CONJUNCTIVE MANAGEMENT OF SURFACE WATER AND

GROUND WATER QUANTITY AND QUALITY:

CONCEPTUAL AND FUNCTIONAL MODELING APPROACH

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Executive Summary

This report discusses how to design a computer model to aid optimizing conjunctive management of groundwater and surface water quantity and quality. The report does not present a completed computer model, but rather discusses how a future model could be developed. The discussed modelling approach is termed PROMOD (PROposed methodology and MODel). Precursors to PROMOD are in current use, but are far from having all the attributes discussed here. The additional capabilities are important to address world needs.

Water management problems are becoming increasing complex. Frequently, managers are attempting to satisfy increasing water needs while reconciling other conflicting goals. Computer models are valuable tools for this effort. Both simulation models (here abbreviated S) and simulation/optimization (S/O) models are needed. They differ in purpose, and utility.

A simulation model is designed to simulate how a physical system will respond to stimulus (groundwater pumping, diversion, among others). This is an important role because one cannot optimize management of a complicated system unless one can predict how the system will respond to management.

A S/O model is designed to compute the best water management strategy[1] for a particular user-specified management problem. A modeller can use a S/O model to calculate a better management strategy than he can develop using a normal simulation (S) model. The difference in meaning between calculate and develop is significant here.

Although normal simulation models have frequently been used to develop water management strategies, the best strategy developed in that way is not really optimal. It is only the best choice from among the strategies assumed and tested by the modeller. On the other hand, a strategy computed by a S/O model can be truly optimal--mathematically the best of an infinite number of possible strategies that will all satisfy the restrictions of a particular scenario. Personal experience has shown improvements of 10-40% in water management strategies between those developed using S/O models versus S models alone.

The discussed PROMOD model will link S and S/O modules with other software modules to aid computing and reporting optimal water management strategies. The resulting PROMOD model will:
■ simulate flow and transport between reservoir, stream, canal and aquifer, and show the effects of water user practices on return flows and concentrations.
■ aid water allocation between agricultural, urban and ecological users on local to regional scales
■ perform multiobjective optimization: simultaneously considering goals of optimizing water use or delivery, crop yield, environmental protection, economic return or combinations.
■ be useful for a wide range of planning horizons

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[1] A 'strategy' is a set of spatially and temporally distributed water fluxes that can be directly managed by man. For example, a conjunctive use strategy might be a set of groundwater pumping and surface water diversion rates. A wastewater loading strategy might be a set of rates of discharges to a stream. A loading and conjunctive use strategy addresses both issues. A management strategy is developed to address a particular management 'scenario' (posed management problem).

PROMOD will:
- integrate the simulation abilities of existing well documented and tested software.
- add extra code to existing software, to provide needed capabilities.
- provide functional relations (mathematical expressions) within a simplified simulation module (SSM) and a simulation/optimization (S/O) module; and compute numerically optimal water management strategies.
- provide the user with alternative equations to employ for the same physical process, so that the model can make best use of available data.
- include the most common computer approaches to allocating use of water resources.
- be mathematically and computationally sufficient for the task. It will include both linear and nonlinear objective functions and constraint equations. To the extent practical, it will utilize linear systems theory and multivariate statistical analysis to develop simplified expressions for describing stream-aquifer system response to management action (stimulus). It will include methods for removing errors introduced by treating nonlinear systems as if they are linear.
- assure that computed optimal strategies satisfy all management goals and constraints to the extent physically possible (for example, preventing unacceptable: salinization, declines or rises in water levels, concentrations, salt water intrusion, contaminant migration, flows or mass flow rates, or related changes in ecological, environmental, social or natural systems), while best achieving the major management objective (for example, maximizing annually supplied water, or production of crops or hydropower).
- be written in a modular fashion to allow easy upgrading.
- be user-friendly, WINDOWS-based, and very useful for training and management.
- be transportable and designed to run on a 386/486/pentium personal computer.

To have the characteristics listed above, PROMOD modules do the following, in approximately the order shown:
- help simulation model calibration by using optimization algorithms.
- select and include proven simulation models as submodules within an integrated simulation module (ISM). The ISM will be able to simulate with varying degrees of accuracy and detail, depending on how much data is available and what the management goals are.
- develop a data base of system responses to stimuli by systematically and recursively simulating flow and transport (using the ISM), for assumed unit stimuli or ranges of stimuli.
- develop simplified expressions that describe system response to appropriate stimuli (i.e, linear influence coefficients or linear or nonlinear expressions) practical for inclusion within a S/O module. The resulting SSM will perform some simulations more quickly on a computer than current available models.
- employ the ISM to simulate system response to an assumed water management strategy. The assumed strategy can be a current water management practice; or the best management strategy the user can determine without using the S/O model.
- compute an optimal water allocation or management strategy for the posed management problem using the S/O module (that couples the normal and simplified simulation expressions with operations research style optimization algorithms). The ISM will simulate system response to implementing the optimal strategy to verify acceptability of accuracy, and

PROMOD will cycle as needed to reduce error and improve reliability of the optimal strategy.

■ provide graphical and tabular results summaries, highlighting the benefits of optimal management. For example, summaries will illustrate the difference between the benefits of an initially assumed (for convenience termed 'nonoptimal') strategy, and an optimal strategy computed by the S/O module.

Expected benefits of an implemented PROMOD model are that:

■ it will be practical to compute optimal water management strategies for complicated water management problems (simultaneously considering policy, sociological, ecological and economic constraints).

■ hands-on training in S/O modelling will become more available.

■ S/O model use will become more common.

■ water management will improve.

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$a_{\bar{o}}$ and $b_{\bar{o}}$ = site specific empirical coefficients.

$a_{\bar{o},i}$ = constant coefficient for the average inflow in i stress period before stress period $k+1$

$\hat{a}$ = index denoting a potential pumping cell.

A^a = concentration of algae [mg-A/L].

$A_{\bar{o}}$ = cell area [L^2]

A_x = cross-sectional area [L^2]

AA, BB, AA' and BB' = regression coefficients.

$b(\hat{a},k)$ = sum of all changes in deep percolation or canal/aquifer interflow that result at cell $\hat{a}$ during stress period k, from the computed optimal management strategy [L^3/T]

$b_{\bar{o},i}$ = constant coefficient for the average inflow in $i+1$ stress period before stress period $k+1$

$B_{\bar{o}}^{sr}$ = elevation of the bottom of the surface water body [L].

c = concentration [$M\ L^{-3}$]

$c^{cat}_{\hat{e},\acute{e},\ddot{e},k}$ = average concentration of water delivered to UCA user $(\hat{e},\acute{e},\ddot{e})$ during the stress period [$M\ L^{-3}$].

$c^{catavg}_{\hat{e},\acute{e},\ddot{e}}$ = average concentration of water delivered to UCA user $(\hat{e},\acute{e},\ddot{e})$ during the planning period [$M\ L^{-3}$].

$c^{crw}_{\hat{e},\acute{e},\ddot{e}}$ = a dimensionless crop loss coefficient. It equals the proportional reduction in the annual potential yield that results from a proportional lack of adequate irrigation water in time step k, known by site-specific studies

c^g = the concentration of dissolved contaminants in groundwater [ML^{-3}]

c^{nonc} = concentration of the nonconservative constituent [m-nonc L^3]

c^g = concentration of contaminants sorbed on the porous medium, [MM^{-1}]

$c_{\ddot{y},k}^{mt}$ = average concentration of water delivered to M&I user $\ddot{y}$ during the stress period [$M\ L^{-3}$]

$c_{\ddot{y}}^{mtavg}$ = average concentration of water delivered to M&I user $\ddot{y}$ during the planning period [$M\ L^{-3}$] and

c^{ssg} = concentration of the sources or sinks [ML^{-3}]

$c^x(i,j)$ = concentration of the jth constituent in the ith reach of the xth source/control location [M/L^3]

cacg(1) = set of all cells belonging in UCAs

casG($\acute{e}$) = set identifying all q^{ca} flows within UCA group $\acute{e}$

catg($\ddot{a}$) = set including all pumping cells of catgg($\ddot{a}$) and all surface flows of catsg($\ddot{a}$).

catgg($\ddot{a}$) = subset (subgroup) identifying each pumping cell, pc($\hat{a}$), providing groundwater to UCA group catg($\ddot{a}$). There are $M^{catgg}(\ddot{a})$ such cells

catsg($\ddot{a}$) = subset (subgroup) identifying each q^{ca} providing any surface water to UCA group catg($\ddot{a}$). There are $M^{catsg}(\ddot{a})$ such flows

$C^{+h}(\hat{o},k)$, $C^{-h}(\hat{o},k)$ = weights assigned to groundwater head over-achievement and under-achievement variables, respectively [dimensionless, or $\$L^{-1}$]

$C^{cr}(\Upsilon)$ = weight assigned to UCA Υ. This can be the economic benefit per unit of crop yield. It can also be a cost per unit crop yield, depending on user intent [M^{-1}].

$C^{HGV}(\grave{o})$ = 1, to control head difference

= L^{δ} , to control hydraulic gradient

= $(L^{\delta} \theta) / J$, to control seepage velocity

= $(L^{\delta} \theta R_f) / J$, to control contaminant velocity

$C^{ip}(\hat{a})$, $C^{id}(\hat{e})$ = respectively, cost of installing a well or diversion structure at locations $\hat{a}$ and $\hat{e}$, respectively [$]

$C^{p}(\hat{a},k)$ = cost or weighting coefficient for managed pumping in cell $\hat{a}$ during stress period k [$ per L^3/T] or [dimensionless]

$C^{p1}(\hat{a},k)$, $C^{p2}(\hat{a},k)$ = respectively, linear and quadratic cost or weighting coefficients for managed pumping [$ per L^3/T $ per L^4/T] or [dimensionless]

$C^{d}(\hat{e},k)$ = cost or weighting coefficient for managed diversion in cell $\hat{e}$ during stress period k [$ per L^3/T] or [dimensionless]

$C^{d1}(\hat{e},k)$, $C^{d2}(\hat{e},k)$ = respectively, linear and quadratic cost or weighting coefficient for managed diversion [$ per L^3/T $ per L^4/T] or [dimensionless] and

CC, DD, CC' and DD' = regression coefficients.

Chl$\underline{a}$ = concentration of chlorophyll $\underline{a}$ [ug-Chl$\underline{a}$ /L]

$d(\hat{e},k)$ = difference between nonoptimal and optimal diversion or reservoir release [L^3/T]

$d^{ete}_{\bar{o}}$ = extinction depth in cell $\bar{o}$ (depth below $h^{etd}_{\bar{o}}$ at which there is no evapotranspiration) [L].

$d^{G}(\hat{e},k)$ = sum of diversion in diversion group $\hat{e}$ in stress period k, [L^3/T]. There are $M^{dg}(\hat{e})$ such cells

$d_{\bar{o},k}$ = diversion from (+) or augmentation to (-) the stream in cell $\bar{o}$ in time k step (+), [L^3T^{-1}]. For a stream reach, the simulation model can compute only one of v^c, and v^o. For a reservoir reach d is a release.

$dg(\hat{e})$ = set identifying each cell, $dc(\hat{e})$, belonging to diversion group $\hat{e}$

$dsfg(\hat{e},\acute{e},0)$ = set of drain, spring or flowing cell cells that provide water to alpha drainage canal $\hat{e},\acute{e}$.

$dsfg(\hat{e},\acute{e},\ddot{e})$ = set of drain, spring or flowing cell cells that provide water to beta drainage canal $\hat{e},\acute{e},\ddot{e}$.

$dsg(\acute{a})$ = set identifying each diversion cell, $dc(\hat{a})$, belonging to pumping-diversion group $pdg(\acute{a})$. There are $M^{dsg}(\acute{a})$ such reaches

D_{ij} = groundwater hydrodynamic dispersion coefficient [L^2T^{-1}

D^{g}_{L} = groundwater dispersion coefficient [$L^2 T^{-1}$]

D^{s}_{L} = surface water dispersion coefficient, [L^2T^{-1}]

$\hat{e}$ = index denoting a potential river water diversion, reach

E^{col} = concentration of coliforms [colonies L^{-3}]

$E^{hp}_{\hat{e},k}(P_{\hat{e},k})$ = energy conversion efficiency as a function of power generation

$E^{ls}_{\hat{e},\acute{e}}$ = conveyance efficiency (as a proportion) of the canal section

$EC^{catavg}_{\hat{e},\acute{e},\ddot{e}}$ = average electrical conductivity value of the irrigation water delivered to the UCA during the planning period [dSm^{-1}]

$EC^{min}_{\hat{e},\acute{e},\ddot{e}}$	= lowest average electrical conductivity value of the irrigation water which will not cause crop yield reduction in the UCA [dSm^{-1}].
$EC^{ymax}_{\hat{e},\acute{e},\ddot{e}}$	= average electrical conductivity value of the irrigation water above which there will be no crop yield in the UCA [dSm^{-1}]
$E^{dpca}_{\hat{e},\acute{e},\ddot{e},\dot{e}}$	= proportion of the water applied to a UCA that becomes deep percolation in cell è. The deep percolation in cell è is the same as the q^{dp} of the groundwater flow equation
$E^{rfca}_{\hat{e},\acute{e},\ddot{e},\dot{e}}$	= proportion of the water applied to the UCA that becomes runoff in cell è.
$E_{\bar{o}}$	= potential evapotranspiration in cell ō [LT^{-1}]
$E^{sac}_{\hat{e},\acute{e},\ddot{e}}$	= assumed proportion of the salt applied to the UCA that remains in the soil profile and does not leach to groundwater or runoff the land during stress period k.
$E^{vr}_{\bar{o},k}$	= proportion of reservoir storage that is lost due to evapotranspiration
FF and FF'	= regression coefficients.
g(â,k)	= p(â,k) + b(â,k) = difference between the nonoptimal and optimal vertical discharge or recharge rate at cell â during stress period k [L^3/T]
$g^{ut}(\hat{a})$	= magnitude of 'unit' discharge or recharge stimulus in cell â [L^3/T]. This does not necessarily have a magnitude of one
h	= aquifer potentiometric surface elevation (head) [L]
h(ô,k)	= groundwater potentiometric surface elevation at head control cell ô by the end of stress period k [L].
$h(\hat{o}_{\grave{o},1},k)$	= potentiometric surface head at point 1 (some cell ô) of HGV pair ò at end of period k, [L]
$h(\hat{o}_{\grave{o},2},k)$	= potentiometric surface head at point 2 (a second cell ô) of HGV pair ò at end of period k, [L]
h^{lp}, h^{ld}	= the head that needs to be overcome for the pumped or diverted (respectively) water to be used. For pumping, the head can be the total dynamic lift. For the diversion, it might be the head needed to push the diverted water to the user [L].
$h^{+}(\hat{o},k)$, $h^{-}(\hat{o},k)$	= groundwater head over-achievement and under-achievement, respectively [h]. Both must be positive, and only one can be nonzero at one stress period for a particular location.
$h^{dsf}_{\bar{o}}$	= elevation of drain base or ground surface for spring or flowing well (L).
$h^{etd}_{\bar{o}}$	= potentiometric surface elevation below which the evapotranspiration rate begins to decrease [L]
h^{non}	= potentiometric surface elevation that results without implementing the optimal strategy, (nonoptimal head) [L]
$h_{\bar{o},k}$	= average potentiometric head in cell ō at end of stress period k [L]
$h^{t}(\hat{o},k)$	= target head (i.e. the head we are trying to achieve)[L].
$H_{\hat{e},k}$	= net head [L]
$I^{p}(\hat{a})$, $I^{p}(\hat{e})$	= respectively, integer variables indicating a well or diversion structure.
II	= a the number of terms in the polynomial expression
J	= average hydraulic conductivity between control pair locations [L/T]
JJ	= the number of terms in the exponential polynomial

