y, is:

$$\phi_y = \mathbf{y}_0^T B_0[\mathbf{1}_y - \mathbf{y}] \tag{10}$$

2. Domestic and industrial consumers, who require treatment of their water, the cost of which is defined at their supply connection. This can be introduced into the model, using functions similar to the above.
3. Consumers with concentration limits, who require that the water quality be within specified limits, with no cost or benefit function for quality being specified. These quality limits are incorporated into the constraints.

Combining all the components yields the total objective function:

$$\min f = t\,\mathbf{w}_s(\mathbf{q}_s)^T\mathbf{q}_s + t\,\mathbf{w}_t(\mathbf{r})^T\mathbf{q}_t + t\,\mathbf{w}_p(\mathbf{q}_a)^T\mathbf{q}_a + \mathbf{y}_0^T B_0[\mathbf{1}_y - \mathbf{y}] \tag{11}$$

Constraints

Mass Conservation Law for Conservative Quality Parameters

This law can be expressed by n_3 (number of primary quality parameters) sets of equations. Each set of equations includes equations for all nodes, except the source nodes.

$$\sum_{(ij)\in E_i} a_{ij}Q_{ij}C_{ijm} + \sum_{(ij)\in E_2} a_{ij}Q_{ij}(1 - R_{ijm})C_{ijm} - d_jC_{jjm} = 0$$
$$\forall\, j \notin N_1 \text{ and } \forall\, m \in M_1 \tag{12}$$

where

a_{ij} – element ij of the adjacency matrix A.
d_j – consumption at node j.
M_1 – primary quality parameters group.
Q_{ij} – flow from node i to j.
C_{ijm} – concentration of primary quality parameter m at the arc between node i and j.
C_{jjm} – concentration of primary quality parameter m at node j.
R_{ijm} – removal ratio of primary quality parameter m, at the treatment plant located between node i and j.

Dilution Condition

The model assumes that total mixing occurs at all nodes resulting in the concentration in all pipes leaving a node being equal. However, since the flow direction in pipes is not known in advance the dilution condition is written as:

$$C_{ijm} = \frac{C_{iim}\exp\{\varpi(a_{ij}Q_{ij})\} + C_{jjm}\exp\{-\varpi(a_{ij}Q_{ij})\}}{\exp\{\varpi(a_{ij}Q_{ij})\} + \exp\{-\varpi(a_{ij}Q_{ij})\}} \quad \forall(ij) \text{ and } \forall m \in M_1 \qquad (13)$$

which uses the exponential smoothing procedure described in the Appendix. This formulation overcomes the difficulty encountered by Sinai *et al.* [25] and Shah and Sinai [22, 23] in specifying the dilution conditions, by allowing the flows to reverse during the solution process.

Quality Parameter Function

According to the definition of dependent quality parameters, each dependent water quality parameter has a function which defines its relationship with primary parameters. An example is SAR, which depends on the concentrations of Ca, Na and Mg. These functions are incorporated as constraints in the following manner:

$$C^d_{jjm} = \xi_{jm}(C_{jj1}, C_{jj2}, \ldots, C_{jjn}) \quad \forall j \in N_2 \text{ and } \forall m \in M_2 \qquad (14)$$

where

M_2 – dependent parameter group.
$\xi_{jm}(.)$ – the relation function between dependent parameter m at node j and the primary parameter at node j.

Pipe Discharge Limits

As indicated earlier, this problem considers a wide feasibility domain from the hydraulic point of view. However, in order to prevent infeasibilities and unreasonable hydraulic conditions, limits are

imposed on the flow in each pipe through:

$$\mathbf{q}'_a \leq \mathbf{q}_a \leq \mathbf{q}''_a \tag{15}$$

where $\mathbf{q}''_a$ and $\mathbf{q}'_a$ are upper and lower discharge limits, respectively. If the flow direction in pipe i is restricted then $(q'_a)_i = 0$, otherwise $(q'_a)_i = -(q''_a)_i$. Equation (15) can be translated using Eq. (1) into constraints on $\mathbf{q}$:

$$\mathbf{q}'_a - \mathbf{q}^0_a \leq L^T\mathbf{q} \leq \mathbf{q}''_a - \mathbf{q}^0_a \tag{16}$$

The velocity in each pipe may also be limited. This limitation has to be expressed as a limit on the discharge, since the diameters of the pipes are given.

Supply Discharge Limits

The discharge supplied from each source may be restricted by an upper limit q''_s and an inability to reverse the flow, *i.e.*,

$$\mathbf{0} \leq \mathbf{q}_s \leq \mathbf{q}''_s \tag{17}$$

Using Eq. (3). Equation (17) translates into constraints on $\mathbf{q}$:

$$-\hat{A}\mathbf{q}^0_a \leq \hat{A}L^T\mathbf{q} \leq \mathbf{q}''_s - \hat{A}\mathbf{q}^0_a \tag{18}$$

Quality Limits

These constraints are introduced for consumers who require that quality be supplied within specified limits, and for whom no cost or benefit function for quality is specified. With respect to the primary parameters, the constraints are:

$$C'_{jjm} \leq C_{jjm} \leq C''_{jjm} \quad \forall j \in N_2 \text{ and } \forall m \in M_1 \tag{19}$$

where C''_{jjm} and C'_{jjm} are upper and lower limits on the quality parameter m at node j, respectively. Similarly for the dependent parameters:

$$C^d_{jjm'} \leq C^d_{jjm} \leq C^d_{jjm''} \quad \forall j \in N_2 \text{ and } \forall m \in M_2 \tag{20}$$

Treatment Limits

Treatment limits are required:

$$R_{ijm'} \leq R_{ijm} \leq R_{ijm''} \quad \forall (ij) \in E_2 \text{ and } \forall m \in M_1 \tag{21}$$

where $R_{ijm''}$ and $R_{ijm'}$ are upper and lower limits on the removal ratio with respect to primary water quality parameter m of treatment plant located between node i and j. Note that according to the definition of the removal ratio $R_{ijm''} \leq 1$.

Problem Properties

The objective function and mass conservation constraints are nonlinear. Avriel [1] (p. 95) has defined sufficient conditions for convexity of constrained optimization. One of these conditions requires equality constraints to be linear. Since the equality constraints in Eq. (12) are nonlinear, the formulation is neither convex nor concave.

A smooth model can be developed from this basic formulation if the dilution equations and the transportation cost are smoothed by the exponential procedure as described in the Appendix. The smoothing also allows the flows to reverse during the solution process, thus permitting the network to be undirected. The ability to handle undirected networks is a substantial expansion of the model capabilities, since until now models for multi-quality systems have only been able to address directed networks, in which the flow directions are selected in advance, and cannot be reversed by the solution algorithm.

Methods of nonlinear optimization are in general sensitive to scaling, which means that difficulties may arise when decision variables and/or their coefficients are on different scales. Transformation of variables has been used for overcoming these difficulties [8 (pp. 273–275)].

Optimization Strategy

The steps discussed in the previous section result in a general nonlinear optimization model, which can be solved directly by using one of the general existing nonlinear programming packages, such as

MINOS [14], SQP [7], or SLP [9]. However, for a network of practical size the optimization model becomes very large, particularly if there are several water quality parameters, in which case it would have hundreds or even thousands of decision variables and constraints, and the solution time would be impracticably large.

It is therefore necessary to exploit special properties of the problem to develop an optimization method which is efficient and practical. First, it should be noted that if the flows and removal ratios are fixed the remaining optimization problem, in which the decision variables are the water quality values throughout the network, called "the internal problem", is quite easy to solve. Now denote the optimization problem of finding the flow distribution and the removal ratios as "the external problem". Recall that the flow distribution in the entire network is defined by the cyclic discharges, **q**. The decision variables in the reduced problem are therefore **q** and **r**, and it is an optimization problem of much lower dimension than the full problem originally defined.

