Seasonal multi-year optimal management of quantities and salinities in regional water supply systems

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ABSTRACT

A seasonal multi-year model for management of water quantities and salinities in regional water supply systems (WSS) was developed and implemented. Water is taken from sources which include aquifers, reservoirs, and desalination plants, and conveyed through a distribution system to consumers who require quantities of water under salinity constraints. The year is partitioned into seasons, and the operation is subject to technological, administrative, and environmental constraints such as water levels and salinities in the aquifers, capacities of the pumping, distribution system, and the desalination plants, and the desalination plants maximum removal ratios. The objective is to operate the system at minimum total cost. The objective function and some of the constraints are nonlinear, leading to a nonlinear optimization problem. The nonlinear optimization problem is solved efficiently by adapting (1) a set of manipulations that reduce the problem size and (2) a novel finite difference scheme for calculating the derivatives required by the optimization solver, entitled the Time-Chained-Method (TCM). The model is demonstrated on a small illustrative example and on a real sized regional water supply system in Israel.

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1. Introduction

Management of water resources systems (WSS) is aided by models of various types, ranging from long-term development of large systems, to detailed operation of smaller parts such as a distribution system or an aquifer. Thus models range from highly aggregate versions of an entire water system to much more detailed models in space and time. It does not seem feasible to create a single tool that covers all levels in time and space simultaneously. The preferred option is to use a suite of models, inter-connected in a hierarchy (Shamir, 1971; Zaide, 2006). Selecting the proper aggregation in time and space for a particular application is one of the most important aspects of modeling. The short-term (weekly to annual) or long-term (years, decades) operation of a large scale WSS can be captured in a model of medium aggregation that is used to manage simultaneously, both the sources and the network (Fisher et al., 2002; Draper et al., 2003, 2004; Jenkins et al., 2004; Watkins et al., 2004). Many models deal with quantities of water to be delivered from sources to demand zones. Some models

consider water quality as well, in particular salinity (Mehrez et al., 1992; Tu et al., 2005; Yates et al., 2005a,b; Zaide, 2006).

The network representation in the model can be classified according to the physical laws that are considered explicitly in the model constraints (Ostfeld and Shamir, 1993a,b; Cohen et al., 2000). According to this classification the proposed models of Tu et al. (2005), Yates et al. (2005a,b) and Zaide (2006) are flow-quality models which consider the balance of the flows and mass of quality parameters, but without explicit inclusion of the hydraulics. The inherent assumption of these models is that the hydraulic operation with the quantities prescribed by the model would be feasible hydraulically. With the inclusion of desalination plants as an important source in WSS, as is the case in Israel, water salinity consideration must be included in the management. It is important and necessary to consider both quantity and salinity in the water sources, in the water supplied to consumers and at nodes of the supply system itself. With the salinity considerations becoming an important part of management models, the complexity of the model evidently increases.

A further consideration is sustainability of the management plan. This implies meeting the needs of the present without reducing the ability of the next generation to meet its needs (Loucks, 2000). Sustainable management requires a perspective with a relatively long time-horizon, and hence the need to develop multi-year flow-quality models for WSS management. The multi-

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year models ensure that the final state of the system at the end of the operating horizon is considered, either as a constraint or having a value in the objective function.

An associated aspect of multi-year water supply management relates to hydrological uncertainty (Ajami et al., 2008), climate change (Brekke et al., 2009; Yates et al., 2005a,b), population growth (Kasprzyk et al., 2009), and the decline of water quality in the sources. The model proposed in this paper is deterministic, with a time horizon of several years, designed to minimize operating costs of an existing physical system. Uncertainty issues are addressed by sensitivity or uncertainty analysis (Lal et al., 1997; Wong and Yeh, 2002; Wu et al., 2006). Water resources management models have been solved by a variety of optimization techniques. Evolutionary Algorithms, including Genetic Algorithms and others, have gained popularity in recent years, as detailed in a recent review paper (Nicklow et al., 2010). However, as will be demonstrated below, our model is developed with structural adaptability and high computational efficiency in mind, so it can be a building-block for a model that takes uncertain considerations into account by an Ensemble or Scenario-based Optimization (Pallottino et al., 2005; Kracman et al., 2006; Mahmoud et al., 2011) or by Implicit Stochastic Optimization (Lund and Ferreira, 1996; Labadie, 2004).

This paper introduces a non-linear seasonal multi-year model for optimal management of both water quantity and salinity, which minimizes the overall cost of the system operation subject to technological, administrative, and environmental constraints. The model does not include hydraulic constraints and does not guarantee required heads at consumer nodes, yet the objective function takes into account the cost of conveyance as a function of the hydraulic properties of the network. It is implicitly assumed that the short-term hydraulic operation is feasible for the seasonal quantities prescribed by the model (Cohen et al., 2000).

1.1. Literature review

Our model differs from others in the literature in several aspects. Fisher et al. (2002) developed a model which considers the optimal water allocation from water sources to consumers through a conveyance system. It is a single-year model and includes neither quality nor hydraulic considerations.

Draper et al. (2004) developed a single time step optimization model for water allocation decisions, while the sequence of monthly time steps are linked by simulation. Water quality considerations are not included explicitly in the model, so it uses an external module which consists of an Artificial Neural Network (ANN) to estimate the water quality in the system. Thus, this model considers in some sense quality and multi-year management but not by simultaneous optimization, as we propose in this work.

Jenkins et al. (2004), Draper et al. (2003) and Watkins et al. (2004) developed and applied optimization models for multi-year management of surface and groundwater sources. The optimization problem was formulated as a linear network flow where convex economic functions are replaced by piecewise linear functions. Moreover, these models are solved only for water quantities; they do not include quality and hydraulic considerations.

Tu et al. (2005) developed a nonlinear optimization model for flow-quality operation of water distribution in regional water supply system with multi-quality sources. However, this model is not multi-year and it only considers a six month horizon with monthly time units, since the optimization problem was solved by Genetic Algorithms which is very expensive computationally.

To the best of our knowledge, the closet formulation to the proposed model is the model developed by Zaide (2006), which does not include hydraulic consideration. Zaide (2006) developed

a model for multi-year combined optimal management of quantity and quality. Both quantity and salinity considerations (in the water sources, supply system and demand zones) are optimized simultaneously for a long time horizon. Since the optimization problem was solved directly without an efficient optimization plan to overcome the computational burden, the formulation had to be reduced by defining "future representative years" where the same decision variables for each "future representative year" were repeated for several years in the future. This relaxation led to a smaller optimization problem but may lead to a suboptimal solution of the original problem.

Here, we modify Zaide's (2006) model by explicit consideration of hydraulics and then an efficient optimization plan is developed to reduce the model size without the need to of the "future representative years". The optimization plan utilizes a new matrix representation of the quality constraints (including the dilution constraints) to extract the quality variables and reduce the optimization problem size.

To solve the optimization problem efficiently we have also developed the Time-Chained-Method (TCM), a novel and efficient scheme for calculating gradients of the objective and of the Jacobian matrix in a time-dependent inventory problem, which can be applied in other problems as well − such as groundwater management and reservoirs operation.

The details of our model and the solution technique are given in the next sections. In Section 2, the formulation of the model (objective function and the constraints) is presented. Section 3 contains the optimization plan, namely structuring the model for the optimization solver. Section 4 describes the optimization tools, including an analysis of the problem properties and how to exploit them in the optimization. Section 5 presents illustrative examples and Section 6 shows performance measures of the optimization technique.

2. Model components

In the seasonal multi-year model for management of water quantity and salinity, water is taken from sources, which include aquifers, reservoirs and desalination plants, conveyed through a distribution system to consumers who require certain quantities of water with specified salinity limits. The small WSS shown in Fig. 1 was used for model development, testing and demonstration; results will be shown (in Section 5) for the WSS shown in Figs. 4 and 5, which is a central part of the Israeli National WSS. The year is divided into seasons (two seasons in this paper, but there could be more, since the computational cost rises only linearly with the number of seasons, as detailed in Section 6 below) and the operation is subject to constraints on water levels and water quality (salinity) in the aquifers, capacities of the pumping and distribution
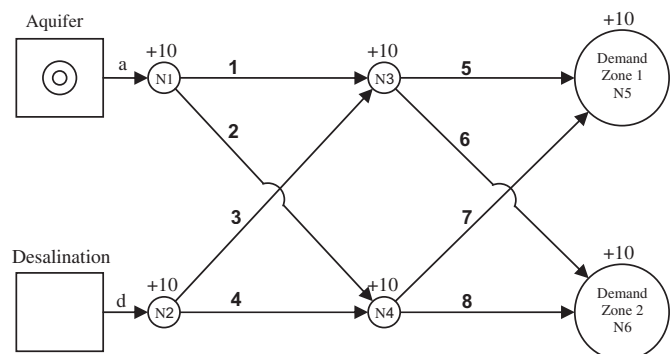

Fig. 1. Illustrative example.

system, capacity of the desalination plants and the salinity removal ratio. Therefore the decision variables in each season are: desalinated water production and salinity removal ratio in the desalination plants, and the water flow and water salinity distribution throughout the network. Two sets of state variables describe the state of the system at the end of each season: water levels and water salinities in the natural resources (aquifers and reservoirs).