k	= index for stress period
$k_{\bar{o}}^{s}$	= linear relation between average flowrate and head in cell $\bar{o}$ for flowrates that are not less than σ^{lin}, $[TL^{-2}]$
K	= total number of stress periods within the optimization (planning) period
K^{ds}	= dispersion constant [dimensionless]
K^{0}_{2}	= the reaeration rate in accordance with the Fickian diffusion analogy [temperature dependent $[day^{-1}]$
K^{col}_{5}	= coliform die-off rate, temperature dependent $[T^{-1}]$.
K^{BOD}_{1}	= carbonaceous BOD deoxygenation rate, temperature dependent $[day^{-1}]$
K^{nonc}_{6}	= decay rate for the constituent, temperature dependent $[T^{-1}]$
K^{O}_{4}	= sediment oxygen demand rate, temperature dependent $[g/ft^{2}$-day]
$L^{lc}_{\hat{e},\acute{e}}$	= length of canal section $\hat{e},\acute{e}$ [L] and
$L^{lc}_{\hat{e},0}$	= total length of alpha canal $\hat{e}$ [L].
L^{BOD}	= concentration of ultimate carbonaceous BOD [mg/L]
$L^{e}_{\bar{o},k}$	= evapotranspiration loss from the reservoir $[L^{3}T^{-1}]$
L^{δ}	= distance between pair of control locations, $\hat{o}_{\delta,1}$ and $\hat{o}_{\delta,2}$ [L]
LI	= number of stress periods lagged inflows and
LQ	= number of stress periods of lagged outflows.
min(q,r)	= an expression stating that the computer model will utilize the smaller of the two values: q and r.
msg($\ddot{Y}$)	= set identifying each surface flow providing water to M&I group $\ddot{Y}$. There are $M^{msg}(\ddot{Y})$ such flows
mtg($\acute{y}$)	= set including all pumping cells of mtgg($\acute{y}$) and all surface flows of mtsg($\acute{y}$).
mtgg($\acute{y}$)	= subset (subgroup) identifying each pumping cell, pc($\hat{a}$), providing groundwater to M&I group mtg($\acute{y}$). There are $M^{mtgg}(\acute{y})$ such cells
mtsg($\acute{y}$)	= subset (subgroup) identifying each q^{m} providing any surface water to M&I group mtg($\acute{y}$). There are $M^{mtsg}(\acute{y})$ such flows
M	= mass [M].
$M^{2s}(\hat{e})$	= set of beta canals receiving water from alpha canal $\hat{e}$.
M^{b}	= total number of cells at which vertical fluxes other than pumping can occur from or to the aquifer.
M^{c}	= the number of reaches at which streamflow concentration is constrained.
$M^{ca}(\hat{e},\acute{e})$	= set of unit command areas served by beta canal $\hat{e},\acute{e}$.
M^{cacG}	= number of cells in all agricultural command areas (UCAs)
M^{CASG}	= the number of groups of UCA surface water inflows considered.
$M^{catgg}(\ddot{a})$	= number of pumping cells providing groundwater to UCA group catg($\ddot{a}$), which is the same number providing groundwater to UCA subroup catgg($\ddot{a}$)
$M^{CATG}(\ddot{a})$	= number of UCA groups to which total water provided in any stress period is bounded
$M^{catsg}(\ddot{a})$	= number of surface flows (q^{ca}) providing water to UCAs in UCA group catsg($\ddot{a}$)
M^{d}	= total number of reaches at which surface water diversion from a stream can be optimized

$M^{dsg}(\acute{a})$	= number of diversion reaches in pumping-diversion group pdg($\acute{a}$).
M^{dvf}	= $M^d + M^v + M^f$
M^{DG}	= the number of groups of diversion reaches considered
M^f	= total number of locations at which changes in canal flow to a stream, (resulting from optimal water management) can occur
M^{mf}	= the number of reaches at which mass flow rate is constrained.
$M^{mtgg}(\acute{y})$	= number of pumping cells providing groundwater to M&I group mtg($\acute{y}$), which is the same number providing groundwater to M&I subroup mtgg($\acute{y}$)
$M^{mtsg}(\acute{y})$	= number of surface flows (q^m) providing water to M&I users in M&I group mtsg($\acute{y}$)
M^{MSG}	= the number of groups of M&I users considered.
$M^{MTG}(\acute{y})$	= number of M&I groups to which total water provided in any stress period is bounded
$M^{\delta}_{\hat{u},\acute{o},\ddot{o}}$	= set of aquifer cells providing water to beta drain $\hat{u},\acute{o},\ddot{o}$.
M^P	= total number of cells at which groundwater pumping will be optimized.
M^{pb}	= $M^P + M^b$ total number of cells at which water can vertically recharge or discharge from the aquifer via optimal pumping, deep percolation that can directly result from water application or use (a decision variable), or canal losses that can result from optimal water management
M^{PDG}	= number of pumping-diversion groups considered
M^{PG}	= the number of groups of pumping cells considered. A group should have either extraction or injection cells in it, but not both
M^s	= number of cells at which stream flow can be constrained.
M^{sr}	= number of cells at which r/ai or s/ai can be constrained
M^{SRG}	= total number of groups of stream or river cells at which total r/ai or s/ai can be constrained.
M^v	= total number of locations at which reservoir release can be optimized
M^{vsg}	= number of reservoir reaches in a particular grouping (there might be more than one reach in one reservoir).
M^{σ}	= number of cells at which stream or reservoir stage can be constrained.
n	= number of the stress period for which system response is being computed
n^m	= Manning's roughness coefficient [dimensionless]
$\tilde{n}$	= mass flow rate (ie., flowrate times concentration) [MT^{-1}]
$\tilde{n}^x(i,j)$	= mass flow rate of the jth constituent in the ith reach of the xth source or control location [M/T]
N_1	= ammonia nitrogen concentration [mg-N/L]
N_2	= nitrite nitrogen concentration [mg-N/L]
$\bar{o}$	= identification number of a cell at a particular horizontal location and in a particular aquifer layer
$\hat{o}$	= index denoting an observation location, at which system response is being evaluated
0	= the concentration of dissolved oxygen [mg/L]
0^*	= the saturation concentration of dissolved oxygen at the local temperature and pressure [mb/L]

$p(\hat{a},k)$	= difference between the nonoptimal and optimal groundwater pumping (extraction, - ; injection, +) rate at cell $\hat{a}$ during stress period k [L^3/T]
p^a	= the local respiration rate of algae, which is temperature dependent, [LT^{-1}]
$P_{\hat{e},k}$	= power generated by q^s flow of water passing through a turbine [KW]
$pdg(\acute{a})$	= set including all pumping cells of psg($\acute{a}$) and all diversion reaches of dsg($\acute{a}$).
$p^G_{\grave{a},k}$	= total groundwater extraction rate from cells in pumping group pg($\grave{a}$) [L^3T^{-1}]
$p^G(\grave{a},k)$	= sum of pumping in pumping group $\grave{a}$ in stress period k, [L^3/T]
$pd^G(\acute{a},k)$	= sum of pumping and diversion in pumping-diversion group $\acute{a}$ in stress period k, [L^3/T]. This is the sum of pumping and diversion in groups psg($\acute{a}$) and dsg($\acute{a}$), respectively, [L^3/T]
$p_{\ddot{o},k}$	= groundwater pumping [L^3T^{-1}]
$pg(\grave{a})$	= set identifying each cell, pc($\hat{a}$), belonging to pumping group $\grave{a}$. There are $M^{pg}(\grave{a})$ such cells
$pg\ (\hat{e},\acute{e},\ddot{e})$	= group of cells extracting groundwater
$psg(\acute{a})$	= set identifying each pumping cell, pc($\hat{a}$), belonging to pumping-diversion group pdg($\acute{a}$). There are $M^{psg}(\acute{a})$ such cells
$q^{SR}(\hat{\imath},k)$	= net r/ai or s/ai in grouping ì and time k [L^3/T]
q^{0d}	= flow moving from a set of drain, spring or flowing well cells into a beta drain [L^3T^{-1}]
$q^b_{\ddot{o},k}$	= known flow across aquifer boundaries (i.e., bedrock recharge, deep percolation) [L^3T^{-1}]
$q^{ca}_{\hat{e},\acute{e},\ddot{e}}$	= surface water flow to unit command area $\hat{e},\acute{e},\ddot{e}$ [L^3T^{-1}]
$q^{cag}_{\hat{e},\acute{e},\ddot{e},k}$	= total groundwater extraction rate from the cells supplying UCA ($\hat{e},\acute{e},\ddot{e}$) [$L^3T^{-1}$].
$q^{casG}(\acute{e},k)$	= sum of surface waters delivered to UCA group $\acute{e}$ in stress period k, [L^3/T]. There are $M^{casg}(\grave{e})$ such flows within that group
$q^{cat}_{\hat{e},\acute{e},\ddot{e},k}$	= average rate of surface water and groundwater provided to UCA ($\hat{e},\acute{e},\ddot{e}$) [$L^3T^{-1}$].
$q^{catG}(\ddot{a},k)$	= sum of groundwater and surface waters delivered to UCA group $\ddot{a}$ in stress period k, [L^3/T]. This is the sum of groundwater pumping and q^{ca} in groups catgg($\ddot{a}$) and catsg($\ddot{a}$), respectively, [L^3/T]. Note that group catgg($\ddot{a}$) is equivalent to one group pg($\grave{a}$)
$q^{dp}_{\ddot{o},k}$	= deep percolation (knowns or unknowns which are a function of management). Aquifer discharges are (-) and recharges are (+) in sign [L^3T^{-1}].
$q^{dpca}_{\hat{e},\acute{e},\ddot{e},k}$	= deep percolation in a UCA served by diversion point $\hat{e}$, offtake $\acute{e}$, turnout $\ddot{e}$, in stress period k [L^3T^{-1}]
$q^{dsf}_{\ddot{o},k}$	= discharge from a drain, spring or naturally flowing well [L^3T^{-1}]
q^{cs}	= external source or sinks [M T^{-1}]
$q^{rfca}_{\hat{e},\acute{e},\ddot{e},k}$	= surface return flow from the UCA
$q^{gh}_{\ddot{o},k}$	= saturated flow between the aquifer and general head boundary cells [L^3T^{-1}]
$q^{mtG}(\acute{y},k)$	= sum of groundwater and surface waters delivered to M&I group $\acute{y}$ in stress period k, [L^3/T]. This is the sum of groundwater pumping and q^m in groups mtgg($\acute{y}$) and mtsg($\acute{y}$), respectively, [L^3/T]. Note that group mtgg($\acute{y}$) is

	equivalent to one group pg(à)
$q^{mt}_{\ddot{y},k}$	= average rate of surface water and groundwater provided to M&I user $\ddot{y}$ during period k $[L^3T^{-1}]$
q^s	= stream flow rate $[L^3/T]$
q^{snon}	= stream flow rate that results without implementing the optimal strategy (nonoptimal stream flow) $[L^3/T]$
$q^s_{\bar{o}}{}''$	= flowrate in cell $\bar{o}$ when the elevation of the river surface is $\sigma^{lin}_{\bar{o}}$, $[L^3T^{-1}]$
$q^s_{\bar{o},k}$	= flow from stream cell $\bar{o}$ via the stream in time step k (+), $[L^3T^{-1}]$
$q^{s'}_{\bar{o},k}$	= flow into the cell from upstream via the stream $\qquad$ (+),$[L^3T^{-1}]$
$q^{sr}(\hat{i},k)$	= rate of r/ai or s/ai at cell $\hat{i}$ by end of stress period k (negative for flow from aquifer to stream or river) $[L^3/T]$
$q^{src}_{\bar{o},k}$	= flow between the aquifer and stream, river or canal $[L^3T^{-1}]$
$q^{sr}_{\bar{o},k}$	= interflow between the surface water and groundwater systems $[L^3T^{-1}]$
$q^{sr}_{\bar{o},k}$	= interflow between stream or reservoir and aquifer, $[L^3T^{-1}]$
q^{ssg}	= volumetric flux of water per unit aquifer volume, due to sources (+) and sinks (-) $[T^{-1}]$. This equals the sum of recharging values of q^b , p, q^z , q^{src} , q^{gh} , and q^{dp}
$q^{ls}_{\hat{e},\acute{e},k}$	= upstream inflow into section $(\hat{e},\acute{e})$ of alpha supply canal $\hat{e}$, which receives water from diversion $\hat{e}$ $[L^3T^{-1}]$
$q^{lsi}_{\hat{e},\acute{e},k}$	= canal/aquifer interflow for section $(\hat{e},\acute{e})$ $[L^3T^{-1}]$
q^{lso}	= inflow from overland flow, surface drainage, or surface return flow, assumed to occur at the upstream end of the section $[L^3T^{-1}]$
$q^{2s}_{\hat{e},\acute{e},1,k}$	= upstream inflow into section $(\hat{e},\acute{e},1)$ of beta canal $(\hat{e},\acute{e})$ $[L^3T^{-1}]$
$q^{msG}(\ddot{Y},k)$	= sum of surface water delivered to M&I group $\ddot{Y}$ in stress period k, $[L^3/T]$
$q^m_{\ddot{y},k}$	= surface water flowing to municipality $\ddot{y}$ $[L^3T^{-1}]$.
$q^t_{\bar{o},k}$	= evapotranspiration from the aquifer $[L^3T^{-1}]$
$q^{vfr}_{\bar{o},k}$	= reduction in vertical flow between cells in layer l and the lower layer l+1 due to drop in head below the top of layer l+1 $[L^3T^{-1}]$
$\Delta q^v_{\bar{o},k}$	= $\{(ST_{\bar{o},k} - ST_{\bar{o},k-1})/\Delta t\}$ = rate of change of volume in storage in the stream or reservoir, $[L^3T^{-1}]$
$q^x(i)$	= flow rate in the ith reach of the xth source or control location $[L^3/T]$.
$q_{\ddot{y},k}{}^{dpm}$	= deep percolation resulting from water used by M&I user $\ddot{y}$ $[L^3T^{-1}]$
$q_{\ddot{y},k}{}^{rfm}$	= surface return flow from M&I user $\ddot{y}$
$q^z_{\bar{o},k}$	= lateral flow across a boundary (which depends on the boundary's fixed head and adjacent heads) $[L^3T^{-1}]$
$q^{xyl}_{\bar{o},k}$	= interflow between a canal of level x (1 = alpha, 2=beta) and type y (s = supply, d= drain)$[L^3T^{-1}]$.
R_f	= the retardation factor:
sri, ov, p	= designate stream/aquifer interflow, overland or source flow, and point source, respectively. Stream/aquifer interflow and point sources are treated as decision variables. Source or overland flows are assumed known
srg(î)	= set identifying all r/ai or s/ai interflow cells, î , belonging to grouping ì. There are $M^{rg}(\hat{i})$ such cells
$S_{\bar{o}}$	= storage coefficient or specific yield for cell $\bar{o}$