The decision variables can be divided into two groups. The first are the control variables **u**, which consist of the vectors **q** and **r**. The variables in the second group are the water quality values throughout the network. The variables in this second group are called the state variables (or resultant variables), and are denoted by **x**. Under this definition, the overall optimization problem has the following general form:

(Problem P_0)

$$\min f_0(\mathbf{x}, \mathbf{u}) \tag{22}$$

$$\text{subject to: } \mathbf{g}(\mathbf{x}, \mathbf{u}) = \mathbf{0} \tag{23a}$$

$$\mathbf{h}' \leq \mathbf{h}(\mathbf{u}) \leq \mathbf{h}'' \tag{23b}$$

$$\mathbf{x}' \leq \mathbf{x} \leq \mathbf{x}'' \tag{23c}$$

where

$f_0(\mathbf{x}, \mathbf{u})$ – objective function given by Eq. (11).
$\mathbf{g}(\mathbf{x}, \mathbf{u})$ – mass conservation equations for the primary water quality parameters, including the dilution conditions for the quality parameters at nodes given by Eqs. (12) and (13).

$\mathbf{h}(\mathbf{u})$ – functions of the cyclic flows and of the removal ratios, which are constrained between bounds $\mathbf{h}'$ and $\mathbf{h}''$. Equations (16) and (18) are related to the cyclic discharges ($\mathbf{q}$), and the functions (21) are related to the removal ratios ($\mathbf{r}$).

$\mathbf{x}'$, $\mathbf{x}''$ – lower and upper bounds, respectively, on water quality at some or all consumer nodes (constraints (19–20)).

Each of the constraints (23c) is expressed as a penalty term:

$$P(x_i) = z_i \exp\{\varpi(z_i)\} \tag{24}$$

where $\varpi(z_i)$ is the normalized function of Eq. (8) with respect to z_i, where z_i is defined by:

$$z_i = (x_i'' - x_i)(x_i - x_i') \tag{25}$$

Denote the penalty cost by $\phi_L(\mathbf{x})$ where:

$$\phi_L(\mathbf{x}) = \Sigma_i P(x_i) = \Sigma_i z_i \exp\{\varpi(z_i)\} \tag{26}$$

Problem P_0 can be transformed into an equivalent problem, by introducing the constraints on the water quality values $\mathbf{x}$ into the objective function as a penalty term:

(Problem P_1)

$$\min f(\mathbf{x}, \mathbf{u}) = f_0(\mathbf{x}, \mathbf{u}) + \phi_L(\mathbf{x}) \tag{27}$$

s.t.

$$\mathbf{g}(\mathbf{x}, \mathbf{u}) = \mathbf{0} \tag{28a}$$

$$\mathbf{h}' \leq \mathbf{h}(\mathbf{u}) \leq \mathbf{h}'' \tag{28b}$$

Problem P_1 can be further transformed into:

(Problem P_2)

$$\min \Psi(\mathbf{u}) = f_0[\mathbf{x}(\mathbf{u}), \mathbf{u}] + \phi_L[\mathbf{x}(\mathbf{u})] \tag{29}$$

$$\text{subject to: } \mathbf{h}' \leq \mathbf{h}(\mathbf{u}) \leq \mathbf{h}'' \tag{30}$$

$\Psi(\mathbf{u})$ is a function of $\mathbf{u}$ and of $\mathbf{x}$, where $\mathbf{x}$ is obtained by solving the equations $\mathbf{g}(\mathbf{x}, \mathbf{u}) = \mathbf{0}$, when $\mathbf{u}$ is given. The gradient of $\Psi(\mathbf{u})$ with

respect to the control variables $\mathbf{u}$, $\nabla_u \Psi$, is:

$$\nabla_u \Psi = \nabla_u f + [\nabla_u \mathbf{g}]^T \beta \tag{31}$$

where $[\nabla_u \mathbf{g}]$ is the Jacobian of Eq. (23a) with respect to $\mathbf{u}$, and the vector β is computed from:

$$[\nabla_x \mathbf{g}]^T \beta = -\nabla_x f \tag{32}$$

In this problem the constraints $\mathbf{h}(\mathbf{u})$ are linear. Consequently, Problem P_2 has *linear constraints* and a nonlinear objective function. The complexity of Problem P_2 is considerably lower than that of the original problem, and therefore is more attractive to solve.

Principles of the Solution Method

The solution of Problem P_2 is based on the projected gradient method. The main steps of the solution are:

1. Computation of $\Psi(\mathbf{u})$.
2. Computation of $\nabla_u \Psi$, and the projected gradient direction.
3. Computation of the projected gradient if, at the current $\mathbf{u}$, there are active constraints.
4. Computation of the modified direction.
5. Updating $\mathbf{u}$ if optimality conditions are not satisfied.

Computation of $\Psi(u)$

For a given $\mathbf{u} = (\mathbf{q}, \mathbf{r})$ the flows in all network arcs are known, and the costs of supply, treatment and transportation can be computed from Eqs. (5), (6) and (9), respectively. The cost of the yield losses ϕ_y and the penalty cost ϕ_L depend on the water quality values which are found by solving the mass conservation equations $\mathbf{g}(\mathbf{x}, \mathbf{u}) = \mathbf{0}$. When $\mathbf{q}$ and $\mathbf{r}$ are given, these equations are linear. Furthermore, these equations can be decomposed into a single set of equations for each water quality parameter. In other words, for each water quality parameter, there is a separate linear system of equations, all with the same matrix, and different right hand vectors. As a result, when $\mathbf{q}$ and $\mathbf{r}$

are given, the equation system $\mathbf{g}(\mathbf{x}, \mathbf{u}) = \mathbf{0}$ has the following form:

$$E\mathbf{c}^m = \mathbf{b}^m \tag{33}$$

where

$\mathbf{c}^m$ – the values of the water quality parameter m at nodes.
E – quality discharge matrix whose components are computed by:

$$\begin{aligned} E_{ij} &= d_{ij}Q_{ij} && \text{if } d_{ij}Q_{ij} \geq 0 \text{ and } i \neq j \\ &= -[\Sigma_k d_{ik}Q_{ik} + d_i] && \text{if } d_{ij}Q_{ij} < 0 \end{aligned} \tag{34}$$

$\mathbf{b}^m$ is a vector of inputs from the sources of primary parameter m. The components of $\mathbf{b}^m$ are computed by:

$$(\mathbf{b}^m)_j = \sum_{s \in N_1} Q_{sj}C_{ssm} \tag{35}$$

where

C_{ssm} – concentration of quality parameter m at source s.
Q_{sj} – flow from source s to node j.

Since each system of the equations has the same matrix, solution by LU decomposition is desirable. That is, the matrix E is first decomposed into E_U (upper triangular matrix) and E_L (lower triangular matrix) such that:

$$E = E_L E_U \tag{36}$$

and the values of the primary water quality parameter m is obtained by solving

$$E_L\mathbf{w}^m = \mathbf{b}^m \tag{37}$$

for $\mathbf{w}^m$ and

$$E_U\mathbf{c}^m = \mathbf{w}^m \tag{38}$$

for $\mathbf{c}^m$. Recall that the matrices E_L and E_U are both triangular thus $\mathbf{w}^m$ and $\mathbf{c}^m$ can be obtained by forward and back substitution, respectively. The distribution of the dependent quality parameters is computed by Eq. (14). The yield loss cost ϕ_y, and the penalty cost ϕ_L are computed by Eqs. (10) and (26), respectively.