The model was developed in two forms, first as an annual model and then it was expanded into a multi-year model. The annual model served as the building block for the multi-year where the state variables linking the seasons and the years (Fig. 2). The annual model has value in itself, as it can be used to determine the coming year's operation with the known initial condition and the desired end-of-year state prescribed. It is also valuable for developing and debugging when new system expansions/modifications are considered.

2.1. Objective function

The objective is to operate the system with minimum total cost of desalination CD, extraction levy from the natural sources CE and conveyance costs CC over the planning horizon T_f.

In the next sections p, a, d, z, S, Y denote pipe, aquifer, desalination plant, demand zone, season and year, respectively.

2.1.1. Conveyance cost

The conveyance cost in a pipe is related to the head loss, given by the Hazen-Williams equation, and the topographical difference between its ends (assuming the same hydraulic head at both ends, a reasonable assumption for a seasonal model).

$$CC_p^{S,Y} = \frac{X_p^{S,Y} \cdot \left(\dfrac{Q_p^{S,Y}}{w^{S,Y}}\right)}{200} \cdot 0.736 \cdot w^{S,Y} \cdot KWHC^{S,Y}$$

$$X_p^{S,Y} = \Delta Z_p + \Delta Hf_p^{S,Y} \tag{1}$$

$$\Delta Hf_p^{S,Y} = 1.526 \times 10^7 \cdot \left(\frac{Q_p^{S,Y}}{w^{S,Y} c_p^Y}\right)^{1.852} \cdot D_p^{-4.87} \cdot L_p$$

where $CC_p^{S,Y}$ is conveyance cost (\$/season); $X_p^{S,Y}$ is head loss (m); $Q_p^{S,Y}$ is discharge (m³/season); $w^{S,Y}$ is number of pumping hours (h/season); $KWHC^{S,Y}$ is pumping cost (\$/kwh); ΔZ_p is elevation difference (m); $\Delta Hf_p^{S,Y}$ is energy head loss (m); c_p^Y is Hazen Williams coefficient (−); D_p is link diameter (cm); and L_p is link length (km).

2.1.2. Extraction levy

The extraction levy depends on the water level in the natural resource. The levy is higher at low water levels, to indicate the increasing value (cost of scarcity) of the resource. The specific levy is expressed as a value per unit volume, so the cost of the extraction levy is:

$$\overline{CE}_a^{S,Y} = \left(1 - \frac{h - h_{\min}}{h_{\max} - h_{\min}}\right)_a^{S,Y} \cdot (\overline{CE}^{\max})_a^{S,Y} \quad CE_a^{S,Y} = \overline{CE}_a^{S,Y} \cdot Q_a^{S,Y} \tag{2}$$

which is a quadratic relationship between of extraction levy and the amount pumped, where $\overline{CE}_a^{S,Y}$ is specific levy (\$/m³); $h_a^{S,Y}$ is

Year 1   Year t Year T_f

Fig. 2. Linkage between seasons and years through state variables.

water level (m); $(h_{\min})_a^{S,Y}$ is minimum allowed water level (m); $(h_{\max})_a^{S,Y}$ is maximum allowed water (m); $(\overline{CE}^{\max})_a^{S,Y}$ is maximum levy (\$/m³); $CE_a^{S,Y}$ is extraction levy (\$/season); and $Q_a^{S,Y}$ is pumping amount (m³/season).

2.1.3. Desalination cost

The desalination cost includes a constant price per unit of desalinated water plus a variable cost of the salinity removal ratio:

$$CD_d^{S,Y} = \left(\alpha_d + \frac{1}{\left(100 - RR_d^{S,Y}\right)^{\beta_d}}\right) \cdot Q_d^{S,Y} \tag{3}$$

where $CD_d^{S,Y}$ is desalination cost (\$/season); α_d is constant (\$/m³); $Q_d^{S,Y}$ is desalination amount (m³/season); and $RR_d^{S,Y}$ is removal ratio (%); β_d is constant (−).

2.1.4. Overall cost

The objective of the multi-year model is to minimize the present value of the total cost of operation over the planning horizon.

$$cost = \sum_Y \frac{\sum_S \left(\sum_p CC_p^{S,Y} + \sum_d CD_d^{S,Y} + \sum_a CE_a^{S,Y}\right)}{(1 + r)^Y} \tag{4}$$

where cost is the total operation cost (\$); r is the annual discount rate (−). Since the objective function is nonlinear, it could be converted into benefit maximization by including the value of the quantity and salinity of the water supplied to consumers (within the specified constraints), if the relevant cost/benefit coefficients are available.

2.2. Constraints

2.2.1. Water conservation law

This law holds for all nodes in the network; source nodes, intermediate nodes and demand nodes. A WSS can be represented as a directed graph consisting of N nodes connected by M edges. The nodes can be grouped into two sub-groups: N_1 are source nodes, such as desalination plant and aquifers, with one outgoing link for each source node and N_2 are junction nodes where two or more edges join i.e., intermediate nodes and demand node. The M edges represent the links between two nodes; links in which the direction of flow is not fixed are represented by two edges, one in each direction. The topology of the network is represented by the junction node connectivity matrix A, where $A \in \mathbf{R}^{N_2 \times M}$ has a row for each node and a column for each edge. The nonzero elements in each row are +1 and −1 for incoming and outgoing edges respectively. The first columns in A correspond to the links which leave source nodes (aquifers and desalination plants), while the last rows correspond to the demand nodes. For each season S in year Y the following linear equation system ensures water conservation at the network nodes.

$$A \cdot Q = b \tag{5}$$

where $Q = [Q_{source}, Q_{pipes}]^T$; $b = [0, Q_{demand}]^T$; Q_{Source} is the vector of discharges leaving source nodes; Q_{pipes} is the vector of discharges in the links which are connected to intermediate nodes excluding the links which are connected to source nodes; Q_{demand} is the vector of outgoing discharges at demand nodes. For example, the water supply network shown in Fig. 1 has 2 source nodes, 4 intermediate nodes and 2 demand nodes. The junction node connectivity matrix for this network is $A \in \mathbf{R}^{6 \times 10}$ and the vectors Q and b are $Q = [Q_a, Q_d, Q_1, ..., Q_8]^T$; $b = [0, ..., 0, Q_{z=1}, Q_{z=2}]^T$.

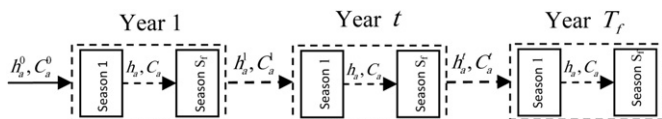### 2.2.2. Mass conservation law

For each season S of year Y the following linear equation system ensures salt mass conservation at network nodes:

$$A^0 \cdot D_Q \cdot C^0 = 0, \quad A^0 \in \mathbf{R}^{N_2 \times (M+n_3)}$$

$$A^0 = \left(A \;\middle|\; \begin{matrix} 0 \\ -I \end{matrix} \right)$$

$$C^0 = [C_{\text{source}}, C_{\text{pipes}}, C_{\text{demand}}]^T \tag{6}$$

$$D_Q \in \mathbf{R}^{(M+n_3) \times (M+n_3)} \quad \text{diagonal matrix}$$

$$D_Q = \text{diag}([Q_{\text{source}}, Q_{\text{pipes}}, Q_{\text{demand}}])$$

where C_{source} is salinity leaving source nodes; C_{pipes} is the salinity in the links which are connected to intermediate nodes excluding the links which are connected to source nodes; C_{demand} is salinity supplied at demand nodes; n_3 number of demand nodes; and $I \in \mathbf{R}^{n_3 \times n_3}$ is the identity matrix. For the network in Fig. 1 $A^0 \in \mathbf{R}^{6 \times 12}$, $D_Q \in \mathbf{R}^{12 \times 12}$ and $C^0 = [C_a, C_d, C_1, \ldots, C_8, C_{z=1}, C_{z=2}]^T$.

2.2.3. Hydrological balance for natural resources

The hydrological water and salinity mass balances ensure that the change in aquifer storage equals the difference between the recharge and withdrawal during the season:

$$R_a^{S,Y} - Q_a^{S,Y} = \text{SA}_a \cdot \left(h_a^{S,Y} - h_a^{(S,Y)-1} \right) \tag{7}$$

$$(C_R)_a^{S,Y} \cdot R_a^{S,Y} - C_a^{(S,Y)-1} \cdot Q_a^{S,Y} = \text{SA}_a \cdot \left(C_a^{S,Y} \cdot h_a^{S,Y} - C_a^{(S,Y)-1} \cdot h_a^{(S,Y)-1} \right) \tag{8}$$

where $R_a^{S,Y}$ is recharge (m³); SA_a is the storativity multiplied by area (m²); $h_a^{S,Y}, C_a^{S,Y}$ are water level and salinity respectively (m), (mgcl/lit); $h_a^{(S,Y)-1}, C_a^{(S,Y)-1}$ are water level and salinity in the previous season respectively (m), (mgcl/lit); and $(C_R)_a^{S,Y}$ is salinity of the recharge water (mgcl/lit).