$ST_{\bar{o},k}$	= storage in reservoir $\bar{o}$ during stress period k [L^3]
t	= time [T]
td1sg	= set of all reaches that divert water to alpha supply canals
Δt_k	= duration of time step or stress period k [T]
tvg	= set of reservoir reaches (a reservoir can consist of more than one reach).
$\bar{u}$	= mean velocity [L T^{-1}]
ü	= index denoting a stream/aquifer interflow observation or control reach
û	= index denoting a stream flow observation or control reach
$u_{\hat{e},\acute{e},\ddot{e}}$	= the volume of unsatisfied water needs in a UCA during stress period k [L^3]
$u_{\hat{e},\acute{e},\ddot{e}}/ w_{\hat{e},\acute{e},\ddot{e}}$	= the proportion of water needs in time step k that are unsatisfied.
$v(\hat{e},k)$	= a decision variable describing some difference in flow from or to a stream between nonoptimal and optimal water management, other than those caused by diversion, reservoir release, or flow from an aquifer [L^3/T].
$v^c_{\bar{o},k}$	= a) for a stream reach, this is canal flow to (-) the stream from a canal that is not modelled in the same level of detail as a stream b) for a reservoir reach, this is spillage ($SP_{\bar{o},k}$) from the reservoir that is lost and does not reenter the modelled system [$L^3 T^{-1}$]
v_i	= seepage or linear pore water velocity [LT^{-1}
$vg(\ae)$	= set of reservoir release reaches .
$v^o_{\bar{o},k}$	= a) for a stream reach, this is flow from (+) or to (-) the stream in time step k, other than that included in other terms, [$L^3 T^{-1}$].
V	= M/c, [LT^{-1}]
$w_{\hat{e},\acute{e},\ddot{e}}$	= water (including irrigation and effective precipitation) required in stress period k in order to produce the maximum potential yield, known, [L^3]
$w^{ymax}_{\hat{e},\acute{e},\ddot{e}}$	= water needed for delivery in the UCA in order to achieve maximum potential crop yield [L^3]
$w^{ymin}_{\hat{e},\acute{e},\ddot{e}}$	= minimum water needed the UCA in order to obtain any crop yield at all [L^3].
$ww(x,k)$	= a nonlinear state variable; examples include: groundwater contaminant concentration, head of an aqueous or nonaqueous phase liquid within an aquifer, area of nonaqueous lens floating on groundwater, volumes of nonaqueous phase liquid as free product, residual within the aquifer, or captured by pumping
x	= distance [L]
X^{hp}	= conversion factor (11.8 to convert from ft-lb to kW)
x_i	= distance along a respective Cartesian coordinate axis [L]
$y_{\hat{e},\acute{e},\ddot{e}}$	= crop yield in UCA ($\hat{e},\acute{e},\ddot{e}$) [M]
$y^{pot}_{\hat{e},\acute{e},\ddot{e}}$	= maximum potential crop yield in UCA ($\hat{e},\acute{e},\ddot{e}$) (assuming adequate water, fertility and trace elements and acceptable salinity) [M]
$z(\hat{e},k)$	= $d(\hat{e},k) + v(\hat{e},k)$ = difference between nonoptimal and optimal diversion, reservoir release or other management decision directly adding water to or removing water from the stream (indirect effects felt through the aquifer are not included) [L^3/T]
$z^{ut}(\hat{e})$	= magnitude of 'unit' diversion, reservoir release, or direct discharge or

source at location ê [L^3/T]. This does not necessarily have a magnitude of one.

Z	= objective function value

$\beta^h(\hat{o},\hat{e},n\text{-}k\text{+}1)$= influence coefficient describing effect of river water diversion or inflow at reach ê or reservoir release at location ê in stress period k, on potentiometric surface elevation at cell ô by the end of period n [L]

α, β = empirical constants derived from stage-discharge rating curves.

α^o_3 = the rate of oxygen production per unit of algal photosynthesis [mg-O/mg-A]

α^o_4 = the rate of oxygen uptake per unit of algae respired [mg-O/mg-A]

α^o_5 = the rate of oxygen uptake per unit of ammonia nitrogen oxidation [mb-O/mg-N]

α^o_6 = the rate of oxygen uptake per unit of nitrite nitrogen oxidation [mb-O/mg-N]

$\beta^o(DOX)$ = regression coefficient describing the contribution of the background concentration of dissolved oxygen to the DOX mass flow rate at reach û, [M/T].

β^o_1 = ammonia oxidation rate coefficient, temperature dependent[day^{-1}]

β^o_2 = nitrite oxidation rate coefficient, temperature dependent [day^{-1}]

$\beta^s(\hat{u},\hat{e},n\text{-}k\text{+}1)$= influence coefficient describing effect of river water diversion or inflow at reach ê or reservoir release at location ê in stress period k, on stream flow rate at reach û by the end of period n [L]

$\beta^{sri}(\ddot{u},\hat{e},n\text{-}k\text{+}1)$= influence coefficient describing effect of river water diversion or inflow at reach ê or reservoir release at location ê in stress period k, on stream flow rate at reach ü by the end of period n [L]

$\beta^x(j)$ = regression coefficient describing the contribution of specific mass flow rate to ñ $^x(i,j)$.

$\Gamma^{dsf}_{\bar{o}}$ = coefficient describing flow from drain, spring, or naturally flowing well as a function of head, [t^2T^{-1}]

$\Gamma_{\bar{o}}$ = hydraulic conductance of the surface water-aquifer interconnection, (including any clogging layer) [L^2T^{-1}]

Δ var = a change in variable bound

μ^a = the local specific growth rate of algae as defined below, which is temperature dependent, [T^{-1}] (DeGroot, 1983; Scavia and Park, 1976; Swartzman and Bentley, 1979)

$\delta^h(\hat{o},\hat{a},n\text{-}k\text{+}1)$= influence coefficient describing effect of ground water pumping at cell â in stress period k, on potentiometric surface elevation at cell ô by the end of period n [L]

$\delta^s(\hat{u},\hat{a},n\text{-}k\text{+}1)$ = influence coefficient describing effect of ground water stimulus at cell â in stress period k, on stream flow at reach û by the end of period n [L]

$\delta^{sri}(\ddot{u},\hat{a},n\text{-}k\text{+}1)$= influence coefficient describing effect of groundwater stimulus at cell â in stress period k, on stream flow at reach ü by the end of period n [L]

$\sigma^{avg}_{\hat{e},k}$ = average reservoir water surface elevation during stress period k [L]

$\sigma^{tavg}_{\hat{e},k}$ = average tailrace water surface elevation below reservoir release ê during stress period k [L]. This is a function of $q^s_{\hat{e},k}$ and water conditions downstream of the release (for example, another reservoir water surface elevation).

σ^d = stream depth [L]

$\sigma^{lin}{}_{\bar{o}}$ = elevation of the river surface above which a linear stage discharge relation is applicable, [L].

α_{oar} = scaled proportion of algae that is chlorophyll $\underline{a}$

$\sigma_{\bar{o},k}$ = elevation of the free water surface in the surface water body [L]

$\sigma_1{}^a$ = the local settling rate of algae, which is temperature dependent, [LT^{-1}]

$\sigma^{nonc}{}_6$ = rate coefficient for constituent settling, temperature dependent [T^{-1}]

$\sigma^{nonc}{}_7$ = benthal source for constituent, temperature dependent [m-nonc L^{-2}T].

θ = porous medium porosity

ρ_b = porous medium bulk density [ML^{-3}]

λ = first-order rate reaction rate constant [T^{-1}]

$v^{ca}{}_{\hat{e},\acute{e},\ddot{e},k}$ = proportion of flow in canal segment $\hat{e},\acute{e},\ddot{e}$ that is diverted to UCA $\hat{e},\acute{e},\ddot{e}$.

$v^{2s}{}_{\hat{e},\acute{e},1,k}$ = proportion of flow in alpha canal section $\hat{e},\acute{e}$ that is diverted to beta canal section $\hat{e},\acute{e},1$

Υ = index referring to a particular UCA. This is an alternative notation to $(\hat{e},\acute{e},\ddot{e})$

I. Introduction

I.1. Statement of Need

As competition for water resources intensifies, it becomes increasingly important to improve coordinated management of water and land resources. This requires the ability to predict the effect of management practices on surface and ground water flow and transport. It also highlights the need to be able to develop optimal management strategies for increasingly complex problems.

Currently, there are a number of well documented, verified and accepted computer models for simulating flow or transport processes in groundwater or surface water resources. However, no existing code addresses all the major processes needed for optimal integrated water resources management in a practical manner. Integrating the outputs or inputs of the disparate codes is not trivial, and has been rarely performed even partially. Furthermore, there is no simulation / optimization (S/O) model that addresses all these flow and transport processes.

Normal simulation models (termed S models here) are frequently used to guide management decisions. In that case, the modeler must assume a water management strategy (set of temporally and spatially distributed pumping, diversion or allocation rates), use the model to predict the consequences of implementing the strategy is the field, and make modifications as necessary. Since there are generally an infinite number of possible management strategies for a situation, the likelihood that the modeler assumes the absolutely best strategy is slight. He eventually stops modelling, selects the best strategy from among those he assumed and tested, and might call it an 'optimal' strategy.

On the other hand, a S/O model, which couples simulation ability and optimization algorithms, can compute the best strategy directly. The user poses for the S/O model the management goal, and restrictions on system responses to that strategy. The model tells the user what pumping, diversion, augmentation and loading rates are best. Table 1 summarizes the differences between a normal simulation model and a S/O model.

For example, assume the management goal is to maximize irrigated crop production in a stream/aquifer system. The manager wants to determine the conjunctive use strategy that maximizes crop production, without causing unacceptable side affects (termed restrictions or constraints). Restrictions might be to assure that:

- downstream municipal and industrial (M&I) users receive prespecified flow rates,
- groundwater levels do not decline unacceptably near wetlands,
- water tables do not rise into the root zone in irrigated areas,
- enough water flows to the coast in all time periods to maintain a fishery, and
- a plume of industrially contaminated groundwater does not reach public supply wells.

A S/O model will compute the temporally and spatially varying groundwater pumping and surface water diversion strategy that will maximize crop production while satisfying the imposed restrictions. Using a S model to attempt to select a suitable conjunctive use strategy can waste manpower and natural resources. A S model is best suited for the task for which it is designed--simulating system response to stimuli. That is different than the task of computing an optimal set of stimuli.

Appendix A illustrates how to solve a simple optimization problem using a graphical approach, and further clarifies the difference between a S model and a S/O model. There, optimal pumping rates are computed for two wells. The example shows what is meant by optimization and demonstrates why a S/O model is needed if optimal rates must be determined for more than a couple wells.

The more complicated the management problem, the more difficult it is for one using a S model to assume a strategy that is close to the actual optimal strategy. As environmental concerns intensify, the need for practical and user-friendly S/O models increases.

This report addresses that need. It builds upon existing proven technology in the manner described below. It proposes a simulation and S/O approach suitable for computing optimal water management strategies on PC-based computers. It proposes software that: is transportable; utilizes data in formats that are currently widely used; aids optimal calibration of simulation models; and provides standardized graphics and tabular products to help managers evaluate and explain optimal strategies and results.

Table I-1.   Partial comparison between inputs & outputs of Simulation &
Simulation/Optimization (S/O) models (modified from Peralta and Aly, 1993)

Model Type	Input Values	Computed Values
Model Type Simulation	Physical system parameters	
	Initial conditions	
	Some boundary flows	Some boundary flows
	Some boundary heads	Heads at 'variable' head cells
	Pumping rates	
(S/O)	Physical system parameters	
	Initial conditions	
	Some boundary flows	Some boundary flows
	Some boundary heads	Optimal heads at 'variable' head cells
	Bounds on pumping, heads, & flows	Optimal pumping, heads, & flows
	Objective function (equation)	Objective function value
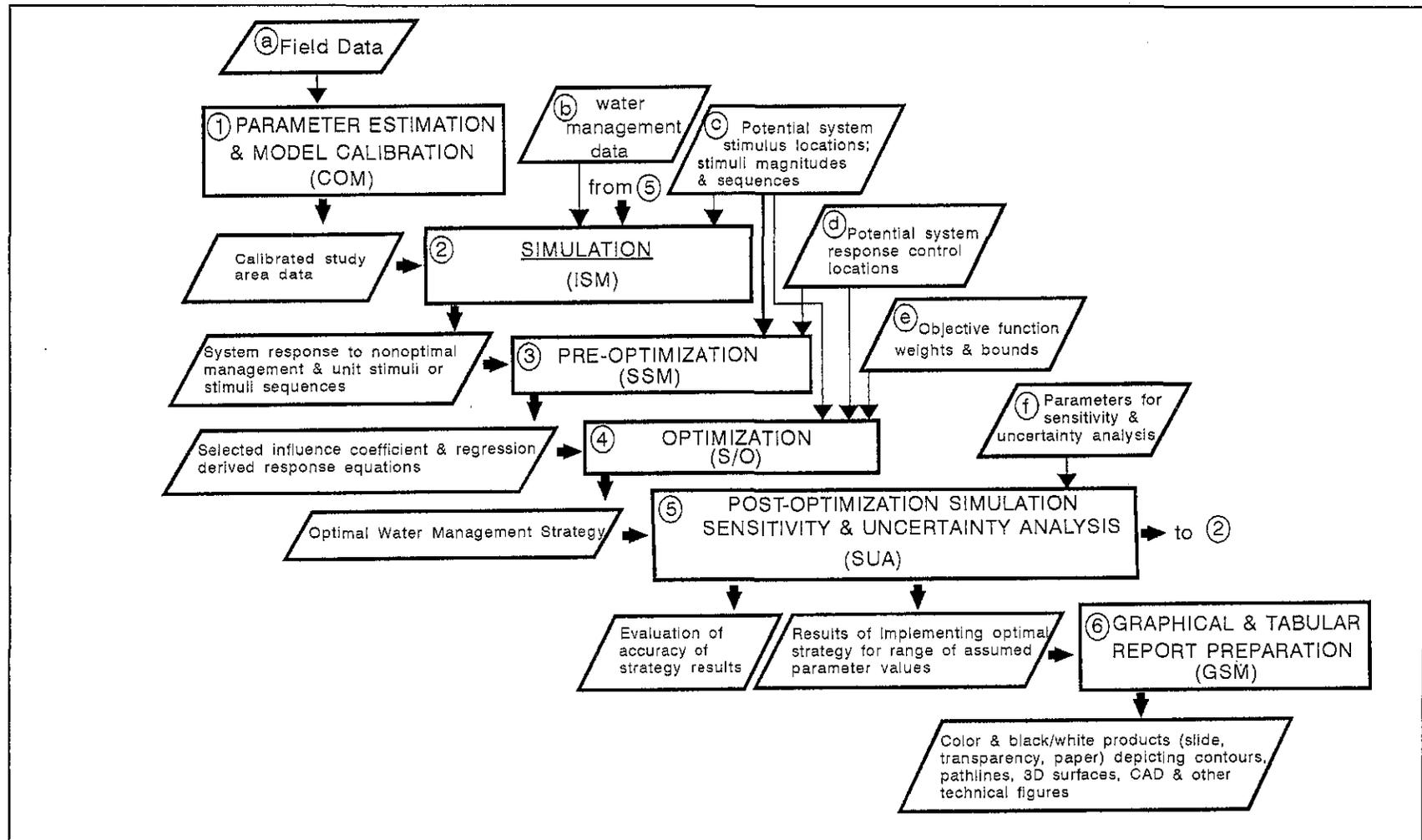
Figure I-1 PROMOD data and process flow diagram