Computation of $\nabla_u \Psi$

The gradient $\nabla_u \Psi$ of the objective function in Problem P_2, depends on $\nabla_u f$ and $\nabla_x f$. $\nabla_x f$ is derived from the gradient of the yield loss cost and from the penalty cost. The gradient $\nabla_x^m \phi_y$ of ϕ_y with respect to primary quality parameter m, is:

$$\nabla_x^m \phi_y = F_y^m + \sum_{j=1}^{n_4} F_D^j F_c^m \tag{39}$$

where

F_y – Jacobian of the relative yield function with respect to the values of the primary water quality parameters at the consumer nodes. Cell im of F_y contains the derivative of the relative yield function at node i with respect to primary parameters m, *i.e.*,

$$(F_y)_{im} = -b_0^i y_0^i \frac{d\mathbf{y}^i}{dc_{im}} \tag{40}$$

It should be noted that F_y^m is the column of the matrix F_y related to primary parameter m. The matrix F_D is related to the dependent quality parameters, and is defined in a similar fashion to the matrix F_y, namely:

$$(F_D)_{im} = -b_0^i y_0^i \frac{d\mathbf{y}^i}{dc_{im}^d} \tag{41}$$

F_c – the Jacobian matrix of the dependent parameters with respect to the primary parameters. The F_c matrix consists of n_3 submatrices. Submatrix i is defined with respect to primary parameter m whose cell ij is:

$$(F_c^m)_{ij} = \frac{d\xi_{ij}}{dc_j^m} \tag{42}$$

The gradient of the penalty cost, ϕ_L, with respect to primary quality parameter m is:

$$\nabla_x^m \phi_L = F_z^m + \sum_{j=1}^{n_4} F_L^j F_c^m \tag{43}$$

where

F_z – the Jacobian of the penalty function ϕ_L with respect to the distribution of primary water quality parameters. Cell ij contains the derivative of ϕ_L with respect to primary water quality parameter m:

$$(F_z)_{im} = \frac{d\phi_L(x_i)}{dc_{im}} = -\exp\{\varpi(z_i)\}\left[1 - \frac{k_p z_i \varepsilon}{z_i^2 + \varepsilon}\right]\left[\left(c''_{im} - c_{im}\right) + \left(c'_{im} - c_{im}\right)\right] \quad (44)$$

The matrix F_L is related to the dependent parameters and is defined in a similar fashion to the matrix F_z:

$$(F_L)_{ij} = \frac{d\phi_L(x_i)}{dc_{ij}^d} = -\exp\{\varpi(z_i)\}\left[1 - \frac{k_p z_i \varepsilon}{z_i^2 + \varepsilon}\right]\left[\left(c_{ij}^{d''} - c_{ij}^d\right) + \left(c_{ij}^{d'} - c_{ij}^d\right)\right] \quad (45)$$

The variables x appear in the objective function f only in the yield loss cost and in the penalty cost. Thus, the gradient of f with respect to the distribution of primary quality parameter m is the summation of Eqs. (39) and (43):

$$\nabla_x^m f = \nabla_x^m \phi_y + \nabla_x^m \phi_L = F_y^m + F_z^m + \sum_{j=1}^{n_4} \left(F_D^j + F_L^j\right) F_c^m \quad (46)$$

Computation of β

The vector β is computed by solving Eq. (32). The matrix $[\nabla_x \mathbf{g}]$ is block diagonal, where the sub-matrix m, $[\nabla_x^m \mathbf{g}]$, is related to primary parameter m. Furthermore, the sub-matrix is the quality input discharge matrix, E, and therefore the vector β can be computed separately:

$$E^T \beta^m = -\nabla_x^m f \quad \forall\, m \in M_1 \quad (47)$$

where β^m is sub-vector of β related to primary quality parameter m. Since E has been decomposed into E_U and E_L, the vector β can be

computed simply by solving:

$$E_U^T \mathbf{w}^m = -\nabla_x^m f \tag{48}$$

for $\mathbf{w}^m$ and then

$$E_L^T \beta^m = \mathbf{w}^m \tag{49}$$

for β^m, by backward and forward substitution, respectively.

Computation of $\nabla_u f$

The gradient of f with respect to $\mathbf{u}$ consists of two sub-vectors: $\nabla_q f$, which relates to the cyclic discharges, and $\nabla_r f$ which relates to the removal ratio in the treatment plants.

$\nabla_q f$ is derived from the gradients of the supply cost (ϕ_s), transportation cost(ϕ_p) and treatment cost(ϕ_t). Using the chain rule for the derivative of ϕ_s with respect to $\mathbf{q}$ yields:

$$\nabla_q \phi_s = tL\hat{A}^T \left[F_s \hat{A}\left(\mathbf{q}_a^0 + L^T \mathbf{q}\right) + \mathbf{w}_s\right] \tag{50}$$

where F_s is the Jacobian of the cost of water at sources, $\mathbf{w}_s(\mathbf{q}_s)$, with respect to the source flows $\mathbf{q}_s$. The matrix F_s is square and diagonal, where element *ii* is:

$$(F_s)_{ii} = d\mathbf{w}_s^i / d\mathbf{q}_s^i \tag{51}$$

note that $F_s = 0$ if $\mathbf{w}_s$ has constant values, and the first term in the square bracket of Eq. (50) is zero. Similarly,

$$\nabla_q \phi_p = tL[F_p \mathbf{q}_a + \mathbf{w}_p] \tag{52}$$

where F_p is the Jacobian of the transportation costs in pipes, $\mathbf{w}_p(\mathbf{q}_a)$, with respect to the pipe flows $\mathbf{q}_a$. The matrix is square and diagonal, where element *ii* is:

$$(F_p)_{ii} = d\mathbf{w}_p^i / d\mathbf{q}_a^i \tag{53}$$

Note that $F_p = 0$ if $\mathbf{w}_p$ has constant values, and the first term in the square brackets of Eq. (52) is zero. Similarly,

$$\nabla_q \phi_t = tLB_t^T \mathbf{w}_t \tag{54}$$

$\nabla_q f$ is thus:

$$\begin{aligned}\nabla_q f &= \nabla_q \phi_s + \nabla_q \phi_t + \nabla_q \phi_p \\ &= tL\hat{A}^T \left[F_s \hat{A}\left(\mathbf{q}_a^0 + L^T\mathbf{q}\right) + \mathbf{w}_s\right] + tL\left[F_p \mathbf{q}_a + \mathbf{w}_p\right] + tLB_t^T \mathbf{w}_t \end{aligned} \quad (55)$$

The gradient $\nabla_r f$ depends on the treatment costs. Using the chain rule for the derivative of ϕ_t with respect to $\mathbf{r}$ yields:

$$\nabla_r \phi_t = tF_r B_t \left[\mathbf{q}_a^0 + L^T\mathbf{q}\right] \quad (56)$$

where F_r is the Jacobian of the treatment costs, $w_t(\mathbf{r})$, with respect to the removal ratios, $\mathbf{r}$. The matrix is diagonal, where element ii is:

$$(F_r)_{ii} = d\mathbf{w}_t^i / d\mathbf{r}^i \quad (57)$$

Since the gradient $\nabla_r f$ depends only on the treatment cost:

$$\nabla_r f = \nabla_r \phi_t = tF_r B_t \left[\mathbf{q}_a^0 + L^T\mathbf{q}\right] \quad (58)$$

The expressions for $\nabla_q f$ and $\nabla_r f$ include many matrix multiplications. However, since most of them are diagonal they are simple.

