INTEGRATION OF WATER QUANTITY/QUALITY
IN RIVER BASIN NETWORK FLOW MODELING

by

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Robert C. Ward, Director
The inseparable interaction of water quantity and quality clearly exists in all river basins. Most river basin management models focus on either water quantity or water quality, with interaction, if any, accounted for by superficial trial and error processes. The MODSIM River Basin Water Rights Planning model developed at Colorado State University is extended in this study to incorporate constraints on water quality loading and concentrations. The new model, MODSIMQ, integrates a Lagrangian relaxation network solver with the Frank-Wolfe nonlinear programming algorithm to directly include conservative routing of water quality constituents, maintenance of salinity load mass balance, and imposition of constraints on water quality concentrations.

MODSIMQ incorporates a generalized model for estimating the quality of irrigation return flows and predicting quality transport mechanisms in groundwater. Routing of streamflow water quality constituents is performed through direct linkage with the EPA QUAL2E streamflow water quality routing model. An iterative procedure between MODSIMQ and QUAL2E assures convergence to solutions that satisfy water right priorities, while attempting to maintain minimum streamflow and water quality requirements. Irrigation return flows, canal seepage, reservoir seepage, deep percolation, and river depletion due to groundwater pumping are modeled using stream-depletion factors (SDF) developed by the U.S. Geological Survey. Water quality constraints can be imposed based on: (i) quality standards for certain river reaches; (ii) irrigation water quality control; (iii) water quality preference for demand nodes; and (iv) groundwater quality rehabilitation.

The Arkansas River Basin in Colorado is selected as a case study for application of MODSIMQ. Particular modeling challenges arise from complex legal and administrative issues governing operation of John Martin Reservoir under the Arkansas River Compact and Agreement B. Up to 45 special storage accounts and pools are defined in John Martin Reservoir using MODSIMQ. These storage accounts are essential to dictating when water users are allowed to place a call above John Martin Reservoir. MODSIMQ successfully models the complex water exchange mechanisms governing use of the many off-stream reservoirs administered in the Arkansas River Basin. Extensive model calibration exercises conducted for the case study area confirm that MODSIMQ reasonably reproduces both historical flows and salinity levels for water year 1988-1989, including consideration of stream-aquifer interactions in the basin.

Application of MODSIMQ to historical conditions of water year 1988-1989 in the lower Arkansas River Basin in Colorado results in satisfaction of all water supply requirements with conjunctive use of surface and groundwater, in contrast with actual historical operations that resulted in shortages to junior water right holders. Unfortunately, both the MODSIMQ and historical operations produce high salinity levels in the lower reaches of the study area. Imposition of water quality constraints in MODSIMQ encourages increased conjunctive use of surface and groundwater resources, resulting in dramatic improvement in water quality conditions, but at the expense of temporal distribution of water supply shortages that differ from those observed historically. These shortages, however, are
consistent in magnitude with estimated shortages that occurred during the historical period. Other scenarios are tested with MODSIMQ, such as assessing impacts of improved irrigation practices and transfer of water rights in the basin resulting in higher water use efficiencies.
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I. INTRODUCTION

1.1 Integrated Water Quantity/Quality Management

The inseparable interaction of water quantity and water quality clearly exists in any water resource system. Unfortunately, the management and regulation of water quantity and quality is not currently treated in an integrated fashion. National policies as reflected in the Clean Water Act of 1970 and the Federal Water Pollution Act of 1972 were established to unify actions affecting water systems by rejecting water policies that do not recognize the importance of all elements. However, current management practice rarely treats water systems as a whole. Many authors believe that fully integrating water quantity and quality issues in water resources management will alleviate many of the problems that exist between water users and water managers/administrators (Shih and Meier, 1972; Dworsky and Allee, 1977; Azevedo, 1994; and Rooy, et al., 1993).

Irrigation practice has been identified as one of the major contributing factors in quality degradation of groundwater and adjacent rivers (Duffy, 1984; Cain, 1984; and Sepehr, et al., 1985). Large downstream increases in salinity have been observed in numerous streams in the U.S., such as: the Colorado River Basin (Duffy, 1984; National Academy of Sciences, 1968), the Sevier River Basin (Sepehr, et al., 1984; Thorne, 1967), the Arkansas River Basin (Cooperative Extension Service, 1977; Cain, 1984; and Konikow and Bredehoeft, 1974), Rio Grande River Basin (Wilcox, 1962), and the lower San Luis Rey River Basin (Labadie and Khan, 1979). Duffy (1984) points out that one of the predominant factors for the trend in downstream salinity is dissolution and weathering of residual salts from soil and geologic strata by infiltration of excess irrigation water.

Although irrigation return flows can contribute significantly to salt loading of rivers and other water bodies, one way of controlling the detrimental effects is to increase irrigation efficiency and consequently reduce the amount of irrigation return flow. Therefore, while irrigation inefficiency is compensated by return flows, it can have serious implications for water quality in streams and connected alluvial aquifers. Poorly managed irrigation can result in environmental problems from transport of pesticides, nutrients, and sediments into water supplies. Repeated diversion and reuse of irrigation drainage results in on-site and downstream salinity degradation in most river basins. Concerns are being raised over crop yield loss and actual loss of land from salinization and rising saline water tables in some areas. Improvements in application efficiency can indeed reduce the amount of water moving through the soil and carrying contaminants into the connected alluvial aquifer and adjacent streams. However, widespread modification of on-farm irrigation technology could completely change the hydrogeologic character of a river system.

These interconnected water quality and quantity issues are a growing concern, and policy makers and producers alike are struggling to find solutions to these problems that are effective, profitable and socially acceptable. Although the Agricultural Chemicals and Groundwater Protection Act (SB 90-126) was established to promote voluntary adoption of
best management practices (BMP's), solutions are obscured by the difficulties in predicting environmental outcomes of the complex systems underlying allocation of water and the fate and transport of contaminants on a regional scale. It is likely that failure to voluntarily reduce adverse impacts on the environment will likely result in regulations that force compliance (Crutchfield, 1989). The public is demanding improvements in the conservation of water quantity and quality. Before policies are promulgated, however, all impacts of proposed policies must be assessed if there is hope of achieving improvement. These impacts must be studied at the regional or river basin scale, and not limited to localized impacts. In addition, evaluation of water rights and interstate compact agreements must be included in policy evaluation, particularly in river basins in the western U.S. governed by some form of the prior appropriation doctrine of water rights.

1.2 Literature Review

Shih and Meier (1972) developed an integrated water quality-quantity management model, involving minimization of the total cost for waste treatment, water treatment, and reservoir operation for water supply. The general approach was based on problem decomposition afforded by application of dynamic programming (DP). However, the model is limited to a dual state variable—single-decision variable problem due to the state dimensionality limitations inherent in the DP algorithm. Furthermore, pertinent components in a river basin such as groundwater supply were not considered. Similar studies have been conducted by Loucks and Jacoby (1972) and Lee, et al. (1993). Most of these studies utilize simplified simulation models, with little inclusion of optimization methods. The integration of water quantity and quality issues greatly magnifies the range and complexity of alternative management strategies, thereby making it essential to incorporate efficient optimization techniques for screening the best solutions.

Loftis, et al. (1985) included both water quantity and quality by combining simulation and nonlinear optimization techniques to determine optimal operational guidelines for a system of lakes. Quantity and quality modules were placed in separate subproblems, and then integrated through iterative procedures converging on target temperature and dissolved oxygen (DO) concentrations for key reaches in the system. Target water quality levels were achieved through regulation of lake operating strategies as well selective withdrawal from various levels in those lakes with the requisite control structures installed.

Liang and Nnaji (1983) utilized linear and separable programming techniques to determine well pumpage schemes to meet target water supply concentration levels. The authors assert that the processes of reducing concentrations of incoming flows are usually too expensive, and hence, mixing waters of differing qualities can produce water of usable quality without resorting to expensive water purification processes. However, the strategy of controlling water quality by mixing water from different sources is not suitable under two conditions: (i) the quality of water from available sources are not sufficiently different, and (ii) sources with suitable water quality are extensive distances from where they will be used. Mehrez, et al. (1992) developed a nonlinear programming model for optimal real-time operation of a regional water supply system. Numerous water sources of varying water
qualities are distributed to a variety of uses with differing flow and quality requirements. The objective is to minimize daily operational expenses of groundwater pumpage, subject to numerous constraints, including predefined consumer water quality and water quantity demands. These hard constraints must be satisfied for a feasible solution, which greatly decreases the flexibility of the model since ideal water user quantity and quality demands may be impossible to achieve in real world systems.

Considerable research has been conducted on development of realistic simulation and optimization models for river basin planning and management. Models employing simulation attempt to describe system behavior and predict consequences of alternative system designs and operational strategies as a basis for rational decision making. Simulation models are not hampered by formal structures required by optimization models, thereby creating the potential for highly accurate modeling of system behavior. The disadvantage is that lack of optimization capability requires specification of restrictive a priori operating rules. HEC-5 (HEC, 1991), one of the most popular river basin simulation models, was developed to assist in planning studies for evaluating proposed reservoirs in a system and assist in sizing flood control and conservation storage requirements for each recommended project for the system. It has also been utilized for selecting reservoir release policies for hydropower, water supply, and flood control, albeit through trial and error mechanisms. Although HEC-5 includes limited optimization capability in maximizing system firm yield, it cannot directly find the most desirable solutions. In addition, administrative and institutional aspects of water allocation, such as assigning water allocation priorities due to water rights, are not considered in HEC-5. A water quality version HEC-5Q (HEC, 1991), incorporates water quality routing into HEC-5. Although water quality targets may be specified in HEC-5Q at certain key control points in a river basin, these targets are achieved through optimization of selective control structure operations. No direct optimization is performed to attain water quality targets through manipulation of reservoir system operating strategies. Both HEC-5 and HEC-5Q are not designed for incorporation of stream-aquifer system interactions in river basin management.

QUAL2E (Brown and Barnwell, 1987) focuses on simulating water quality impacts of streamflows based on given river system regulation policies. The model is incapable of optimizing regulation policies to achieve desired water quality targets, although trial-and-error procedures can be utilized to interactively assess the impacts of changes in river regulation policies. Streamflow water quality conditions can be simulated in QUAL2E under both steady-state and dynamic scenarios. The model is capable of simulating stream water quality conditions under both steady-state and dynamic conditions. Due to the comprehensiveness and versatility of the model, it has been widely utilized in numerous studies (e.g., Todd and Bediant, 1985; Tischler et al., 1984; and Cubillo et al., 1992).

A more accurate means of predicting the quality of irrigation return flow is to use finite difference methods to solve the advection-dispersion equations of the transport mechanisms in groundwater. Various solution techniques such as: explicit, implicit and Crank-Nicholson schemes can be used to solve the aforementioned equations. Mackay and Sriley (1993) showed that both implicit and Crank-Nicholson can provide accurate solutions
when compared to analytical solutions. Several models are presented in Ahuja et al., (1995) as possible tools for predicting the quality of irrigation return flows using numerical models. These include: CMLS, EPIC, GLEMS, NLEAP, RZWQM, and UNSATCHM. These models can be utilized for analyzing the quality of return flows resulting from complex agricultural practices. However, some of these models are limited to modeling certain specific water quality constituents. For example, NLEAP is only capable of modeling the leaching mechanisms of nitrates. Moreover, most of these models require extensive field data, which is impractical for studying large-scale river basin systems.

1.3 Objectives of Study

A comprehensive river basin network flow and water rights simulation model is needed that can be incorporated into a decision support system for simultaneously assessing water quantity and quality impacts in both surface water and groundwater, while analyzing the effects of implementing improved irrigation practices on total flows in the river, water quality and water rights. Presented herein is an integrated water quantity/quality river basin management model MODSIMQ that is comprised of two existing models: MODSIM (Labadie, 1995) and QUAL2E (Brown and Barnwell, 1987), along with a soil column model for predicting salinity loadings in irrigation return flows. An iterative procedure based on the Frank-Wolfe nonlinear programming algorithm links MODSIMQ and the water quality models to assure convergence to solutions satisfying water right priorities, while attempting to maintain minimum water quality requirements. Unlike other integrated water quality and water quantity models, MODSIMQ has the ability to optimally allocate water subject to water quality restrictions and water quantity demands based on administrative priorities, water rights, or other ranking mechanisms such as economic evaluation. Irrigation return flows, canal seepage, reservoir seepage, deep percolation, and river depletion due to pumping are modeled using stream depletion factors developed by the U.S. Geological Survey. MODSIMQ successfully models the complex water exchange mechanisms governing use of off-stream reservoirs and conjunctive use of surface and groundwater resources.

MODSIMQ employs a state-of-the-art network flow optimization algorithm for simultaneously assuring that water is allocated according to physical, hydrological, and institutional/administrative aspects of river basin management. The underlying principle in the operation of MODSIMQ is that most complex water resource systems can be simulated as capacitated flow networks which can be solved by efficient minimum cost network flow algorithms. The components of the system are represented in the network as nodes, both storage (e.g., reservoirs, groundwater basins, and storage right accounts) and non-storage (e.g., river confluences, diversion points, and demand locations); and links or arcs (e.g., canals, pipelines, natural river reaches, and decreed water rights) connecting the nodes.

A real-world case study is presented to fully demonstrate the functionality and capability of MODSIMQ. The case study area chosen for this demonstration is the lower Arkansas River Basin in Colorado. Many attempts have been made to model the Arkansas River Basin (Burns, 1989; Cain, 1987; Cain, et al., 1980; McGuckin, 1977; Cain 1984; Abbott, 1986; Kuhn, 1987). However, due to the complexity and dimensions of the basin,
most of the aforementioned research either involved development of customized, nongeneralized models, or was limited to superficial treatment of the basin hydrologic/hydraulic/administrative features. Although MODSIMQ is capable of simulating up to 15 water quality constituents, including conservative and nonconservative elements, this case study on the Arkansas River Basin focuses on control of salinity in the basin. According to research conducted by Colorado State University and EPA (Cooperative Extension Service, 1977), the Arkansas Valley of Colorado had the U.S. Laboratory's highest classification of salinity hazard, thereby causing several million dollars of damage each year.

The water quality impacts of irrigation return flows (both as tailwater and deep percolation) represent an important factor in the existing salinity problem. The purpose of utilizing MODSIMQ for a river basin such as Arkansas River Basin, is to examine possible ways of alleviating existing water quality problems without violating any legal operational agreements, including modification of river operations, innovative water exchange mechanisms resulting in improvement in water quality conditions, conjunctive use of groundwater and surface water, and improvement in irrigation efficiency. The focus of this study is on the physical, hydrologic, and administrative feasibility of improving water quality conditions in the basin. Comprehensive economic analysis of feasible alternatives is left for future work.
II. WATER QUANTITY MODULE

2.1 Background

The water quantity module within MODSIMQ is based on the generalized river basin network flow model MODSIM developed at Colorado State University (Labadie, 1995). The underlying assumption of MODSIM is that most complex river basin systems can be accurately and efficiently represented in a network flow structure consisting of nodes and links. Nodes serve to represent storage components in a river basin such as reservoirs and aquifer storage; as well as nonstorage points of inflow, demand, diversion, and river confluence. Links connecting the nodes define river reaches, pipelines, canals, and stream-aquifer interconnections representing stream depletions from pumping and return flows from seepage and water applications. Links in a network flow model are required to be both unidirectional and capacitated, which means that every link in the system must have a predetermined flow direction with flows restricted to specified lower and upper bounds.

Links and nodes in MODSIM are not confined to representing physical components of a river basin system, but may also be utilized to symbolize artificial and conceptual elements for modeling complex administrative and legal mechanisms governing water allocation. In addition to the links and nodes defined by users, several accounting nodes and links are automatically created in MODSIM, as shown in Fig. 2.1. These nodes and links are

![Figure 2.1. Illustration of MODSIM Network Structure with Accounting Nodes and Links](image)

Figure 2.1. Illustration of MODSIM Network Structure with Accounting Nodes and Links
essential to satisfying the fully circulating network requirement imposed by the network flow algorithm. Once the network is constructed, a highly efficient network flow optimization algorithm is employed in MODSIM, providing solutions which simulate the allocation of water in a river basin according to water rights and other priority structures.

MODSIM has been successfully applied to numerous river basins, such as: the Piracicaba River Basin (Azevedo, 1994); Rio Grande River Basin (Graham, et al., 1986); Nile River Basin (El-Beshri and Labadie, 1994); Cumberland River Basin (Labadie, 1983); South Platte River Basin (Fredericks and Labadie, 1995); Upper Colorado River Basin (Law and Brown, 1989); Upper Pampanga River Basin, Philippines (Faux, et. al., 1983); Poudre River Basin, Colorado (Labadie, et. al., 1986); and the Upper Snake River Basin (Frevert, et. al., 1994). This study applies MODSIM, as embodied in MODSIMQ, to the lower Arkansas River basin in Colorado, with consideration of both water quantity and quality.