I.2. Objective

The objective of this report is to describe a framework and strategy for computer modelling that can help development and management of a surface water/groundwater system. Included are the flow and transport processes needing consideration for best management of water quantity and quality. Proposed is a modeling methodology practical for international use. The presented deterministic simulation and S/O methodology:

○ represents the flow and transport features most essential for managers of systems containing hydraulically connected or unconnected rivers, canals and aquifers. It is applicable to many irrigated or otherwise developed areas, especially those overlying alluvial deposits. Canal systems of potential application include those within the Nile, Indus, Yellow, Mekong, Mississippi, Amazon and other river systems.

○ uses simulation modules of proven and wide-spread acceptance.

○ links the simulation modules in a practical manner for microcomputer processing.

○ provides the simulation basis for an advanced S/O model. The S/O model permits efficient computation of optimal conjunctive use strategies that address water quantity and quality.

○ is applicable to systems having a range of data availability (at one extreme, system response to stimulus might be spatially distributed in a grid and computed by detailed numerical model; at the other extreme, system response might be empirically created and manually input for control locations within a branching water distribution network).

○ emphasizes fluxes in a stream/aquifer system. Fluxes entering that system in response to land management practices are assumed as knowns in the simulation model or as bounded variables in the s/o model.

○ aids model calibration and prepares materials for persuasively presenting model results.

○ is suitable for use on pc computers worldwide.

NOTE: The proposed methodology and model are together termed PROMOD. For ease of expression and liveliness this report (from Chapter I through Section VII.1.4.) is written as if PROMOD exists. For example, we state that 'PROMOD includes this option' or 'PROMOD does this', instead of 'PROMOD will include this option' and 'PROMOD will do this'. Technically our wording is accurate, the PROMOD methodology exists because it is written in this report. The PROMOD program does not exist. Hopefully, the report will generate sufficient interest for PROMOD to be coded and implemented.

I.3. Overview of Addressed Flow and Transport Processes and Management Goals

Part of the PROMOD approach involves integrating proven simulation models, and using them to develop simplified simulation functions that can practicably be included within a simulation/optimization module. PROMOD is designed to simulate the following physical processes within both normal and simplified simulation modules:

■ Steady and transient flow in streams or canals in response to surface water diversions and inflows and groundwater pumping in a hydraulically connected aquifer. Although simulations can be performed using daily time discretization, weekly, monthly or seasonal discretizations are more likely.

■ Steady and transient advective-dispersive transport of dissolved contaminants in an open channel experiencing steady flow. The system might or might not be in hydraulic connection with an aquifer. Contaminants include dissolved oxygen (DO), biochemical oxygen demand (BOD), nitrogen in its various forms, salinity and other conservative contaminants. Reactions between constituents are modelled. Transport is simulated only for periods of steady flow.

■ Steady and transient interflow between surface water body (stream, river, canal or lake) and groundwater. In one case stream stage is affected by groundwater pumping and aquifer head is affected by river water diversions. In another case river stage is assumed unaffected by groundwater pumping and river flow is not explicitly modelled. The ability to handle either situation helps promote more widespread use than would otherwise be possible.

■ Steady and transient groundwater flow in a multilayer heterogeneous aquifer. Periods of uniform stimulus will probably be weekly, monthly or seasonal, although longer planning periods will be modelable.

■ Steady and transient advective-dispersive contaminant transport in a multilayer heterogeneous aquifer (river stages are assumed known and unaffected by pumping). Contaminants include salinity and conservative contaminants and those describable by equilibrium controlled linear or nonlinear sorption and first order irreversible decay or biodegradation and sorption.

■ Flow and transport into surface water or ground water systems resulting from land management practices. The entering flow and transport are treated as knowns. They can be estimated empirically or computed exernally. In the subsequently developed S/O model these fluxes can be treated as bounded variables, the values of which are optimized. In this way the effect of land management practices can be linked with water management.

■ Water release from reservoirs, changes in reservoir storage, and effect of releases.

The PROMOD approach does <u>not</u>:

■ represent flow and transport in sufficient detail to predict system response to individual rainfalls, storms or similar events.

■ compute erosion, scouring, or sediment transport within the surface water resources.

■ include an event watershed runoff model.

■ simulate reservoir water quality changes.

■ emphasize equilibrium chemistry. Those processes are included only to the extent that they are already incorporated within selected flow and transport simulation models. This increases practical usability of the ultimate model product. (Integrated transport and equilibrium

chemistry models are not common, and agency acceptance is even less usual.)

PROMOD addresses the management problems more directly with a S/O module than with the simulation modules. To explain this, we first define as 'decision variables', those variables subject to direct control and management by man. Decision variables include groundwater pumping, surface water diversion or augmentation, reservoir release, water delivered to agricultural, municipal or industrial users, and mass loading rates of contaminated water to surface or ground waters. 'Implementing' an optimal strategy refers to the act of stressing the actual physical system in accordance with the values of the decision variables computed by the S/O model.

'State variables' describe the condition or state of the physical system, usually resulting from the decision variables (changes resulting from management). State variables include: ground and surface water levels, pressures, heads, head gradients, velocities and flowrates; and contaminant concentrations, velocities and mass flow rates; over-and under-achievement variables (from goal-programming equations described later) used to describe how close variables can be brought to predetermined target values .

PROMOD computes strategies (sets of decision variables) that maximize (or minimize if so desired) the value of the user-selected objective function. The objective function is an equation that describes some combination of decision and state variables. In PROMOD, there are over 50 possible objective functions from which to choose. These include summations of: groups of or all decision variables or state variables; combinations of decision variables and some achievement variables; or combinations of several objective functions. Variables in the objective function can be weighted with dimensionless or dimensioned coefficients. Using cost coefficients allows the model to perform economic optimization.

PROMOD can perform multiobjective optimization using either weighting or E-constraint methods. Alternative objectives can be linear or nonlinear.

I.4. PROMOD Organization and Report Overview

Figure I-1 illustrates the modules included within PROMOD, and data flows between them. These include:

■ Calibration Optimization Module (COM), which uses optimization methods to estimate the physical system parameters needed to appropriately calibrate the simulation modules for field problems.

■ Integrated Simulation Module (ISM), which contains as sub-modules, public-domain simulation models of proven and widespread use, plus other necessary software.

■ Simplified Simulation Module (SSM), which contains simplified simulation expressions. It performs some of the same simulations as the ISM, but more rapidly and with acceptable accuracy. This semi-automatically stresses each pertinent ISM sub-module with a range of assumed stimuli; analyzes system responses; and develops concise response equations which can be readily included within the S/O module. These equations are developed using the most practical combination of response matrix, embedding, regression and related approaches.

■ Simulation/Optimization Module (S/O), which permits the user to compute optimal water management strategies for posed problems. It contains a range of management objective functions, constraint equations (including simplified simulation expressions), and bounds on decision and state variables. It includes as constraints equations from both the ISM and SSM. ■ Sensitivity and Uncertainty Analysis Module (SUA), which facilitates rapid and systematic analysis of the effects of uncertain knowledge of system parameters. It evaluates: (1) the effect of inaccurate knowledge of system parameters on the consequences that will result in the field of implementing an optimal strategy computed using S/O; and (2) the effect of changing assumed parameter values on the strategy computed by the S/O.

■ Graphical and Summary Module (GSM), which aids preparing standardized tabular and graphical representations of strategy results.

To explain PROMOD in a systematic manner, the report contains:

■ conceptual overview of the system flows and transports being considered.

■ overview of the most significant functions (equations) used in simulation models appropriate for inclusion in the ISM.

■ discussion of conventional approaches for simulating system response to stimulus within S/O models, and justification for the approaches selected for PROMOD.

■ detailed explanation of how simplified expressions can be used to represent (within the SSM and the S/O) the same processes modelled by the ISM.

■ overview of S/O module objective functions and additional constraint and bound equations. ■ selected examples of applying S/O models to study areas. Illustrated are highlights demonstrating application to:

     o maximize total delivered groundwater and surface water during 8 stress periods, subject to lower bounds on streamflow and aquifer head. (A stress period is a period of uniform stimulus--others might call this a time step.)

     o maximize municipal wastewater loading to a stream while trying to maximize conjunctive water use from a hydraulically connected stream aquifer system, subject to restrictions on the downstream water quality. These objectives conflict since the stream is initially gaining water from the aquifer. Increasing groundwater pumping

reduces that dilution, causing downstream contaminant concentrations to increase.
○ maximize sustained groundwater yield from a multilayer aquifer. This illustrates PROMOD applicability but also shows that an alternative constraint approach is preferred for some situations.

■ other module functions and pertinent topics, including: model calibration: uncertainty analysis; options for graphical and tabular reports preparation; and achieving solution optimality.

■ summary and recommendations

■ cited references.

■ explanation of the difference between simulation and simulation/optimization models, an example of the benefits of using a S/O model versus using a simulation model, and discussion of two types of multiobjective optimization.

Hopefully, this report will increase interest in integrating simulation and S/O modelling efforts. Support is needed to produce a quality, well-documented, easily used, and transportable PROMOD model. Once developed, PROMOD will compute numerically optimal management strategies which integrate conjunctive use of available water resources with water quality management. It will address a range of planning horizons to enhance its use as an operational as well as sustained yield planning tool.

II. Conceptual Representation of Addressed Systems

Figure II-1 illustrates the types of flows and storage loci that can be considered by PROMOD:

- inflows from the atmosphere (rainfall to reservoir, stream), and external groundwater and surface water supplies,
- water storage in aquifer, reservoir, and surface water system,
- flows between storage loci, and
- losses from the system.

PROMOD can address a system containing several reservoirs and one aquifer. Depending on management goals and area size and complexity, PROMOD can model a large system en toto or just a portion of the system, as long as subsystem boundary conditions can be appropriately specified.

Figures II-2, II-3 and II-4 illustrate a representative PROMOD study area. Together, the figures show that PROMOD considers those flows needed for conjunctive water management. For now, we use q^x to depict the xth type of flow. Later, we use subscripts or arguments that place those flows in time and space. PROMOD also keeps track of the contaminants that move with these flows.

A multi-layer aquifer can underlie all or part of a study area. Arrows in Figure II-2 indicate groundwater flow in a water table aquifer. PROMOD simulates all groundwater movement in all aquifer layers underlying the area.

Horizontal groundwater flow can enter the system at rates that are independent (q^b) or dependent on head. It can also leave at rates that are independent or dependent (q^z) on head.

Aquifer head is a function of all groundwater discharges and recharges, including boundary flow, evaporation, flow to surface water bodies, and pumping. Because the aquifer can be affected by the stream system, aquifer head is also affected by stream discharges and recharges.

In Figure II-2, the aquifer is gaining water from the reservoir and stream (q^{src}), from a beta canal (q^{2sl}), from deep percolation at an agricultural command area (q^{dpca}), and from deep percolation from a municipal and industrial (M&I) user (q^{dpm}). The aquifer is losing water to an alpha drainage canal (q^{1dl}) and a beta drainage canal (q^{2dl}). It is losing water due to extraction from wells within a group of pumping cells, totalling (q^G). It is also losing water due to natural flow to drains in a group of drain cells, totalling (q^{0d}).

Figure II-3 illustrates the larger surface water flows and storages from upstream inflows to downstream outflows. Surface water systems might branch out as a 'supply' canal system; or might branch in as a 'drainage' canal system.

Surface water flow entering the system is the only q^s that is input information. Other streamflow(s) can be affected by all groundwater and surface water discharges and recharges.

Streamflow might enter a reservoir, and be stored or released as needed. It can be augmented by precipitation or flow from the aquifer, or diminished by evapotranspiration or deep percolation. Streamflow can diminish or increase due stream/aquifer interflow (q^{src}), diversions or augmentations.

Surface water can flow from streams to other streams or canals. Here, the arbitrary difference between a stream and a canal is the amount of information used for modelling--more data is used for a stream. The water leaving or entering the stream (through diversion or augmentation) is termed d.

Figure II-3 identifies alpha supply canals as those that branch from a stream, and beta supply canals as those that branch from alpha supply canals. Beta canals provide water to agricultural unit command areas (UCAs).

Water flowing from stream to alpha canal is termed d when it leaves the stream, but q^{1s} when it enters the alpha canal. (Both names are needed. This permits water to be diverted from the stream with or without flowing into an alpha canal. In some cases, the management objective is to simply maximize the sum of diversions and groundwater pumping, and no alpha or beta canal modelling is needed.) Water leaves an alpha canal as q^{2s} to enter a beta canal. Alpha and beta canals can both gain or loose water from the aquifer (q^{1dl} and q^{2dl} respectively).

Figure II-4 shows how water ultimately reaches the water users. Water can flow from stream, alpha, or beta canal to an M&I user (q^{m}). That water is joined by groundwater pumping from a specified number of pumping locations (p^{G}). A specified proportion of the water provided for M&I use is consumed. Other proportions return to the aquifer as deep percolation (q^{dpm}, seen previously), or runoff to a surface water body (q^{rfm}). After water has reached the aquifer it can reemerge as surface water.

Surface water reaches an agricultural command area by first flowing through stream, alpha canal and beta canal (Figure II-4). This q^{ca} flow entering an agricultural unit command area can be augmented by the total groundwater pumped from a group of cells (p^{G}). Prespecified proportions of the water percolate to the aquifer (q^{dpa}, seen previously) or become surface water return flow (q^{rfa}).