2.2.4. Desalinated water salinity

$$C_d^{S,Y} = C_{\text{sea}} \cdot \left(\frac{100 - \text{RR}_d^{S,Y}}{100} \right) \tag{9}$$

where $C_d^{S,Y}$ is desalinated water salinity (mgcl/lit); C_{sea} is sea water salinity (27,000 mgcl/lit); and $\text{RR}_d^{S,Y}$ is the removal ratio (%).

2.2.5. Dilution condition

The model assumes total mixing at all nodes, so the salinity in all links leaving a node is equal. This dilution condition is given by the linear equation system:

$$B^0 \cdot C^0 = 0 \tag{10}$$

Each row of B^0 indicates equal salinity for two outgoing edges which share the same inflow node, i.e. each row has only two non-zero elements $+1$ and -1; when three links leave the same node there are two rows, each with two non-zero elements $+1$ and -1.

2.2.6. Flow constraints

Inequality constraints are imposed on the flow variables of the model: (a) on pipe flows (11) and (b) on the extraction from the natural sources (12) and the desalination plants (13).

The lower bounds in (11) and (12) are set to zero since the flow direction is fixed whereas the lower bounds in (13) represent a condition of the contract with the desalination plant concessions.

The discharge in the pipes is limited by upper bounds, to prevent infeasibilities of hydraulic conditions. The extraction from natural resources is limited by an upper bound, reflecting various hydrological and hydraulic considerations. The amount of desalinated water from each plant is limited by an upper bound which represents plant capacity.

$$0 \le Q_p^{S,Y} \le (Q_{\text{max}})_p^{S,Y} \tag{11}$$

$$0 \le Q_a^{S,Y} \le (Q_{\text{max}})_a^{S,Y} \tag{12}$$

$$(Q_{\text{min}})_d^{S,Y} \le Q_d^{S,Y} \le (Q_{\text{max}})_d^{S,Y} \tag{13}$$

where $(Q_{\text{max}})_p^{S,Y}$ is the maximum discharge allowed (m³/season); $(Q_{\text{max}})_a^{S,Y}$ is the maximum admissible/feasible withdrawal (m³/season); $(Q_{\text{max}})_d^{S,Y}$, $(Q_{\text{min}})_d^{S,Y}$ are maximum and minimum supply of desalinated water (m³/season), respectively.

2.2.7. Removal ratio limits

Salinity removal limits reflect the plant technology and its overall system design:

$$(\text{RR}_{\text{min}})_d^{S,Y} \le \text{RR}_d^{S,Y} \le (\text{RR}_{\text{max}})_d^{S,Y} \tag{14}$$

where $\text{RR}_d^{S,Y}$ is removal ratio (%); $(\text{RR}_{\text{min}})_d^{S,Y}$ and $(\text{RR}_{\text{max}})_d^{S,Y}$ are minimum and maximum removal ratios (%), respectively.

2.2.8. Water levels in the sources

Constraints on water levels in the natural resources reflect policy and operational limits.

$$(h_{\text{min}})_a^{S,Y} \le h_a^{S,Y} \le (h_{\text{max}})_a^{S,Y} \tag{15}$$

where $h_a^{S,Y}$ is water level (m); $(h_{\text{min}})_a^{S,Y}$ and $(h_{\text{max}})_a^{S,Y}$ are minimum and maximum allowed water levels (m), respectively.

2.2.9. Salinity levels in the sources

Constraints on admissible source salinity reflect source management policies, especially for preventing excessive water salinity.

$$(C_{\text{min}})_a^{S,Y} \le C_a^{S,Y} \le (C_{\text{max}})_a^{S,Y} \tag{16}$$

where $C_a^{S,Y}$ is water salinity in (mgcl/lit); $(C_{\text{min}})_a^{S,Y}$ is minimum salinity (mgcl/lit) (which may be zero); and $(C_{\text{max}})_a^{S,Y}$ is maximum admissible salinity (mgcl/lit).

2.2.10. Demand salinity constraints

Ensuring salinity of supply water within bounds:

$$(C_{\text{min}})_z^{S,Y} \le C_z^{S,Y} \le (C_{\text{max}})_z^{S,Y} \tag{17}$$

where $C_z^{S,Y}$ is water salinity supplied for demand zone z (mgcl/lit); $(C_{\text{min}})_z^{S,Y}$ and $(C_{\text{max}})_z^{S,Y}$ are minimum and maximum salinities (mgcl/lit), respectively.

3. Optimization plan

The mathematical formulation of the optimization model determines its suitability for solution by an optimization algorithm and the resultant computational efficiency. Since we intend to run the model many times, in interactive mode with decision making, and later as a kernel of models for management under uncertainty, we have developed a set of manipulations that improve substantially the solvability and efficiency of the model.

The model formulated in Section 2 can be solved directly, namely, by considering the flow variables and the quality variables as decision variables and accounting for all the equality constraints in the model. However, solving the model directly by taking both the flow and quality variables as decision variables and taking all the equality constraints into consideration will increase the optimization problem size dramatically, especially when the time horizon is long. In this Section we present an efficient optimization strategy in which we reduce the optimization problem size by extracting all the quality variables and part of the flow variables, so the number of decision variables after the size reduction is orders of magnitude smaller than the problem obtained when solving the optimization problem directly. Moreover, this strategy will produce an optimization problem without equality constraints.

The attempt of Zaide (2006) to solve a similar model directly has led to a very large optimization problem; hence to reduce the computational burden Zaide (2006) solved an approximation of the original optimization which does not contain the detailed management in the future.

The optimization plan developed here reduces the size of the optimization problem without the need to approximate the future decisions hence, the optimal solution provides detailed management policy for each of the years considered in the management horizon.

3.1. Eliminating dependent variables

To reduce the model size we extract one dependent decision variable from each equality constraint. Then the dependent variables are substituted in the objective function and the inequality constraints to obtain a smaller model (fewer decision variables) without equality constraints. In the linear equality constraints set obtained from the water balance requirement (Equation 5):

$$A \cdot Q = b \tag{18}$$

The reduction is achieved by solving the linear equation system. This system is most likely underdetermined since we have more edges than nodes $M > N_2$, and the rank of the matrix A is therefore N_2 (Boulos and Altman, 1991). The general solution of the underdetermined system (18) is given by:

$$Q_{dep} = A_1^{-1} \cdot \left(b - A_2 \cdot Q_{indep}\right) \tag{19}$$

where A_1 is a matrix of N_2 independent columns of A; A_2 is a matrix of $M - N_2$ dependent columns of A; $()_{dep}$ is the vector of dependent decision variables; $()_{indep}$ is the vector of independent decision variables.

In graph theory this is related to the spanning tree (ST); a ST of a connected graph is defined as a maximal set of edges that contains no cycle, i.e. the graph matrix of the ST has full rank. Thus finding the dependent columns of the matrix A is equivalent to finding the non-ST edges of the graph. In a connected graph there are many STs, and any of these can indicate which columns in A are dependent and which are not. To generate a ST one can use the Breadth-First-Search algorithm (BFS) (Boulos et al., 2006), or simply by calculating the reduced echelon form of A using Gauss Jordan elimination with partial pivoting. In the reduced echelon form the columns which are related to ST edges construct the standard basis.

The inequality constraints (11)–(13) define lower and upper bounds for the vector Q. Substituting the dependent variables in the inequality constraints (11)–(13) leads to:

$$\begin{aligned} (Q_{min})_{dep} &\leq A_1^{-1} \cdot \left(b - A_2 \cdot Q_{indep}\right) \leq (Q_{max})_{dep} \\ b - A_1 \cdot (Q_{max})_{dep} &\leq A_2 \cdot Q_{indep} \leq b - A_1 \cdot (Q_{min})_{dep} \end{aligned} \tag{20}$$

Constraint (20) with the following bound replaces constraints (11)–(13):

$$(Q_{min})_{indep} \leq Q_{indep} \leq (Q_{max})_{indep} \tag{21}$$

For the WSS model shown in Fig. 1, one possible ST is defined by the edges $\{a, d, 1, 2, 5, 7\}$. Thus $Q_{indep}^S = [Q_3^S, Q_4^S, Q_6^S, Q_8^S]^T$, $Q_{dep}^S = [Q_a^S, Q_d^S, Q_1^S, Q_2^S, Q_5^S, Q_7^S]^T$, A_2 contains columns $\{3, 4, 6, 8\}$ of A and A_1 contains columns $\{a, d, 1, 2, 5, 7\}$.

3.2. Resultant variables

A special and useful property of our model is that equality constraints (6), (9), (10) and the hydrological constraints (7) and (8) imply that for fixed values of the flows and removal ratios the salinity variables C and the state variables of the natural resources h_a, C_a are also fixed (resultant variables). This property ensures the ability to evaluate the objective function and all the constraints for predetermined Q_{indep} and RR, since the remaining flows are dependent and the other variables are resultant variables which can be evaluated directly.