2.2 Network Flow Optimization Problem

MODSIM simulates water allocation mechanisms in a river basin through sequential solution of the following generalized network flow optimization problem for each successive time period $t$:

$$\text{minimize } \sum_{\ell \in A} w_{\ell t} q_{\ell}$$

subject to:

$$\sum_{k \in O_i} q_k - \sum_{\ell \in I_i} q_{\ell} = b_{it} \quad \text{for all nodes } i \in N$$

$$l_{\ell t} \leq q_{\ell t} \leq u_{\ell t} \quad \text{for all links } \ell \in A$$

where $A$ is the set of all arcs or links in the network; $N$ is the set of all nodes; $O_i$ is the set of all links originating at node $i$ (i.e., outflow links); $I_i$ is the set of all links terminating at node $i$ (i.e., inflow links); $b_{it}$ is the (positive) supply or (negative) demand at node $i$; $q_{\ell t}$ flow rate in link $\ell$; $w_{\ell t}$ are costs, weighing factors, or water right priorities per unit flow rate in link $\ell$, which in some cases can vary with time $t$; and $l_{\ell t}$ and $u_{\ell t}$ are specified lower and upper bounds, respectively, on flow in link $\ell$. The network flow optimization problem represented by Eqs. 2.1 to 2.3 is solved with a highly efficient Lagrangian relaxation algorithm based on dual coordinate ascent called RELAX-IV (Bertsekas and Tseng, 1994), which is up to two orders of magnitude faster than the revised simplex method of linear programming. Comparative studies by Kuczera (1993) and Ardekaaniaan and Moin (1995) have shown the RELAX algorithm to be the most efficient network solver, as compared to primal-based algorithms and variations of the out-of-kilter method.
The network topology and object characteristics are completely defined by the sets \( N \), \( O \), \( I \), and arc parameters \([l_{it}, u_{it}, w_{it}]\) for each arc or link \( t \), for each time period \( t \).

Solution of Eqs. 2.1-2.3 is executed period by period, rather than as a fully dynamic optimization. Flows in the carryover storage arcs shown in Fig. 2.1 become initial storage levels for the next period optimization. In this way, the optimization performed in MODSIM is primarily a means of accurately simulating the allocation of water resources according to water rights and other ranking mechanisms, which may include economic factors. An object oriented graphical user interface included with MODSIM allows creation of the network topology and data base through simple point and click mouse control operations on desktop computers under MS Windows. Execution of the network optimization model is launched within the graphical user interface, along with graphical output of solution results.

2.3 River Basin Components as Network Elements

2.3.1 Unregulated Inflows and Basin Import

Since MODSIM does not include a watershed runoff model, all system inflows are precalculated and input to MODSIM. Unregulated inflows may be based on historical data, future forecasts, drought scenarios, or synthetic generation of streamflows. They are assigned as right-hand-side constants in Eq. 2.2 for both storage and nonstorage nodes:

\[
b_{it} = I_{it} + S_{it} \quad \text{for storage node } i \\
b_{it} = I_{it} \quad \text{for nonstorage node } i
\]

where \( I_{it} \) is the inflow to node \( i \) during period \( t \) and \( S_{it} \) is the storage in reservoir node \( i \) at the beginning of period \( t \). MODSIM allows consideration of import nodes, representing nodes receiving water from transbasin diversion projects. In contrast with unregulated inflows, imported water is entered as annual, quarterly, or weekly total flows, with corresponding monthly, weekly, or daily fractional coefficients entered to represent the temporal distribution of imported water.

2.3.2 Reservoir Operating Targets

Carryover storage accounting links originate at each reservoir and accumulate at the accounting carryover storage node \( S \), as shown in Fig. 1. They include an accounting active storage link and an accounting flood storage link with the following arc parameters:

\[
[S_{i,\text{min}}, T_{it}; w_{it}] \quad \text{for accounting active storage link } \ell=[i,S]_1 \text{ originating at storage node } i \text{ and terminating at node } S.
\]

\[
[0, S_{i,\text{max}} - T_{it}; 0] \quad \text{for accounting flood storage link } \ell=[i,S]_2 \text{ also originating at storage node } i \text{ and terminating at node } S
\]
where \( S_{i,\text{min}} \) is the minimum allowable storage in node \( i \), \( S_{i,\text{max}} \) is the maximum allowable storage in node \( i \), \( T_{it} \) is the ideal target storage level for active storage node \( i \) for the current period \( t \), and
\[
w_{it} = -\left(50000 - 10 \cdot OPRP_i\right)
\]
for accounting active storage link \( \ell = [i,S]_t \) (2.4)

where \( OPRP_i \) is a water rights priority ranking between 1 and 50000, where a lower number indicates a higher ranking. Alternatively, the user may enter a storage right decree date, which is then automatically translated into a priority ranking in MODSIM. Again, priority \( w_{it} \) is shown as a function of \( t \) since, in some cases, priorities may vary with time. Notice that these rankings are translated into negative weights or costs in Eq. 2.4 which are assigned to the accounting active storage links. Since the accounting flood storage link is assigned a weight of 0, the negative weight on the accounting active storage link insures that it is always filled first in the network flow cost minimization algorithm.

2.3.3 Evaporation Loss

Evaporation loss is calculated in MODSIM as a function of average surface area in the reservoir over the current period. Since average surface area in a reservoir is normally unknown until calculations are completed for the current period, an iterative process requiring successive solutions of the model is usually required for accurate calculation of evaporation loss. A procedure is adopted in MODSIM, however, which does not require successive iterations to estimate evaporation loss. For each reservoir \( i \), compute:

\[
E_{i,\text{max}} = e_u \cdot \left[A_i(S_u) + A_i(S_{i,\text{max}})\right]/2
\]

\[
E_{i,\text{min}} = e_u \cdot \left[A_i(S_u) + A_i(S_{i,\text{min}})\right]/2
\]

\[
E_{i,\text{target}} = e_u \cdot \left[A_i(S_u) + A_i(T_u)\right]/2
\]

where \( e_u \) is net evaporation rate (i.e., evaporation rate less rainfall rate) for reservoir \( i \) (e.g., feet per month) for the current period; \( A_i(S_u) \) is the (interpolated) area-capacity table for reservoir \( i \), \( S_u \) is storage at the beginning of the current period \( t \), \( S_{i,\text{max}} \) is the maximum capacity, \( S_{i,\text{min}} \) is dead storage, and \( T_u \) is user supplied target level.

The storage link parameters are then adjusted as follows:

for active storage links:
\[
[0, (S_{i,\text{max}} - T_u) + (E_{i,\text{max}} - E_{i,\text{target}}), 0]
\]

for flood storage links:
\[
[(S_{i,\text{min}} + E_{i,\text{min}}), (T_u + E_{i,\text{target}}), w_{it}] \text{ for link } \ell = [i,S]_t
\]

In this formulation, link upper bounds are adjusted to carry sufficient flow to include evaporation loss, and the lower bound on the active storage link is increased such that when
evaporation is removed, it will not be violated. After calculations for the current period are completed, flows in the carryover storage links (i.e., the total end-of-period storage, plus evaporation loss) are adjusted such that evaporation loss is removed so as to provide carryover storage for the next period:

1. An initial guess $EVP_i$ of evaporation loss is first made. The total carryover storage in reservoir node $i$, including evaporation loss, is: 
   
   $$q_{i, \text{total}} = (q_{i, \text{active}} + q_{i, \text{flood}})$$

2. The current estimate of actual end-of-period storage is
   
   $$S_{i, \text{final}} = q_{i, \text{total}} - EVP_i$$

3. Compute the average surface area $A_{i, \text{ave}}$ over the period for each reservoir $i$:
   
   $$A_{i, \text{ave}} = 0.5 \cdot [A_i(S_{i, \text{begin}}) + A_i(S_{i, \text{end}})]$$

   and update the evaporation estimate $EVP_i$ as
   
   $$EVP_i = e_i \cdot A_{i, \text{ave}}$$

4. Return to Step 2 and repeat until successive evaporation estimates converge within a predefined error tolerance.

Evaporation loss is not directly calculated for other water bodies such as streams in MODSIM. For streams, however, channel loss coefficients may be appropriately increased to account evaporation losses, or properly adjusted to consider a net loss term which includes rainfall. Since channel loss coefficients are allowed to vary seasonally (e.g., monthly), adjustments for evaporation and rainfall can also be made seasonally.

2.3.4 Consumptive Demands

MODSIM automatically creates accounting demand links which originate at each demand node and accumulate at a single accounting demand node $D$, as seen in Fig. 2.1. The parameters for the accounting demand links are defined as:

$$[0, D_i, w_{\ell}]$$ for accounting demand link $\ell = [i, D]$ originating from demand node $i$

where demands $D_i$ may be defined as: historical diversions, decreed water right amounts, predicted agricultural demands based on consumptive use calculations (performed outside the model), or projected municipal and industrial demands. The link weights or costs on the accounting demand links are calculated as follows:

$$w_{\ell} = -(50000 - 10 \cdot DEMR_i)$$ for accounting demand link $\ell = [i, D]$ (2.8)

where, as with reservoir storage priorities $OPRR_i$, the user selects priorities $DEMR_i$ for demands between 0 and 50000, with lower numbers representing higher priorities. These
priorities must be selected in relation to the reservoir storage priorities and may also be entered as water right decree dates. If shortages must occur, then demands with lower priority (i.e., junior water rights) are denied flow first in the optimization since they have a less negative weight. For inefficient water application, MODSIM is capable of calculating return flows via groundwater or tailwater as surface drainage.

Although Fig. 2.1 shows a single diversion link to the demand at node 3, a particular demand may own several direct diversion rights on natural flow in the river. In this case, the user may specify several diversion links to the same demand node, with the capacity of each link corresponding to the decreed amount for each water right. Time variable decrees may be specified through use of variable capacity links. As shown in Fig. 2.1, it is usual to specify a final demand node at the farthest downstream drainage point in the basin which is assigned a large demand to account for the highest possible downstream flows. However, these demands are assigned the lowest priority in the basin so that all water is first allocated upstream, unless there are higher priority downstream rights.

2.3.5 Instream Flow Requirements

As illustrated in Fig. 2.2, MODSIM also provides for demands which are not consumptive; i.e., instream flow demands which flow through the demand node and remain in the network for possible downstream diversion. In effect, this corresponds to demands with 100% return flow which is unlagged. This includes demands for instream flow uses for navigation, water pollution control, fish and wildlife maintenance and recreation. Flow-through demands are also useful for augmentation plans, exchanges between basin water users, and development of reservoir release operating rules. Although minimum streamflow

\[
q^{(k)}_\ell = \text{Flow in link } \ell = [2,D] \\
\text{for iteration } k
\]

\[
[q^{(k-1)}_\ell, q^{(k-1)}_\ell, 0]
\]

Flow-through demand

\[
[0, D_2, w_2]
\]

\[
D
\]

**Figure 2.2.** Illustration of Flow-Through Demand for Instream Flow Uses
requirements could be set by assigning a minimum flow $l_{2t} = D_{2t}$ to link 2, where $D_{2t}$ is the minimum streamflow requirement, there are two disadvantages to this approach: (1) the instream flow demand implicitly has the highest priority in the basin in this case since the lower bound constitutes a **hard** constraint; and (2) there is increased danger of infeasible network solutions if a hydrologic period is encountered with insufficient flow to maintain the instream flow requirement.

The **flow-through demand** operates by iteratively removing flow as a demand from the network, but then replacing the flow to any downstream node(s) specified by the user. For purposes of instream flow requirements, usually only one downstream **accrual node** is specified. It should be emphasized that, in effect, it is as if the flow was never actually removed from link 2. The **superscript k** in Fig. 2.2 represents an iteration counter, since flow-through demand returns must be calculated iteratively through successive solutions of the network. In the first iteration $k=0$, the demand is treated as a consumptive demand and flow is delivered according to priority through solution of the network algorithm. At the next iteration, the flow $q^{(0)}_t$ actually observed to have been delivered in link $t = [2, D]$ is then added to the bounds of the **accounting inflow link** returning flow to accrual node 4, and the network is solved once again. This solution process continues until successive estimates of returns to node 4 agree. Notice that this iterative scheme prevents complications in setting priorities to instream flow requirements. Otherwise, the priority assigned to the instream flow demand would have to exceed the total priority of all downstream junior rights for the allocation to perform correctly.

### 2.3.6 Link Capacities and Losses

MODSIM includes the capability of allowing users to input a constant bound for each link, or varying daily, weekly or monthly maximum flow limits for certain specified **variable capacity** links. The latter are useful for considering seasonal influences in canal capacities and maintenance schedules. In addition to variable capacity links, MODSIM allows specification of **seasonal capacity links**, whereby a total seasonal maximum flow through a particular link may be specified. Once the seasonal maximum is exceeded, the link is effectively **turned off** for that season, and no further diversions can be made through the current season. For monthly time steps, for example, a season would be considered as one year in length. **Minimum flow capacities** may also be assigned to any link in the network, but care must be taken since improperly assigned minimum and maximum flow capacities on links are the major reasons for network solutions terminating in infeasibility errors.

An iterative procedure is employed in MODSIM for calculating channel losses, as illustrated in Fig. 2.3. First, network flows are initially solved via the network optimization algorithm with **no losses** assumed. The losses in each link are then computed by multiplying the loss coefficient $cl_i$ by the calculated flows from the initial solution. This loss is removed during the next iteration by an accounting link to the **accounting groundwater node** $GW$ with both lower and upper bounds set to the amount of loss. The network flow algorithm is then solved again. If current flows in the reach agree with those found in the previous iteration,
then convergence has occurred. Otherwise, the procedure is repeated with channel losses defined on the bounds of the accounting link updated to reflect current flows in the real link.

As an alternative to this iterative approach to computing channel losses, networks-with-gains algorithms can be employed which allow specification of channel loss factors directly in the network link characteristics. This is particularly useful if a portion of the channel losses can reappear as lagged return flows to specified downstream nodes. A network-with-gains algorithm is not employed in MODSIM for the following reasons. Once a direct connection between losses and return flows occur as variable links, complications arise in setting allocation priorities. A simple ranking mechanism setting, for example, \( w_{lt} < w_{mt} < w_{nt} \) is not necessarily sufficient to guarantee that flow in link \( \ell \) has higher priority than flow in link \( m \), which in turn is ranked higher than flow in link \( n \). In addition, networks-with-gains algorithms are more computationally time consuming than the pure network algorithm employed in MODSIM, which may balance the computational cost of several iterations.

### 2.4 Reservoir Storage Rights and Exchanges

For reservoirs with storage right accounts, it is necessary to treat them as offstream reservoirs, even if they are actually on-stream reservoirs. As shown in Fig. 2.4, the reservoir is represented as off-stream storage, with accrual links diverting flow to each storage account and release links returning to the river. Each storage account in the reservoir is treated as a separate account reservoir. The account reservoir should not be confused with the terms accounting nodes and links, since the former is a real node which is supplied by the user. Notice that flow must be allowed to bypass the reservoir, which, for an on-stream reservoir, represents flow passing through the reservoir to satisfy senior demands downstream. In effect, nodes 2, 3, and 4 combine to represent a single physical reservoir containing two storage accounts.
The accrual links in Fig. 2.4 are assigned negative costs as related to fill decree priorities. They can be specified as variable capacity links if there are time limitations on the fill period. Zero capacities can be set for those periods where the reservoir is not allowed to fill. In addition, the accrual link can be specified as a seasonal capacity link, with the seasonal capacity corresponding to the amount of the fill decree. Storage refill priorities may also be specified in MODSIM.

Since storage account volume generally depends on reservoir evaporation, the account reservoirs are associated with a parent reservoir that adjusts water right account storage volumes for total reservoir evaporation. Evaporation data are read in for the parent reservoir, as well as the area-capacity-elevation tables. Total volume is determined from the volumes of the storage account child reservoirs attached to the parent reservoir. It is not necessary to provide formal links connecting the parent reservoir to the system network or to its associated storage account reservoirs. All network linkages are directed to and from the child or storage account reservoirs. Total evaporation loss calculated in the parent reservoir is debited from each storage account according to the fraction of contents in each account in relation to total contents in the reservoir at the beginning of the period.

Although accrual to the storage accounts via the accrual links in Fig. 2.4 are governed by the normal, priority based allocation process of MODSIM, once water is available in a storage account, it must be released to the owner as needed to satisfy demands. This implies a process which is not governed by priority-based network flow allocation. The storage ownership link shown in Fig. 2.4 is related to one of the accrual links to the child account reservoirs. This guarantees that the owner of the storage right receives water from the correct account. In order to allow for allocation of releases from storage accounts to the owners of those accounts, MODSIM includes an additional iterative step which is performed after
allocation of all natural flows or direct diversions according to water right priority. The storage allocation step follows the natural flow allocation step in MODSIM. During the natural flow allocation step, releases are not allowed from the storage accounts, and diversions to the storage ownership links are also temporarily turned off. MODSIM evaluates the volume available in the storage account, and releases via the outflow links an amount which is the lower of the volume available versus the shortage incurred by the storage account owner. This is accomplished by executing the network flow algorithm with storage account outflow link bounds fixed to assure release of the correct amount of water. Demands may of course have several storage ownerships as well as several natural flow rights.

The ability for water users to formulate exchange agreements and plans for augmentation have become an important part of water administration in many highly appropriated river basins. For example, a water user may own storage rights in a reservoir from which it is physically impossible for the owner to directly receive releases. In this case, MODSIM allows exchange mechanisms to take place whereby releases are made to downstream senior water right holders, and in return, the storage right owner is allowed to divert water out of priority. Since all natural flow links are fixed to the allocations obtained during the natural flow allocation step, there is no danger of senior water right holders being injured by this procedure. Although a storage owner has a certain amount of water available for release for exchange purpose, there may be insufficient flow available for upstream diversion to the storage right owner. In this case, MODSIM monitors how much flow the storage owner was actually able to divert, and then reduces the amount available to be released from the storage account accordingly during the next cycle of iterations.

2.5 Stream-Aquifer Modeling Components

2.5.1 Background

The stream-aquifer module within MODSIM allows consideration of reservoir seepage, irrigation infiltration, pumping, channel losses, return flows, river depletion due to pumping, and aquifer storage. Stream-aquifer return/depletion flows are simulated using response coefficients calculated using the one dimensional equations developed by Maasland (1959), Glover (1977), and McWhorter (1972). Alternatively, groundwater response coefficients estimated from other methods such as the stream depletion factor (SDF) method (Jenkins, 1968), the three-dimensional finite difference groundwater model MODRSP/MODFLOW (Maddock and Lacher, 1991), or the discrete kernel generator GENSAM (Morel-Seytoux and Restrepo, 1987), can be read into MODSIM from external data files.