Drainage systems branch in a manner opposite to supply canal systems. Drainage systems begin with: flow from drain cells that receive groundwater from the aquifer as a function of head; flow from known sources at user-specified rates; or return flow from M&I or agricultural users. Drainage water enters beta drainage canals, flows to alpha drainage canals and discharges to the more explicity modelled streams. Surface return flow can also enter alpha canals directly, without first passing through beta canals.

PROMOD computes the flowrates of groundwater (q^{z} and others) or surface water (q^{s}) departing the system.
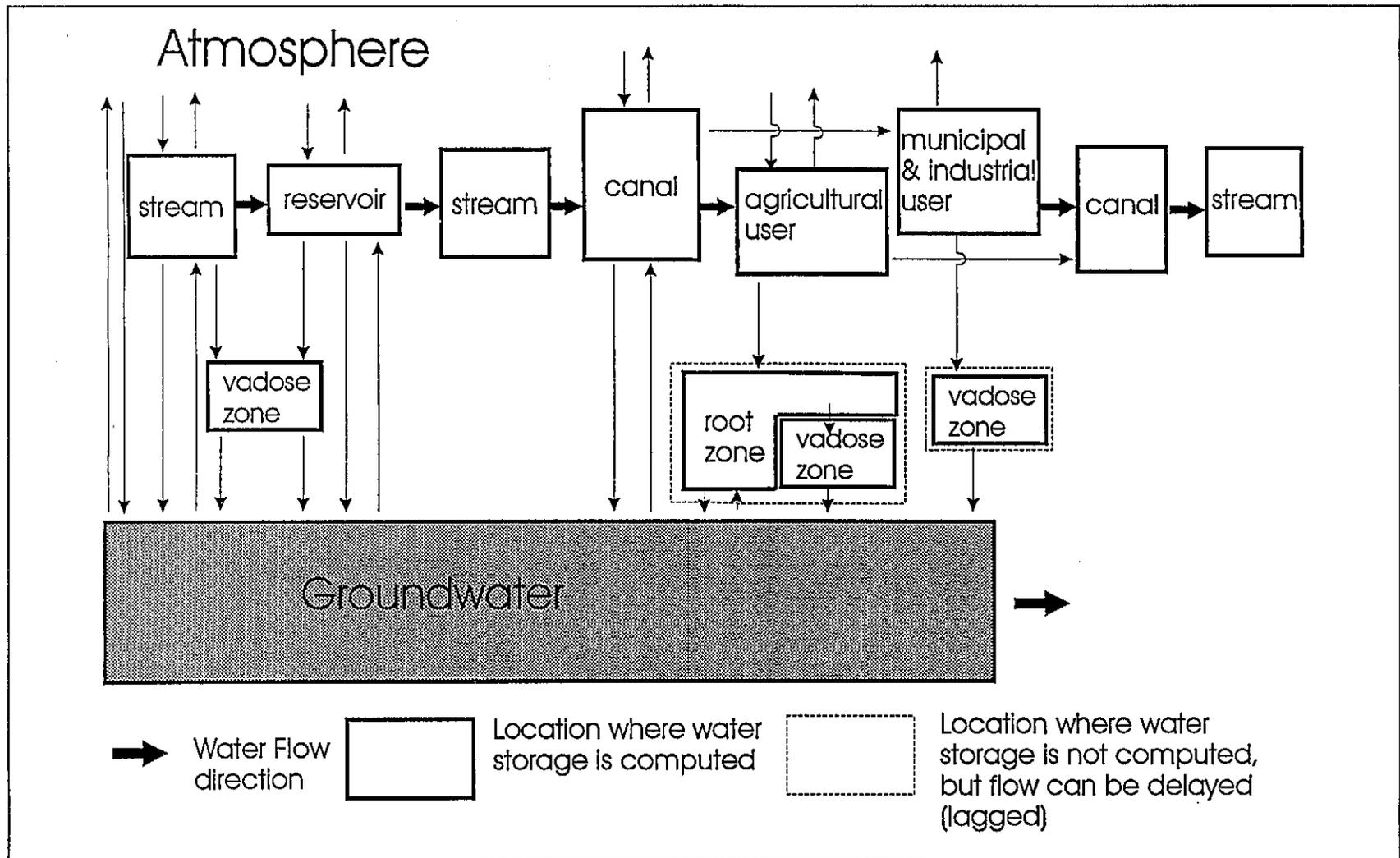
Figure II-1 Considered water storage loci and flow directions.
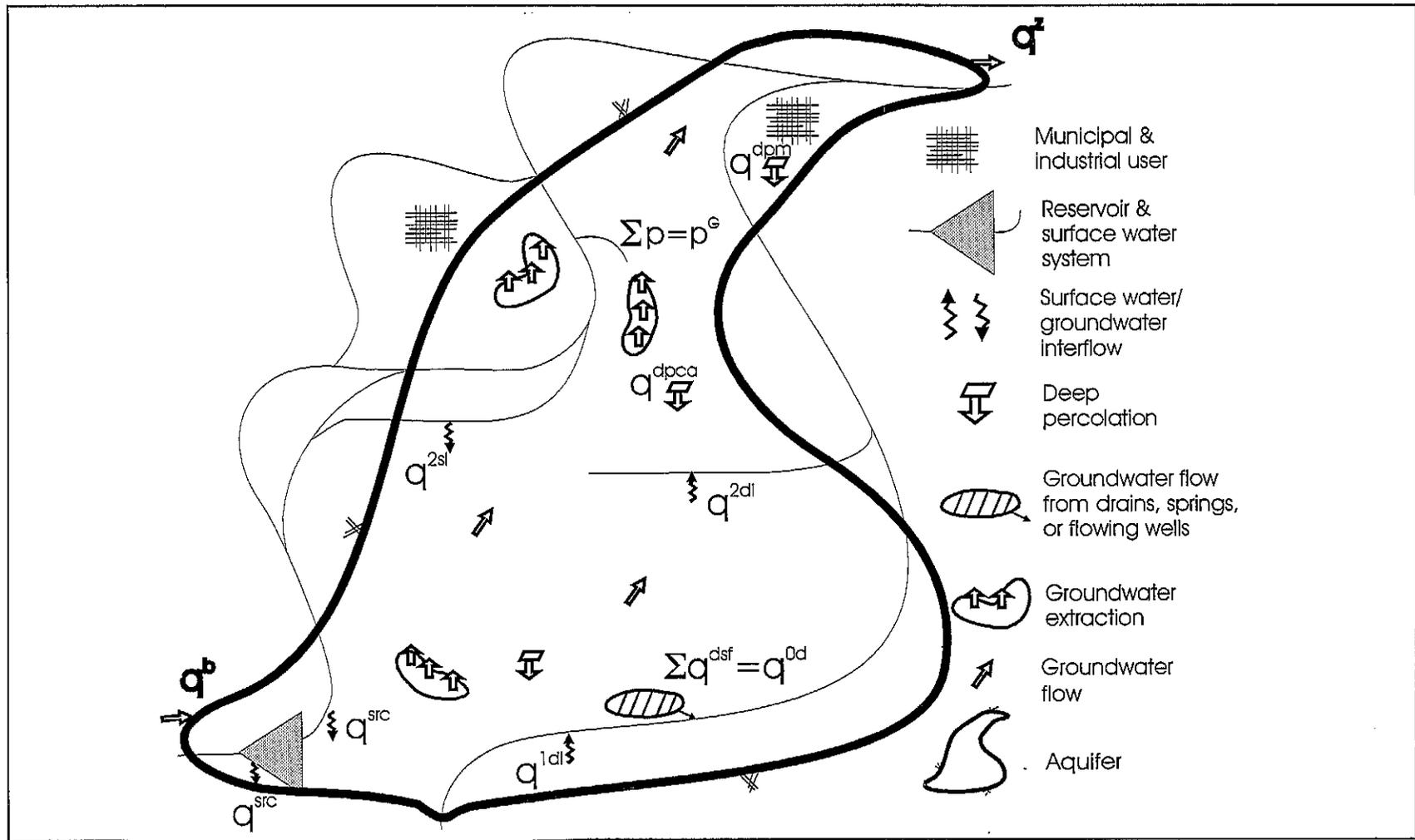
Figure II-2 Representative study area: aquifer, groundwater flows and surface water/aquifer interflows.
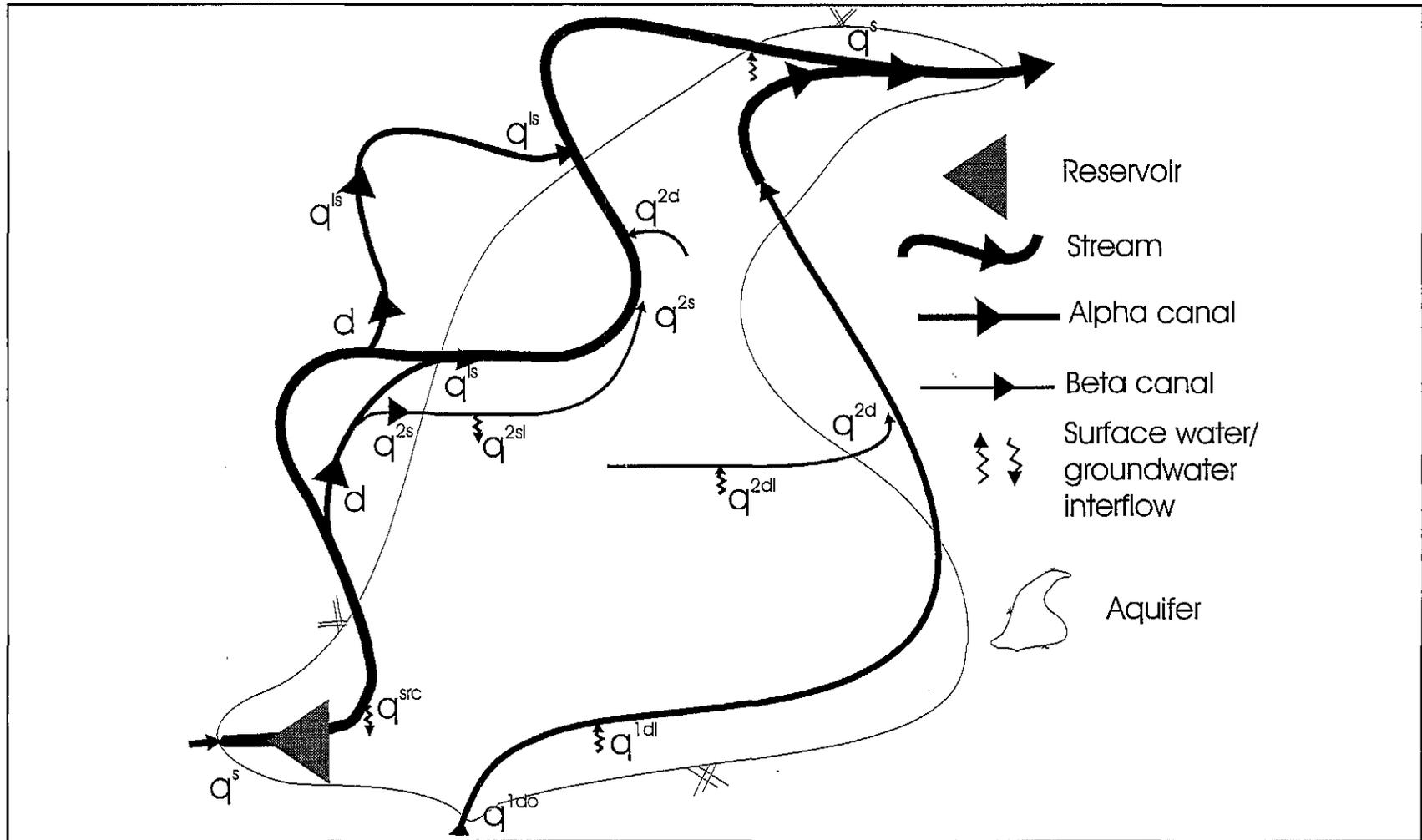
Figure II-3 Representative study area: surface water distribution system.
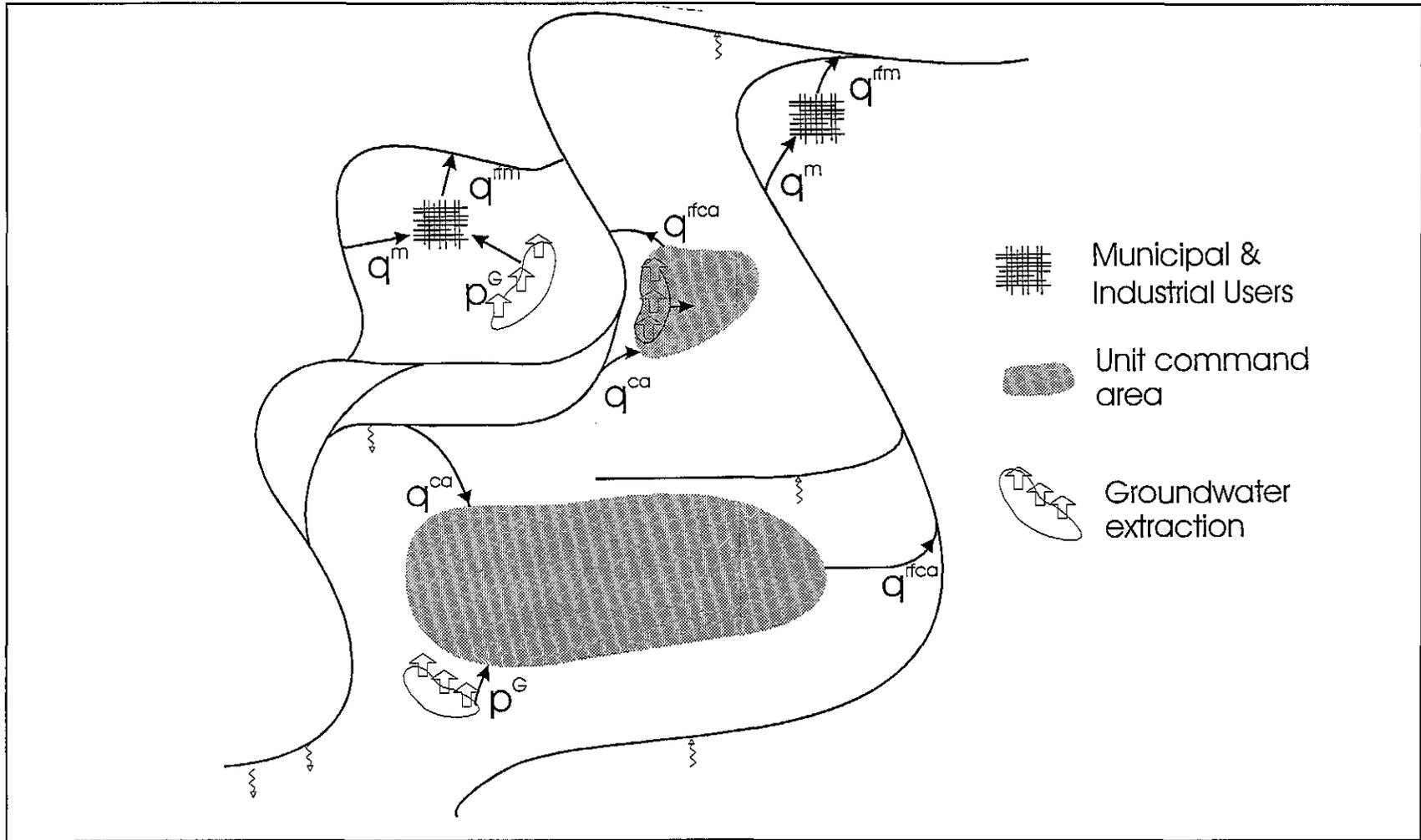
Figure II-**4** Representative study area: water users and their surface water flows.