Computation of the Projected Gradient

Assume that, at the current, $\mathbf{u}$, there are a_1 active constraints related to the cyclic discharges, and e active constraints related to the removal ratios. Denote by A_a the coefficient matrix of the active set related to $\mathbf{q}$, and by J_e the coefficient matrix of the active constraints related to $\mathbf{r}$.

The projected gradient, s_u, is derived [18]:

$$\mathbf{s}_u = -\left[\nabla_u \Psi + N_a^T \lambda\right] \quad (59)$$

where N_a is the coefficient matrix of the active constraints, and the multiplier vector λ is obtained by solving:

$$N_a^T N_a \lambda = -N_a^T \nabla_u \Psi \quad (60)$$

In our problem N_a has the form:

$$\left[\begin{array}{cc} A_a & 0 \\ \hline 0 & J_e \end{array}\right] \quad (61)$$

and $\nabla_u \Psi = [\nabla_q \Psi; \nabla_r \Psi]$, thus the system described by Eq. (60) is decomposable into the following two sub-systems:

$$A_a A_a^T \lambda_1 = -A_a \nabla_q \Psi \tag{62}$$

$$J_e J_e^T \lambda_2 = -J_e \nabla_r \Psi \tag{63}$$

where λ_1 and λ_2 are sub-vectors of λ. λ_1 is related to the cyclic discharge active constraints and λ_2 to the removal ratio active constraints. Substituting the solution of Eqs. (62) and (63) into (59) and arranging yields the projected gradient with respect to cyclic discharges, $\mathbf{s}_q$:

$$\mathbf{s}_q = -[I - (A_a A_a^T)^{-1} A_a] \nabla_q \Psi \tag{64}$$

and the projected gradient with respect to the removal ratios, $\mathbf{s}_r$:

$$\mathbf{s}_r = -[I - (J_e J_e^T)^{-1} J_e] \nabla_r \Psi \tag{65}$$

Since the constraints on the removal ratios are simple bounds:

$$J_e J_e^T = I \tag{66}$$

substituting into Eq. (65) yields:

$$\mathbf{s}_r = -(I - J_e^T J_e) \nabla_r \Psi \tag{67}$$

The relations described in Eqs. (63) and (67) imply the following:

(a) The computations of $\mathbf{s}_q$ and of $\mathbf{s}_r$ are independent.

(b) $J_e^T J_e$ is a diagonal matrix of 1 or 0. Element i is 1 if r_i is at one of its bounds (r_i' or r_i'') and is included in the active set. It is zero either when r_i is between its bounds or r_i is equal to one of its bounds but it has been omitted from the active set. Therefore Eq. (67) can be reduced to:

$$\begin{aligned} \mathbf{s}_r^i &= 0 \qquad \text{if } i \in J_r \\ \mathbf{s}_r^i &= -\nabla_r \Psi \quad \text{if } i \notin J_r \end{aligned} \tag{68}$$

where J_r is the active set with respect to $\mathbf{r}$.

(c) Equations (63) and (66) imply that $\lambda_2 = -\nabla_r \Psi$.

Now return to Eq. (64), which may be solved in a number of ways. The basic method uses Eq. (64) where the multiplier of $\nabla_q \Psi$ is the projection matrix, which projects the gradient $\nabla_q \Psi$ on to the manifold of the active constraints. The computation of the projection matrix requires considerable computation effort, since it has to be done every time the contents of the active set are changed. However, since the change in the active set always involves either adding or omitting only one constraint, it is preferable to update the matrix instead of recomputing. Avriel [1] (pp. 427–428) describes a method for updating the matrix $(A_a A_a^T)^{-1}$ in such cases. Jacoby *et al.* [11] (p. 217) state that numerical difficulties may arise in this updating process when the matrix is ill-conditioned. Jacoby *et al.* [11] claim that the method of Bartles *et al.* (cited in [11]) which uses the QR decomposition of Householder and then updates the matrices Q and R, is stable numerically.

These methods focus on computation of the projection matrix. However, Eq. (64) can be derived from the solution of Eq. (62), using the LU-decomposition method. First the matrix $(A_a A_a^T)$ is decomposed into A_L (lower triangular) and A_U (upper triangular) such that:

$$A_L A_U = A_a A_a^T \tag{69}$$

λ_1 is then obtained by the following steps.

Compute $\mathbf{w}$ from:

$$A_L \mathbf{w} = -A_a \nabla_q \Psi \tag{70}$$

then compute λ_1 from:

$$A_U \lambda_1 = \mathbf{w} \tag{71}$$

by backward and forward substitution, respectively. Substituting λ_1 into Eq. (59) with respect to $\mathbf{q}$ yields $\mathbf{s}_q$.

As long as the active set does not change, the decomposition matrices remain constant, and are computed from Eqs. (70) and (71). When a constraint is added to the active set, A_L and A_U are updated as follows. The matrix $(A_{a+1} A_{a+1}^T)$ remains symmetric and is given by:

$$(A_{a+1} A_{a+1}^T) = \left[\begin{array}{cc} A_a A_a^T & \mathbf{a}_5 \\ \mathbf{a}_5^T & \alpha_0 \end{array}\right] \tag{72}$$

where $\mathbf{a}_5$ is

$$\mathbf{a}_5 = A_a \mathbf{a}_4 \tag{73}$$

$\mathbf{a}_4$ is a vector whose elements are the coefficients of the active constraint being added. α_0 is a scalar obtained from:

$$\alpha_0 = \mathbf{a}_4^T \mathbf{a}_4 \tag{74}$$

The new decomposition matrices $\tilde{A}_L$ are also triangular, of the form:

$$\tilde{A}_L = \left[\begin{array}{cc} A_L & 0 \\ \hline \mathbf{a}_L^T & \alpha_L \end{array}\right] \tag{74a}$$

$$\tilde{A}_U = \left[\begin{array}{cc} A_U & \mathbf{a}_U \\ \hline 0 & \alpha_U \end{array}\right] \tag{74b}$$

where $\mathbf{a}_U$, $\mathbf{a}_L$, α_U and α_L are obtained from:

$$A_L \mathbf{a}_U = \mathbf{a}_5 \tag{75}$$

$$A_U \mathbf{a}_L = \mathbf{a}_5 \tag{76}$$

$$\alpha_L = \mathbf{a}_L^T \mathbf{a}_U - \alpha_0 \tag{77}$$

$\mathbf{a}_U$ and $\mathbf{a}_L$ are obtained by forward and backward substitutions, respectively.

The decomposition is performed only when the active set is changed, which is only when the current $\|\mathbf{s}_q\|$ equals zero, and then by updating A_L and A_U directly. This approach reduces the computational burden substantially.

Computation of the Modified Projected Gradient

Recall that the removal ratios at the treatment plants are in the range [0, 1], whereas the cyclic discharge can be of the order of tens, hundreds and even thousands. Furthermore, the effect of a unit change in a removal ratio is much greater than the effect of a unit change in the cyclic discharge. As a result, there is a scaling problem between **r**

and **q**. Methods for nonlinear optimization are in general sensitive to scaling, and especially the projected gradient which is an extension of steepest decent. Transformation of the variables is the method suggested by Gill *et al.* [8] (pp. 273–275) to overcome these difficulties. In the problem described in this paper, transformation of the variables leads to defining r in percent (%) when the circular discharge is in the order of hundreds, or in parts per thousand (‰) when the circular discharge is in the order of thousands. However attempts to apply this approach to our problem were not successful, and the computational difficulties remained.