By using the equality constraints (7) and (8) we can extract the state variables of the natural resources h_a, C_a as a function of Q_{indep}. The salinity variables of the desalination plants nodes given in (9) could also be calculated by given Q_{indep} and RR. Hence, C_{source} is a function of Q_{indep} and RR. After calculating the state variables of the natural resources the objective function and the inequality constraints (15) and (16) can also be evaluated.[3]

To extract the salinity variables, constraints (6) and (10) can be joined to form the following:

$$K \cdot C^0 = 0 \tag{22}$$

where K is a block matrix defined as $K = (A^0 \cdot D_Q / B^0)$. When C_{source} is determined using the salinity state variables C_a and the desalination plants salinity C_d given in (9), the first columns corresponding to the sources are moved to the RHS of the equation system to form the following:

$$K_1 \cdot C = -K_2 \cdot C_{source} \tag{23}$$

where $C = [C_{pipes}, C_{demand}]^T$, K_1 is a square and full rank matrix, hence the resultant salinity variables are:

$$C = -K_1^{-1} \cdot K_2 \cdot C_{source} \tag{24}$$

The matrices K_1, K_2 are functions of the flows, i.e. functions of the independent decision variables Q_{indep}. Since the salinity variables are a product of the inverse of K_1 and K_2, this creates a nonlinear relationship between the salinity variables and Q_{indep}. As a consequence, the inequality constraint (17) is nonlinear.

Regarding the WSS shown in Fig. 1, for predetermined $Q_{indep} = [Q_3, Q_4, Q_6, Q_8]^T$ and RR_d; the vector $C_{source} = [C_a, C_d]^T$ is determined using (8) and (9). Hence, the vector $C = [C_1, ..., C_8, C_{z=1}, C_{z=2}]^T$ can be obtained by (24), where $K_2 \in \mathbf{R}^{2 \times 10}$ is the matrix combining the first columns (corresponding to the sources) of the matrix K and $K_1 \in \mathbf{R}^{10 \times 10}$ is the matrix of the remaining columns of K.

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[3] Note that in our formulation the objective function does not depend directly on water salinity in the system (it does, however, reflect the cost of desalination, which is required in order to meet salinity constraints). Constraint (15) is linear in the given formulation, but when the aquifers are represented by a finite differences model or a simulation program this constraint is nonlinear.

3.3. Evaluating the objective function and the constraints

The dependent variables Q_{dep} and the resultant variables are function of the decision variables Q_{indep} and RR. Hence, the objective function and all the constraints can be evaluated for pre-determined decision variables Q_{indep} and RR. The seasonal evaluation scheme is depicted in Fig. 3, where: (a) The flow distribution in the network (5) and the source limitations (11)–(13) are integrated by the inequality linear constraints (20) and the bounds (21), (b) Evaluation of the objective function does not require the salinity calculations in the system, since it depends only on the removal ratios of the desalination plants, and (c) The remaining inequality constraints (15)–(17) are nonlinear in the general case (discussed in the previous section).

4. The optimization solver

4.1. The time-chained-method (TCM)

The steps described in the previous sections result in a general nonlinear optimization, which can be solved with one of the existing general nonlinear programming solvers, such as SQP (Fletcher, 1985) or interior point algorithm (Waltz et al., 2006; Byrd et al., 2000). These solvers use the gradient of the objective and the Jacobian matrix of the nonlinear constraints.

The efficient optimization plan in Section 3 reduces the problem size. But on the other hand it generates new non-linear relations in the optimization problem, for example in Eq. (24) the matrices K_1, K_2 are functions of the flows, i.e. functions of the independent decision variables Q_{indep}. Since the salinity variables are a product of the inverse of K_1 and K_2, this creates a nonlinear relationship between the salinity variables and Q_{indep}. As a consequence, the inequality constraints related to quality would be non-linear. The calculation of the analytical derivatives for these constraints is computationally demanding since they depend on the product of the inverse of K_1 and K_2, which depend on the flow and the network graph matrix A.

When calculation of the analytical derivatives is computationally demanding, a finite differences scheme can be used to give an estimation of the derivatives. However, for a water supply network of practical size the optimization model becomes very large, particularly for long-term multi-stage operation problems, so this numerical approximation is very cumbersome.

We have therefore developed the Time-Chained-Method (TCM), an efficient finite differences scheme designed for our model's multi-stage structure, which reduces the computation time from $O(T_f^2)$ to $O(T_f)$ where T_f is the number of stages. See Section 6 for numerical example and Appendix A for the general proof.

The TCM utilize the structure of the optimization problem depicted in Fig. 2 where each stage is linked with the past and future stages by the state variables.

For example to approximate the derivative of the cost function of the last stage T_f, i.e. $\text{cost}^{\text{stage}=T_f}$ with respect to (w.r.t) the first decision variables in the first stage, $x^{\text{stage}=1}_{\text{decision}=1}$, the change in $\text{cost}^{\text{stage}=T_f}$ should be evaluated for small change in $x^{\text{stage}=1}_{\text{decision}=1}$.

Without the TCM to evaluate $\text{cost}^{\text{stage}=T_f}$ for small change in $x^{\text{stage}=1}_{\text{decision}=1}$ one should evaluate all the stages $1..T_f$ corresponding to the change in $x^{\text{stage}=1}_{\text{decision}=1}$ in order to get the change in $\text{cost}^{\text{stage}=T_f}$. However, the TCM recognize that stage T_f is linked to first stage by the state variables hence the change in $\text{cost}^{\text{stage}=T_f}$ is obtained by evaluating the change of sate 1 w.r.t the change in $x^{\text{stage}=1}_{\text{decision}=1}$, the change of state 2 w.r.t the change of state 1, state 3 w.r.t state 2, etc., up to the change of $\text{cost}^{\text{stage}=T_f}$ w.r.t the state $T_f - 1$. Thus, we do not have to evaluate all the stages. The technical detailed description of the TCM method appears in Appendix A.

Nonlinear optimization solvers are sensitive to scaling (Betts, 2004), which means that the solver may encounter difficulties when decision variables have different scale. To overcome these difficulties a transformation of variables should be used. Details about the scaling procedure appear in Appendix A.

4.2. Optimization software

Due to the general structure of the objective function and constraints in our model a general nonlinear optimization solver is required. Our model was programmed in MATLAB and uses the interior point algorithm with conjugate gradient of the FMINCON nonlinear optimization suite.

5. Large scale water supply system (WSS) example

The small system shown in Fig. 1 was used in the development phase of the research. Extensive sensitivity analysis was used to test and verify the model's performance, which was then applied to a larger and more realistic WSS.
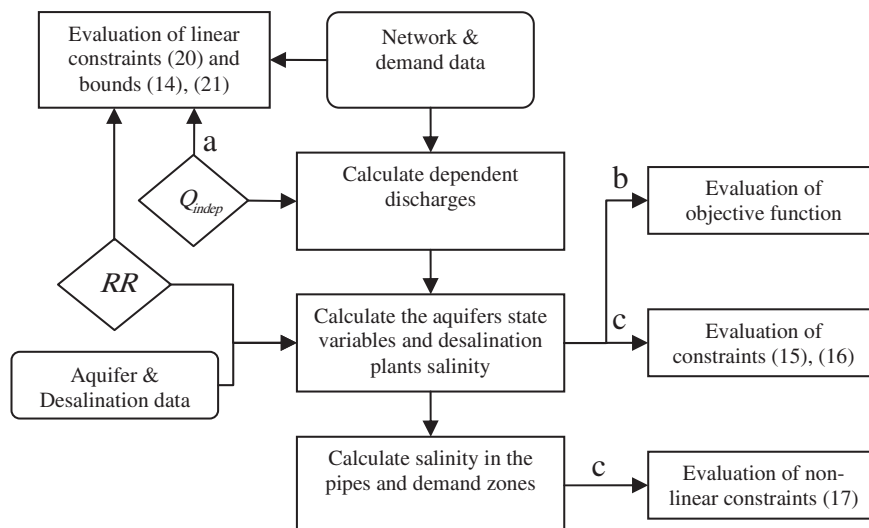