III. Functional Expressions needed for the Integrated Simulation Module (ISM)

III.1. Processes Needing Simulation and Existing Models That Can Be Included With/Without Modification

Concerning flow, the ISM and S/O must be able to calculate:
- the effect of pumping, recharge and interflow on aquifer heads. They must be able to compute the head change anywhere caused by all recharges or discharges that might be part of an assumed or computed management strategy (pumping) or result from such a strategy (interflow, deep percolation, evaporation).
- the effect of diversion, inflow and interflow on streamflow and stream stage. They must be able to compute streamflow changes caused by all assumed or computed diversions or any augmentations or interflows resulting from implementing a management strategy.

Concerning transport, the ISM and S/O must be able to calculate:
- the effect of groundwater recharges and discharges, and surface water diversions and augmentations on contaminant concentrations within the aquifer and the stream.
- the effect of surface water diversions and loadings (augmentations) on contaminant concentrations within the aquifer and the stream.

Concerning other processes and issues, the ISM and S/O must be able to compute or consider:
- hydropower production from reservoir release.
- distribution of water and a conservative contaminant through the canal system.
- deep percolation and surface water return flow resulting from water management on the ground surface (for example, irrigation)
- contaminant movement to groundwater and surface water.
- crop yield resulting from irrigation (or lack thereof) and salinity.

These desired simulation abilities are provided using equations such as those shown in the next sections. Some of these equations are used in many simulation models. However, four public domain codes in particular contain most of the simulation abilities mentioned in the first two paragraphs above. These four codes, which are widely used and available to anyone worldwide are:

■ MODFLOW, Modular Three Dimensional Finite-Difference Ground-water Flow Model (McDonald and Harbaugh, 1984), is perhaps the most widely used groundwater modelling program in the world. MODFLOW data sets exist for many aquifers. Many training materials have been developed for the code (including those by Andersen, 1993).

■ STR, a stream routing code, is becoming widely used for dynamic stream-aquifer interflow modelling and stream routing (Prudic, 1989). STR has the advantage of interfacing seamlessly with MODFLOW. It permits groundwater pumping to affect stream stage and stream diversions and augmentations to affect groundwater levels--something very few groundwater models do.

■ MT3D, Modular Three-Dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems (Zheng, 1990),

is an increasingly popular groundwater transport model. MT3D accepts as input, the heads and flow velocities computed by MODFLOW.

■ QUAL2E, Enhanced Stream Water Quality Model (Brown and Barnwell, 1987) is the most widely used program in the US for assessing the contaminant concentrations that will result in a stream due to loadings and discharges.

Some simulation equations are needed in addition to those found in the four cited models. The following enhancements should be made to the selected codes.
- Modifying STR to permit:
    - the designation of some stream reaches as reservoir reaches;
    - the ability to use hydrologic routing (for example, via Muskingum method), lag times and storage changes with time within reservoir or stream reaches.
- Modifying MT3D to permit contaminant to flow between a stream (modelled with STR and QUAL2E) and the aquifer.

Simulation abilities which must be gained, but can be kept separate of the cited models include:
- distribution and use of water in areas where data is insufficient to justify use of detailed stream routing with steam stage computation (i.e. through alpha and beta supply and drainage systems);
- distribution of water after discharge from an aquifer through drains, springs or naturally flowing wells;
- hydropower production in response to discharge from a reservoir;
- expressions relating chemical movement to groundwater and surface water response to irrigation;
- crop yield production; and
- economic benefits of water management.

In summary, the needed simulation abilities can be garnered by linking enhanced versions of existing codes with additional equations. We propose the four programs mentioned above. Although many software codes provide simulation abilities needed for PROMOD. However, not all are as freely available, thoroughly tested, or widely used as those listed above. The above programs are available to anyone for the cost of reproduction, and have been proven for a wide range of conditions. Linking them and their abilities within PROMOD will probably provide greater benefit than utilizing other codes that do not have those attributes.

III.2. Groundwater Flow Equations

Groundwater flow is modelled via a quasi 3-D numerical representation of the linearized Boussinesq equation. Any of several numerical schemes can be utilized. For a polygon or cell, the right hand side of the flow equation can be represented by Equation III-1. For brevity, we use the term cell here. In this and subsequent sections we use the term stress period to indicate a period of uniform stress. Others might call this time step.

(III-1)

$$\frac{S_{\bar{o}} A_{\bar{o}}}{\Delta t_k} \left(h_{\bar{o},k} - h_{\bar{o},k-1} \right) + q^b_{\bar{o},k} + p_{\bar{o},k} + q^{dsf}_{\bar{o},k} + q^t_{\bar{o},k} + q^z_{\bar{o},k}$$
$$+ q^{src}_{\bar{o},k} + q^{gh}_{\bar{o},k} + q^{vfr}_{\bar{o},k} + q^{dp}_{\bar{o},k} \qquad \text{for } \bar{o} \in M, \; k \in K$$

where

$\bar{o}$ = identification number of a cell at a particular horizontal location and in a particular aquifer layer;

$S_{\bar{o}}$ = storage coefficient or specific yield for cell $\bar{o}$;

$A_{\bar{o}}$ = cell area $[L^2]$;

Δt_k = duration of time step or stress period k [T];

$h_{\bar{o},k}$ = average potentiometric head in cell $\bar{o}$ at end of stress period k [L];

$q^b_{\bar{o},k}$ = known flow across aquifer boundaries (i.e., bedrock recharge, deep percolation) $[L^3T^{-1}]$;

$p_{\bar{o},k}$ = groundwater pumping $[L^3T^{-1}]$;

$q^{dsf}_{\bar{o},k}$ = discharge from a drain, spring or naturally flowing well $[L^3T^{-1}]$;

$q^t_{\bar{o},k}$ = evapotranspiration from the aquifer $[L^3T^{-1}]$;

$q^z_{\bar{o},k}$ = lateral flow across a boundary (which depends on the boundary's fixed head and adjacent heads) $[L^3T^{-1}]$;

$q^{src}_{\bar{o},k}$ = flow between the aquifer and stream, river or canal $[L^3T^{-1}]$;

$q^{gh}_{\bar{o},k}$ = saturated flow between the aquifer and general head boundary cells $[L^3T^{-1}]$;

$q^{vfr}_{\bar{o},k}$ = reduction in vertical flow between cells in layer 1 and the lower layer 1+1 due to drop in head below the top of layer 1+1 $[L^3T^{-1}]$; and

$q^{dp}_{\bar{o},k}$ = deep percolation (knowns or unknowns which are a function of management). Aquifer discharges are (-) and recharges are (+) in sign $[L^3T^{-1}]$.

Flow from a drain or spring is described by:

$$q^{dsf}_{\bar{o}} = \Gamma^{dsf}_{\bar{o}} \left(h_{\bar{o}} - h^{dsf}_{\bar{o}} \right) \qquad \text{for } h_{\bar{o}} \geq h^{dsf}_{\bar{o}}$$
$$= 0 \qquad\qquad\qquad\quad \text{for } h_{\bar{o}} < h^{dsf}_{\bar{o}}$$

(III-2)

where

$\Gamma^{dsf}_{\bar{o}}$ = coefficient describing flow from drain, spring, or naturally flowing well as a function of head, $[t^2 T^{-1}]$; and

$h^{dsf}\bar{o}$ = elevation of drain base or ground surface for spring or flowing well (L).

Groundwater discharge due to evapotranspiration is (McDonald and Harbaugh, 1984):

$$q^{et}_{\bar{o},k} = E_{\bar{o}} \, A_{\bar{o}} \qquad\qquad \text{for} \quad h^{etd}_{\bar{o}} < h_{\bar{o},k}$$

$$q^{t}_{\bar{o},k} = E_{\bar{o}} \, A_{\bar{o}} \, \frac{(h_{\bar{o},k} - (h^{etd}_{\bar{o}} - d^{ete}_{\bar{o}}))}{d^{ete}_{\bar{o}}} \qquad \text{for} \quad h^{etd}_{\bar{o}} - d^{ete}_{\bar{o}} < h_{\bar{o},k} \leq h^{etd}_{\bar{o}} \qquad \textbf{(III-3)}$$

$$q^{t}_{\bar{o},k} = 0 \qquad\qquad \text{for} \quad h_{\bar{o},k} \leq h^{etd}_{\bar{o}} - d^{ete}_{\bar{o}}$$

where

$E_{\bar{o}}$ = potential evapotranspiration in cell $\bar{o}$ $[LT^{-1}]$;

$h^{etd}_{\bar{o}}$ = potentiometric surface elevation below which the evapotranspiration rate begins to decrease [L]; and

$d^{ete}_{\bar{o}}$ = extinction depth in cell $\bar{o}$ (depth below $h^{etd}_{\bar{o}}$ at which there is no evapotranspiration) [L].

In PROMOD, interflow between a surface water resource and the aquifer can be of three types.

■ 'River/aquifer' interflow (r/ai) results when river stage is assumed unaffected by modellable groundwater pumping or diversion. That is an acceptable assumption when rivers are large or data availability does not justify a more precise representation. R/AI is computed for each cell.

■ 'Stream/aquifer' or reservoir/aquifer interflow (s/ai) results when the surface water stage is affected by groundwater pumping. Modeling s/ai is more precise than r/ai modeling, and requires computation of both aquifer and stream heads. S/AI is computed the same as r/ai, except that stream stage is a variable instead of a known. S/AI is computed for each reach. In PROMOD there can be several stream or reservoir reaches per cell. However, no reach can include more than one cell. (For convenience in presenting the equations below, we refer to a reach consisting of one cell.) A reservoir is simply a special type of stream reach. With a stage-discharge relation, we can compute stream stage if we know streamflow, or vice versa.

■ 'Canal/aquifer interflow (c/ai) is used when the surface resource is insufficiently large to permit treating it as having a known head (ruling out the r/ai approach), and there is no stage-discharge relation available (ruling out the s/ai approach). Such surface water bodies are here termed as 'canals'. We term their segments as 'sections' rather than reaches.

In PROMOD, the river, stream and canal nomenclature has little relation to the size of the surface water body. Instead it has to do with data availability and how the body can best be treated in the model. Interflow between the surface water body and the aquifer (from the groundwater flow equation) is defined as:

$$q_{\bar{o},k}^{src} = q_{\bar{o},k}^{sr} + q_{\bar{o},k}^{1sl} + q_{\bar{o},k}^{2sl} + q_{\bar{o},k}^{1dl} + q_{\bar{o},k}^{2dl} \tag{III-4}$$

where

$q_{\bar{o},k}^{sr}$ = interflow between the surface water and groundwater systems $[L^3T^{-1}]$; and

$q_{\bar{o},k}^{xyl}$ = interflow between a canal of level x (1 = alpha, 2=beta) and type y (s = supply, d = drain)$[L^3T^{-1}]$.

The expressions for saturated and unsaturated interflow are shown below. These are the same whether the interflow is between a river and aquifer, stream and aquifer, or reservoir and aquifer.

$$q_{\bar{o},k}^{sr} = \Gamma_{\bar{o}}^{sr} (\sigma_{\bar{o},k} - h_{\bar{o},k}) \qquad \text{for } h_{\bar{o},k} \geq B_{\bar{o}}^{sr}$$

$$q_{\bar{o},k}^{sr} = \Gamma_{\bar{o}_{sr}} (\sigma_{\bar{o},k} - B_{\bar{o}}^{sr}) \qquad \text{for } h_{\bar{o},k} < B_{\bar{o}}^{sr} \tag{III-5}$$

where

$\Gamma_{\bar{o}}$ = hydraulic conductance of the surface water-aquifer interconnection, (including any clogging layer) $[L^2T^{-1}]$;

$\sigma_{\bar{o},k}$ = elevation of the free water surface in the surface water body [L]; and

$B_{\bar{o}}^{sr}$ = elevation of the bottom of the surface water body [L].

Clearly, to compute q^{sr}, an interflow conductance value is needed. To estimate interflow between canals and aquifers, an efficiency factor is used instead. This is explained in the next section.

III.3. Basic Surface Water Flow Equations

The stream or reservoir reach continuity expression is:

$$q^{s'}_{\bar{o},k} - q^{s}_{\bar{o},k} - \Delta q^{v}_{\bar{o},k} = d_{\bar{o},k} + q^{sr}_{\bar{o},k} + v^{c}_{\bar{o},k} + v^{o}_{\bar{o},k} \qquad \text{(III-6)}$$

where

$q^{s}_{\bar{o},k}$ = flow from stream cell $\bar{o}$ via the stream in time step k (+), $[L^3T^{-1}]$;

$q^{s'}_{\bar{o},k}$ = flow into the cell from upstream via the stream (+), $[L^3T^{-1}]$;

$\Delta q^{v}_{\bar{o},k}$ = $\{(ST_{\bar{o},k} - ST_{\bar{o},k-1})/\Delta t\}$ = rate of change of volume in storage in the stream or reservoir, $[L^3T^{-1}]$;

$ST_{\bar{o},k}$ = storage in reservoir $\bar{o}$ during stress period k $[L^3]$;

$q^{sr}_{\bar{o},k}$ = interflow between stream or reservoir and aquifer, $[L^3T^{-1}]$;

$d_{\bar{o},k}$ = diversion from (+) or augmentation to (-) the stream in cell $\bar{o}$ in time k step (+), $[L^3T^{-1}]$. For a stream reach, the simulation model can compute only one of v^c, and v^o. For a reservoir reach d is a release.;

$v^{c}_{\bar{o},k}$ = a) for a stream reach, this is canal flow to (-) the stream from a canal that is not modelled in the same level of detail as a stream;
b) for a reservoir reach, this is spillage ($SP_{\bar{o},k}$) from the reservoir that is lost and does not reenter the modelled system $[L^3T^{-1}]$;

$v^{o}_{\bar{o},k}$ = a) for a stream reach, this is flow from (+) or to (-) the stream in time step k, other than that included in other terms, $[L^3T^{-1}]$. This can include overland flow, precipitation, flow through marshes, flow that might be a function of water used on land, and evapotranspiration losses.
b) for a reservoir reach, this is primarily evapotranspiration and precipitation.