An alternative method which overcomes the scaling problem is described in Algorithm TF below. This uses the fact that, for a separable quadratic problem, the optimal solution can be reached in one iteration, independent of the initial point and the order of the scaling. As seen above, $\mathbf{s}_q$ and $\mathbf{s}_r$ are orthogonal. The problem is therefore separable with respect to **q** and **r** and the modified projected gradient direction is derived as follows:

Algorithm TF (Two Phases)

Step a Assume an initial search direction for **q**, $\mathbf{d}'_q = \mathbf{s}_q$, and for **r**, $\mathbf{d}'_r = \mathbf{s}_r$.

Step b Compute α''_q, the maximum step along $\mathbf{d}'_q$ and α''_r, the maximum step along $\mathbf{d}'_r$, such that $(\mathbf{q} + \alpha''_q \mathbf{d}'_q)$ and $(\mathbf{r} + \alpha''_r \mathbf{d}'_r)$ meet a constraint which is not included in the active set.

Step c Compute α^*_q, the optimal step length along $\mathbf{d}'_q$:

$$\Psi(\mathbf{q} + \alpha^*_q \mathbf{d}'_q, \mathbf{r}) = \min\{\Psi(\mathbf{q} + \alpha_q \mathbf{d}'_q, \mathbf{r}) \mid 0 \leq \alpha_q \leq \alpha''_q\}$$

Step d Compute, using a method to be discussed below, α^*_r, the optimal step length along $\mathbf{d}'_r$:

$$\Psi(\mathbf{q}, \mathbf{r} + \alpha^*_r \mathbf{d}'_r) = \min\{\Psi(\mathbf{q}, \mathbf{r} + \alpha_r \mathbf{d}'_r) \mid 0 \leq \alpha_r \leq \alpha''_r\}$$

It is important to note that one dimensional search along **q** and **r** separately remains on the manifold of the active set.

Step e Compute the norm of the updated direction, **s**:

$$\|\mathbf{s}\| = \left[\alpha^*_q (\mathbf{d}'_q)^T \mathbf{d}'_q + \alpha^*_r (\mathbf{d}'_r)^T \mathbf{d}'_r\right]^{1/2}$$

Step f Compute $\mathbf{d}_q$, the normalized modified projected gradient direction related to $\mathbf{q}$:

$$\mathbf{s}_q := \alpha_q^* \mathbf{d}_q' / \|\mathbf{s}\|$$

Step g Compute $\mathbf{d}_r$, the normalized modified projected gradient direction related to $\mathbf{r}$:

$$\mathbf{s}_r := \alpha_r^* \mathbf{d}_r' / \|\mathbf{s}\|$$

(Note that $\mathbf{d}_r = \mathbf{d}_r'$ if $\mathbf{s}_q = \mathbf{0}$ and $\mathbf{d}_q = \mathbf{d}_q'$ if $\mathbf{s}_r = 0$)

It should be recognized that the optimal step size could be determined by one of the exact methods for one dimensional search, such as the Powell or Davidson methods in Ref. [1] (pp. 221–240). However, the computation of Ψ and $\nabla\Psi$ can be expensive and therefore a nonexact search method is preferable. As a result, the efficiency of the scaling method is probably reduced, since its efficiency is actually based upon an exact one dimensional search. The efficiency reduction resulting from the nonexact one dimensional search was examined by Cohen [4] and Cohen *et al.* [5] in a wide range of examples, and it was found that the reduction is negligible.

Termination Criteria

When the relative change of the objective function at two successive points is less than an arbitrary small parameter ε_c and/or the relative change in the decision variables at two successive iterations is less than an arbitrary small parameter ε_v, then the Kuhn-Tucker optimality condition is satisfied if the multipliers with respect to the active constraints at their upper bounds are nonnegative, and nonpositive for the active constraints at their lower bounds. Otherwise, the active constraint having the multiplier with maximal absolute value is dropped from the set, and the solution process continues with respect to the updated active set.

Algorithm Q-C

The entire set of steps detailed above is summarized as follows:

Initialize Assume initial value $\mathbf{u}^0 := \{\mathbf{q}^0, \mathbf{r}^0\}$. Initialize the iteration counter $k = 0$.

Step 1 Compute the distribution of the primary quality parameters by solving

$$E\,\mathbf{c}^m = \mathbf{b}^m \quad m = 1, 2, \ldots, M$$

Step 2 Compute the distribution of the dependent quality parameter by using the relation functions:

$$\mathbf{c}^d = \xi(\mathbf{c}^1, \mathbf{c}^2, \ldots, \mathbf{c}^n)$$

Step 3 Compute the value of the objective function at the current $\mathbf{u}^k$, $\Psi(\mathbf{u}^k)$.

Step 4 Compute $\nabla_x f$ from Eq. (46).

Step 5 Compute β^m by solving:

$$E^T\beta^m = -\nabla_x m_f \quad m = 1, 2, \ldots, M$$

Step 6 Compute $\nabla_q f$ and $\nabla_r f$ from Eqs. (55) and (58), respectively.

Step 7 Compute $\nabla_q \Psi$ and $\nabla_r \Psi$ from:

$$\nabla_q \Psi := \nabla_q f + [\nabla_q \mathbf{g}]^T \beta$$
$$\nabla_r \Psi := \nabla_q f + [\nabla_r \mathbf{g}]^T \beta$$

Step 8 Compute λ_1 by solving:

$$A_L A_U \lambda_1 = -A_a \nabla_q \Psi$$

Step 9 Compute λ_2 from:

$$\lambda_2 = -\nabla_r \Psi$$

Step 10 Compute the projected gradient with respect to $\mathbf{q}$ from:

$$\mathbf{s}_q = -\left[\nabla_q \Psi + A_a^T \lambda_1\right]$$

and with respect to $\mathbf{r}$ from

$$\mathbf{s}_r^j = 0 \qquad \text{if } j \in J_r$$
$$\mathbf{s}_r^j = -\nabla_r \Psi \quad \text{if } j \notin J_r$$

Step 11 Compute the modified projected gradient as described in steps *a* to *g* of Algorithm TF.

Step 12 Compute the optimal step length along the modified projected gradient, α^*.

Step 13 Check the optimality conditions. If they are satisfied, the current $\mathbf{u}^k$ is the optimal solution, otherwise, update $\mathbf{q}$ and $\mathbf{r}$ from: $\mathbf{q}^{k+1} := \mathbf{q}^k + \alpha^* \mathbf{d}_q$, $\mathbf{r}^{k+1} := \mathbf{r}^k + \alpha^* \mathbf{d}_r$, update the iteration counter: $k := k + 1$, and return to Step 2.