Fig. 3. Scheme for evaluation of the constraints and objective function with a given set of decision variables Q_{indep} and RR
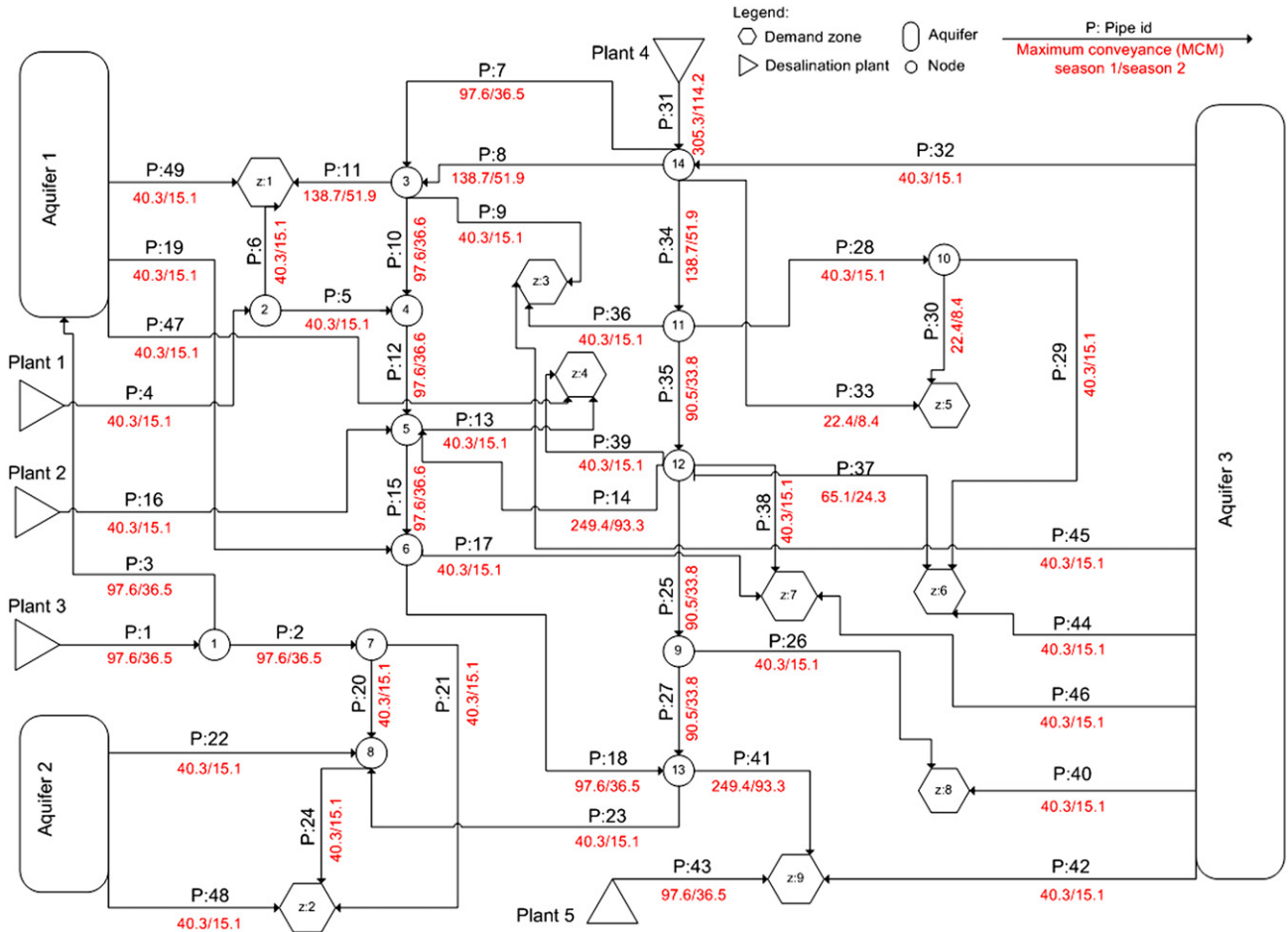
Fig. 4. Large WSS layout and conveyance capacity in seasons 1 and 2. (MCM, rounded to one decimal place).

5.1. Problem parameters

A water system with 9 demand zones, 3 aquifers, 5 desalination plants and 49 pipes (Fig. 4) has been solved in this example; the structure of this system mimics a part of the Israeli National Water System. The year is divided into two seasons, which can be called "winter" (lower demands, 265 days) and "summer" (high demands, 90 days).

The daily pumping hours are 14, 16 (h/day) respectively for the first and the second season, hence the seasonal pumping hours are: $w^{S=1} = 3710$ (h/season), $w^{S=2} = 1440$ (h/season). The seasonal capacities of the pipes are shown in Fig. 4, based on pipe diameters, lengths, Hazen Williams coefficients, topographic difference and a hydraulic loss of 4‰. The energy cost for the first season is $KWHC^{S=1} = 0.09$($/kwh) and for the second season is $KWHC^{S=2} = 0.11$($/kwh).

The seasonal demands for the 9 demand zones are given in Table 1. The maximum allowed water salinity in all zones is set to 220 (mgcl/lit). The maximum desalination amount for plants 1 to 5 are $(Q_{max})_d^S = [30, 100, 100, 200, 100]$ (MCM) respectively, while all the desalination plants have no obligation for a minimal supply requirement i.e. $(Q_{min})_d^S = 0$ (MCM). The removal ratio of the plants is between $(RR_{max})_d^S = 99.95$(%) and $(RR_{min})_d^S = 99.75$(%), yielding a product salinity in the range 13.5–67.5 (mgcl/lit). The desalination cost parameters are: $\alpha_d = 0.7$(M$/MCM) and $\beta_d = -10^6$ (−) which implies constant desalination cost per (MCM) in all the plants. Data for the three aquifers are given in Table 2. The maximum allowed salinity in all aquifers is set to 350 (mgcl/lit).

5.2. Base run and sensitivity analysis

The model was run for a single year: a Base Run (BR) and four Sensitivity Analysis runs (SA1–SA4), each with certain data modified, to examine its performance under various conditions (detailed below). Tables 3 and 4 show the quantities taken from sources, aquifer levels and salinities, the cost components and the total cost for each run.

5.2.1. Base run

In the base run we solve the model for one year with the data given in Fig. 4, Tables 1 and 2, and no extraction levy from the aquifers. The optimal quantity and salinity distribution in the network for the 1st season are shown in Fig. 5. The objective value (total cost) is 295 (M$) comprised of 56 (M$) conveyance and 239 (M$) desalination Since there is no extraction levy cost the optimal

Table 1
Demand data for the large WSS.

Demand z	Season 1 (MCM)	Season 2 (MCM)
1	116.9	50.1
2	9.1	3.9
3	53.9	23.1
4	36.4	15.6
5	18.2	7.8
6	90.3	38.7
7	9.1	3.9
8	18.2	7.8
9	198.1	84.9

Table 2
Aquifer data for the large WSS.

Aquifer $a = 1\ldots3$	$(Q_{\max})_a^S$ (MCM)	$(h_{\max})_a^S$ (m)	$(h_{\min})_a^S$ (m)	h_a^0 (m)	C_a^0 (mgcl/lit)	SA (MCM/m)	$R_a^{S=1\,a}$ (MCM)
1	130	33	1	2	300	65	210
2	111	50	1	3	300	37	100
3	290	50	17	19	150	25	360

[a] The recharge salinity is 150 (mgcl/lit), recharge in the second season is 0.

solution preferred water from the aquifers to desalinated water. However, the extraction from the aquifers did not reach the maximum possible amounts stated in Table 2 since there are other constraints that became binding. The results for season 1 (Fig. 5) are used to explain the logic of the optimal solution that has been reached, concentrating especially on the role of salinity in determining the outcome.

The flow capacities of the pipes leading from aquifer 1 are all $40.3 \cdot 3 = 120.9$ (MCM) but the flow in pipe 47 cannot reach 40.3 (MCM) since this is a direct pipe to demand zone 4 and the initial water salinity in the aquifer does not meet the water salinity requirement in demand zone 4. Hence the need for some desalinated water in order to meet the salinity requirement, which is brought via pipes 13 and/or 39. The optimal solution is expected to result in maximum allowed salinity in demand zone 4 (to reduce cost), so the three flows and salinities to demand zone 4 are set to match the demand 36.4 (MCM) and maximum salinity of 220 (mgcl/lit). The optimal allocation is: pipe 39 carries no flow, pipe 13 carries 10.2 (MCM) with salinity 13.5 (mgcl/lit), while pipe 47 carries 26.2 (MCM) with the salinity of aquifer 1, i.e. 300 (mgcl/lit).

Aquifer 2, with salinity 300 (mgcl/lit), is connected directly to demand node 2, whose demand is 9.1 (MCM), and supplies to it only 6.6 (MCM) while pipes 20 and 21 brings the remainder as desalinated water to meet the salinity limit in demand zone 2.

In aquifer 3 the initial water salinity is 150 (mgcl/lit) which is below the demand requirement, hence the only limitation is the conveyance capacity of the pipes leaving the aquifer i.e. 40.3 (MCM). The flows reached the maximum conveyance in pipes 32, 42, 44 and 45, while in pipes 40 and 46 that are connected directly to demand zones the flows are 18.2 and 9.1 (MCM).

5.2.2. Sensitivity analysis

Out of the many sensitivity runs that have been conducted we show here four, which were selected to demonstrate the response of the model to changes in the parameters of the objective function and the constraints. Sensitivity analysis SA1 introduces an extraction levy as defined in Eq. (2) with maximum specific levy $(\overline{CE}^{\max})_a^S$ (M$/MCM) equal to the desalination cost of 1 (MCM) i.e. 0.7

(M$/MCM). As a result, the model takes less water from aquifers 1 and 3 and the total cost is increased compared to the BR, as seen in Table 4. Because of the extraction levy, the optimal solution keeps more water in aquifers 1 and 3, while the same amount is extracted from aquifer 2 with and without the extraction levy, hence the state of the this aquifer remains as in the BR. Another notable characteristic of this run is the flow in pipe 3 that takes desalinated water from node 1 to aquifer 1. Desalinated water is brought via pipe 3 to dilute the aquifer water down to the allowed 220 (mgcl/lit). In this case, demand node 4 takes all its needs through pipe 47 with salinity of 220 (mgcl/lit).

In sensitivity analysis SA2 we modify SA1 by modeling desalination plant 4 as a large and free-of-charge water source with fixed salinity of 180 (mgcl/lit). This is accomplished by: (a) fixing the maximum production of plant 4 to a high value of 1000 (MCM), (b) fixing its removal ratio bound to 99.33 (%) and (c) fixing the desalination cost parameter $\alpha_4 = 0$ (M$/MCM). The total cost decreases compared to BR and SA1, as seen in Table 4. The results show that the model keeps more water in aquifer 1 and 3, while in aquifer 2 the same amount is extracted and the state of the this aquifer does not change compared to BR and SA1. Pipe 3 conveys low salinity water in order to dilute the aquifer water to the required level. Moreover, part of the pipes out of aquifer 1 carry no flow, since supply from the free plant 4 is preferred to extraction from the aquifers.