The interaction of a water table aquifer receiving recharge from irrigation and precipitation, and an interconnected stream can be modeled utilizing the method developed by Maasland (1959). This method was developed for a parallel drain system and can be applied to a stream-aquifer system as well. Assuming height $h$ above the original saturated thickness $d$ is small, the linearized form of the original nonlinear partial differential equation for one-dimensional groundwater flow is
\[
\frac{\alpha \partial^2 h}{\partial x^2} = \frac{\partial h}{\partial t}
\]  
(2.9)

for \( \alpha = T/S \), where transmissivity \( T \) equals \( K \cdot d \); \( K \) is aquifer permeability; \( S \) is specific yield; \( x \) is distance measured along the path of flow; and \( t \) is time. Maasland (1959) obtained the solution

\[
h = \frac{4H}{\pi} \sum_{n=1,3,5,...}^{\infty} \frac{1}{n} \exp\left(-n^2 \pi^2 \frac{\alpha t}{L^2}\right) \sin\left(\frac{n\pi x}{L}\right)
\]
(2.10)

for boundary conditions: \( h = 0 \) @ \( x = 0 \), \( t > 0 \); \( h = 0 \) @ \( x = L \), \( t > 0 \); and \( h = H \) @ \( 0 < x < L \), \( t = 0 \); where \( H \) is initial uniform height of recharge water and \( L \) is spacing of the lateral drains. The fraction of total initially drainable volume in the aquifer at the end of time \( t \) available for flow to the drains is:

\[
F = \frac{8}{\pi^2} \sum_{n=1,3,5,...}^{\infty} \frac{1}{n^2} \exp\left(-n^2 \pi^2 \frac{\alpha t}{L^2}\right)
\]
(2.11)

### 2.5.2 Return Flow Calculations

Consider the idealized stream-aquifer system as shown in Fig. 2.5. The solution described above can be applied directly with drain spacing \( L \) equal to the valley width since the middle section of the parallel drains is a no-flow boundary and is analogous to either the left boundary or right boundary of the stream-aquifer system. If the parallel drain system is

![Figure 2.5. Idealization of Stream-Aquifer System (Glover, 1977)](image-url)
divided in half at the no flow boundary and rearranged to bring the drains into coincidence, the direct analogy with the stream-aquifer system is evident. The drains are replaced by the river and flow to the drains represents return flow to the river. When the river is not located at the center of the valley, the above solution (Eq. 2.11) is still applicable with $L$ equal to twice the width $W$ of either side of the valley (i.e., $L^2 = 4W^2$). Fraction $F$ can be determined for each side of the valley and return flows computed separately.

Let $N$ be the total number of time intervals of length $\Delta t$ and $I_k$ the recharge rate during the $k$-th time interval, where $k < N$. The fraction of return flow to the river during time interval $k$ is

$$\delta_k = F_{k-1} - F_k = \frac{8}{n^2} \left[ \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^2} \exp \left( -n^2 \pi^2 \frac{\alpha(k-1)\Delta t}{L^2} \right) 
- \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^2} \exp \left( -n^2 \pi^2 \frac{\alpha k \Delta t}{L^2} \right) \right]$$

(2.12)

where $\delta_k$ is defined as a unit response or discrete kernel for a recharge rate $I$ of unity. The total return flow $IRF_{ik}$ from previous and current time periods due to groundwater recharge at node $i$ is

$$IRF_{ik} = \sum_{\tau=1}^{k} I_{\tau} \cdot \delta_{i,k-\tau+1} ; \quad \delta_{i,k-\tau+1} = 0 \text{ for } k-\tau+1 > N$$

(2.13)

In MODSIM, upper bounds on accounting return flow links (Fig. 2.1) are adjusted iteratively. In the first iteration, lower and upper bounds are set equal to return flows computed from previous activities, which can be read in as input data since return flow from current activities are as yet unknown. MODSIM is now run for the current period using these bounds. Return flows from all sources are recomputed using diversions obtained from this solution. If changes in return flow estimates are within specified tolerance limits, the solution is assumed to have been found; otherwise bounds on the accounting return flow links are updated and the procedure repeated until convergence is achieved.

Since return flows are treated as natural flows returning to the river, and are not directly included as variable links in the network flow algorithm, complications associated with assigning water right priorities to diversions contributing to return flows are avoided. And yet, this iterative procedure converges to the same solution that would be obtained by using less efficient network-with-gains algorithms which would directly include return flows as variable links. The iterative process is a contractive mapping which always converges since return flow coefficients (i.e., calculated fractions of diverted flows returning during the current or future periods) are less than one.
2.5.3 Stream Depletion from Pumping

The same approach used for calculating return flows is also applied to calculation of stream depletion due to pumping:

\[
PSD_{ik} = \sum_{\tau=1}^{k} P_{ir} \cdot \beta_{l,k-\tau+1} ; \quad \beta_{l,k-\tau+1} = 0 \text{ for } k-\tau+1 > N \tag{2.14}
\]

In the case of groundwater withdrawal \( P_{ir} \), the same principles described above are applicable to determining response coefficient kernels \( \beta_{l,k-\tau+1} \). Here, it is river depletion that is considered rather than return flows to the river. Since the computation is sequentially carried out period by period in MODSIM, the current period stream-aquifer interactions are contingent upon stresses during previous periods. These can be provided as an input data file, or MODSIM can be run for an initial \( N \) periods for start-up or initialization purposes, such that after \( N \) periods, the model output can be trusted to properly account for past history.

2.5.4 Canal Seepage

Seepage from a canal or a stream is assumed to correspond to a line source of recharge water following the development of McWhorter (1972). After termination of the line source, the residual effect still contributes flow to the adjacent stream. The residual is taken into account by assuming an imaginary pumping source at the same location and initiating pumpage at the same rate as the recharge source from the time recharge terminates. The volume ratio at any time after recharge ceases is the difference between the volume ratio obtained if recharge had continued and the volume ratio obtained from pumping of the imaginary pumping source. For a discrete time interval, if the applied line source volume equals one, the volume ratio is in essence the unit response of line source or canal seepage.

If \( \varphi \) represents the unit response coefficient for canal link \( l \), the total return flow \( CRF_{lk} \) from canal seepage \( CS_{l1}, CS_{l2}, ..., CS_{lk} \) during each time interval \( k \) is

\[
CRF_{lk} = \sum_{\tau=1}^{k} CS_{l\tau} \cdot \phi_{l,k-\tau+1} ; \quad \phi_{l,k-\tau+1} = 0 \text{ for } k-\tau+1 > N \tag{2.15}
\]

As before, accounting return flow link bounds in MODSIM are adjusted iteratively to account for return flows from canal seepage.

2.5.5 Stream Depletion Factor

In calculating the unit response coefficients for return flows, stream depletions, and canal seepage, the aquifer parameters can be combined into an aggregate term called the stream depletion factor (SDF), where

\[
SDF = \frac{L^2S}{T} \tag{2.16}
\]

where \( L \) is the average lateral distance from the recharge source, canal source, or pumping well, to the adjacent stream. If distance \( L \) is in units of feet, and transmissivity \( T \) is in units
of ft$^2$/day, then $SDF$ is in units of days, which Jenkins (1968) has shown represents the time in days where the volume of stream depletion (or return flow) is 28% of the net volume pumped (or recharged) during time $t$. In a complex stream-aquifer system, the value of $SDF$ at any location depends on the integrated effects of irregular impermeable boundaries, stream meanders, aquifer properties, areal variation, distance from the stream, and hydraulic connection between stream and aquifer. The U.S. Geological Survey has developed maps and tables of $SDF$ coefficients for several basins, which are sufficient for computing the response coefficients utilized in MODSIM.
3.1 Introduction

Stream water quality models are important in helping decision makers to alleviate and improve many existing water quality problems. In general, water quality models can be grouped into four different classes as follows, in increasing complexity (McCutcheon, 1989): (i) zero-dimensional models, where a segment of the stream is described by a single computational element, ignoring any lateral, vertical, and longitudinal variation that may occur; (ii) one-dimensional models, where lateral and vertical variations are ignored, and the stream is described by a series of computational elements extending downstream and describing the longitudinal gradients that are prevalent in streams; (iii) two-dimensional models describing lateral and longitudinal gradients and assuming vertical variations are unimportant; and (iv) three-dimensional models describing vertical, lateral, and longitudinal gradients of water quality parameters.

These classifications are based on the way the stream is divided into computational elements and the way relevant equations are represented. Three-dimensional models are the most complex and thorough models, but are far too data intensive to be computational efficient for simulating stream water quality conditions in large river basin networks. On the other hand, the simplest zero-dimensional models are only applicable for screening-level analysis in a mixing zone. The less precise two- and one-dimensional models are the most common and practical approaches to simulating stream water quality conditions. Two-dimensional models require a more extensive data base for model calibration. Lacking the requisite data requirements for two-dimensional models, one-dimensional models may be more appropriate, particularly for streams where longitudinal gradients dominate vertical variations.

All of these aforementioned modeling approaches share a common basic principle: conservation of mass. Conservation is often applied by first defining a control region in the space to be analyzed. The following materials balance equation is written for each constituent over the control section:

$$Q_o C_o = Q_i C_i - \text{Decay Rate} - \text{Accumulation Rate}$$  \hspace{1cm} (3.1)

where $Q_o$ is outgoing flow rate from the control section; $Q_i$ is incoming flow rate; $C_o$ is constituent concentration of outgoing flow; and $C_i$ is constituent concentration of incoming flow.

The term "accumulation rate" in Eq. 3.1 is used to further classify water quality models into steady-state models and dynamic models. When accumulation rate is set to zero, the equation is used to describe steady-state or equilibrium conditions. The term "decay rate" in Eq. 3.1 is used to identify the constituents to be simulated. For conservative constituents, "decay rate" is set to zero; otherwise, the constituents are defined as nonconservative.
Examination of Eq. 3.1 reveals five actions that can be taken to reduce $C_o$ (outgoing concentration): (i) increase outgoing flow rate $Q_o$, (ii) reduce $Q_i$ (incoming flow rate), (iii) reduce $C_i$ (incoming concentration), (iv) increase decay rate, and (v) increase the accumulation rate. Reducing the amount of irrigation return flow can be an effective means of controlling water quality in receiving streams. Water quality models are essential to both describing and predicting the behavior of water quality conditions in a river basin. Furthermore, with advances in computer technologies and water quality modeling techniques, larger and more complex models can be constructed to accurately describe various stream conditions.

3.2 One-dimensional Stream Water Quality Modeling

One-dimensional stream water quality models are the most common and practical approaches to routing water quality constituents in a stream. The stream is discretized into a series of subreaches or computational elements extending downstream, ignoring any lateral and vertical variation that may occur, as shown in Fig. 3.1. Each computational element is visualized as a completely mixed reactor that is linked to adjacent computational elements via two mechanisms: transport by advection ($Q \cdot C$ in Fig. 3.1) and transport by dispersion ($A \cdot D_L \cdot \frac{\partial C}{\partial x}$ in Fig. 3.1). These two transport mechanisms move mass along the stream axis; however, mass can also be moved into or out of the subreach via two additional processes: external sources or sinks ($Q \cdot C_x$ in Fig. 3.1), and internal sources or sinks ($s$ in Fig. 3.1). With these four processes clearly defined, the basic equation for a one-dimensional stream water quality can be written as:

$$\frac{\partial M}{\partial t} = \frac{\partial (A_x D_L \frac{\partial C}{\partial x})}{\partial x} dx - \frac{\partial (A_x \bar{u} C)}{\partial x} dx + (A_x \frac{dx}{dt}) \frac{dC}{dt} + \frac{s}{dx}$$

where $M$ is mass; $x$ is distance; $t$ is time; $C$ is concentration, $A_x$ is cross-sectional area, $D_L$ is dispersion coefficient, $\bar{u}$ is mean velocity, and $s$ is internal source or sinks.

One dimensional models may be further classified into two categories: dendritic stream networks and branched stream networks. Dendritic refers to networks with flows in two or more branches combined at a node and leaving the node in a single branch. The entire flow of the system must be combined and leave the system in a single channel, as illustrated in Fig. 3.2. Branched stream networks, on the other hand, can handle networks with more complexity. Branched stream networks refer to networks with channels that diverge into more than one branches, and need not rejoin and leave the system with only one channel, as illustrated in Fig. 3.2.
3.3 Stream Water Quality Model QUAL2E

3.3.1 Introduction
QUAL2E is a one-dimensional stream water quality model developed by the U.S. Environmental Protection Agency (EPA). The model began with development of the QUAL-I model by Texas Water Development Board in the late 1960s (Texas Water Development Board, 1971). The original QUAL-I model was developed to simulate conservative constituents, temperature, biochemical oxygen demand, and DO in a one-dimensional steady flow river. Later, the model was enhanced by the EPA to include additional constituents such as: ammonia, nitrate, coliform, phosphate, and algae. The modified model of QUAL-I
was then generally referred to as QUAL-II. Moreover, with advance in the understanding of algal, nutrient, and light interactions, the QUAL-II model was further improved by the National Council for Air and Stream Improvement (NCASI) and given the acronym QUAL2E (Brown and Barnwell, 1987). The QUAL2E model has been widely utilized and tested for numerous river basins, such as: major rivers of the Comunidad de Madrid in Spain (Cubillo et. al., 1992), Buffalo Bayou in Houston, Texas (Todd and Bedient, 1985), and the Han River in Korea (Tischler et al., 1984).

The comprehensiveness and the versatility of QUAL2E has enabled the program to be utilized to simulate up to 15 water quality constituents in any desired combination, including:

1. Dissolved oxygen
2. Biochemical oxygen demand
3. Temperature
4. Algae as chlorophyll A
5. Organic nitrogen as N
6. Ammonia as N
7. Nitrite as N
8. Nitrate as N
9. Organic phosphorus as P
10. Dissolved phosphorus as P
11. Coliform
12. Arbitrary nonconservative constituent
13. Three conservative constituents

As a one-dimensional stream water quality model, QUAL2E assumes that the major transport mechanisms (advection and dispersion) are only significant along the axis of the main direction of flow, allowing QUAL2E to be implemented and solved utilizing the basic functional representation of one-dimensional stream water quality models.

### 3.3.2 Functional Representation

As mentioned previously, Eq. 3.2 is the most fundamental equation for all standard one-dimensional stream water quality models, and hence is also the equation utilized in QUAL2E. However, QUAL2E further simplifies Eq. 3.2 by assuming steady flow conditions in the stream where \( \frac{\partial Q}{\partial t} = 0 \). This simplified form of Eq. 3.2 is written as:

\[
\frac{\partial C}{\partial t} = \frac{\partial (A_x D_x \frac{\partial C}{\partial x})}{A_x \frac{\partial x}{\partial t}} - \frac{\partial (A_x \bar{u} C)}{A_x \frac{\partial x}{\partial t}} \frac{dC}{dt} + \frac{s}{V}
\]  

where

\[
M = VC
\]

\[
V = A_x \Delta x = \text{incremental volume (L}^3)\]

For steady-state conditions, the local derivative \( \frac{\partial C}{\partial t} \) is assumed to vanish. In QUAL2E, Eq. 3.3 is solved by numerically integrating the equation over space and time for each water quality constituent. The numerical solution technique requires this equation to be written for each of the computational elements in the network at each time step, and for each constituent. However, under most prototype conditions, analytical solutions cannot be derived for these aforementioned equations. According to the documentation of QUAL2E (Brown and Barnwell, 1987) a finite difference method (classical implicit backward difference method) is therefore applied to obtaining solutions. The accuracy of the numerical method used in QUAL2E has been confirmed by McCutcheon (1983), who compared the QUAL2E numerical solution to an analytical solution of the classical Streeter-Phelps equation under an extensive range of actual field conditions and found insignificant discrepancies. A detailed description of the numerical solution procedure for QUAL2E can be found in Brown and Barnwell (1987).

### 3.3.3 Computational Representation

The basic functional representation discussed in the previous section provides a fundamental methodology for constructing a river basin water quality model. However, in order to utilize the functional formulation of a one dimensional river quality model, an ordinary river network must be transformed into a certain format, where the spatial and temporal characteristics of the basin are represented by a series of computational elements.
**Computational representation** is the process of translating the network into a number of basic building blocks or computational elements.

The first step involved in the process of computational representation is to subdivide the stream system into a network of reaches, which are essentially sections of stream where the assumption of *uniform hydraulic characteristics* can be made. Each reach is then divided into computational elements of equal length. All reaches must consist of an integer number of computational elements with the same length; however, reaches in the network are not required to have the same length. Fig. 3.3 illustrates a portion of a river system being represented with a network of numbered reaches and computational elements.

The requirement that all computational elements in the same reach must be the same length, as one may argue, can present some difficulties when trying to accurately represent the spatial characteristic of a stream. However, by reducing the length of the computational elements, these difficulties can be eliminated.

### 3.3.4 Classification of Computational Elements

After subdividing a reach into a series of computational elements, QUAL2E requires each computational element to be identified as one of the predefined elements in QUAL2E. There are seven element types allowed, as listed below (Brown and Barnwell, 1987):

1. **Headwater source element:** The first element in a headwater reach for every tributary and main river system.
2. **Standard element:** An element that does not qualify as one of the remaining six element types. Incremental inflow/outflow are permitted in a standard element.
3. **Element on main stream immediately upstream of a junction:** Utilized to indicate an element on the mainstem situated just upstream of a junction.
4. **Junction element:** An element which receives flow from a simulated tributary.
5. **Most downstream element:** The last computational element in the river system; every river system must have one and only one of element type 5.
6. **Input (point source) element:** Indicates an element which has inputs.
7. **Withdrawal element:** Indicates an element which has withdrawals.