EXAMPLE

Use of the method described in the previous section is demonstrated by application to the example network shown in Figure 1. These data are taken from a water supply system in the Arava Valley in Southern Israel. The system is located in a region which lies 200–250 m below sea level. It is fed from two constant head reservoirs at nodes 8 and 9, and delivers to consumers at nodes 4, 5, 6 and 7. It consists of 9 pipes and 9 nodes. The system is operated 2000 hours per year and the cost

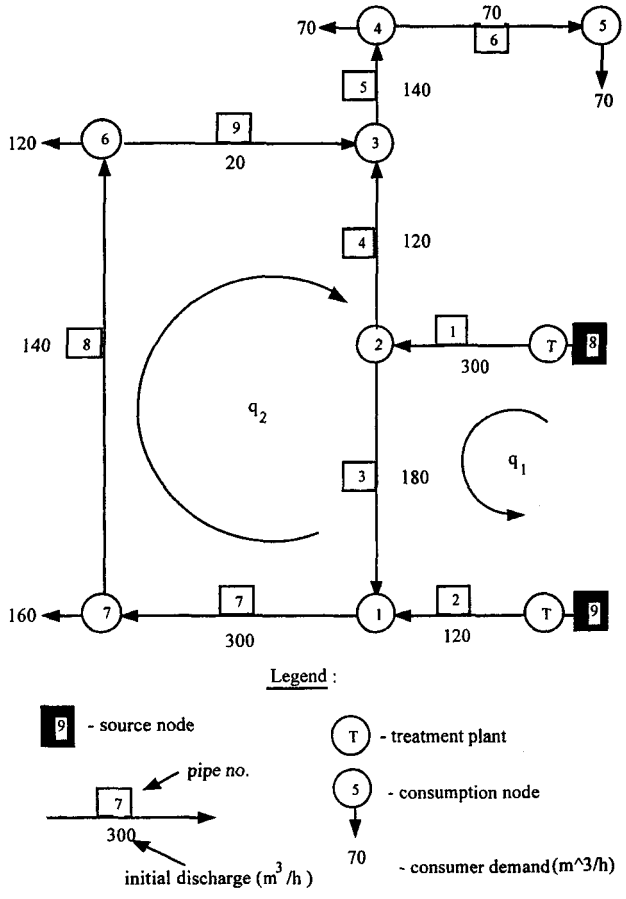

FIGURE 1 Schematic description of the network.

per unit energy is 0.22 NIS/kWh (1$ = ~3.6 NIS (NIS = New Israeli Shekel)).

The water quality parameters of importance to this system are salinity, magnesium and sulphur. The relevant water quality data for the sources are given in Table I.

At the consumption nodes 4, 5 and 6 a quadratic yield function of the form $y = a_0 + a_1 c + a_2 c^2$ is defined to model the impact of salinity on yield, where y is the relative yield, c is the salinity in mgcl/l, and a_0, a_1 and a_2 are constants given in Table II. Upper limits are defined for the other parameters. At node 7 all the quality parameters are limited by the upper limits given in Table II. $b_0 * y_0$ is defined as the entire income at the node when there is no yield loss due to water quality.

Treatment plants for salinity and magnesium are located on pipe 2, and a treatment plant for sulphur is located on pipe 1. The specific treatment costs with respect to reducing salinity are

$$w_t = 2.151 * 10^{-4} r^2 \quad r \leq 0.75$$

and with respect to magnesium and sulphur is:

$$w_t = 1.32 * 10^{-4} r^2 \quad r \leq 0.75$$

TABLE I Data for sources

Node –	*Specific cost* NIS/m^3	*Elevation* m	*Maximum discharge* m^3/h	*Water quality*		
				Salinity $mgcl/l$	*Magnesium* mg/l	*Sulphur* mg/l
8	0.638	2.5	325	450	140	500
9	0.256	0	700	860	250	300

TABLE II Data for consumption nodes with respect to quality

Node	$b_0 * y_0$ $NIS * 10^8$	*Coefficients of the yield function*			*Upper limits for water quality*		
		a_0	$a_1 * 10^5$	$a_2 * 10^8$	*Salinity* $mgcl/l$	*Magnesium* mg/l	*Sulphur* mg/l
4	0.700	1	1.250	−2.707	–	250	500
5	0.448	1	−3.06	−3.890	–	200	500
6	1.200	1	1.250	−2.707	–	200	450
7	–	–	–	–	600	170	450

where w_t is the specific cost in NIS/m^3 and r is the removal ratio in %. All the removal ratios are limited to 75%. Recall that the transportation cost in each pipe is related to the energy losses. Thus, w_p^i, the transportation specific cost function of pipe i, is:

$$w_p^i = \mu_i (q_a^i)^{1.852}$$

where w_p^i is in (NIS $*$ h/m^3), q_a^i (in m^3/h) is defined from Eq. (7), and μ_i is computed from:

$$\mu_i = 2.726 * 10^{-3} k_e \, \mathrm{Chw}_i^{-1.852} (d_a^i)^{-4.87} l_a^i$$

where k_e is the cost per unit energy (NIS/kWh), Chw_i is the Hazen Williams coefficient for pipe i, d_a^i is the diameter (mm) and l_a^i is the length (m), respectively for pipe i.

The relevant pipe data for the system are given in Table III.

All pipes have Chw = 120. The network consists of 2 loops: one closed loop of pipes 3, 7, 8, 9 and 4 and one pseudo-loop between the nodes 8 and 9 which includes pipes 1, 2 and 3. The initial flows, the positive directions of the pipe flows and of the circular flows are shown in Figure 1.

The optimal solution is $f^* = 4162303.2$ NIS, and the optimal circular flows are $q_1^* = 25$, $q_2^* = 40.33\,\mathrm{m}^3/\mathrm{h}$ (flows relative to those in Fig. 1). The optimal removal ratios of salinity and magnesium in the treatment plants placed on pipe 2 are zero and 11%, respectively. The optimal removal ratio of sulphur in the treatment plant placed on pipe 1 is zero. The optimal distributions of flows and quality parameters are given in Figure 2.

This solution was obtained after 10 iterations in 1.49 sec on an IBM-3081 computer. The values of the objective function during the solution process are shown in Figure 3.

TABLE III Pipe data for the example problem

Pipe	1	2	3	4	5	6	7	8	9
Length (m)	400	1300	3700	1000	4300	2600	800	5000	3500
Diameter (mm)	250	250	300	250	300	250	250	250	250
Initial flow (m^3/h)	300	120	180	120	140	70	300	140	20
μ_i ($*10^{-4}$)	0.22	0.71	0.83	0.54	0.96	1.41	0.43	2.71	1.90
Maximum flow (m^3/h)	530	530	763	530	763	530	530	530	530