Sensitivity analysis SA3 and SA4 demonstrate how to eliminate parts of the model in order to use it as a tool to check planning alternatives. SA3 modifies SA1 by eliminating desalination plant 2, this is achieved by fixing its maximum flow to 0. In SA1 plant 2 produced 24.3 (MCM) which was conveyed through pipes 16, 15, 18 and 41 to demand node 9. After eliminating plant 2 the model produces more water in desalination plants 4 and 5. The additional water from plant 4 is distributed in the network through different routes to demand node 9 in order to minimize the conveyance cost. SA4 modifies SA1 by eliminating pipe 3 which connects desalination plant 3 with aquifer 1, implemented by fixing the maximum conveyance capacity to 0. In SA1 the model used pipe 3 to dilute aquifer 1 water from salinity of 300 (mgcl/lit) to the required 220

Table 3
Flow and salinity from the sources (MCM), (mgcl/lit) respectively. The values in the parentheses are the salinities. (All values have been rounded to one decimal place).

Run	S	Aquifer extraction, $a = 1\ldots3$			Aquifer water level,[a] $a = 1\ldots3$			Desalination plants, $d = 1\ldots5$				
		1	2	3	1	2	3	1	2	3	4	5
(BR)	1	106.8(300)	6.6(300)	188.5(150)	3.6(164.9)	5.5(226.6)	25.9(150)	7.5(28.4)	33.5(13.5)	2.5(13.5)	110.7(30.5)	94.2(40.5)
	2	45.2(164.9)	3.8(226.6)	72(150)	2.9(164.9)	5.4(226.6)	23(150)	5.3(41.3)	15.1(40.2)	0.1(14.3)	57.8(44.6)	36.5(41)
SA1	1	84.3(220)	6.6(300)	168.9(150)	3.9(176.8)	5.5(226.6)	26.6(150)	7.7(40.2)	24.3(38.6)	35.2(13.5)	130(43.5)	93.2(41)
	2	45.2(176.8)	3.8(226.6)	72(150)	3.2(176.8)	5.4(226.6)	23.8(150)	5.3(40.8)	15.1(40.2)	0.1(19.4)	57.8(44.8)	36.5(41.3)
SA2	1	53.8(220)	4.5(300)	142.1(150)	4.4(189.9)	5.6(227.4)	27.7(150)	0(36.5)	0(37.3)	22.2(13.5)	305.3(180.9)	22.2(40)
	2	30.1(189.9)	3.5(227.4)	72(150)	3.9(189.9)	5.5(227.4)	24.8(150)	0(39.4)	0(40.2)	0.1(38.1)	114.2(180.9)	15.9(41)
SA3	1	84.3(220)	6.5(300)	169(150)	3.9(176.8)	5.5(226.6)	26.6(150)	11.3(40.2)	0(67.5)	35.2(13.5)	146.3(42.1)	97.6(40.8)
	2	45.2(176.8)	3.8(226.6)	72(150)	3.2(176.8)	5.4(226.6)	23.8(150)	10(40.5)	0(67.5)	0.1(28.1)	68.2(44)	36.5(41)
SA4	1	106.8(300)	6.5(300)	168.9(150)	3.6(164.9)	5.5(226.6)	26.6(150)	7.7(37.8)	33.4(13.5)	2.5(14)	130.1(38.1)	94.2(39.1)
	2	45.2(164.9)	3.8(226.6)	72(150)	2.9(164.9)	5.4(226.6)	23.8(150)	5.3(41.6)	15.1(40.8)	0.1(19.2)	57.8(43.5)	36.5(41.3)

[a] Aquifer water levels (m), and salinities (in parentheses) (mgcl/lit) at the end of the season.

Table 4
Component and total costs (M$) of the large WSS − base run and 4 sensitivity analyses. (All the values have been rounded to two decimal places).

Run	Annual cost (M$)			
	Extraction	Desalination	Conveyance	Total
(BR)	0.00	238.69	56.43	295.12
SA1	135.48	266.39	54.97	456.84
SA2	89.55	39.76	67.47	196.78
SA3	135.49	266.38	56.08	457.95
SA4	149.98	251.61	56.41	458.00

Table 5
The recharge in the three aquifers.

Year	Recharge (MCM)[a]		
	Aquifer 1	Aquifer 2	Aquifer 3
1	117	58	139
2	188	94	304
3	172	86	264
4	195	97	409
5	252	126	520
6	182	91	262
7	200	100	340
8	200	100	260
9	222	111	292
10	174	87	230

[a] The second season recharge is 0.

(mgcl/lit). After elimination of pipe 3, aquifer 2 and plant 3 can only convey water to demand node 2, hence the extraction in aquifer 1 and the production in plant 2 has to increase significantly compared to SA1, as seen in Table 3.

5.3. Multi-year run

Two 10-year runs with 6.5% discount rate are compared, with and without extraction levy. The first is based on the BR parameters and the second on SA1 parameters, and the maximum water level in the aquifers is changed to $(h_{max})_a^S = 100 (m)$ to ensure no spill/overflow from the aquifers. The same data are repeated year after year for 10 years in both runs, except that the aquifer recharges in the first season ("winter") $R_a^{S=1}$ (MCM) are the last 10 years' recharge data from the hydrological data of Israel (Table 5).

The water level trajectories in the three aquifers for both runs are shown in Fig. 6. The results demonstrate that the extraction levy encourages preserving high water levels in aquifer 1 and 3. In aquifer 2 practically the same trajectory is obtained in both runs, since aquifer 2 is limited to supplying demand zone 2 and therefore the same amount is extracted with and without the extraction levy.

The extraction levy is a value assigned to water in storage, representing a policy of sustainable management. Runs with different extraction levy values can be used to show the tradeoff between storage in the aquifers at the end of the management horizon and the costs of desalination and conveyance, which rise as
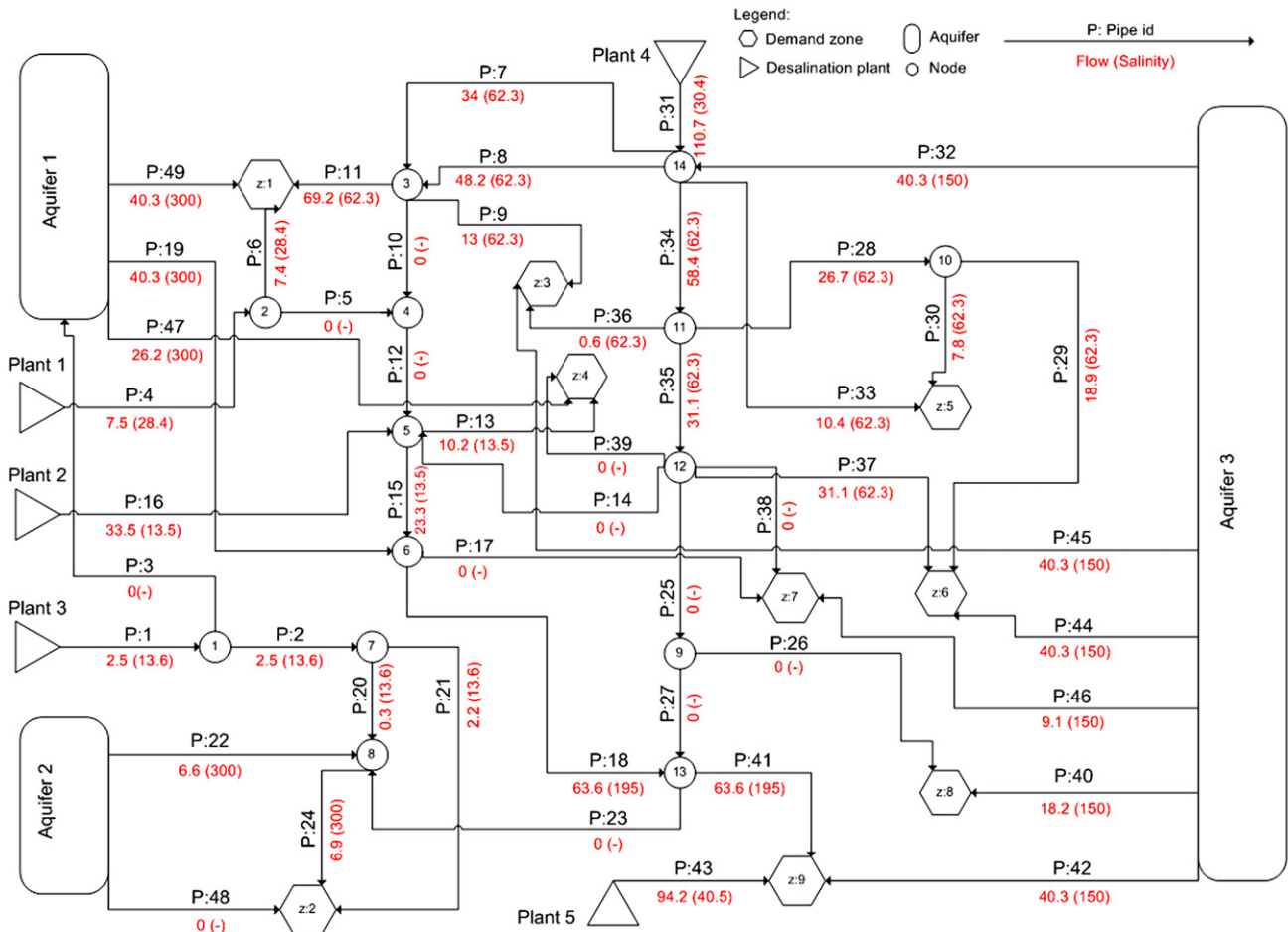
Fig. 5. Base run Season 1 results − flow (MCM) and salinity (mgcl/lit) distribution. (All values have been rounded to one decimal place).
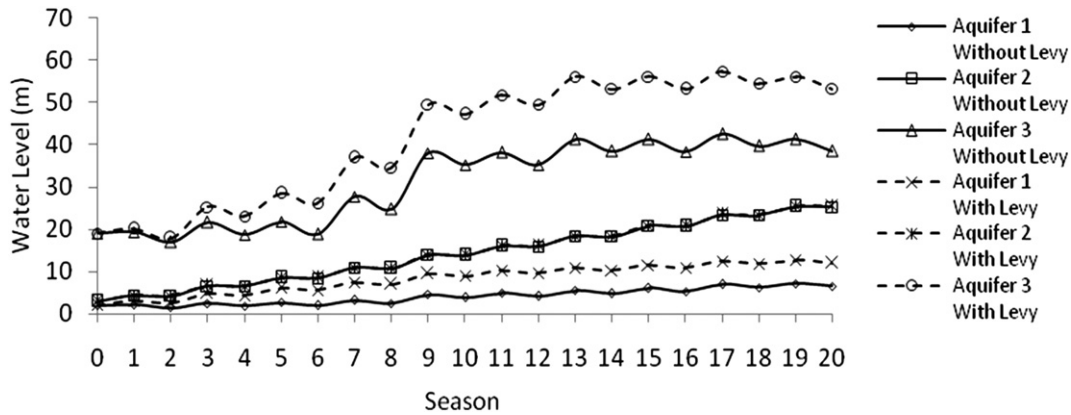
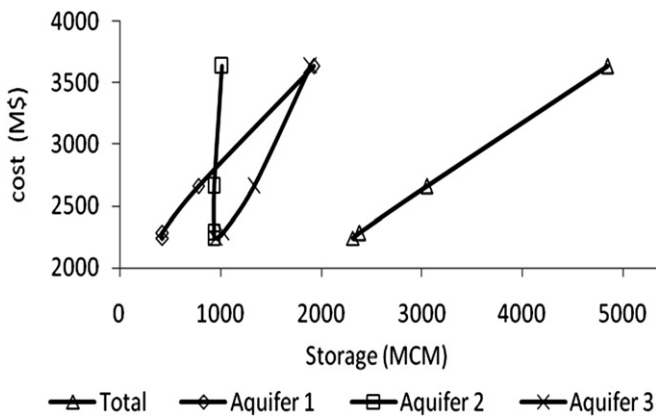Fig. 6. Water level trajectories with and without extraction Levy.