These elements are further exemplified in Fig. 3.4.
Figure 3.3. Stream Network of Computational Elements and Reaches (Brown and Barnwell, 1987).
3.3.5 QUAL2E Limitations

In order to achieve the full potential of QUAL2E, the limitations must also be carefully examined. The dimensional limitations of the program are as follows (Brown and Barnwell, 1987):

- Reaches: maximum of 25
- Computational elements: no more than 20 per reach or 250 total
- Headwater elements: maximum of 7
- Junction elements: maximum of 7
- Input and withdrawal elements: a maximum of 25 in total

An additional limitation of QUAL2E is related to the complexity of networks it can handle. As mentioned previously, one-dimensional models may be described by the manner in which complex networks can be simulated, as illustrated in Fig. 3.2. QUAL2E is limited to simulating dendritic streams, which means that the entire flow of the system must be combined and leave the system in a single channel.

In the process of developing an integrated water quality and quantity model, QUAL2E is required to interact with the water allocation model MODSIM. However, incompatibilities were encountered between the two models with respect to network representation. For example, Fig. 3.5 gives an example stream network with two reaches (links 1 and 2) with dissimilar hydraulic characteristics, and a diversion at node 1. This network can be easily represented in MODSIM with little difficulty. However, when this simple network is represented in QUAL2E, the last computational element for link 1 must be an element of type 3 (i.e., element just upstream from a junction) and the first computational element for link 2 must be an element type 4 (i.e., junction element). This means that the diversion cannot be placed at the intersection since a computational element in a reach can not be both a junction element and a withdrawal element. To overcome this situation...
problem, one may either change the way MODSIM represents this network or reconfigure the network to be compatible with QUAL2E. However, both of these approaches can be cumbersome and inaccurate.

### 3.4 Modification of QUAL2E

To overcome the aforementioned limitations of QUAL2E, it was necessary to make several modifications to the program code. After a careful study of the program, it was clear that retaining the integrity and the efficiency of the program is the most important factor, which means that any changes made to the program must be simple and effective.

The first enhancement incorporated into the program was the utilization of an algorithm, similar to that proposed by Lanfear (1990), to determine the proper stream order for the network. The term *proper stream order* is used here to describe a numbering scheme, whereby each link is assigned a unique order number starting with number one and ending with a number equal to the number of stream reaches in the network. Furthermore, the number increases as it proceeds downstream. For example, if reach number 5 is downstream of reach number 6, then the order number for reach number 5 must have a higher order number than reach number 6. A simple example of this numbering scheme is illustrated in Fig. 3.6, and the flow chart for the algorithm is illustrated in Fig. 3.7.
Once the stream order is established, QUAL2E is then utilized to calculate the water qualities for each reach, individually starting from the upstream reaches of the network and proceeds downstream. However, in order to connect the individual reaches as a whole, some modifications were made to the numerical solution technique used in QUAL2E.

Before any alteration was made to the program, QUAL2E (Brown and Barnwell, 1987) uses the following finite difference method to describe the spatial and temporal configuration of the system. The finite difference scheme is formulated by considering the constituent concentration $C$ at four points in the mnemonic scheme, as show in Fig. 3.8. Three points are required at time $n+1$ to approximate the spatial derivatives. The temporal derivative is approximated at distance step $i$.

The modification made to the program uses exactly the same method to determine the constituent concentration for the entire segment of the reach, however, at the end of the reach a different method, zero gradient assumption (Arden and Astill, 1970), is utilize to calculate the constituent concentration for the most downstream element of the reach. This approach simply inserts an imaginary computational element at the end of the reach with the same constituent concentration as the last computational element of the reach. In other words, when calculating the $C_i$ for the very downstream of a reach, $C_{i+1}$ is replaced with $C_{i+1}$. 

Figure 3.6. Example of the Proposed Stream Reach Numbering Scheme
Figure 3.7. Flow Chart for Proposed Numbering Algorithm

Figure 3.8. Classical Implicit Nodal Scheme (Brown and Barnwell, 1987)

Now, when calculating the quality conditions for the stream reach downstream of the reach segment already examined, the model feeds the constituent concentration in that imaginary computational element into the current reach as a fixed headwater source. The graphical
representation of this scheme is illustrated in Fig. 3.9. Similar approaches have also been proposed and proven to provide a satisfactory result by a number of researchers (Grimsrud et al., 1976; Hydroscience, Inc., 1972; Bartholow, 1995; Theurer and Voos, 1982, Theurer, et al., 1982, and 1984; and Rinaldi et al., 1979).

Modifying the program code as proposed herein permits the handling of large-scale, complex networks, such as the current study. Furthermore, the aforementioned incompatibilities between QUAL2E and MODSIM are effectively eliminated with these current enhancements.
IV. RETURN FLOW QUALITY MODULE

4.1 Introduction

It has been observed that substantial changes occur in drainage water quality as it percolates through the soil into groundwater. Moreover, excess water from irrigation practice has been criticized as one of the predominant factors in degradation of groundwater supplies. When quality conditions change in groundwater systems, there are similar impacts on water quality conditions in hydraulically connected streams. QUAL2E, as discussed previously, is designed for routing constituent concentrations in a stream; however, it is incapable of simulating water quality conditions in return flows. For the purposes of this study, it is therefore necessary to develop a module for predicting the quality of return flows, with the flow characteristics of return flows modeled using the previously discussed stream-aquifer components in the MODSIM model. Although a number of models are available (e.g., Bresler and Hanks, 1969; Konikow and Bredehoeft, 1974; and Sepehr et al., 1985), it is believed that the best approach is to develop a generalized model capable of estimating concentrations for a variety of constituents, thereby allowing direct interaction with the stream water quality model QUAL2E.

Another approach to predicting the quality of water as it percolates through the soil profile is to examine the processes of ion exchange and adsorption of solutes. Ion exchange is a process of a simultaneous transfer of ions in the solution and ions adsorbed on soil particles. Adsorption of solutes is a process by which the solid components in the soil are being adsorbed or released from or to the soil solution. Considerable research in developing models based on ion exchange and adsorption theories has been conducted by Dutt (1962a, 1962b), Dutt and Tanji (1962), Dutt and Doneen (1963), and Dutt, et al. (1972). These studies effectively model the complex chemical changes between excess irrigation water and soil particles. The fundamental solution techniques used to simulate ionic activities are based on theory originally derived by Gapon (1933) and the Debye-Hückel formula (Glasstone, 1947). Similar studies have also been conducted by a number of other researchers (Tanji et al., 1967a, 1967b; Thomas et al., 1971; Margheim, 1967; and Sylvester et al., 1963). Since the case study to be presented subsequently requires accurate estimates of salinity, a specialized model is developed for specifically predicting the salinity of irrigation return flows as an alternative to the generalized model.

4.2 Generalized Model

4.2.1 Transport Processes in Groundwater

The movement of constituents in the saturated zone of a phreatic aquifer can be modeled utilizing the method developed by Mackay and Riley (1993). The basic transport mechanisms in groundwater are advection and dispersion, but unlike surface water, advection is not simply the flow rate of the water. In groundwater, advective velocity \( u \) is defined as follows:
\[ u = \frac{1}{n_e} q \]  \hspace{1cm} (4.1)

where \( q \) is the specific discharge or groundwater volume flux and \( n_e \) is the kinematic or effective porosity of a volume of aquifer, which can be written as:

\[ n_e = \frac{\text{volume occupied by movable water}}{\text{total volume}} \]  \hspace{1cm} (4.2)

Furthermore, the advective mass flux \( J^a \) of dimension \( \frac{M}{L^2 T} \) is written as:

\[ J^a = n_e c u \]  \hspace{1cm} (4.3)

where \( c \) is the constituent concentration.

Dispersion is the process whereby the constituents migrate in nonparallel directions to the direction of advection. The directions of dispersion are related to two constants \( \alpha_L \) and \( \alpha_T \); the longitudinal and transverse dispersivities, respectively. The mechanical dispersion tensor \( D_y^{mn} \) is written as:

\[ D_y^{mn} = n_e \left( \alpha_L \delta_{ij} + (\alpha_L - \alpha_T) \frac{u_j u_i}{u} \right) \]  \hspace{1cm} (4.4)

where \( \delta_{ij} \) is the Kronecker delta (\( \delta_{ij} = 1 \) if \( i = j \); 0 otherwise). The total hydrodynamic dispersive flux \( J^D \) is the sum of the mechanical dispersive flux and the molecular diffusive flux, which can be shown to be:

\[ J^D_i = -D_y^{ij} \frac{\partial c}{\partial x_j} \]  \hspace{1cm} (4.5)

where \( J^D_i \) is the \( i \)th component of the hydrodynamic dispersive flux; \( D_y = D_y^{mn} + d_e \) is the \( ij \)th component of the hydrodynamic dispersion coefficient matrix \( D \); \( d_e = d_o n \chi \) is the effective or intrinsic coefficient of molecular diffusion; \( d_o \) is the free water diffusion coefficient; \( n = \frac{\text{total volume of void space}}{\text{total volume}} \) is the total or bulk porosity; and \( \chi \) is the tortuosity factor accounting for pore geometry.

With the establishment of the total hydrodynamic dispersive flux, it is now possible to fully describe the transport processes of water under both dispersion and advection as:

\[ \frac{\partial}{\partial t} (nc) = \frac{\partial}{\partial x_i} \left( D_y^{ij} \frac{\partial c}{\partial x_j} - n_e c u_i \right) \]  \hspace{1cm} (4.6)

### 4.2.2 Computational Procedure

Due to the complexity of groundwater quality modeling, it has been shown that the most appropriate approach is to utilize numerical solution techniques rather than analytical approaches. In fact, analytical solutions to groundwater flow and transport problems are available only for a limited number of simple cases (Mackay and Riley, 1993). To facilitate
application of numerical solution techniques, the advection-dispersion equation of Eq. 4.6 is rearranged into the following format:

\[
\frac{\partial c}{\partial t} = \frac{D}{n_x} \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x}
\] (4.7)

This one-dimensional structure is consistent with the link-node network structure associated with the stream-aquifer components of the MODSIM model. Eq. 4.7 is solved for each return flow link in MODSIM under specified network flow conditions. Several important assumptions are required for efficient solution of this problem via numerical methods. Both the density and viscosity of the pore water are assumed to be constant and unaffected by the constituent concentration. The one-dimensional structure requires the assumption that the source of contaminant enters the system at the first computational element. An additional assumption is that the initial groundwater concentration distribution is uniform. Based on these assumptions, the program predicts the constituent concentration at each computational element for each specified time period.

4.3 Salinity Model

4.3.1 Ion Exchange and Adsorption of Solutes

The salinity of return flows can be modeled utilizing the method developed by Dutt (1962a). The prediction of the mineral composition of water as it percolates through the soil profile is based on examining the processes of ion exchange and adsorption of solutes. The mineral surfaces of a soil profile have the ability to attract oppositely charged ions, commonly called the exchangeable ions, to maintain neutrality. The term exchangeable ions is given since as a solution is brought into contact with these minerals, the exchangeable ions are free to exchange with ions of the same charge in the solution. The chemical reaction describing this particular process for the adsorbed cations on the mineral surface, calcium (Ca\(^{++}\)), and the cations in the solution, magnesium (Mg\(^{++}\)), can be written as:

\[
Ca_a^{++} + Mg_s^{++} \rightleftharpoons Mg_a^{++} + Ca_s^{++}
\] (4.8)

where the subscript \(s\) represents the cations in the solution and the subscript \(a\) represents the adsorbed cations on the mineral surface. Furthermore, the equilibrium expression for the above reaction (4.8) can be written as:

\[
\frac{[Ca_s^{++}]}{[Mg_s^{++}]} = K \frac{[Ca_a^{++}]}{[Mg_a^{++}]}
\] (4.9)

where the solid square brackets ([ ]) indicate the concentrations of the chemical species at equilibrium, in moles per liter, the hollow square brackets (| |) indicate the concentrations of the chemical species at equilibrium, in moles per gram, and \(K\) is a constant called the equilibrium constant with no units.

Let \(y\) be the number of moles of Mg\(^{++}\) per gram of soil leaving or entering an exchange complex. Then:
where \( \beta \) is the ratio of the gram of soil to the liters of the solution, and the subscript 0 refers to the initial condition. Combining Eqs. 4.10, 4.11, 4.12, and 4.13 with Eq. 4.9 gives:

\[
\beta (1 - K) y^2 + \beta ([Mg_a]_0 + K[Ca_a]_0) + [Ca_s]_0 - K[Mg_s]_0 \cdot y + [Ca_s]_0[Mg_a]_0 - K[Mg_s]_0[Ca_a]_0 = 0
\]  

(4.14)

Gypsum, or \( CaSO_4 \), commonly found in the soil is another important factor that can determine the salinity of return flows. Gypsum is considered to be a slightly soluble salt, which means that it is only sparingly soluble in water and leaches slowly from soils. The reaction of this particular salt with the solution can be expressed by the equation:

\[
CaSO_4 \rightleftharpoons Ca^{++} + SO_4^{--}
\]  

(4.15)

The solubility of a moderately soluble salt is adequately described by the solubility product concept. In the case of \( CaSO_4 \), the solubility product \( K_{sp} \) is:

\[
K_{sp} = [Ca_s] [SO_4_s] \gamma^2
\]  

(4.16)

where \( \gamma \) represents the activity coefficient. Let \( X \) be the number of moles per liter of \( Ca^{++} \) and \( SO_4^{--} \) which dissolve or precipitate when a solution whose initial concentration of \( Ca^{++} \) and \( SO_4^{--} \) is \([Ca_a]_0\) and \([SO_4_s]_0\), then:

\[
[Ca_s] = [Ca_s]_0 + X
\]  

(4.17)

\[
[SO_4_s] = [Ca_sSO_4_s]_0 + X
\]  

(4.18)

Combining Eqs. 4.17 and 4.18 with Eq. 4.16 yields:

\[
X^2 + ([Ca_s]_0 + [SO_4_s]_0)X + ([Ca_s]_0[SO_4_s]_0 - \frac{K_{sp}}{\gamma^2}) = 0
\]  

(4.19)

The activity coefficient may be approximated from an extension of the Debye-Hückel theory (Glasstone, 1947):

\[
\log \gamma = - \frac{0.509 Z^2 \sqrt{\mu}}{1 + \sqrt{\mu}}
\]  

(4.20)

where \( Z \) is the valence of the ion and \( \mu \) is the ionic strength as defined by:
\[ \mu = \frac{1}{2} \sum_{i=1}^{n} C_i Z_i^2 \]  

(4.21)

where \( C \) represents the molar concentration of each ion, and the subscript \( i \) denotes all of the different ionic species present in the solution. Finally, combining Eqs. 4.19 and 4.20 gives:

\[
X^2 + \left( [Ca]_0 + [SO_4]_0 \right) X + \left( [Ca]_0 [SO_4]_0 - K_{sp} \frac{4.072 \sqrt{\mu}}{1 + \sqrt{\mu}} \right) = 0
\]

(4.22)

The above theoretical derivations are essentially taken from the study conducted by Dutt (1962a, 1962b). The original documentation can be consulted for a more detailed presentation. However, it should be noted that there are several errors in the original paper. For example, the negative sign in Eq. 4.20 is missing in the original documentation, which cannot possibly be used to combine with Eq. 4.19 to derive Eq. 4.22. Furthermore, Eq. 4.22 is presented differently by Dutt (1962a, 1962b) as follows:

\[
X^2 + \left( [Ca]_0 + [SO_4]_0 \right) X + \left( [Ca]_0 [SO_4]_0 - K_{sp} \frac{9.336 \sqrt{\mu}}{1 + \sqrt{\mu}} \right) = 0
\]

(4.23)

Eqs. 4.22 and 4.23 should be mathematically identical, but they are not, since the number 9.336 in Eq. 4.23 should have been 9.366. There are several other errors in the original paper (i.e., Figure 1, Figure 2 and Eq. 15) that are important to note.

4.3.2 Computational Procedure

The basic approach in the computational procedure is to subdivide the soil column into a series of segments. Starting from the top most layer, each layer is brought into equilibrium utilizing successive approximation calculations between Eq. 4.14 and Eq. 4.22, which is necessary since both equations are dependent on the concentration of \( Ca^{++} \). Furthermore, one may notice from Eq. 4.22 that change \( X \) in \( Ca^{++} \) and \( SO_4^{--} \) in the solution is dependent on \( \mu \), which in turn is a function of the equilibrium of \( Ca^{++} \) and \( SO_4^{--} \) concentrations, as shown in Eq. 4.21. Therefore, calculation of \( X \) also needs to be accomplished by successive approximations. Once a segment of the soil equilibrium state is determined, salinity conditions from the current segment are provided to the next segment as input to calculate the equilibrium state for this segment. This process is repeated until all of the segments have been equilibrated with the solution.

4.4 Network Representation

Fig. 4.1 exemplifies a network involving return flows, with river reaches and canals shown with solid lines with arrows representing the direction of flow, and return flows depicted with dash lines. Non storage node \textit{Node} #1 receives return flows from three different sources: \textit{Demand Node} #1, \textit{Demand Node} #2, and \textit{Demand Node} #3.
As discussed earlier, in addition to the links and nodes defined by the users, several accounting nodes and links are automatically constructed by the water allocation model MODSIM. One such accounting nodes created by MODSIM is the accounting groundwater node, which reconstructs the network of Fig. 4.1 into the configuration shown in Fig. 4.2.