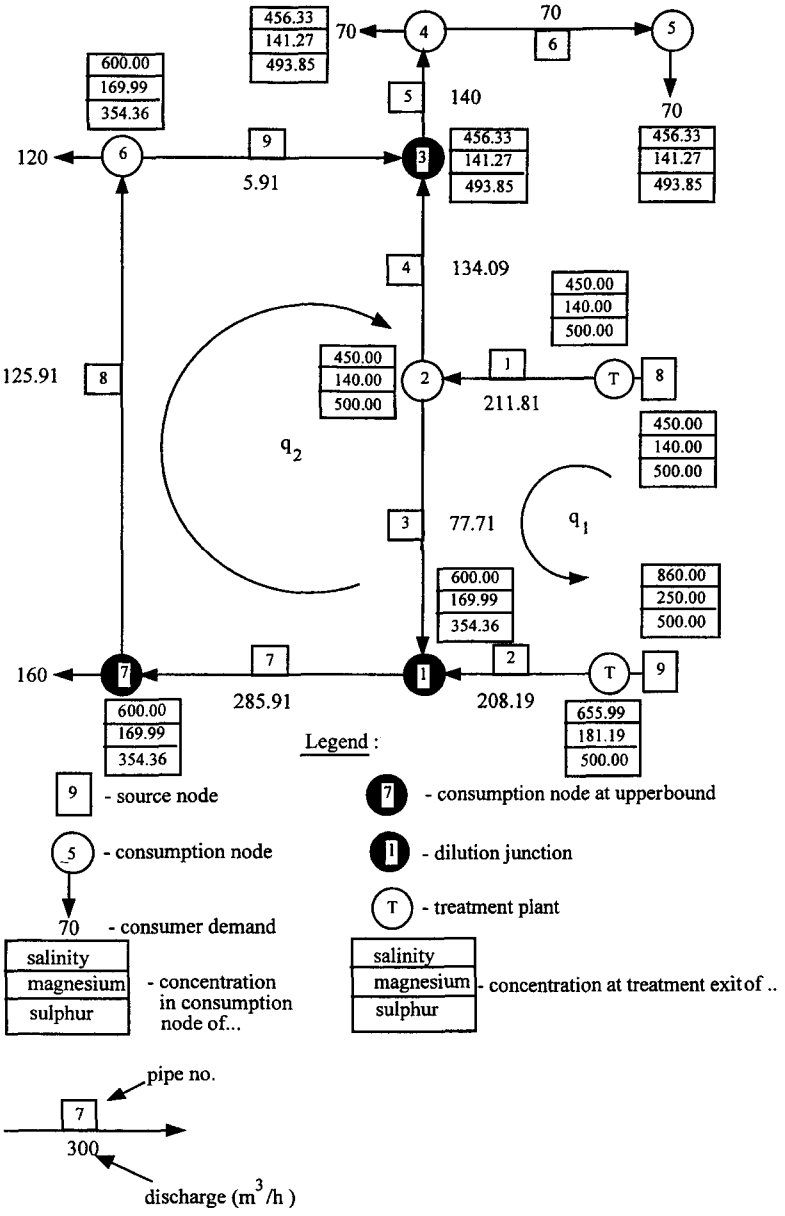

FIGURE 2 Optimal distribution of flows and quality parameters.

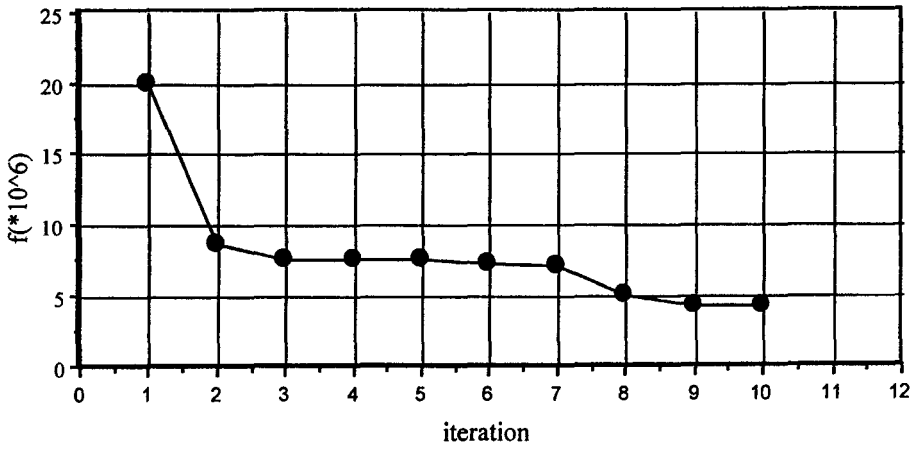

FIGURE 3 The values of the objective function during the solution process.

The value at zero iteration is omitted because it contains a large penalty value.

The utility of the method for a more realistically sized network was examined by application to the water distribution system of Central Arava Region, which supplies an area in the southern region of Israel. This system has 38 nodes, 39 pipes, 11 wells, 14 aggregated consumers and 7 treatment plants located at the sources, where the product water is pumped into the distribution system. Four nodes supply domestic consumers while the others supply agriculture. Water quality in the system is expressed in terms of 3 parameters: salinity, magnesium and sulphur, all of which are assumed to be conservative, *i.e.*, they do not decompose or interact, only dilute by flow and mixing. For the domestic consumers the quality parameters are restricted by upper limits, determined by water quality standards. At the agricultural nodes, net income and reduction yield with respect to salinity are defined. These functions reflect the sensitivity of crops. The other water quality parameters at these nodes are restricted by upper limits. The solution for this larger network was obtained after 42 iterations in 18.95 sec on an IBM-3081 computer.

SUMMARY

A new model for the optimal operation of a multi-quality water distribution network is proposed. The model determines optimal operating decisions for what is termed the Q-C (flow-quality) problem, for a single loading condition. Continuity of flows and solute transport are satisfied explicitly in the model, while the hydraulics of the system are addressed implicitly by transportation limits and costs.

The characteristics of the Q-C model are:

* The objective is minimization of total operating cost, which includes cost of water at the sources + treatment, cost of transportation, loss of income due to low water quality.
* The optimization problem is solved by decomposing the problem into inner–outer problems when the outer problem is solved by the projected gradient method combined with special consideration of scaling problems of the decision variables. The decomposition enables problems with many water quality parameters to be solved.

* The non-smooth functions are smoothed by an approach developed specifically for this application.
* The flow directions in the pipes do not have to be specified in advance, and are determined as part of the solution. This property is enabled by the smoothed functions.
* Transportation cost can be defined as nonlinear with flow. The capacities of the pipes in the system are introduced as limits to assist in defining the feasible region with respect to hydraulic conditions.

The *Q-C* model is applicable in its current form to systems where the hydraulics of the operation are not a significant determinant, and it can be assumed that the operation of the system is feasible within a wide range of hydraulic conditions. The model is, however, one of two components of a more complete full flow-quality-head (*Q-C-H*) model (which is the subject of a companion paper), in which the solute transport and the hydraulic constraints are combined, using the *Q-C* based approach of this paper and a *Q-H* model described in a second companion paper in this series.

References

[1] Avriel, M. (1976). *Nonlinear Programming: Analysis and Methods.* Prentice-Hall, Inc, N.J.
[2] Clark, R. M., Grayman, W. M., Goodrich, J. A., Deininger, R. A. and Skov, K. (1994). Measuring and modeling chlorine propagation in water distribution systems. *J. Water Resour. Plng. Mgmt., ASCE,* **120**(6), 871–887.
[3] Clark, R. M., Rossman, L. A. and Wymer, L. J. (1995). Modeling distribution systems water quality: Regulatory implications. *J. Water Resour. Plng. Mgmt., ASCE,* **121**(6), 423–428.
[4] Cohen, D. (1991). *Optimal operation of multi-quality networks. D.Sc. Thesis,* Faculty of Agricultural Engineering, Technion, Israel (In Hebrew).
[5] Cohen, D., Shamir, U. and Sinai, G. (1999). *Optimal operation of multi-quality water supply systems.* Report to Water Research Institute, Technion, Haifa, Israel.
[6] Feinerman, E. and Yaron, D. (1983). Economics of irrigation water mixing within a farm framework. *Water Resour. Res.*, **19**(2), 337–345.
[7] Fletcher, R. (1980). *Practical Methods of Optimization.* John Wiley and Sons, N.Y.
[8] Gill, P. E., Murray, W. and Wright, M. H. (1981). *Practical Optimization.* Academic Press, N.Y.
[9] Gomez, P. F., Lasdon, L. and Engquist, M. (1982). Nonlinear optimization by successive linear programming. *Management Science J.*, **28**(10), 1106–1120.
[10] Grayman, W. M., Clark, R. M. and Males, R. M. (1988). Modeling distribution system water quality-dynamic approach. *J. Water Resour. Plng. and Mgmt.*, **114**(3), 295–312.
[11] Jacoby, S. L. S., Kowalik, J. S. and Pizzo, J. T. (1972). *Iterative methods for nonlinear optimization problems.* Prentice-Hall Inc., N.J.