Fig. 7. Tradeoff curves of desalination + conveyance cost vs. final storage; each curve has points corresponding to four values of the maximum specific extraction levy (from bottom to top on each curve) [0,0.4,0.7,1] (M$/MCM).

less water is taken from the aquifers with increasing values of the levy. Fig. 7 shows this tradeoff between storage in the aquifers at the end of 10 year horizon and the desalination and conveyance cost, for different maximum specific levy values.

$(\overline{CE}^{max})_a^S = [0, 0.4, 0.7, 1](M\$/MCM)$. The tradeoff shows that increasing the maximum specific levy from 0 to 0.4 (M$/MCM) (lowest two points on each curve) does not change the optimal solution markedly, resulting in small changes in the cost and the final total storage. While by increasing the maximum specific levy from 0.4 to 0.7 (M$/MCM) the model preserves 30% more water in storage with a 16% increment of desalination and conveyance costs.

The linear tradeoff of the total storage indicates that each additional (MCM) of storage at the end of year 10 costs almost the same as the present value cost of 1 (MCM) desalinated water. This is particularly true because the conveyance cost did not change significantly among the runs with different levy values. The tradeoff of aquifer 2 shows a small change in storage, due to the limited conveyance network in the vicinity of aquifer 2. The allocation of additional storage between aquifers 1 and aquifer 3 changes for different values of the maximum specific levy. For 0.4–0.7 the allocation is 54% in aquifer 1 and 46% in aquifer 3, while for 0.7–1 the allocation is 67% in aquifer 1 and 33% in aquifer 3.

6. Efficiency of the TCM scheme

This section presents the computational efficiency of the Time-Chained-Method (TCM) compared with the conventional

approach of calculating the derivatives at each stage separately. The results are shown for the multi-year base run from section 5.3 where for the single year run we use the first year's recharge value, for two years the first two, and so on. Each year in the planning horizon has 62 decision variables, 124 linear inequalities and 60 nonlinear inequalities, and a nonlinear objective function. Fig. 8 presents the computational time to reach an optimal solution for a planning horizon ranging from 1 to 10 years. Each additional year expands the problem size, so that for 10 years it has 620 variables, 1240 linear inequalities, and 600 nonlinear inequalities.

Two model forms are compared, one with the standard gradient calculations of the objective function and Jacobian, the other with the TCM scheme. These results show the linear rise with TCM versus the quadratic rise with the conventional method, as predicted by Eqs. (A3) and (A10) in Appendix A.

Each run was started from the same initial guess of the decision variables and exactly the same final solution was obtained. The results demonstrate the dramatic reduction in computation time achieved by the TCM. For a 10 year operation horizon the ratio is 11,200/1750 = 6.4 and it would rise further for a longer horizon. For 2–5 years the ratio is less significant, but still ranges between 2.5 and 4.5. This computational efficiency will be most significant when the model is extended to deal with uncertainty, where multiple optimization solutions are required as explained in the introduction.
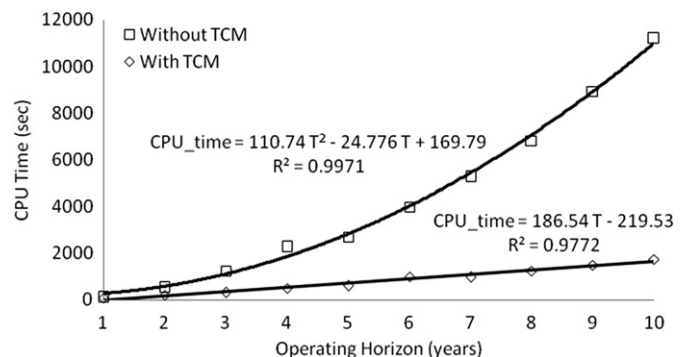

Fig. 8. Computation time as a function of planning horizon, comparing with and without the TCM procedure (on an Intel Core i7 M620 2.67 GHz laptop).

7. Summary and conclusions

The model developed in this work determines the optimal flow and salinity distribution in each season of a multi-year planning horizon for a WSS that is fed from aquifers (could also be lakes or reservoirs) and desalination plants and supplies to consumers through a hydraulic system. The objective is to minimize the total net present value of the cost, which includes the cost of water at the sources and the cost of conveyance, to supply prescribed quantities within salinity limits to all consumers. The algorithm handles a non-linear objective function, so objectives other than the one formulated in this paper can also be considered.

Flexibility in model building, ease of use, and computational efficiency are important properties for its application in the deterministic form presented herein, for evaluation of proposed system developments. These properties are even more important when the model will be used for management of the WSS under uncertainty, where many optimization solutions are required with variable data.

Computational efficiency of the optimization model has been achieved through mathematical development and implementation of several strategies: (a) extracting dependent and resultant variables, thereby reducing the size of optimization problem, (b) matrix formulation of quality and the dilution constraints which allows extraction of all the quality variables (Section 2.2.5), (c) extraction of the dependent discharges, which facilitates their scaling to ensure solvability, (d) an efficient scheme of evaluating the objective and constraints, (e) a novel and efficient scheme for calculating gradients of the objective and of the Jacobian matrix in a time-dependent inventory problem (TCM). These strategies, combined, result in a model that is tractable even for a large water system, as shown above. Due to this efficiency, the time horizon can be expanded and/or the year can be subdivided into more periods, for example four seasons per year, at the cost of a linearly increasing computation time (as seen in Fig. 8). Since the model examines a long time horizon it facilitates the search for sustainable management policies.

General efficacy and applicability of the model is achieved by a user-oriented front-end processor (the technical details of which are outside the scope of this paper); it receives the system data in a concise format and "spreads out" the model. This enables easy evaluation of modifications and expansions of the system, using the difference in the optimal cost between the new/proposed system and the existing one to determine the justification for the proposed addition/expansion/change. As a consequence, the model can be used in interactive mode with the decision maker to evaluate alternatives.

The development of the model is demonstrated on a small system, and its efficacy is proven on a large WSS that emulates the central part of the Israeli National Water System with several aquifers and desalination plants, using a 10-year historical time series of aquifer recharge. Sensitivity runs are used to indicate the robustness of the methodology and its application for testing proposed modifications in the system.