When calculating the constituent concentration of return flows terminating at Node #1, which is the constituent concentration of Link #4 in Fig. 4.2, the model is applied in the following manner: either the generalized model (discussed in Section 4.2) or the salinity model (discussed in Section 4.3), based on the type of constituent, is applied to Links #1, #2, and #3 to determine their constituent concentrations. Then, the constituent concentration of Link #4 is calculated based on the flow rates and constituent concentrations of Links #1, #2, and #3 with the following equation:
where $\overline{C}_{s,j}$ is the concentration for constituent $j$ of link $s$, originating at the accounting groundwater node and terminating at node $i$; $R_i$ is the set of all links originating at nodes that contribute return flows to node $i$ and terminating at the accounting groundwater node. Therefore, prior to calculating the constituent concentration of return flows terminating at a particular node, it is necessary to determine the constituent concentrations of return flows for all nodes contributing return flows to that particular node. Eq. 4.24 is then utilized to calculate the constituent concentration of return flows terminating at that particular node.
V. INTEGRATION OF WATER QUANTITY AND QUALITY MODULES: MODSIMQ

5.1 Introduction

The integration of water quantity and quality in river basin network flow modeling is challenging due to the nonlinearity and nonconvexity of the problem. This has made it difficult to analyze water quality criteria and water quantity criteria simultaneously. To overcome these difficulties, a nonlinear programming algorithm is utilized to simultaneously perform optimization on both water quality and quantity in river basin management, while still retaining the efficient network structure of MODSIM. The resulting model MODSIMQ inherits much of its structure and assumptions from MODSIM, and continues to utilize the powerful minimum cost network flow algorithm based on Lagrangian relaxation.

MODSIMQ extends the network structure of MODSIM to include additional link parameters representing upper bounds for each water quality constituent. Other than the upper bound on flow capacity for each link, 15 additional upper bounds are imposed on every physical link in the system corresponding to the 15 quality constituents included in the streamflow quality routing model QUAL2E. These upper bounds can be utilized to represent a number of quality criteria, including:

- numeric quality standards for any segment of river reach
- irrigation water quality control
- water quality preferences for a demand node
- groundwater quality rehabilitation

There are essentially no limitations on the usage of these upper bounds on water quality, and they are not restricted to representing only the physical components of a river basin system. They can also be utilized to represent artificial and conceptual elements of a river basin system if desired.

5.2 Problem Formulation

MODSIMQ solves a network flow optimization problem similar to the MODSIM model, as defined by Eqs. 2.1 to 2.3, but with the following additional water quality constraints included:

\[
\sum_{t \in t_i} c_{tm}q_t \leq c_{km}^{\text{max}} \quad \text{for all nodes} \quad i \in N
\]

\[
\sum_{t \in t_i} q_t \leq c_{km}^{\text{max}} \quad \text{for all nodes} \quad i \in N
\]

\[
c_{km}^{\text{max}} = \left[ \min_{t \in t_i \to O_i} c_{tm}^{\text{max}} \right] \quad \text{for all nodes} \quad i \in N
\]

\[
\text{for all links} \quad k \in O_i, \text{for all constituents} \quad m \in B
\]
where $B$ is the set of all quality constituents; $c_{tm}$ is the concentration of water quality constituent $m$ in link $l$; $c_{tm}^{\text{max}}$ is the specified upper bound on water quality constituent $m$ in link $l$; $I_i$ is the set of all links terminating at node $i$ (i.e., inflow links); $O_i$ is the set of all links originating at node $i$ (i.e., outflow links); and complete mixing is assumed to occur at each node.

With the constraints of Eq. 5.1 now included in the optimization problem, and concentrations $c_{tm}$ treated as variables in this formulation, this problem now violates the network problem structure and is highly nonlinear. A successive relaxation computational procedure is invoked whereby the water quality concentrations are temporarily relaxed as decision variables and supplied to MODSIMQ as initial estimates from the water quality module, which is then solved under these assumed concentrations. The resulting network flow solution from MODSIMQ is then input back into the water quality module, which results in updated water quality concentration estimates over the operational horizon. The water quality module ensures that mass balance constraints on each constituent at each node are satisfied based on link flows supplied from MODSIMQ. This is why it is unnecessary to include constituent mass balance equations in the network optimization model. These updated water quality concentrations are returned to MODSIMQ for subsequent solution, with these iterations repeated until all water quality concentrations converge to stable values. It is believed that this iterative process is a contractive mapping that will always converge since $\|\partial c_{km}\| < 1$. That is, normed changes in link flows produce smaller normed changes in water quality concentrations in the network.

In order to retain the highly efficient pure network structure of the problem, the water quality constraints (Eq. 5.1) are added to the objective function (Eq. 2.1) using penalty coefficients $P_m$:

\[
\minimize f(q) = \sum_{\ell \in A} w_{\ell} q_{\ell} + \sum_{m \in B} P_m \left( \frac{\sum_{k \in D_\ell} c_{km} q_k}{\sum_{k \in D_\ell} q_k} - c_{tm}^{\text{max}} \right)^2 \quad \text{if} \quad \frac{\sum_{k \in D_\ell} c_{km} q_k}{\sum_{k \in D_\ell} q_k} > c_{tm}^{\text{max}}; \quad \sum q_k > 0
\]  

(5.2)

using where $D_\ell$ is the set of all links terminating at the same node as link $\ell$. By incorporating Eq. 5.1 into the objective function, water quality constraints are now indirectly maintained through the penalty term. This means that the water quality constraints can be
softened or hardened by altering the penalty coefficients. Again, strict imposition of water quality constraints may result in infeasible solutions.

5.3 Solution Algorithm

A solution algorithm is desired that can minimize the nonlinear objective function of Eq. 5.2 without altering the efficient network structure embodied in Eqs. 2.2 and 2.3. One of the few nonlinear programming methods which does not alter the original constraint set is the Frank-Wolfe algorithm (Kennington and Helgason, 1980). The Frank-Wolfe algorithm is a feasible direction method that improves an initial feasible solution by solving a linearized objective function using the truncated Taylor series expansion. The solution to the linearized network flow problem only serves to provide a new improving direction for a constrained one-dimensional optimal search on the original nonlinear optimization problem. The updated link flows are now input into the water quality module to provide updated estimates of concentrations of water quality constituents in all network links. The objective function is again linearized around the new improved solution (flows and concentrations), and the procedure continues until convergence. An advantage of this method is that arbitrary trust regions or step bounds need not be applied to step sizes since they are calculated through the one dimensional search on the original nonlinear problem. The execution sequences for MODSIMQ are presented in a flow chart in Fig. 5.1.

The following objective function is the linearization of Eq. 5.2 expanded around a given set of feasible link flows \( q^{(n)} \) and current estimates of concentrations \( c^{(n)}_{lm} \) at iteration \( n \):

\[
\minimize \quad \nabla f(q^{(n)})^T q = \sum_{m \in A} \left[ \sum_{k \in D_l} \frac{C_{km}^{(n)} q_k^{(n)}}{\sum_{k \in D_l} q_k^{(n)}} - C_{tm}^{max} \frac{\sum_{k \in D_l} q_k^{(n)}}{\sum_{k \in D_l} q_k^{(n)}} \right] q_l
\]

where since Eqs. 2.2 and 2.3 constitute a convex set, it is guaranteed that the solution
Figure 5.1. Flow Chart for Program MODSIMQ

\[ q^{(n)} + \alpha [q^* - q^{(n)}] \] is feasible for all step sizes \( \alpha \in [0,1] \) since each solution \( q^{(n)} \) and \( q^* \) is also feasible. The problem of Eq. 5.4 is easily solved by an efficient one-dimensional search algorithm, which gives the new solution:

where \( \alpha^* \) is the optimal step size found from solution of Eq. 5.4 such that

\[ f(q^{(n+1)}) < f(q^{(n)}) \]. This new solution \( q^{(n+1)} \) of link flows is then input into the water quality module, producing updated estimates of concentrations \( c^{(n+1)} \). The linearized
objective function of Eq. 5.3 is now expanded around new link flows $q^{(n+1)}$ and concentrations $c^{(n+1)}$ and the procedure repeats until convergence to a Karush-Kuhn-Tucker optimal solution. Since the original objective function is nonlinear, it is unlikely that the solution obtained from MODSIM will occur at an extreme point of the convex set defined by Eqs. 2.2 and 2.3. The extreme point solution $q^*$ found from the linearized problem of Eq. 5.3 primarily provides a direction search for finding the solution to the original nonlinear problem. It is significant that solution of the linearized problem of Eq. 5.3 subject to Eqs. 2.2 and 2.3 fully conforms to the minimum cost network flow problem of MODSIM, and can be solved with the efficient Lagrangian relaxation procedure. Solution of Eq. 5.4 is easily accomplished with an efficient one-dimensional search algorithm.

Insights can be gained by noting that the second term in Eq. 5.3 represents how much the original cost term $w$ is altered as a result of incorporation of the water quality constraints in the penalty function. It can be seen that:

1. Link cost increases if violation in downstream water quality constraints increase.
2. Link cost increases if the quality in link $i$ is poorer than the current downstream water quality conditions.
3. Link costs either increase and decrease inversely with the amount of water flowing into the downstream node.
VI. APPLICATION TO LOWER ARKANSAS RIVER BASIN IN COLORADO

6.1 Introduction

Several attempts have been made to model operations in the Arkansas River Basin in Colorado. The lower Arkansas River in Colorado is selected as the case study to demonstrate the functionality and capabilities of MODSIMQ. Many attempts have been made to model the Arkansas River Basin (McGuckin, 1977; Cain et al., 1980; Cain 1984; Abbott, 1986; Kuhn, 1987; Cain, 1987; and Burns, 1989). However, due to the complexity and dimensions of the basin, most of the aforementioned research utilized specialized models, or only modeled the basin superficially.

As an example, Burns (1989) developed the interactive accounting model (IAM) to simulate dissolved solids, streamflow, and water-supply operations in a river basin, although it was primarily designed for the Arkansas River Basin. Linear regression equations are utilized which aggregate water quality impacts from both natural and agricultural activities. Moreover, many of the pertinent basin operational complexities, such as water exchanges between users and satisfaction of the Arkansas River Interstate Compact, are not considered. More recently, the HIM model was developed by the State of Kansas in support of a lawsuit against Colorado claiming violation of the Arkansas River Compact (Simpson, 1996), but treats water quantity issues only. Detailed modeling for localized areas in the basin was performed by Konikow and Bredehoeft (1974) and Konikow and Person (1985). McLin (1981) favorably compared results from a lumped hydrosalinity model with the more detailed, spatially distributed model of Konikow and Bredehoeft (1974), providing encouragement for use of basin-wide models such as MODSIMQ.

6.2 Description of Study Area

Attempts were originally made to include the Arkansas River basin in Colorado, starting from the headwaters, which includes 74 water users, 11 reservoirs, and 29 gaging stations. However, after examination of the operations of the water systems and geophysical characteristics of the basin, it was decided to limit the case study to the portion downstream of Pueblo Reservoir. Due to the physiographical setting of the basin, return flow patterns and irrigation practices above the Pueblo Reservoir are quite different from those areas below Pueblo Reservoir. Furthermore, Pueblo Reservoir, situated near the city of Pueblo, is used to store water during the winter and flood periods for later release, which regulates the amount of water available for the study area. Therefore, it is both reasonable and practical to limit the current study to the area downstream of Pueblo Reservoir. However, pertinent connections between water uses upstream of Pueblo Reservoir and those downstream are not neglected. This means that even though releases from Pueblo Reservoir are treated as headwaters for the study area, they are divided into several portions for different downstream users, based on the operational plans implemented in Pueblo Reservoir during the winter storage period. Other
studies, such as the one conducted by Cain (1985), and models developed for litigation on the Arkansas River Interstate Compact, are also limited to areas downstream of Pueblo Reservoir.

The lower Arkansas River Basin in Colorado extends from just below Pueblo Reservoir to the Colorado-Kansas State line, as illustrated in Fig. 6.1. The Geographical setting of the basin area is described by several authors (Abbott, 1986; Cain, 1984 and 1987; and Burns, 1989). The Arkansas River Basin in Colorado is located between 37° and 39° latitude and 102° and 106° longitude, and composes approximately the entire southeastern one-quarter of the State. Headwaters of the Arkansas River are located in the 14,000 foot peaks of the Sawatch Range of central Colorado, where they gather the primary source of streamflow from melting of snow accumulated in the mountain area during October to May. The climate in the Arkansas River Basin in Colorado is greatly influenced by the elevation;

Figure 6.1. Location of Study Area (Cain, 1984)
the mean annual precipitation ranges from less than 10 inches on the plains to more than 40 inches in the mountain region, as illustrated on Fig. 6.2.

Figure 6.2. Mean Annual Precipitation in the Arkansas River Basin (Abbott, 1986)

Due to the lack of natural precipitation in the study area, diversion of streamflow and groundwater pumpage are common practices to accommodate agricultural irrigation demands. Water development in the Arkansas River Basin of Colorado can be divided into five chronological phases:

1. Development of direct diversions: starting around 1860, small ditches were developed to divert water to irrigate small plots on the flood plain of the river.
2. Development of water storage: to further utilize streamflow at times other than the irrigation season, off-stream reservoirs were constructed during the 1890's.
3. Importation of water by transmountain diversion: as early as the 1960's, importation of water by transmountain diversions was established from the Rio Grande and Colorado River Basins.
4. Development of groundwater: in addition to the usage of surface water, during the 1940's to 1960's, many groundwater wells were drilled in the alluvial aquifer adjacent to the river.

The Arkansas River serves as a conduit that carries pristine waters from the snowbelt originating from the mountain region to the eastern part of the State, where it is utilized to convert fertile but dry lands into productive agricultural areas. In the process of diverting the streamflow for irrigation purposes, canal leakage and irrigation return flows also increase. Infiltration of excess irrigation water eventually recharges the alluvial aquifer connected to the stream system. Return flows replenish some of the flow in the stream, particularly late in the irrigation season, which provides water to downstream users. This process of use and reuse of stream water eventually degrades the quality of the stream as it moves downstream. Moreover, in areas where groundwater is utilized for irrigation, the quality of return flows is further degraded. With establishment of complex conjunctive use systems, winter water storage plans, and transmountain importations, it is clear that proper modeling of the study area requires consideration of several pertinent hydrological components simultaneously.

6.3 Water Systems Operations

6.3.1 Direct Diversions

The area under current study includes three Water Districts, 14, 17, and 67 with 16 major and several minor direct diversion systems: Bessemer, Hamp-Bel, West Pueblo, Pueblo Waterworks, Riverside, Booth Orchard, St. Charles Mesa, Excelsior, Collier, Colorado Canal, Highline, Oxford Farmers, Otero, Baldwin-Stubs, Catlin, Holbrook, Rocky Ford, Fort Lyon, Las Animas Town, Fort Bent, Keesee, Amity, Lamar, Hyde, Manvel, X-Y and Graham, Buffalo, and Sisson and Stubs. The amount of water a particular diversion system can remove from the river is governed by the Prior-Appropriation Doctrine, which is found in most states in the Western U.S. This legal doctrine enforces water rights on how much and when a ditch can divert water from a river. Some ditches may own more than one diversion right, such as the two water rights owned by the X-Y and Graham ditch: 69 cfs with an appropriation date of July 22, 1889, and 61 cfs with an appropriation date of August 24, 1891. Manvel, on the other hand, only has one right: 54 cfs with an appropriation date of October 14, 1890. This means that X-Y and Graham has the right to divert up to a flow rate of 69 cfs from the river before Manvel can divert any water from the river. However, since the second water right of X-Y and Graham comes after Manvel's water right, X-Y and Graham cannot divert any additional water from the river before Manvel diverts its share.

These water rights are only applicable to native waters, which are defined as waters occurring naturally in the basin where they originate, and not imported from outside the basin. However, some of these ditches have additional rights to divert water from transmountain importations. Highline, for example, has the right to divert not only native waters of the basin, but also shares a portion of the water from the Busk-Ivanhoe transmountain diversion. Catlin Canal is another example, which owns part of the water from the Larkspur transmountain diversion. Other than direct diversion from the stream either from native waters or transmountain importations, a number of ditches also can perform exchanges with other water systems, as examined subsequently.
6.3.2 Off-Stream Reservoirs

Several off-stream reservoirs exist in the study area: Lake Henry, Lake Meredith, Dye Reservoir, Holbrook Reservoir, the Great Plains Reservoir system, Horse Creek Reservoir, and Adobe Creek Reservoir. These reservoirs are utilized to store water during the winter when irrigation is not taking place so as to provide releases during the growing season to meet irrigation demands. Some of these reservoirs, however, are topographically too low to irrigate lands by gravity flow, and an exchange process must be initiated to use waters stored in them.

Lake Henry and Lake Meredith reservoirs are owned by the Colorado Canal, with Colorado Canal topographically situated above Lake Meredith and below Lake Henry. This enables Lake Henry to deliver flows into Lake Meredith and Colorado Canal through direct gravity release; however, Lake Meredith is topographically too low to release waters into Colorado Canal. An exchange with Holbrook Canal, the Fort Lyon Storage Canal, or the Arkansas River is necessary to enable the Colorado Canal to utilize waters stored in Lake Meredith. The outlet of Lake Meredith crosses both the Holbrook Canal and the Fort Lyon Storage Canal prior to discharging into the Arkansas River. Therefore, depending on which canal is in priority at the time, the exchange process is accomplished by releasing water from Lake Meredith into the receiving channel, and diverting a like quantity directly from the Arkansas River into the Colorado Canal. However, this exchange process can only be accomplished if there is sufficient water left in the river at the headgate of the Colorado Canal to satisfy all senior rights between the headgate and the confluent point of outflow from Lake Meredith.

As mentioned previously, Holbrook Canal has the ability to both divert water directly from the river and from releases from Lake Meredith. Furthermore, Holbrook Canal can store the diverted water in either Dye Reservoir or Holbrook Reservoir. However, neither reservoir can normally release water directly back to Holbrook Canal for irrigation purposes. Therefore, a similar exchange process must be performed between Rocky Ford Ditch and Holbrook Canal, so that Holbrook Canal can utilize the water stored in these two reservoirs.