Evapotranspiration from surface water bodies can be input as known values. Alternatively, evapotranspiration from reservoirs is defined as:

$$L^{e}_{\bar{o},k} = E^{evr}_{\bar{o},k}\frac{(ST_{\bar{o},k} + ST_{\bar{o},k+1})}{2} \qquad \text{for } \bar{o} \in tvg \qquad \text{(III-7)}$$

where
$L^{c}_{\bar{o},k}$ = evapotranspiration loss from the reservoir $[L^3T^{-1}]$; and
$E^{vr}_{\bar{o},k}$ = proportion of reservoir storage that is lost due to evapotranspiration
tvg   = set of reservoir reaches (a reservoir can consist of more than one reach).

To reflect the time lags common in larger rivers, PROMOD can use a hydrologic approach, representing outflow for a time period as a function of the average inflows and outflows for the previous periods. The general linear expression is:

$$q_{\bar{o},k+1}^{s} = \sum_{i=0}^{LI} a_{\bar{o},i} \, q_{\bar{o},k+1-i}^{s\prime} + \sum_{i=0}^{LQ} b_{\bar{o},i} \, q_{\bar{o},k-i}^{s} \tag{III-8}$$

where

$a_{\bar{o},i}$ = constant coefficient for the average inflow in i stress period before stress period k+1;

$b_{\bar{o},i}$ = constant coefficient for the average inflow in i+1 stress period before stress period k+1;

LI = number of stress periods lagged inflows; and

LQ = number of stress periods of lagged outflows.

PROMOD implements this expression using Muskingum routing (Chow, 1959; Gavilan and Houck, 1985; Martin, 1986). Combining equations 6 and 8 yields the volume of water in storage. Equation 9 determines reservoir stage as a function of reservoir storage. Reservoir stage is used to compute reservoir/aquifer interflow (q^{sr}, using Equation III-5).

$$\sigma_{\bar{o},k} - B_{\bar{o},k}^{sr} = a_{\bar{o}} \, (ST_{\bar{o},k})^{b_{\bar{o}}} \tag{III-9}$$

where

$a_{\bar{o}}$ and $b_{\bar{o}}$ = site specific empirical coefficients.

Within a stream reach, PROMOD can use steady or transient approaches to compute the stage needed to estimate stream/aquifer interflow. For steady flow conditions, PROMOD uses a hydraulic routing approach, converting stream flow into flow depth using the Manning Equation. Adding the flow depth to the stream bottom elevation yields an elevation with which to compute stream-aquifer interflow.

Alternatively, PROMOD can convert flow to head using a linear relation, if the expression is acceptable, and calibratable, for the range of expected river stages. In other cases a nonlinear river stage-discharge relation is adopted, or linearized (Loucks and others, 1981). One linear approach is (Peralta et al, 1990):

$$\sigma_{\bar{o},k}^{s} = k_{\bar{o}}^{s} \left((q_{\bar{o},k}^{s} + q_{\bar{o},k}^{s\prime}) / 2 - q_{\bar{o},k}^{s\prime\prime} \right) + \sigma_{\bar{o}}^{lin} \tag{III-10}$$

where

$k_{\bar{o}}^{s}$ = linear relation between average flowrate and head in cell $\bar{o}$ for flowrates that are not less than σ^{lin}, [TL^{-2}];

$q_{\bar{o}}^{s\prime\prime}$ = flowrate in cell $\bar{o}$ when the elevation of the river surface is $\sigma_{\bar{o}}^{lin}$, [$L^{3}T^{-1}$]; and

$\sigma_{\bar{o}}^{lin}$ = elevation of the river surface above which a linear stage discharge relation is applicable, [L].

III.4. Additional Expressions for Water Distribution and Management

Water leaving a stream by diversion can enter a canal. Canal reaches end and begin at a point source or discharge, or where the proportion of canal/aquifer interflow changes significantly. Canal flow can discharge into a stream directly (ie rejoin a stream from which it was initially diverted).

PROMOD assumes that storage changes with time in the canals are insignificant for our purposes. During each stress period, a steady-state volume balance is used for both alpha (Equation III-11) and beta (Equation III-13) canals. In these canals, c/ai is some fixed proportion of the water flowing into the canal section.

$$q^{1s}_{\hat{e},\acute{e},k} = q^{1si}_{\hat{e},\acute{e},k} + q^{1so}_{\hat{e},\acute{e},k} + q^{2s}_{\hat{e},\acute{e},1,k} + q^{1s}_{\hat{e},\acute{e}+1,k}$$ (III-11)

$$\text{for } \hat{e} \in \text{td1sg}; \ \acute{e}=1..M^{2s}(\hat{e}); \ k=1..K$$

where
$q^{1s}_{\hat{e},\acute{e},k}$ = upstream inflow into section $(\hat{e},\acute{e})$ of alpha supply canal $\hat{e}$, which receives water from diversion $\hat{e}$ [L^3T^{-1}];

$q^{1si}_{\hat{e},\acute{e},k}$ = canal/aquifer interflow for section $(\hat{e},\acute{e})$ [L^3T^{-1}];

q^{1so} = inflow from overland flow, surface drainage, or surface return flow, assumed to occur at the upstream end of the section [L^3T^{-1}];

$q^{2s}_{\hat{e},\acute{e},1,k}$ = upstream inflow into section $(\hat{e},\acute{e},1)$ of beta canal $(\hat{e},\acute{e})$ [L^3T^{-1}];

td1sg = set of all reaches that divert water to alpha supply canals; and

$M^{2s}(\hat{e})$ = set of beta canals receiving water from alpha canal $\hat{e}$.

Canal section indices are the same as those of the structure (diversion or inflow) that exists at their lower end. At the end of section $(\hat{e},\acute{e})$ is offtake $(\hat{e},\acute{e})$, which diverts water to reach 1 of beta canal $(\hat{e},\acute{e})$. Similarly, $q^{2s}_{\hat{e},\acute{e},1,k}$ is upstream inflow into section $(\hat{e},\acute{e},1)$ of beta canal $(\hat{e},\acute{e})$. Near the end of this section is turnout $(\hat{e},\acute{e},\ddot{e})$, which supplies surface water to unit command area $(\hat{e},\acute{e},\ddot{e})$.

PROMOD estimates C/AI ($q^{1si}_{\hat{e},\acute{e},k}$, canal/aquifer interflow) for section $(\hat{e},\acute{e})$ as a function of average canal conveyance efficiency, the length of the particular canal section in relation to the total canal length, and the inflow to that section.

$$q^{1si}_{\hat{e},\acute{e},k} = q^{1s}_{\hat{e},\acute{e},k} (1 - E^{1s}_{\hat{e},\acute{e}}) L^{1s}_{\hat{e},\acute{e}} / L^{1s}_{\hat{e}}$$ (III-12)

where:
$E^{1s}_{\hat{e},\acute{e}}$ = conveyance efficiency (as a proportion) of the canal section;

$L^{1c}_{\hat{e},\acute{e}}$ = length of canal section $\hat{e},\acute{e}$ [L]; and

$L^{1c}_{\hat{e},0}$ = total length of alpha canal $\hat{e}$ [L].

The volume balance in a beta canal is similar to that for an alpha canal, and uses analagous variable names (the major difference being that a 2 replaces a 1 in the superscript):

$$q^{2s}_{\hat{e},\acute{e},\ddot{e},k} = q^{2si}_{\hat{e},\acute{e},\ddot{e},k} + q^{2so}_{\hat{e},\acute{e},\ddot{e},k} + q^{ca}_{\hat{e},\acute{e},\ddot{e},k} + q^{2s}_{\hat{e},\acute{e},\ddot{e}+1,k} \quad \text{for } \ddot{e}=1..M^{ca}(\hat{e},\acute{e}) \tag{III-13}$$

where

$q^{ca}_{\hat{e},\acute{e},\ddot{e}}$ = surface water flow to unit command area $\hat{e},\acute{e},\ddot{e}$ $[L^3T^{-1}]$; and

$M^{ca}(\hat{e},\acute{e})$ = set of unit command areas served by beta canal $\hat{e},\acute{e}$.

Flow that is diverted from a canal section is either some proportion of the flow entering the section, or a flowrate input by the user.

$$q^{2s}_{\hat{e},\acute{e},1,k} = v^{2s}_{\hat{e},\acute{e},1,k} \; q^{1c}_{\hat{e},\acute{e},k} \text{ , or an input value} \tag{III-14}$$

$$q^{ca}_{\hat{e},\acute{e},\ddot{e},k} = v^{ca}_{\hat{e},\acute{e},\ddot{e},k} \; q^{2s}_{\hat{e},\acute{e},\ddot{e},k} \text{ , or an input value} \tag{III-15}$$

where

$v^{2s}_{\hat{e},\acute{e},1,k}$ = proportion of flow in alpha canal section $\hat{e},\acute{e}$ that is diverted to beta canal section $\hat{e},\acute{e},1$; and

$v^{ca}_{\hat{e},\acute{e},\ddot{e},k}$ = proportion of flow in canal segment $\hat{e},\acute{e},\ddot{e}$ that is diverted to UCA $\hat{e},\acute{e},\ddot{e}$.

Flow from a group of drain or spring cells is indexed slightly differently depending on whether it enters an alpha or a beta canal. However, in both cases, the flow entering a canal section can be the sum of drainage flows from a group of cells containing drains (or springs or flowing wells), an input value, or the return flow from a UCA or municipality:

$$q^{1so}_{\hat{e},\acute{e},k} = \sum_{\bar{o} \, \in \, dsfg(\hat{e},\acute{e},0)} q^{dsf}_{\bar{o}} \text{ , an input value, } q^{rfca}, \text{ or } q^{rfm} \tag{III-16}$$

$$q^{2so}_{\hat{e},\acute{e},k} = \sum_{\bar{o} \, \in \, dsfg(\hat{e},\acute{e},\ddot{e})} q^{dsf}_{\bar{o}} \text{ , an input value, } q^{rfca}, \text{ or } q^{rfm} \tag{III-17}$$

where

dsfg($\hat{e},\acute{e}$,0) = set of drain, spring or flowing cell cells that provide water to alpha drainage canal $\hat{e},\acute{e}$.

dsfg($\hat{e},\acute{e},\ddot{e}$) = set of drain, spring or flowing cell cells that provide water to beta drainage canal $\hat{e},\acute{e},\ddot{e}$.

q^{2so} serves the same function as q^{1so}, but for a beta supply canal; q^{1do} is for an alpha drain canal; and q^{2do} is for a beta drain canal. There must also be a $q^{2s}_{\hat{e},\acute{e},1,k}$ at the downstream end of the same section, even if the q^{2s} value is zero.

We can deliver surface water to an M&I user directly from a stream or from an alpha canal. Depending on the location,

$$q^m_{\ddot{y},k} = \text{one of } d_{x,k} \; q^{1s}_{x,k}, \; q^{2s}_{x,k}, \; q^{1d}_{x,k}, \; q^{2d}_{x,k} \qquad \text{(III-18)}$$

where

$q^m_{\ddot{y},k}=$ surface water flowing to municipality $\ddot{y}$ [L³T⁻¹].

Water can be delivered to M&I or agricultural users from groundwater as well as surface water. The rate of groundwater delivery is the sum of the extraction from a prespecified group of groundwater pumping cells.

$$p^G_{\hat{a},k} = \sum_{\hat{a} \in pg(\grave{a})} g_{\hat{a},k} = q^{mg}_{\ddot{y},k}, \; q^{cag}_{\hat{a},\acute{e},\ddot{a}}, \text{ or other total} \qquad \text{(III-19)}$$

assuming $\grave{a}$ contains all pumping cells of city ($\ddot{y}$), UCA ($\hat{e},\grave{e},\ddot{e}$), or other grouping

where

$p^G_{\hat{a},k}$	= total groundwater extraction rate from cells in pumping group pg($\grave{a}$) [L³T⁻¹];
pg ($\hat{e},\acute{e},\ddot{e}$)	= group of cells extracting groundwater;
$q^{mg}_{\ddot{y},k}$	= total groundwater extraction rate from the cells supplying M&I user $\ddot{y}$ [L³T⁻¹]; and
$q^{cag}_{\hat{e},\acute{e},\ddot{e},k}$	= total groundwater extraction rate from the cells supplying UCA ($\hat{e},\acute{e},\ddot{e}$) [L³T⁻¹].

The total rate of surface water and groundwater delivered to a municipality or UCA in period k are defined as:

$$q^{mt}_{\ddot{y},k} = q^m_{\ddot{y},k} + q^{mg}_{\ddot{y},k} \qquad \text{(III-20)}$$

$$q^{cat}_{\hat{e},\acute{e},\ddot{e},k} = q^{ca}_{\hat{e},\acute{e},\ddot{e},k} + q^{cag}_{\hat{e},\acute{e},\ddot{e},k} \qquad \text{(III-21)}$$

where

$q^{mt}_{\ddot{y},k}$	= average rate of surface water and groundwater provided to M&I user $\ddot{y}$ during period k [L³T⁻¹]; and
$q^{cat}_{\hat{e},\acute{e},\ddot{e},k}$	= average rate of surface water and groundwater provided to UCA ($\hat{e},\acute{e},\ddot{e}$) [L³T⁻¹].

Both M&I and agricultural users consume some of the water. The rest percolates to the aquifer, or departs as flow through a surface water body. The proportions of each are assumed known apriori.

Deep percolation in a UCA is a proportion of the total water delivered to the UCA.

$$q^{dpca}_{\hat{e},\acute{e},\ddot{e},\grave{e},k} = q^{cat}_{\hat{e},\acute{e},\ddot{e},k} \; E^{dpca}_{\hat{e},\acute{e},\ddot{e},\grave{e}} \qquad \text{(III-22)}$$

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where

$q^{dpca}_{\hat{e},\acute{e},\ddot{e},k}$ = deep percolation in a UCA served by diversion point $\hat{e}$, offtake $\acute{e}$, turnout $\ddot{e}$, in stress period k [L^3T^{-1}];

$E^{dpca}_{\hat{e},\acute{e},\ddot{e},\grave{e}}$ = proportion of the water applied to a UCA that becomes deep percolation in cell $\grave{e}$. The deep percolation in cell $\grave{e}$ is the same as the q^{dp} of the groundwater flow equation; and

A proportion of the water applied in a UCA returns directly to a surface water body.

$$q^{rfca}_{\hat{e},\acute{e},\ddot{e},k} = q^{cat}_{\hat{e},\acute{e},\ddot{e},k} \sum_{\grave{e}=1}^{M^{\grave{e}}_{\hat{e},\acute{e},\grave{e}}} (E^{rfca}_{\hat{e},\acute{e},\ddot{e},\grave{e}}) \qquad \text{(III-23)}$$

where

$q_{\hat{e},\acute{e},\ddot{e},k}{}^{rfca}$ = surface return flow from the UCA; and

$E^{rfca}_{\hat{e},\acute{e},\ddot{e},\grave{e}}$ = proportion of the water applied to the UCA that becomes runoff in cell $\grave{e}$.