Appendix A

The model can be formulated as the following nonlinear optimization problem:

$$\min_{u^t \forall t} F = \sum_{t=1}^{T_f} f(x^{t-1}, u^t, p^t)$$

s.t.

$$
\left.
\begin{array}{l}
x_r^t = W(x_r^{t-1}, u^t, p^t) \quad \forall r = 1...n_1 \\
y_r^t = V(y_r^{t-1}, x_r^{t-1}, x_r^t, u^t, p^t) \quad \forall r = 1...n_1 \\
A^t \cdot u^t \leq b^t \\
g_j(y^{t-1}, x^{t-1}, u^t, p^t) \leq 0 \quad \forall j = 1...m \\
\mathrm{LB}_i^t \leq u_i^t \leq \mathrm{UB}_i^t \quad \forall i = 1...n
\end{array}
\right\} \forall t = 1...T_f
$$

$$(A1)$$

where t is the stage index $t \in [1, T_f]$; $u^t \in R^n$ is vector of decision variables; $x^t \in R^{n_1}, y^t \in R^{n_1}$ are two vectors of state variables corresponding to the aquifers state variables (n_1 is number of aquifers); p^t is a vector of parameters; $f, W, V, g_j \ \forall j$ are nonlinear functions; A^t is a rectangular coefficient matrix; b^t is RHS vector; $\mathrm{LB}^t \in R^n, \mathrm{UB}^t \in R^n$ are lower and upper bounds respectively.

Each of the T_f stages has its contribution to the objective function f^t, set of constraints $g_{j=1...m}^t \leq 0$, decision variables $u_{i=1...n}^t$ and state variables $x_{r=1...n_1}^t$, $y_{r=1...n_1}^t$, where f^t, g^t denote $f(x^{t-1}, u^t, p^t)$ and $g(y^{t-1}, x^{t-1}, u^t, p^t)$ ' respectively. The overall objective is to minimize $F = \sum_{t=1}^{T_f} f^t$ satisfying the constraints $\forall t = 1...T_f$ while the decision variables are $u_{i=1...n}^{\forall t=1...T_f}$.

The time-chained-method (TCM)

A finite difference scheme provides estimations for $\nabla F \in R^{1 \times n \cdot T_f}$ and of the Jacobian matrix of the nonlinear constraints $J \in R^{n \cdot T_f \times m \cdot T_f}$. The central finite differences scheme to calculate an approximation of ∇F is:

$$\frac{\partial F}{\partial U_v} \approx \frac{F(U + \delta_v \cdot e_v) - F(U + \delta_v \cdot e_v)}{2 \cdot \delta_v} \quad \forall v = 1...n \cdot T_f \quad (A2)$$

where U is the multi-year vector of decision variables that contains the annual decision vectors $u^t \ \forall t$ i.e. $U = [u^1, ..., u^{T_f}]$; δ_v is a perturbation step of variable v; e_v is the unit vector in direction v.

Estimation of ∇F requires $2 \cdot n \cdot T_f$ evaluations of the function F and the state equation of x, each evaluation needs the computation for all T_f stages. Suppose S_{time} is the computation time for one stage, therefore the total computation time is:

$$
\begin{aligned}
\mathrm{Time} &= 2 \cdot n \cdot T_f^2 \cdot S_{\mathrm{time}} \\
\mathrm{Time} &= O\left(T_f^2\right)
\end{aligned}
\quad (A3)
$$

For brevity, only the estimation of ∇F is presented; the calculation of the Jacobian matrix of the constraints follows the same logic.

Efficient estimating of ∇F

Each stage t is linked to the previous stages through the state variable so that the derivatives of the objective function with respect to (w.r.t.) former decisions can be calculated using the derivative of the objective function w.r.t. its own input state variable and the derivatives of these state variable w.r.t. previous decisions. For example, to calculate the derivative of the objective function of stage 3 with respect to the decisions of stage 1, u^1, we can use the derivatives of f^3 w.r.t. x^2, derivatives of x^2 w.r.t. x^1 and derivatives of x^1 w.r.t. u^1 as depicted in Fig. A1.
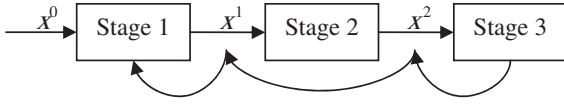
Fig. A1. Scheme of TCM for 3 stages.

The following steps take advantage of two properties of the model: (a) $\nabla F = \sum_{t=1}^{T_f} \nabla f^t$ i.e., the objective function is additive, (b) the functions of stage t do not depend (obviously) on decision variables of later stages thus:

$$\frac{\partial f^t}{\partial u_i^k} = 0 \quad \forall k = t+1\ldots T_f \quad \forall i = 1\ldots n \tag{A4}$$

For each function f^t we have to estimate $(\partial f^t/\partial u_i^k)$ $\forall k = 1\ldots t$ $\forall i = 1\ldots n$.

For the n derivatives $(\partial f^t/\partial u_i^t)$ $\forall i = 1\ldots n$:

$$\frac{\partial f^t}{\partial u_i^t} \approx \frac{f(x^{t-1}, u^t + \delta_i e_i, p^t) - f(x^{t-1}, u^t - \delta_i e_i, p^t)}{2 \cdot \delta_i} \quad \forall i = 1\ldots n \tag{A5}$$

We can also estimate the derivatives $(\partial f^t/\partial x_r^{t-1})$, $(\partial x_r^t/\partial u_i^t)$ and $(\partial x_r^t/\partial x_r^{t-1})$

$$\frac{\partial f^t}{\partial x_r^{t-1}} \approx \frac{f(x^{t-1} + \delta_r e_r, u^t, p^t) - f(x^{t-1} - \delta_r e_r, u^t, p^t)}{2 \cdot \delta_r} \quad \forall r = 1\ldots n_1 \tag{A6}$$

$$\frac{\partial x_r^t}{\partial u_i^t} \approx \frac{W(x^{t-1}, u^t + \delta_i e_i, p^t) - W(x^{t-1}, u^t - \delta_i e_i, p^t)}{2 \cdot \delta_i} \tag{A7}$$

$$\forall r = 1\ldots n_1 \quad \forall i = 1\ldots n$$

$$\frac{\partial x_r^t}{\partial x_r^{t-1}} \approx \frac{W(x^{t-1} + \delta_r, u^t, p^t) - W(x^{t-1} - \delta_r, u^t, p^t)}{2 \cdot \delta_r} \quad \forall r = 1\ldots n_1 \tag{A8}$$

The component r of x^t (i.e. x_r^t) is only dependent on x_r^{t-1}, then $(\partial x_{r=r'}^t/\partial x_{r=r''}^{t-1}) = 0 \quad \forall r' \neq r''$.

The remaining derivatives $(\partial f^t/\partial u_i^k)$ $\forall k = 1\ldots t-1$ $\forall i = 1\ldots n$ are given by the chain rule:

$$\frac{\partial f^t}{\partial u_i^k} = \sum_{r=1}^{n_1} \left(\frac{\partial f^t}{\partial x_r^t} \underbrace{\left(\prod_{j=k+1}^{t-1} \frac{\partial x_r^j}{\partial x_r^{j-1}} \right)}_{(k=t-1) \to 1} \frac{\partial x_r^k}{\partial u_i^k} \right) \quad \forall k = 1\ldots t-1 \quad \forall i = 1\ldots n \tag{A9}$$

Thus we need $2 \cdot (n + n_1)$ evaluations of the function f^t and the state equation of x in order to estimate ∇f^t and the linking derivatives, each of these evaluations needs only the computation of stage t.

Suppose S_{time} is the stage computation time, then the computation time for ∇f^t and the linking derivatives is $2 \cdot (n + n_1) \cdot S_{\text{time}}$.

Recalling that $\nabla F = \sum_{t=1}^{T_f} \nabla f^t$ hence the computation time for ∇F is:

$$\text{Time} = 2 \cdot (n + n_1) \cdot S_{\text{time}} \cdot T_f$$
$$\text{Time} = O\left(T_f\right) \tag{A10}$$

This procedure has been entitled the Time-Chained-Method (TCM).

Scaling

Solvers of nonlinear optimization are sensitive to scaling; one way to scale a problem is to introduce a linear transformation of the decision variables, of the form

$$\tilde{u}_i^t = a_i^t \cdot u_i^t + b_i^t \tag{A11}$$

where $a_{i=1\ldots n}^{\forall t=1\ldots T_f}$ are the scale weights and $b_{i=1\ldots n}^{\forall t=1\ldots T_f}$ are the shifts. In our problem the decisions variables are bounded, so we can normalize to the range [0 1] by

$$\tilde{u}_i^t = \frac{u_i^t - LB_i^t}{UB_i^t - LB_i^t} \tag{A12}$$

As a result of this transformation the linear constraints $A^t \cdot u^t \leq b^t$ should also be scaled.

The scaled linear constraints are:

$$A^t \cdot D^t \cdot \tilde{u}^t \leq b^t - A^t \cdot LB^t \tag{A13}$$

where D^t is a diagonal $n \times n$ matrix, $D^t = \text{diag}(UB^t - LB^t)$.

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