Amity Canal, owner of the Great Plains Reservoir system, is situated downstream of John Martin Dam and the outlets of the Great Plains Reservoirs. The reservoirs in the Great Plains Reservoir system are broad, shallow lakes with large surface-area-to-capacity ratio, which means that these reservoirs have significant evaporation rates. Therefore, whenever possible, Amity Canal stores its water in John Martin Reservoir instead of the Great Plains Reservoirs.

6.3.3 In-Stream Reservoir

The only in-stream reservoir in the study area is John Martin Reservoir, constructed by the U.S. Army Corps of Engineers in 1948 with a capacity of 701,775 acre-feet. The reservoir is situated about 58 miles west of the Colorado-Kansas State line. The major purposes of this reservoir are: flood control, irrigation-water conservation, and maintaining a recreation pool. Water stored in the reservoir for irrigation purposes basically follows the agreement established in December 1948 between the States of Colorado and Kansas, called the Arkansas River Compact (Terms of the Arkansas River Compact can be found in a
compilation by Radosevich, et al. (1975)). Generally, these terms provide for a winter and summer storage period.

In practice, operations formally dictated by the Compact provided unsatisfactory results, such as emptying reservoir storage too early in the irrigation season. Subsequently, two additional resolutions, Resolution Concerning an Operation Plan for John Martin Reservoir and Agreement "B", were reached to further enhance operation of John Martin Reservoir. Currently, the reservoir is operated under these two agreements.

In practice, these agreements govern the operation of John Martin Reservoir in the following manner:

- During the winter-storage period between November 1 and March 31, all inflows are required to be stored in the winter conservation pool.
- Beginning on April 1, water in winter conservation storage is released and distributed, with 40 percent going to the Kansas account and 60 percent to Colorado Water District 67 ditches as winter stored water according to the following percentages of a total rate of 1250 cfs:
  
<table>
<thead>
<tr>
<th>Ditch</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fort Bent</td>
<td>9.90%</td>
</tr>
<tr>
<td>Keesee</td>
<td>2.30%</td>
</tr>
<tr>
<td>Amity</td>
<td>49.50%</td>
</tr>
<tr>
<td>Lamar</td>
<td>19.80%</td>
</tr>
<tr>
<td>Hyde</td>
<td>1.30%</td>
</tr>
<tr>
<td>Manvel</td>
<td>2.40%</td>
</tr>
<tr>
<td>X-Y and Graham</td>
<td>5.10%</td>
</tr>
<tr>
<td>Buffalo</td>
<td>8.50%</td>
</tr>
<tr>
<td>Sisson-Stubbs</td>
<td>1.20%</td>
</tr>
</tbody>
</table>

- During the summer-storage period between April 1 and October 31, all inflows are required to be stored in each of the Colorado Water District 67 ditch accounts as summer stored water and Kansas account, following the aforementioned percentages.
- If any entity has designated winter stored water in its account beyond May 1st of the succeeding year, these waters become summer stored water for that particular user.
- As long as an entity has any summer stored water in its account, it cannot place a call above John Martin for its priority on the river.
- Amity may store water in its other water account in John Martin Reservoir as it could otherwise be diverted from the Arkansas River for storage in the Great Plains Reservoir systems.
- Fort Lyon Canal also has an other water account for up to 200,000 acre-feet, and Fort Lyon Canal may deliver water into this account under an approved Pueblo winter storage plan.
- Las Animas Consolidated Canal also has an other water account for up to 5,000 acre-feet for storing water delivered under an approved Pueblo winter storage plan.
35 percent of water delivered into all of the other water accounts is transferred into the transit loss account.

Other important issues regarding operation of John Martin Reservoir include transfer of water from the transit loss account to the winter stored water account on November 1st. Since MODSIMQ is utilized to simulate operation of the basin for a period of one year starting November 1st, any transfer of water that takes place at the beginning of the simulation period is simply viewed as initial conditions for the relevant accounts.

6.4 Network Configuration

Fig. 6.3 shows the overall configuration of the network representation of the study area for MODSIMQ. The network is constructed through simple point and click operations in the graphical user interface for MODSIMQ, and is composed of demand nodes, confluence/diversion points, reservoirs, stream gaging points, river reaches, diversion ditches, and return flow arcs or links. Return flow arcs are not since they are represented as artificial or accounting links, but ascertained through the spreadsheet interface to the data base. Spreadsheet style data base windows for each data object in the network are accessed through simple mouse control operations. Notice that the river basin network is wrapped around in order to display the entire network on one screen. The dimensionality and complexity of this basin requires 160 nodes and 300 links to accurately represent the system, not including the accounting nodes and links. Several of these components of the network are not shown in Fig. 6.3 in order to improve legibility of the schematic diagram, but are described in more detail subsequently.

There are two kinds of demand nodes: those with access to groundwater and those without, as seen in Fig. 6.3. As mentioned previously, some demand nodes have more than one water right. For example, Excelsior at demand node 90 has two water rights: 20 cfs at May 1, 1887 and 40 cfs at January 6, 1890. Demand nodes represent a point of a known quantity of demand, which can vary from period to period. All demand nodes are numbered as illustrated in Fig. 6.3 with the names of these demand nodes listed in Table 6.1. Table 6.1 also gives the ID number, which is the official reference number used by the U.S. Geological Survey.

As mentioned previously, some demand nodes have more than one water right. For example, demand node 90, Excelsior, has two water rights - 20 cfs at May 1, 1887 and 40 cfs at January 6, 1890. In Fig. 6.3, only one link is shown connecting the diversion point, node 89, and demand node 90. There are actually two links connecting them, indicated by the notation $x^2$ next to that particular link. The two links that connect the demand node represent two water rights owned by demand node 90. These two links are assigned different capacities and priorities (i.e., negative costs), corresponding to the amounts and priorities of these rights. Similarly, every demand node owning more than one water right has as many links connecting it from the diversion point as the number of water rights owned.
Figure 6.3. Lower Arkansas River Basin Network Configuration in Graphical User Interface for MODSIMQ
Table 6.1. Demand Node Names and Numbers

<table>
<thead>
<tr>
<th>ID #</th>
<th>Node Name</th>
<th>Node #</th>
</tr>
</thead>
<tbody>
<tr>
<td>1401</td>
<td>Bessemer</td>
<td>78</td>
</tr>
<tr>
<td>1402</td>
<td>St. Charles Mesa</td>
<td>87</td>
</tr>
<tr>
<td>1404</td>
<td>Hampbell</td>
<td>79</td>
</tr>
<tr>
<td>1407</td>
<td>West Pueblo</td>
<td>81</td>
</tr>
<tr>
<td>1410</td>
<td>Pueblo Waterworks</td>
<td>83</td>
</tr>
<tr>
<td>1416</td>
<td>Riverside Dairy</td>
<td>84</td>
</tr>
<tr>
<td>1419</td>
<td>Booth Orchard</td>
<td>85</td>
</tr>
<tr>
<td>1422</td>
<td>Excelsior</td>
<td>90</td>
</tr>
<tr>
<td>1425</td>
<td>Collier</td>
<td>94</td>
</tr>
<tr>
<td>1428</td>
<td>Colorado Canal</td>
<td>96</td>
</tr>
<tr>
<td>1431</td>
<td>Highline</td>
<td>99</td>
</tr>
<tr>
<td>1434</td>
<td>Oxford Farmers</td>
<td>102</td>
</tr>
<tr>
<td>1701</td>
<td>Otero</td>
<td>104</td>
</tr>
<tr>
<td>1703</td>
<td>Baldwin-Stubbs</td>
<td>105</td>
</tr>
<tr>
<td>1704</td>
<td>Catlin</td>
<td>108</td>
</tr>
<tr>
<td>1707</td>
<td>Holbrook</td>
<td>110</td>
</tr>
<tr>
<td>1710</td>
<td>Rocky Ford</td>
<td>112</td>
</tr>
<tr>
<td>1716</td>
<td>Fort Lyon</td>
<td>115</td>
</tr>
<tr>
<td>1719</td>
<td>Las Animas Town</td>
<td>118</td>
</tr>
<tr>
<td>6701</td>
<td>Keesee</td>
<td>124</td>
</tr>
<tr>
<td>6704</td>
<td>Fort Bent</td>
<td>123</td>
</tr>
<tr>
<td>6707</td>
<td>Amity</td>
<td>126</td>
</tr>
<tr>
<td>6710</td>
<td>Lamar</td>
<td>128</td>
</tr>
<tr>
<td>6713</td>
<td>Hyde</td>
<td>130</td>
</tr>
<tr>
<td>6716</td>
<td>Manvel</td>
<td>131</td>
</tr>
<tr>
<td>6719</td>
<td>X-Y and Graham</td>
<td>134</td>
</tr>
<tr>
<td>6722</td>
<td>Buffalo</td>
<td>135</td>
</tr>
<tr>
<td>6725</td>
<td>Sisson and Stubbs</td>
<td>137</td>
</tr>
<tr>
<td>99</td>
<td>Kansas</td>
<td>140</td>
</tr>
</tbody>
</table>

Stream gaging points are used to monitor flow conditions and to calibrate the model with historical data. All stream gaging points are numbered as illustrated in Fig. 6.3, with names shown in Table 6.2. Furthermore, Table 6.2 provides the ID number as an official reference number used by the USGS. Reservoirs are another important component of the network. Reservoirs in the study area, both off-stream and in-stream, are generally utilized to store water during the winter months and provide releases during the irrigation season. Table 6.3 lists the node numbers and names of the reservoirs in the study area.
Table 6.2. Number and Name of Stream Gaging Points

<table>
<thead>
<tr>
<th>ID #</th>
<th>Stream Gaging Name</th>
<th>Node #</th>
</tr>
</thead>
<tbody>
<tr>
<td>994</td>
<td>Arkansas River above Pueblo</td>
<td>82</td>
</tr>
<tr>
<td>1065</td>
<td>Fountain Creek at Pueblo</td>
<td>88</td>
</tr>
<tr>
<td>1090</td>
<td>St. Charles River</td>
<td>91</td>
</tr>
<tr>
<td>1095</td>
<td>Arkansas River at Avondale</td>
<td>92</td>
</tr>
<tr>
<td>1160</td>
<td>Huerfano River</td>
<td>97</td>
</tr>
<tr>
<td>1170</td>
<td>Arkansas River near Nepesta</td>
<td>100</td>
</tr>
<tr>
<td>1195</td>
<td>Apishapa River near Fowler</td>
<td>106</td>
</tr>
<tr>
<td>1197</td>
<td>Arkansas River at Catlin</td>
<td>107</td>
</tr>
<tr>
<td>1230</td>
<td>Arkansas River at La Junta</td>
<td>116</td>
</tr>
<tr>
<td>1240</td>
<td>Arkansas River at Las Animas</td>
<td>119</td>
</tr>
<tr>
<td>1285</td>
<td>Purgatoire River near Las Animas</td>
<td>121</td>
</tr>
<tr>
<td>1305</td>
<td>Arkansas River below John Martin Reservoir</td>
<td>122</td>
</tr>
<tr>
<td>1330</td>
<td>Arkansas River at Lamar</td>
<td>129</td>
</tr>
<tr>
<td>1341</td>
<td>Big Sandy Creek</td>
<td>132</td>
</tr>
<tr>
<td>1375</td>
<td>Arkansas River near Coolidge</td>
<td>139</td>
</tr>
</tbody>
</table>

Table 6.3. Numbers and Names of Reservoirs

<table>
<thead>
<tr>
<th>Node #</th>
<th>Reservoir Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>Lake Henry</td>
</tr>
<tr>
<td>5</td>
<td>Lake Meredith</td>
</tr>
<tr>
<td>6</td>
<td>Dye Reservoir</td>
</tr>
<tr>
<td>7</td>
<td>Holbrook Reservoir</td>
</tr>
<tr>
<td>8</td>
<td>Great Plains Reservoir System</td>
</tr>
<tr>
<td>9</td>
<td>Horse Creek Reservoir</td>
</tr>
<tr>
<td>10</td>
<td>Adobe Creek Reservoir</td>
</tr>
<tr>
<td>11</td>
<td>John Martin Reservoir</td>
</tr>
</tbody>
</table>

56
6.5 Storage Accounts

A number of parent/child reservoir systems are set up in the network to model reservoir storage rights and accounts that exist in some of the reservoirs in the study area. Similar to a diversion right, these reservoirs have more than one storage right. For example, Adobe Creek Reservoir has two storage rights: 61575 acre-feet in January 25, 1906 and 25425 acre-feet in December 29,1908. In order to allow a reservoir to have more than one account, it is necessary to represent the reservoir with a parent/child reservoir structure. Using the example of Adobe Creek Reservoir with two storage rights, it can be represented as illustrated in Figure 6.4. The parent reservoir is not connected to any links and its only purpose is to keep track of total storage in all of the child reservoirs, thus enabling calculation of total evaporation loss from the reservoir. Storage capacity in the child reservoirs is set equal to the actual storage right of that particular account. Accrual links are assigned negative costs related to fill decree priorities.

Figure 6.4. Parent/Child Reservoir for Adobe Creek Reservoir

Similarly, this parent/child reservoir structure is set up for other reservoirs in the system with more than one storage account. Lake Henry, Holbrook Reservoir, Horse Creek Reservoir, and Adobe Reservoir all have two storage accounts; therefore, they are all composed of one parent reservoir and two child reservoirs.

John Martin Reservoir, on the other hand, is composed of several child reservoirs. Figure 6.5 illustrates the major components of the parent/child reservoir structure of John Martin Reservoir consisting the following elements and operation rules:
Child reservoir $A$ is the winter conservation storage pool.
Child reservoir $B$ is the summer conservation storage pool.
Child reservoir $C$ is the winter water account.
Child reservoir $G$ is the Kansas account.
Child reservoir $H$ is the winter stored water account.
Child reservoir $I$ is the summer stored water account.
Child reservoir $J$ is the winter stored water account from the previous year.
Child reservoir $K$ is the transit loss account.
Child reservoir $L$ is the other water account.
Nodes $D$, $E$, and $F$ are distribution nodes which allocate the proper percentages of water into the appropriate accounts.
Since there are nine Colorado Water District 67 ditches, there are nine sets of child reservoirs $H$, $I$, and $J$.
Since there are three other water accounts, there are three sets of distribution nodes $F$ and child reservoir $L$.
Link 1 serves to transfers water in the winter conservation storage pool to the appropriate accounts on April 1 and is therefore assigned a zero capacity prior to April 1; after April 1, water is transferred from the winter conservation storage pool.
storage pool to the winter stored water accounts and Kansas account at a total rate of 1250 cfs.

- Link 2 transfers water in the summer conservation storage pool to the summer stored water accounts and Kansas account, with capacity of this link set equal to that of link 1.
- Link 3 transfers water stored in the winter water account to the other water accounts and transit loss accounts, and has a zero capacity, except in March.
- Link 8 is assigned to transfer all waters in the winter stored water accounts from the previous year to the summer stored water accounts on May 1, and therefore has a zero capacity except in May.
- All links used to transfer water at certain times of the year are assigned a high negative cost to ensure the transfer process occurs.

6.6 Data Organization and Model Calibration

As an initial calibration effort on MODSIMQ, it was decided to use the water year starting November 1, 1988 and ending at October 31, 1989. This time frame coincides with operation plans of John Martin Reservoir, which enables several account transferring processes to be accepted as initial conditions. Furthermore, during this water year, all of the major changes to the operation of John Martin Reservoir would have been in existence prior to this period. For future work, a more extensive calibration period is required.

In essence, the goal of the calibration procedure is to duplicate historical streamflow data for both water quantity and quality. To ensure calibration runs are unbiased, streamflow data at several locations throughout the study area are used, as taken from the Water Resources Data, Colorado (USGS, 1989, 1990). Table 6.4 gives gaged historical flow data in the stream, while Table 6.5 provides historical water quality data. Figure 6.6 illustrates average salinity \( \mu \) of the stream, along with \( \mu + \sigma \) and \( \mu - \sigma \) standard deviations from the mean (Cain 1987).

6.6.1 Demands

The data used for the demand nodes are based on studies conducted by Burns (1989). In general, water users are classified into five categories: agricultural, municipal, industrial, in stream and reservoir operator. These five types of users have differing fractional distributions of demand, as illustrated in Table 6.6.