[12] Maas, E. V. and Hoffman, G. J. (1977). Crop salt tolerance–current assessment. *Journal of Irrigation and Drainage, ASCE*, **103**, 115–134.
[13] Males, R. M., Clark, R. M., Wherman, P. J. and Gates, W. E. (1985). Algorithm for mixing problems in the water system. *Jour. Hydraulic Engineering, ASCE*, **111**(2), 206–219.
[14] Murtagh, B. A. and Saunders, M. A. (1982). A projected Lagrangian algorithm and its implementation for sparse nonlinear constraints. *Mathematical Programming Study*, **16**, 84–117.
[15] Ostfeld, A. and Shamir, U. (1993). Modeling multi-quality networks. *Proc. AWWA Annual Conference*, San Antonio, Texas, June, pp. 151–160.
[16] Ostfeld, A. and Shamir, U. (1993). Optimal operation of multi-quality networks I: Steady state conditions. *J. Water Resour. Plng. Mgmt., ASCE*, **119**(6), 645–662.
[17] Ostfeld, A. and Shamir, U. (1993). Optimal operation of multi-quality networks II: Unsteady conditions. *J. Water Resour. Plng. Mgmt., ASCE*, **119**(6), 663–684.
[18] Rosen, J. B. (1960). The gradient projection method for nonlinear programming. *SIAM Journal*, **8**(1), 181–216.
[19] Rossman, L. A., Clark, R. M. and Grayman, W. M. (1994). Modeling chlorine residuals in drinking water distribution systems. *J. Envir. Eng., ASCE*, **120**(4), 803–820.
[20] Rossman, L. A. and Boulos, P. F. (1996). Numerical methods for modeling water quality in distribution systems: A comparison. *J. Water Resour. Plng. Mgmt., ASCE*, **122**(2), 137–146.
[21] Schwartz, J., Meidad, N. and Shamir, U. (1985). Water quality management in regional systems. *Proc. of Jerusalem Symp. on Scientific Basis for Water Resources Management*, IAHS Pub. 153, pp. 341–349.
[22] Shah, M. and Sinai, G. (1985). Salinity control in multi-quality irrigation networks–Kibbutz Hamadia feasibility study. *Agric. Water Mgmt.*, **10**, 235–252.
[23] Shah, M. and Sinai, G. (1988). A steady state model for dilution in water networks. *Journal of Hydraulic Eng., ASCE*, **114**(2), 192–206.
[24] Shamir, U. and Howard, C. D. D. (1991). Topics in modeling water quality in distribution systems. *Proceedings of the Conference on Water Quality Modeling in Distribution Systems, EPA and AWWA*, Cincinnati, Ohio, Grayman, W., Males, R. M. and Clark, R. (Eds.).
[25] Sinai, G., Koch, E. and Farbman, M. (1985). Dilution of brackish water in irrigation networks-an analytic approach. *Irr. Sci.*, **6**, 191–200.
[26] Sinai, G., Shina, G., Kitai, E. and Shah, M. (1987). Physical and computer models of multi-quality networks. *J. Water Resour. Plng. and Mgmt., ASCE*, **113**(6), 745–760.

APPENDIX SMOOTHING

Mathematical models of multi-quality networks generally contain discontinuous functions arising from dilution conditions which depend on flow direction, and from discrete pump operating functions. Such discontinuities can be introduced into the optimization model by use of integer variables. However, this process would result in non-linear integer models, which are notoriously difficult to solve. A smoothing technique, which makes it possible to formulate a non-linear model with continuous variables only is proposed here. The technique is

demonstrated for a discontinuous function of the form:

$$g(x) = \left\{ \begin{array}{ll} a & \text{if } x > 0 \\ b & \text{if } x < 0 \\ 0.5(a+b) & \text{if } x = 0 \end{array} \right\} \tag{I-1}$$

This form is typical of issues relating to the concentration of water quality parameters in a pipe. The value of the function depends on the direction of flow: it is equal to the value of the concentration at the upstream end when there is flow, and to the average of the two when there is no flow. The following smooth approximation of $g(x)$ is used:

$$f(x) = \frac{a\exp\{\varpi(x)\} + b\exp\{-\varpi(x)\}}{\exp\{\varpi(x)\} + \exp\{-\varpi(x)\}} \tag{I-2}$$

in which:

$$\varpi(x) = k_p \frac{x}{\sqrt{x^2 + \varepsilon}} \tag{I-3}$$

k_p is a "gain factor", and ε is an arbitrary small number, used to prevent division by zero.

When $x > 0$ the second terms in the numerator and dominator are negligible compared to the first terms, and then $f(x) = a$. When $x < 0$ the first terms are negligible compared to the second terms, and then $f(x) = b$. When $x = 0$, $\exp\{\varpi(x)\} = \exp\{-\varpi(x)\} = 1$, and $f(x) = (a+b)/2$.

Now consider how Eqs. (I-2) and (I-3) can be used to model dilution conditions. Consider the concentration in a pipe connecting nodes i and j, at which the concentrations of some constituent are c_i and c_j, respectively. The concentration in the pipe itself, c_{ij}, will be that of the upstream node. If the direction of flow is not known in advance, and the model is to have the ability to reverse the direction in the process of the solution, it is necessary to use an expression of the form (I-2) namely:

$$c_{ij} = \frac{c_i\exp\{\varpi(Q_{ij})\} + c_j\exp\{-\varpi(Q_{ij})\}}{\exp\{\varpi(Q_{ij})\} + \exp\{-\varpi(Q_{ij})\}} \tag{I-4}$$

in which Q_{ij} is the flow in the pipe, defined as positive when the flow is from i to j. $\varpi(Q_{ij})$ is defined by (I-3) with $x = Q_{ij}$.

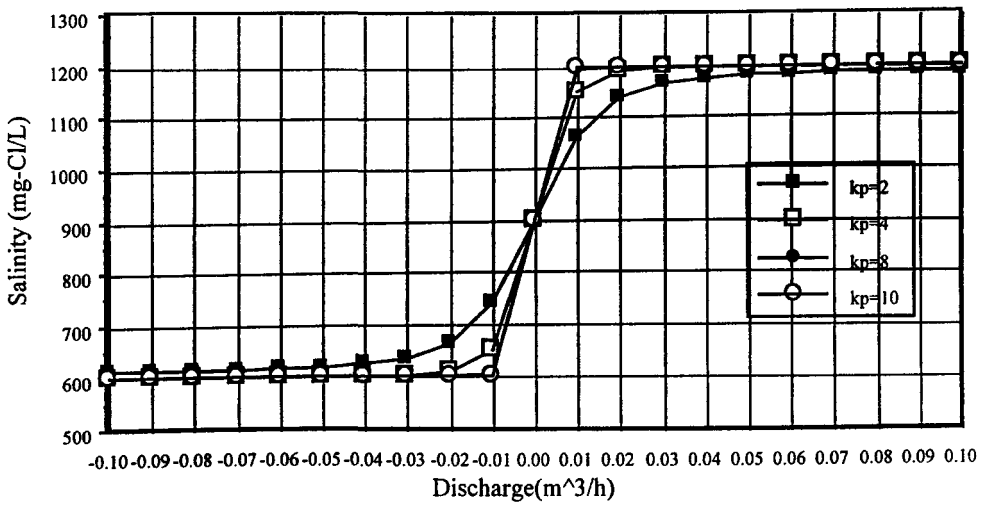

FIGURE I-1 A smooth representation of the dilution condition near zero discharge.

Figure I-1 shows the results of Eq. (I-4) for $c_i = 600\,\text{mg/l}$, $c_j = 1200\,\text{mg/l}$, $k_p = 2, 4, 8, 10$ and $\varepsilon = 0.001$.

The results show that the approximation is good, and can be made as accurate as desired by changing k_p. Experimentation with the optimization technique showed that it is not sensitive to the value of k_p in that range.