For agricultural users, there are two additional distribution patterns, as shown in table 6.6. The column pet are demand distribution patterns based on the monthly potential evapotranspiration, and the column agad are demand distribution patterns based on the monthly agricultural irrigation demand. Using the fractional distributions of demand given in Table 6.6 and a demand factor, a total demand can be derived for each user, as shown in Table 6.7. In Table 6.7, the column Type stands for the type of the demand node and column Distrib. stands for the distribution pattern corresponding to the distribution pattern shown in Table 6.6.
<table>
<thead>
<tr>
<th>Table 6.4. Streamflow Quantity Data (Nov 88-Oct 89)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Streamflow (acre-feet/month)</strong></td>
</tr>
<tr>
<td><strong>Gage</strong></td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td>994</td>
</tr>
<tr>
<td>1065</td>
</tr>
<tr>
<td>1090</td>
</tr>
<tr>
<td>1095</td>
</tr>
<tr>
<td>1160</td>
</tr>
<tr>
<td>1170</td>
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<tr>
<td>1195</td>
</tr>
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<td>1197</td>
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<tr>
<td>1341</td>
</tr>
<tr>
<td>1375</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 6.5. Streamflow Quality Data (Nov 88-Oct 89)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Specific Conductance (microseimens/cm)</strong></td>
</tr>
<tr>
<td><strong>Gage</strong></td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td>994</td>
</tr>
<tr>
<td>1095</td>
</tr>
<tr>
<td>1170</td>
</tr>
<tr>
<td>1197</td>
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<tr>
<td>1230</td>
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<td>1330</td>
</tr>
<tr>
<td>1375</td>
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</tbody>
</table>

60
Figure 6.6. Average Specific Conductance of Study area

Table 6.6. Fractional Distributions of Demand Over 12 Months

<table>
<thead>
<tr>
<th>Month</th>
<th>Agricultural</th>
<th></th>
<th></th>
<th>Industrial and In-stream</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PET</td>
<td>AGAD</td>
<td>Municipal</td>
<td></td>
</tr>
<tr>
<td>Nov</td>
<td>0.000</td>
<td>0.025</td>
<td>0.042</td>
<td>0.083</td>
</tr>
<tr>
<td>Dec</td>
<td>0.000</td>
<td>0.030</td>
<td>0.046</td>
<td>0.083</td>
</tr>
<tr>
<td>Jan</td>
<td>0.000</td>
<td>0.050</td>
<td>0.060</td>
<td>0.083</td>
</tr>
<tr>
<td>Feb</td>
<td>0.048</td>
<td>0.074</td>
<td>0.077</td>
<td>0.083</td>
</tr>
<tr>
<td>Mar</td>
<td>0.159</td>
<td>0.110</td>
<td>0.102</td>
<td>0.084</td>
</tr>
<tr>
<td>Apr</td>
<td>0.207</td>
<td>0.143</td>
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</tr>
<tr>
<td>May</td>
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<td>0.084</td>
</tr>
<tr>
<td>Jun</td>
<td>0.207</td>
<td>0.143</td>
<td>0.125</td>
<td>0.084</td>
</tr>
<tr>
<td>Jul</td>
<td>0.136</td>
<td>0.094</td>
<td>0.091</td>
<td>0.083</td>
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<td>0.068</td>
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<td>0.039</td>
<td>0.052</td>
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Table 6.7. Demand Values and Patterns

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<td>Pueblo Waterworks</td>
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<td>Riverside Dairy</td>
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Groundwater/surface water interactions at the demand nodes in the study area are shown in Table 6.8, obtained from Burns (1989). In Table 6.8, the columns Return-Node and Return-Dist represent the return node number and distance respectively; Inf. Rate represents the infiltration rate; Capacity represents the groundwater pumping capacity; Transmissivity represents the groundwater transmissivity; and Depletion-Node and Depletion-Dist. represent the depletion node number and distance, respectively.
Table 6.8. Return Flow and Stream Depletion Characteristics

<table>
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<tr>
<th>Node #</th>
<th>Return Node</th>
<th>Dist. (ft)</th>
<th>Inf. Rate (fraction)</th>
<th>Capacity (ac-ft/mon)</th>
<th>Transmissivity (gal/d/ft x 1000)</th>
<th>Depletion Node</th>
<th>Dist. (ft)</th>
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Accurately estimating the demand and the demand distribution patterns is essential in analyzing and evaluating system performance. However, to properly initiate model calibration, it is necessary to obtain data on the actual amount of water diverted by each user. Actual diversion records were obtained from the Office of the Colorado State Engineer. Groundwater pumpage data are also needed for model calibration, and were likewise obtained from the State Engineer. Unfortunately, the accuracy of these data are questionable, since
these values are often not actual measurements but rather are estimated based on energy-consumption data using methods such as developed by Hurr and Litke (1989). Similarly, reservoir storage volumes are also acquired from the State Engineer, although volumes for individual accounts in John Martin Reservoir are from the *Annual Report of the Operations Secretary, Concerning the Operation of John Martin Reservoir* (Witte, 1989 and 1990).

### 6.6.2 Return Flow Salinity

Data used for calculating the salinity of return flows are based on work conducted by Cain (1987). To estimate the salinity of return flows, it is necessary to provide:

1. relations of specific conductance to major-ion concentrations for the surface water system.
2. relations of specific conductance to major-ion concentrations for the groundwater system.

Once this information is provided, it can be utilized to interpolate concentrations of Ca$^{++}$, Mg$^{++}$, and SO$_4^{--}$ in both surface water and groundwater.

Figures 6.7, 6.8, 6.9, and 6.10 from Cain (1987) graphically illustrate the regression relationships between specific conductance and the major-ion concentrations for the surface water system and groundwater system, respectively. The coefficients of determination ($r^2$) indicate that the regression equations provide adequate estimations (Cain, 1987). Mean groundwater specific conductances, as shown in Figure 6.11, are utilized for setting initial salinity levels for the groundwater system. Initial groundwater storage volumes are estimated based on work conducted by Burns (1989), as shown in Figure 6.12.

![Specific Conductance vs Concentration](image)

*Figure 6.7. Relations of Specific Conductance to Major-Ion Concentrations for the Arkansas River at Canon City (Cain, 1987)*
Figure 6.8. Relations of Specific Conductance to Major-Ion Concentrations for the Arkansas River at Canon City (Cain, 1987)

Figure 6.9. Relations of Specific Conductance to Major-Ion Concentrations for Groundwater in Alluvial Aquifers along the Arkansas River (Cain, 1987)
Figure 6.9. Relations of Specific Conductance to Major-Ion Concentrations for Groundwater in Alluvial Aquifers along the Arkansas River (Cain, 1987)

Figure 6.11. Downstream Increase in Specific Conductance of Groundwater in Alluvial Aquifers along the Arkansas River (Cain, 1987)
6.6.3 Quality Standards

Water quality criteria are easily introduced by using numerical standards, such as the Arkansas River Basin, Adopted Stream Classifications and Standards (Division of Planning, Pueblo Area Council of Governments). Figure 6.13 gives the standards utilized to construct water quality criteria in this current study. It is clear from Figure 6.13 describe that when salinity of irrigation water exceeds 2250 μS, it is classified as very high salinity hazard. It is evident from Figure 6.6 that average salinity in the lower Arkansas River in Colorado exceeds the standard given in Figure 6.13.

6.6.4 Model Calibration and Estimation of Unregulated Inflows

Model calibration is accomplished by first executing the model without any water quality components. During this run, several link upper and lower bounds are set to historical flow rates. By doing so, it is possible to maintain storage volumes in all of the reservoirs in the system model to historically measured levels, enabling evaporation rates to be accurately estimated. During this phase, unregulated inflows must also be estimated where direct measurements are unavailable. Several methods for estimating unregulated inflows have been examined, including watershed runoff models utilizing historical measured precipitation data and basin geometry to determined the quantity of unregulated inflow. However, due to insufficient rainfall records, mathematical rainfall-runoff models are not applicable for the study area. With a limited number of rainfall gaging stations available in Arkansas River Basin, basin-wide rainfall patterns cannot be adequately interpolated. Furthermore, complete precipitation data, including intensity and duration of rainfall, are also unavailable, making it difficult to estimate the runoff response resulting from the precipitation.
Figure 6.13. Hazzard Classification of Irrigation Waters (Margheim, 1967)
The approach adopted in this study is to utilize historical measurements at stream gaging stations, measured diversions, and estimated groundwater pumpage. Unregulated inflows are then estimated from mass balance calculations applied to individual sections of the stream extending from one gaging station to the next downstream gaging station. Inflows into each control section consist of upstream gaged inflows, groundwater return flows, and unregulated inflows. Outflows from each control section consist of diversions, groundwater depletions, and downstream gaged outflows. Spatial distributions of unregulated inflows within each section of the stream are assumed to be correlated with the incremental drainage areas tabulated in Table 6.9.

To estimate the contribution of groundwater return flows, it is necessary to estimate both groundwater and surface water activities prior to the current simulation period. This is accomplished by executing MODSIMQ over two successive simulation periods using the same inflow and demand data. Results from the first period are essentially viewed as initial conditions for the second period (current simulation period). This provides a means of estimating lagged groundwater contributions and impacts from prior operations, while eliminating the need for collecting data and running the model over two consecutive periods.

In order to ensure that calibration produces the same flow rates as historically observed, the stream gage nodes are replaced with flow-through demand nodes, with flow-through demands set equal to the historical flow rates. Furthermore, an artificial reservoir is introduced to simulate the effects of unregulated inflow. This artificial reservoir is assigned with a large initial volume of water and connected to every node in the main stream, enabling it to release sufficient amounts of water to match the historical flow rates in all gaging stations. The quantity of water released from the artificial reservoir to each node is then utilized as unregulated inflows. This approach effectively employs the optimization algorithm embedded in MODSIMQ to determine the quantity of unregulated inflows, thereby eliminating the trial and error process otherwise needed.

Figures 6.14, 6.15, and 6.16 illustrate the results of the calibration run, which are compared with the estimated historical runoff. The estimated historical surface runoff are calculated using the average annual unregulated inflow estimated by Miles (1977), while taking precipitation data (USGS, 1989, 1990) of the simulation period into consideration. The locations of rainfall gages and corresponding monthly precipitation for the simulation period are shown in Figures 6.17 and 6.18. The estimated historical surface runoff values are calculated by first utilizing the Thiessen method (Chow, et al., 1988) to determine average monthly rainfall. Average monthly rainfall is then employed as fractional distributions of annual runoff to calculate the monthly estimated historical surface runoff. Due to the lack of adequate precipitation information, however, estimated historical surface runoff values can only be considered as rough estimates for comparing the results of the simulation runs.
Table 6.9. Incremental Drainage Area of Arkansas River in Colorado (Cain, 1987)

<table>
<thead>
<tr>
<th>Station number</th>
<th>Station name</th>
<th>River miles upstream from Coolidge, Kans.</th>
<th>Altitude (feet above sea level)</th>
<th>Drainage area (square miles)</th>
<th>Number of measurements</th>
<th>Period of record</th>
</tr>
</thead>
<tbody>
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<td>07079200</td>
<td>Leadville Drain at Leadville</td>
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<td>10,400</td>
<td>-</td>
<td>60</td>
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<td>Arkansas River near Leadville</td>
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<td>California Gulch at Malta</td>
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<td>-</td>
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<td>Halfmoon Creek near Malta</td>
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<td>24</td>
<td>238</td>
<td>1965-84</td>
</tr>
<tr>
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<td>Arkansas River near Malta</td>
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<td>228</td>
<td>150</td>
<td>1964-83</td>
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<td>Arkansas River at Buena Vista</td>
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<td>611</td>
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<td>214</td>
<td>4,740</td>
<td>4,670</td>
<td>3,089</td>
<td>1966-82</td>
</tr>
<tr>
<td>07099500</td>
<td>Arkansas River near Pueblo</td>
<td>209</td>
<td>4,690</td>
<td>4,686</td>
<td>60</td>
<td>1963-80</td>
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<tr>
<td>07103700</td>
<td>Fountain Creek near Colorado Springs</td>
<td>-</td>
<td>6,110</td>
<td>103</td>
<td>228</td>
<td>1971-84</td>
</tr>
<tr>
<td>07103747</td>
<td>Monument Creek at Palmer Lake</td>
<td>-</td>
<td>6,950</td>
<td>26</td>
<td>142</td>
<td>1976-84</td>
</tr>
<tr>
<td>07103750</td>
<td>Monument Creek at Monument</td>
<td>-</td>
<td>6,925</td>
<td>29</td>
<td>28</td>
<td>1975-77</td>
</tr>
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<td>07103800</td>
<td>West Monument Creek at Air Force Academy</td>
<td>-</td>
<td>7,180</td>
<td>15</td>
<td>187</td>
<td>1970-83</td>
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<tr>
<td>07103950</td>
<td>Kettle Creek near Black Forest</td>
<td>-</td>
<td>6,980</td>
<td>9.0</td>
<td>112</td>
<td>1976-83</td>
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<tr>
<td>07104400</td>
<td>Monument Creek at Pikeview</td>
<td>-</td>
<td>6,203</td>
<td>204</td>
<td>205</td>
<td>1973-84</td>
</tr>
<tr>
<td>07104900</td>
<td>Monument Creek at Cache La Poudre Street, at Colorado Springs</td>
<td>-</td>
<td>5,990</td>
<td>-</td>
<td>42</td>
<td>1976-79</td>
</tr>
<tr>
<td>07104905</td>
<td>Monument Creek at Bijou Street, at Colorado Springs</td>
<td>-</td>
<td>5,970</td>
<td>-</td>
<td>52</td>
<td>1979-84</td>
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<td>07105530</td>
<td>Fountain Creek at Colorado Springs</td>
<td>-</td>
<td>5,900</td>
<td>392</td>
<td>265</td>
<td>1970-84</td>
</tr>
<tr>
<td>07105530</td>
<td>Fountain Creek below Janitell Road, below Colorado Springs</td>
<td>-</td>
<td>5,840</td>
<td>-</td>
<td>74</td>
<td>1975-84</td>
</tr>
<tr>
<td>07105780</td>
<td>B Ditch Drain near Security</td>
<td>-</td>
<td>5,724</td>
<td>3.2</td>
<td>46</td>
<td>1981-84</td>
</tr>
<tr>
<td>07105800</td>
<td>Fountain Creek at Security</td>
<td>-</td>
<td>5,640</td>
<td>495</td>
<td>226</td>
<td>1970-83</td>
</tr>
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</table>
Table 6.9. Incremental Drainage Area of Arkansas River in Colorado  
(Cain, 1987) -- Continued

<table>
<thead>
<tr>
<th>Station number</th>
<th>Station name</th>
<th>River miles upstream from Coolidge, Kansas</th>
<th>Altitude (feet above sea level)</th>
<th>Drainage area (square miles)</th>
<th>Number of measurements</th>
<th>Period of record</th>
</tr>
</thead>
<tbody>
<tr>
<td>07105822</td>
<td>Clover Ditch Drain near Widefield</td>
<td>5,620</td>
<td>46</td>
<td>1981-84</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07105825</td>
<td>Fountain Creek below Widefield</td>
<td>5,610</td>
<td>42</td>
<td>1979-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07105900</td>
<td>Jimmy Camp Creek at Fountain</td>
<td>5,530</td>
<td>66</td>
<td>1976-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07105905</td>
<td>Fountain Creek above Little Fountain Creek, below Fountain</td>
<td>5,400</td>
<td>100</td>
<td>1975-84</td>
<td></td>
<td></td>
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<tr>
<td>07105920</td>
<td>Little Fountain Creek above Keaton Reservoir, near Fort Carson</td>
<td>6,430</td>
<td>11</td>
<td>1978-82</td>
<td></td>
<td></td>
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<tr>
<td>07105928</td>
<td>Little Fountain Creek near Fort Carson</td>
<td>6,360</td>
<td>12</td>
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<td>07105940</td>
<td>Little Fountain Creek near Fountain</td>
<td>5,560</td>
<td>27</td>
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<td>07105945</td>
<td>Rock Creek above Fort Carson</td>
<td>6,390</td>
<td>7.8</td>
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<td>07105950</td>
<td>Rock Creek near Fort Carson</td>
<td>5,600</td>
<td>17</td>
<td>1978-83</td>
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<td>07105960</td>
<td>Rock Creek near Fountain</td>
<td>5,630</td>
<td>30</td>
<td>1973-80</td>
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<tr>
<td>07106500</td>
<td>Fountain Creek near Pino</td>
<td>4,475</td>
<td>926</td>
<td>1963-84</td>
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<tr>
<td>07107900</td>
<td>Greenhorn Creek near Rye</td>
<td>7,220</td>
<td>10</td>
<td>1973-80</td>
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<tr>
<td>07108050</td>
<td>Greenhorn Creek near Colorado City</td>
<td>5,630</td>
<td>30</td>
<td>1973-80</td>
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<tr>
<td>07108900</td>
<td>St. Charles River at Vineland</td>
<td>4,585</td>
<td>474</td>
<td>1971-83</td>
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<tr>
<td>07109500</td>
<td>Arkansas River near Avondale</td>
<td>4,510</td>
<td>6,327</td>
<td>1983-83</td>
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<td></td>
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<tr>
<td>07116500</td>
<td>Huerfano River near Boone</td>
<td>4,450</td>
<td>1,875</td>
<td>1976-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07117000</td>
<td>Arkansas River near Nepesta</td>
<td>4,585</td>
<td>9,345</td>
<td>1963-80</td>
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<td></td>
</tr>
<tr>
<td>07117600</td>
<td>Chicosa Creek near Fowler</td>
<td>4,335</td>
<td>109</td>
<td>1968-76</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07118500</td>
<td>Apishapa River at Aguilar</td>
<td>6,335</td>
<td>149</td>
<td>1979-81</td>
<td></td>
<td></td>
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<tr>
<td>07119500</td>
<td>Apishapa River near Fowler</td>
<td>4,317</td>
<td>1,125</td>
<td>1963-83</td>
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<td></td>
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<tr>
<td>07119700</td>
<td>Arkansas River at Catlin Dam, near Fowler</td>
<td>4,246</td>
<td>10,991</td>
<td>1968-79</td>
<td></td>
<td></td>
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<tr>
<td>07121500</td>
<td>Timpas Creek at mouth near Swink</td>
<td>4,113</td>
<td>496</td>
<td>1967-83</td>
<td></td>
<td></td>
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<tr>
<td>07122000</td>
<td>Arkansas River near La Junta</td>
<td>4,080</td>
<td>12,000</td>
<td>1964-67</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07122400</td>
<td>Crooked Arroyo near Swink</td>
<td>4,100</td>
<td>108</td>
<td>1968-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07123675</td>
<td>Horse Creek near Las Animas</td>
<td>3,970</td>
<td>1,265</td>
<td>1961-83</td>
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<td></td>
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<tr>
<td>07124000</td>
<td>Arkansas River at Las Animas</td>
<td>3,884</td>
<td>16,417</td>
<td>1945-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07124050</td>
<td>Middle Fork Purgatoire River at Stonewall</td>
<td>7,710</td>
<td>52</td>
<td>1978-81</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07124200</td>
<td>Purgatoire River at Madrid</td>
<td>6,262</td>
<td>550</td>
<td>1972-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07124300</td>
<td>Long Canyon Creek near Madrid</td>
<td>6,259</td>
<td>100</td>
<td>1972-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07124410</td>
<td>Purgatoire River below Trinidad Lake</td>
<td>6,974</td>
<td>672</td>
<td>1977-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07126200</td>
<td>Van Bremo Arroyo near Model</td>
<td>4,960</td>
<td>168</td>
<td>1968-84</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07126300</td>
<td>Purgatoire River near Thatcher</td>
<td>4,750</td>
<td>1,935</td>
<td>1968-84</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07128500</td>
<td>Purgatoire River near Las Animas</td>
<td>3,875</td>
<td>3,503</td>
<td>1961-83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07130500</td>
<td>Arkansas River below John Martin Reservoir</td>
<td>3,737</td>
<td>18,915</td>
<td>1951-81</td>
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<td></td>
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<tr>
<td>07133000</td>
<td>Arkansas River at Lamar</td>
<td>3,597</td>
<td>19,780</td>
<td>1963-83</td>
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<td></td>
</tr>
<tr>
<td>07134100</td>
<td>Big Sandy Creek near Lamar</td>
<td>3,545</td>
<td>3,307</td>
<td>1968-82</td>
<td></td>
<td></td>
</tr>
<tr>
<td>07137500</td>
<td>Arkansas River near Coolidge, Kans.</td>
<td>3,331</td>
<td>25,410</td>
<td>1963-84</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 6.14. Calibration Results of Estimated Total Unregulated Inflow from Tributaries Between Node 80 and Node 100

Figure 6.15. Calibration Results of Estimated Total Unregulated Inflow from Tributaries Between Node 100 and Node 116
Once water quantity is fully calibrated, water quality is introduced into the model. Figures 6.19 and 6.20 provide some limited calibration results for the return flow salinity model, showing that it is giving reasonable relationship between the quality of irrigation water and the quality of return flows. Due to the complexity of return flow quality modeling and the unavailability of pertinent field data, however, the accuracy of the return flow salinity model remains to be proven. Figure 6.21 gives final results of the calibration run.

6.7 Simulation Results with MODSIMQ

6.7.1 Introduction

A number of actions can be taken to decrease the problem of salinity in the lower Arkansas River in Colorado. However, the complexity and the size of the basin makes it difficult to predict the outcomes of any actions taken to correct the hazard of high salinity. Another issue which further complicates the situation is the high demand for water during the irrigation season. Excess water from irrigation practice tends to degrade the quality of irrigation return flows, and coupled with the downstream use and reuse of return flows, irrigated agriculture is a major contributor to salinization of the Arkansas River.

After successfully estimating the required parameters and unregulated inflows through the calibration runs, the next step is to execute the model with the optimization capability enabled. Based on a careful review of the case study problem, it was determined that MODSIMQ should be run under four scenarios, as outlined in Table 6.10.
Figure 6.17. Locations of Rainfall Gages and Corresponding Precipitation for Water Year 1989 (USGS, 1989)
Figure 6.18. Locations of Rainfall Gages and Corresponding Monthly Precipitation for Water Year 1990 (USGS, 1990)
Figure 6.19. Calibration Results of Return Flow Salinity with Groundwater Salinity Set at 4000 μS

Figure 6.20. Calibration Results of Return Flow Salinity with Surface Water Salinity Set at 2500 μS
Figure 6.21. Comparison of MODSIMQ Simulated Average Salinity in the Arkansas River over the Simulation Period with Historical Data

Table 6.10. MODSIMQ Salinity Management Scenarios for Case Study

<table>
<thead>
<tr>
<th>Scenario</th>
<th>John Martin Reservoir Set to Historical Levels</th>
<th>Water Quality Constraints Included</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scenario 1</td>
<td>YES</td>
<td>NO</td>
</tr>
<tr>
<td>Scenario 2</td>
<td>YES</td>
<td>YES</td>
</tr>
<tr>
<td>Scenario 3</td>
<td>NO</td>
<td>NO</td>
</tr>
<tr>
<td>Scenario 4</td>
<td>NO</td>
<td>YES</td>
</tr>
</tbody>
</table>

Examining the case study under these four scenarios aids in revealing the intricate relationships between demands for water, amounts of water diverted, water use efficiency, and corresponding changes in water quality. The ultimate goal is to provide a means of predicting the consequences of different options that decision makers may wish to exercise.
6.7.2 Scenario 1

As detailed previously, John Martin Reservoir is operated under strict guidelines dictated through several complex legal agreements. Examining the case study under Scenario 1 does not imply that operation of John Martin Reservoir is ignored. Rather, Scenario 1 is established to ensure water storage patterns in John Martin Reservoir follow the historical pattern by setting upper and lower bounds for all accrual links in John Martin Reservoir to historical flow rates. Under this scenario, although storage rights in John Martin Reservoir are essentially removed from the stream, exclusive rights are assigned to it for filling all child account reservoirs as consistent with historical records. By doing so, various other operational strategies can be explored without concern about possible impacts on John Martin Reservoir. Furthermore, the water quality constraints are removed under Scenario 1, allowing MODSIMQ to provide important information on the stream water quality conditions without imposition of any water quality constraints.

Results derived from Scenario 1 are important to understanding operations in the study area since they describe the system response when water quantity criteria dominate the solution and inflows to John Martin Reservoir are set to the historical inflow pattern. Figure 6.22 gives the results of Scenario 1 for the ditches in Water District 67 by comparing historical water consumption, estimated water demand, and the optimized MODSIMQ solution. This figure clearly illustrates the advantage of utilizing an optimization model. The model successfully reduces total demand shortages by utilizing both surface water and groundwater in the most efficient manner. Furthermore, since the model also incorporates all the water rights for each user, no water rights are harmed in the search for the optimal solution.

![Figure 6.22. Water Quantity Results for Scenario 1](image-url)
6.7.3 Scenario 2

Similar to Scenario 1, Scenario 2 also limits the inflow accrual amounts to John Martin Reservoir to duplicate the historical record. However, Scenario 2 incorporates the water quality constraints, which were not considered in Scenario 1. In this case, the model utilizes the embedded optimization techniques to derive solutions based on both the water quality and water quantity criteria. In effect, the penalty coefficient \( P_n \) in Eq. 5.2 serves to evaluate tradeoffs between satisfying the water quantity demands and meeting the water quality constraints, since they are not maintained as explicit constraints in this formulation. Employing the same water right priorities \( w_i \) utilized in Scenario 1, a value of penalty \( P_n \) is selected that provides a compromise solution between the two criteria.

As expected, the MODSIMQ solution results in higher demand shortages for certain months (Figure 6.23), but with improved stream water quality conditions as averaged over the year (Figure 6.24). It is interesting, however, that solutions generated by MODSIMQ still provide less total demand shortages over the year when compared with historical shortages. The results shown in Figure 6.24 clearly indicate that flow patterns can be altered to produce solutions more appropriate for water quality criteria as specified by the decision makers. In this figure, results generated from Scenario 2 are compared to both the historical record and the results generated from Scenario 1.

![Figure 6.23. Water Quantity Results for Scenario 2](image-url)
6.7.4 Scenario 3

In Scenario 3, upper and lower bounds on accrual links to all child accounts in John Martin Reservoir are no longer set to the historical fill record. Unlike Scenarios 1 and 2, storage rights in John Martin Reservoir must compete with other water rights in the basin. Additionally, this alternative also eliminates the water quality constraints. Comparing the results of Figure 6.25 with those in Figure 6.22, it can be seen that solutions derived from
Scenario 3 have higher demand shortages than solutions generated under Scenario 1. This is due to John Martin Reservoir having one of the lowest water storage priorities in the entire basin. Therefore, with specification of fixed accrued inflows into John Martin Reservoir removed, less water is available for storage as compared with Scenario 1. The reduction in storage in John Martin Reservoir consequently reduces the water available for users in Water District 67. The reduction in storage in John Martin Reservoir is illustrated in Figure 6.26.

6.7.5 Scenario 4

Similar to Scenario 3, Scenario 4 also eliminates the restriction of setting inflow accruals to John Martin Reservoir at historical levels, but with incorporation of the water quality constraints. Similar to the results of Scenario, imposition of water quality constraints results in increased shortages, as shown in Figure 6.27. As expected, results derived under Scenario 4 produce lower salinity levels when compared with Scenario 3, as seen in Figure 6.28. As a consequence of lowering the salinity of the Arkansas River, users in the Water District 67 are required to divert less water for irrigation purposes. Furthermore, Figure 6.29 shows drastic reductions in storage volume in John Martin Reservoir as a result of imposition of the water quality constraints, which is necessary in order to lower streamflow salinity downstream of the reservoir.

6.7.6 Improvement in Irrigation Efficiency

Changes in irrigation efficiencies impact the quantities of return flows and diversion requirements for irrigation, which can in turn dramatically alter the stream water quality. For example, if means are available for increasing the efficiency of irrigation, then the amounts of water needed for irrigation can be reduced, which also reduces irrigation return flows back
Figure 6.27. Water Quantity Results for Scenario 4

Figure 6.28. Water Quality Results for Scenario 4
into the stream. Broner and Valliant (1995) have shown that by utilizing an irrigation method called surge irrigation, the amounts of water needed can be greatly reduced. Furthermore, surge irrigation is observed to be as effective as conventional irrigation practices. If one desires to analyze the impact of special irrigation practices, such as surge irrigation, MODSIMQ can be utilized to perform such an analysis. In MODSIMQ, two parameters can easily be altered to reflect the impact of different irrigation practices: the demand and the infiltration rate.

A scenario of improved irrigation efficiency can be modeled using the following equations:

\[
D_C = D^0 (1 - \alpha^0)
\]

(6.1)

where

- \(D_C\) = consumptive demand
- \(D^0\) = demand before irrigation efficiency is improved
- \(\alpha^0\) = infiltration rate before irrigation efficiency is improved

If the irrigation is improved by reducing the infiltration rate to a new rate \(\alpha^1\) then Eq. 6.1 can be rewritten with the new demand \(D^i\) as:

\[
D_C = D^i (1 - \alpha^1)
\]

(6.2)
By assuming the consumptive demand $D_C$ remains the same, then Eqs. 6.1 and 6.2 can be combined to calculate the new demand $D'$ as:

$$D' = \frac{(1 - \alpha^0)}{(1 - \alpha^1)}$$

(6.3)

Using Eq. 6.3, the case study was reconstructed to simulate the effects of improved irrigation efficiency. The new infiltration rate $\alpha'$ was assumed to be 0.15 basin wide. This $\alpha'$ reflects some of the more efficient irrigation methods, such as sprinkler systems. The new demand $D'$ for each user is then calculated using Eq. 6.3.

Under the assumption of improved irrigation efficiency on a basin wide basis, several interesting results are obtained. Figure 6.30 illustrates the estimated water demand for both current and improved irrigation practices, as well as the optimal water usages calculated by MODSIMQ. Note that the optimal solutions are unable to satisfy the demands in a reasonable manner. This results from the fact that groundwater storage acts as a reservoir, and when infiltration rates are decreased, the amounts of water stored in the groundwater system and ultimately returned to the stream are also decreased. Since less water is returned to the stream, amounts of water available in the stream for irrigation practices also decreases, particularly late in the irrigation season. This is the primary reason for the demand shortage increases as shown in Figure 6.30.

![Figure 6.30. Water Quantity Results under Increased Irrigation Efficiency](image_url)
Even though demand shortages increase as a result of improved irrigation efficiency, a trade off is observed in Figure 6.31. When irrigation efficiency is improved, the amounts of return flow decrease; but since the return flow is generally of poorer quality than the receiving stream, the stream water quality is improved, as illustrated in Figure 6.31. This means that increasing irrigation efficiency can both improve stream water quality and decrease the irrigation demand, although, it can also decrease the amount of water available in the stream for diversion by irrigators.

![Graph showing water quality results](image)

**Figure 6.31.** Water Quality Results Showing the Effects of Improved Irrigation Efficiency

### 6.7.7 Analysis of Results

When MODSIMQ is applied to the case study, two relationships have been observed confirming the theoretical considerations of the model. The first one is the upstream / downstream relationship. When a quality constraint is violated downstream, the model equally penalizes all users regardless of their location. This means that the model does not favor users upstream of the system, and penalize users close to where violations are observed. The following example, illustrated in Figure 6.32, shows how MODSIMQ equally penalizes all users regardless of their location.

In Figure 6.32, if it is assumed that increasing flows in link #2 can improve water quality in link #1, which is violating the water quality constraint, then the model will try to decrease the "cost" for link #2 making it act like a flow-through demand, and forcing both user #1 and user #2 to decrease the quantity of their diversion in an unbiased fashion.
Figure 6.32. Example of Upstream /Downstream and Senior User/Junior User Relationships in MODSIMQ

The second relationship observed is the senior user /junior user relationship. When a quality constraint is violated downstream, the model again equally penalizes all users. This means that the model does not change a junior user to a senior user or vice versa. Using the aforementioned example, it is clear that if link #1 is violating the quality constraint, the model again equally penalizes user #1 and user #2 regardless of their seniority. However, in one special instance, the model can reverse the seniorities between two users. For example, using figure 7.35, assume user #2 is a senior user and user #1 is a junior user. Moreover, link #3 is violating the quality constraint and increasing flows in link #4 improves water quality in link #3. This means that the model will try to increase the flows in link #4 and decrease the flows to user #2, thus making user #2 become a junior user when compared to user #1. This simple example demonstrates that the model can actually reverse the seniorities between two users; however, in reality, this reversal of seniorities is the most logical approach to improve quality conditions in link #3. Since user #1 is situated downstream of link #3, altering flows to user #1 has no impact on the quality conditions of link #3, thus it makes sense that user #1 shouldn't be punished for quality violations taking place upstream. In fact, in this example, all users downstream of link #3 are not penalized and all users upstream of link #3 are penalized. This means seniorities between users downstream of link #3 and between users upstream of link #3 are preserved the way it should be in MODSIMQ.

Based on the results generated from the various scenario presented in this chapter, it is clear that there is a strong relationship between the quality of the stream and the amount of diversion for irrigation practices. This relationship plays an important role in determining the most appropriate way of managing a river system, such that both the quality criteria and the quantity criteria are considered unbiasedly. However, in a complex and large river basin, it is often difficult to manage the system effectively. Therefore, in order to properly manage a system while considering individual components of a river basin in an integrated manner, it is necessary to utilize a DDS such as MODSIMQ.
VII. CONCLUSIONS AND RECOMMENDATIONS

7.1 Summary and Conclusions

An integrated water quantity/quality river basin network flow model called MODSIMQ, is developed and incorporated into a decision support system (DSS). The DSS provides users with an intuitive and comprehensive tool for analyzing complex river basin problems. MODSIMQ is capable of simultaneously model water quality and quantity elements in a river basin under various interconnected and rule-driven components. Furthermore, MODSIMQ is a generalized network model, enabling it to be applied to a wide range of river basin configurations.

MODSIMQ incorporates two reliable and well tested modes, MODSIM and QUAL2E in its structure. MODSIM is essentially a river basin network model, which is integrated into MODSIMQ to perform simulation and optimization on the quantity aspects of river basin problems. MODSIM also has a comprehensive submodel capable of simulating interactions between groundwater and surface water systems. QUAL2E is an one dimensional stream water quality model which simulates water quality dynamics in a river basin, including conservative and nonconservative constituents. However, QUAL2E lacks the ability to simulate the quality of return flows. An additional module is therefore developed for MODSIMQ to simulate the movement of groundwater quality constituents.

The ultimate goal of the current study was to combine models that deal with water quality and quantity in a fully integrative fashion. This was accomplished by utilizing the Frank-Wolfe algorithm, which ensures the solution to be optimal for both the water quality and water quantity. The Frank-Wolfe involves combining linear approximations of the objective function (which enables it to be solved efficiently with the network optimization algorithm embedded in MODSIM) with one-dimensional search procedures.

To provide a user-friendly interface for the program, a window based operating shell is been developed which adopts all the standard Microsoft Windows conventions; thereby allowing the user to operate in a familiar and intuitive environment.

A case study is initiated to fully demonstrate the functionality and capabilities of MODSIMQ. The case study selected for the current research is the lower Arkansas River Basin in Colorado. The complex hydrologic systems and legal structures of the study area are comprehensively modeled utilizing MODSIMQ.

Results from case study demonstrate the validity of MODSIMQ, and provide evidence that the theoretical foundations of MODSIMQ successfully incorporates the water quality and water quantity aspects of a river basin in an integrative and systematic manner. The results also reveal the intricate relationships between water quality and water quantity in a river basin. This relationship plays an important role in determining the most appropriate way of
managing a river system, such that both the quality criteria and the quantity criteria are considered in an unbiased fashion.

7.2 Recommendations for Future Work

Recommended future research work on MODSIMQ are listed follows:

1. Integration of the current window based user interface with the most updated user interface of MODSIM. By keeping the Qua-file editor embedded in MODSIMQ and replacing the current ADA-file editor and ORG-file editor in MODSIMQ with the newer interface, the model can take full advantage of the capabilities of drawing and editing system features in an intuitive fashion.

2. Development of a more comprehensive generalized return flow quality model, or separate detailed models for different quality constituents. The current model has a generalized return flow quality model that can provide adequate estimations for all quality constituents. However, if intensive on-site data are available, more comprehensive models can be developed to provide detailed analysis of the movement of groundwater quality constituents.

3. Utilizing MODSIMQ for long term simulations for the case study area. Many groundwater impacts are long term oriented, therefore, it is beneficial to examine the case study area for more than one year.

4. Utilizing MODSIMQ for daily simulations for the case study area. By reducing the duration of simulation periods, it is possible to analyze the system in greater detail. Examining the study area on a daily time frame also tends to increase the accuracy of results.
REFERENCES