Expressions similar to Equations III-22 and III-23 are used to define the deep percolation and surface return flow from M&I users in city $\ddot{y}$,

where

$q_{\ddot{y},k}{}^{dpm}$ = deep percolation resulting from water used by M&I user $\ddot{y}$ [L^3T^{-1}]

$q_{\ddot{y},k}{}^{rfm}$ = surface return flow from M&I user $\ddot{y}$

Water entering the aquifer becomes groundwater, but can leave the aquifer through drains. Water leaving the aquifer through drains, springs or naturally flowing wells enters a beta or alpha drain before it can enter a stream.

$$q^{0d}_{\hat{u},\acute{o},\ddot{o},k} = \sum_{\bar{o}\in M_{\hat{u},\acute{o},\ddot{o}}{}^{\bar{o}}} q^{dsf}_{\bar{o},k} \qquad \text{(III-24)}$$

where

q^{0d} = flow moving from a set of drain, spring or flowing well cells into a beta drain [L^3T^{-1}];

$M^{\bar{o}}_{\hat{u},\acute{o},\ddot{o}}$ = set of aquifer cells providing water to beta drain $\hat{u},\acute{o},\ddot{o}$.

Volume balance equations for beta and alpha drainage canals are analagous to those for alpha and beta supply canals, but have a d in the superscript instead of an s. For example q^{1do} is analagous to q^{1so}. Drain canals can receive water from known flows, variable surface water return flows, and drain, spring or flowing well cells identified in the groundwater model. They differ from supply canals in their manner of branching.

III.5. Hydropower Production

Hydropower can be produced by the release of water from the reservoirs. Hydropower production is expressed as:

$$P_{\hat{e},k} = E_{\hat{e}}^{hp}(P_{\hat{e},k})\ q_{\hat{e},k}^{s}\ H_{\hat{e},k}\ /\ X^{hp} \qquad \text{for } \hat{e} \in vg(\text{æ})$$ (III-25)

where

$P_{\hat{e},k}$ = power generated by q^s flow of water passing through a turbine [KW];

$E_{\hat{e},k}^{hp}(P_{\hat{e},k})$ = energy conversion efficiency as a function of power generation;

X^{hp} = conversion factor (11.8 to convert from ft-lb to kW);

$H_{\hat{e},k}$ = net head [L]; and

$vg(\text{æ})$ = set of reservoir release reaches .

Head is defined as:

$$H_{\hat{e},k} = \sigma_{\hat{e},k}^{avg} - \sigma_{\hat{e},k}^{tavg}$$ (III-26)

where

$\sigma_{\hat{e},k}^{avg}$ = average reservoir water surface elevation during stress period k [L]; and

$\sigma_{\hat{e},k}^{tavg}$ = average tailrace water surface elevation below reservoir release ê during stress period k [L]. This is a function of $q_{\hat{e},k}^s$ and water conditions downstream of the release (for example, another reservoir water surface elevation).

III.6. Groundwater Transport and Chemical Reaction Equations

The groundwater contaminant transport equation can be expressed as (Zheng, 1990):

$$R \frac{\partial c^g}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}^g \frac{\partial c^g}{\partial x} \right) - \frac{\partial}{\partial x_i}(v_i c^g) + \frac{q^{ssg}}{\theta} c^{ssg} - \lambda\left(c^g + \frac{\rho_b}{\theta}\overline{c}^g \right) \qquad \textbf{(III-28)}$$

where

c^g = the concentration of dissolved contaminants in groundwater $[ML^{-3}]$;

t = time $[T]$;

x_i = distance along a respective Cartesian coordinate axis $[L]$;

D_{ij}^g = groundwater hydrodynamic dispersion coefficient $[L^2 T^{-1}$;

v_i = seepage or linear pore water velocity $[LT^{-1}$;

q^{ssg} = volumetric flux of water per unit aquifer volume, due to sources (+) and sinks (-) $[T^{-1}]$. This equals the sum of recharging values of q^b , p, q^z , q^{src} , q^{gh} , and q^{dp};

c^{ssg} = concentration of the sources or sinks $[ML^{-3}]$;

θ = porous medium porosity;

ρ_b = porous medium bulk density $[ML^{-3}]$;

$\overline{c}^g$ = concentration of contaminants sorbed on the porous medium, $[MM^{-1}]$;

λ = first-order rate reaction rate constant $[T^{-1}]$; and

R_f = the retardation factor:

$$R_f = 1 + \frac{\rho_b}{\theta} \frac{\partial \overline{c}^g}{\partial c} \qquad \textbf{(III-29)}$$

In the RHS of Equation III-29, the first term represents dispersion, the second represents advection, the third represents sources and sinks, and the fourth represents reactions. PROMOD features include equilibrium-controlled linear sorption, non-linear (Freundlich and Langmuir) sorption, and first-order irreversible rate reactions (radioactive decay and biodegradation). It can use different rate constants for the dissolved and sorbed phases. PROMOD uses a method of characteristics approach to advective transport, and so reduces numerical dispersion.

III.7. Surface Water Transport and Chemical Reaction Equations for Streams

To simulate the consequences of discharging contaminated water to streams, or diverting from streams, the following equations are needed. These, and others, are included within the QUAL2E stream water quality model (Brown and Barnwell, 1987). These expressions are appropriate for all reaches in which stream stage is computed as a function of flowrate.

QUAL2E can simulate up to 15 water quality constituents, including dissolved oxygen (DOX), biochemical oxygen demand (BOD), temperature, algae as Chlorophyll $\underline{a}$, total organic nitrogen as N (TON), ammonia as N (N-NH$_3$), nitrite as N (N-NO$_2$), nitrate as N (N-NO$_3$), organic phosphorus as P (OGP), dissolved phosphorus as P (DSP), total phosphorus (TOP), coliforms, an arbitrary nonconservative constituent, and three conservative contaminants (such as salt).

The model is appropriate for well mixed dendritic streams. It assumes one dimensional advective and dispersive transport. It permits multiple waste discharges, withdrawals, tributary flows and incremental inflows and outflows (such as can occur via stream/aquifer interflow or overland inflow). Although it simulates transient transport, it is appropriate only for periods of steady stream flow. This is sufficient for most canal system management evaluations.

The following one-dimensional advection-dispersion mass transport equation is solved numerically for each water quality consitutent (Brown and Barnwell, 1987).

$$\frac{\partial c}{\partial t} = \frac{\partial (A_x D_L^g \frac{\partial c}{\partial X})}{A_x \, \partial X} - \frac{\partial (A_x \bar{u} c)}{A_x \, \partial x} + \frac{dc}{dt} + \frac{q^{es}}{V} \qquad \text{(III-30)}$$

where

c	=concentration [M L^{-3}];
A$_x$	=cross-sectional area [L^2];
D$_L^g$	=groundwater dispersion coefficient [L^2 T^{-1}];
x	=distance [L];
$\bar{u}$	=mean velocity [L T^{-1}];
q^{es}	=external source or sinks [M T^{-1}];
V	= M/c, [LT^{-1}]; and
M	=mass [M].

The terms on the right-hand side (RHS) represent dispersion, advection, constituent changes, external sources/sinks, and dilution, respectively. Here, dc/dt represents constituent changes (decay and growth), and is not the same as the partial of c with respect to t, which is the local concentration gradient. Under steady-state conditions, the left-hand side (LHS) equals zero. Constituent reactions are illustrated in Figure III-1.
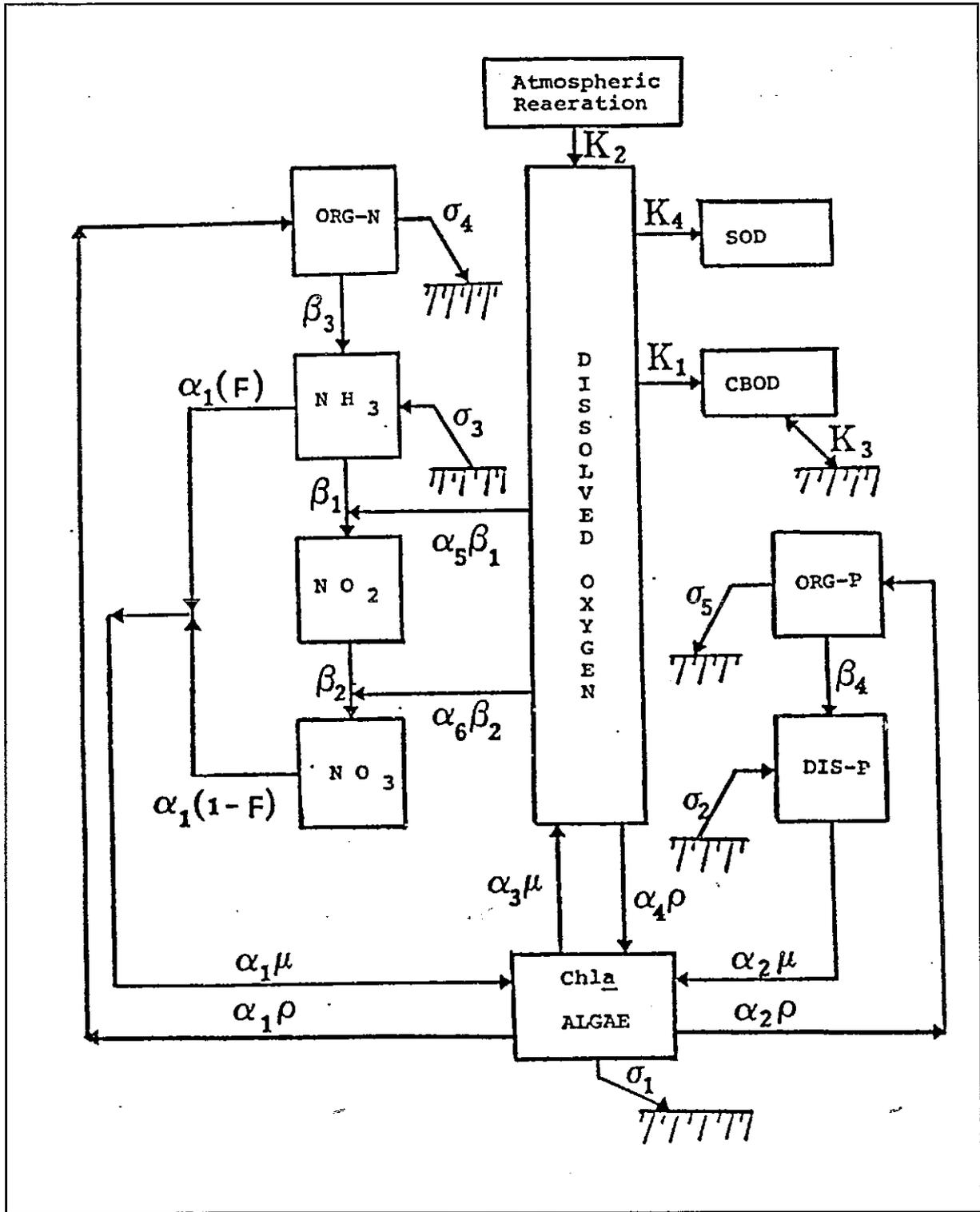
Figure III-1. Constituent reactions and interrelations (Brown and Barnwell, 1987).

Stream depth can be related to stream flow either via the Manning equation, or as (Brown and Barnwell, 1987):

$$\sigma^d = \alpha (q^s)^{\beta}$$

(III-31)

where

σ^d = stream depth [L]; and

α, β = empirical constants derived from stage-discharge rating curves.

Longitudinal dispersion refers to transport resulting from spatially averaged velocity variation. Longitudinal dispersion differs from diffusion, which refers to transport resulting from time-averaged velocity fluctuations. Longitudinal dispersion is computed here as:

$$D_L^s = 3.82 \ K \ n^m \ \bar{u} \ (d^s)^{5/6}$$

(III-32)

where

D_L^s = surface water longitudinal dispersion coefficient, $[L^2 T^{-1}]$

K = dispersion constant [dimensionless];

n^m = Manning's roughness coefficient [dimensionless].

The concentration of chlorophyll a is assumed directly proportional to the concentration of phytoplanktonic algal biomass.

$$Chl\underline{a} = \alpha_{oa} \ A^a$$

(III-33)

where

Chl$\underline{a}$ = concentration of chlorophyll $\underline{a}$ [ug-Chl$\underline{a}$ /L];

α_{oa} = scaled proportion of algae that is chlorophyll $\underline{a}$; and

A^a = concentration of algae [mg-A/L].

Production of algae is defined as:

$$\frac{dA^a}{dt} = \mu^a \ A^a - \rho^a \ A^a - \frac{\sigma_1^a}{\sigma^d} \ A^a$$

(III-34)

where

μ^a = the local specific growth rate of algae as defined below, which is temperature dependent, $[T^{-1}]$ (DeGroot, 1983; Scavia and Park, 1976; Swartzman and Bentley, 1979);

ρ^a = the local respiration rate of algae, which is temperature dependent, $[LT^{-1}]$;

σ_I^a = the local settling rate of algae, which is temperature dependent, $[LT^{-1}]$;

The algal respiration rate includes endogenous respiration, conversion of algal phosphorus to organic phosphorus and the conversion of algal nitrogen to organic nitrogen.

The local specific growth rate is affected by the availability of nitrogen, phosphorus and light. The interaction between these factors can be modelled: multiplicatively; restricted by the most limited nutrient; or as a harmonic mean between the other approaches. The algal growth limitation due to light can be computed using a Monod half-saturation method, Smith's function (Smith, 1936), or Steele's equation (Steele, 1962). Some of the other modelled processes for algae are:

- self shading (JRB Associates, 1983; Bowie et al, 1985);
- growth limitation due to lack of nitrogen and phosphorus;
- use of ammonia and nitrate as a source of inorganic nitrogen;
- temperature dependence of algal growth and death rates;
- nitrogen cycle transformations from organic nitrogen to ammonia, to nitrite and to nitrate;
- inhibition of nitrification at low values of dissolved oxygen;
- phosphorus cycle transformations from organic phosphorus to dissolved inorganic phosphorus, to algal mass and back to organic phosphorus; and
- deoxygenation of carbonaceous BOD (Thomas, 1948).

The oxygen balance in the stream depends on the streams reaeration capacity--a function of advection, diffusion, and sources and sinks (Bowie et al, 1985; APHA, 1985). This is described using:

$$\frac{dO}{dt} = K_2^O (O^* - O) + (\alpha_3^O \mu^a - \alpha_4^O \rho^a) A - K_1^{BOD} L^{BOD} - \frac{K_4^O}{\sigma^d} - \alpha_5^O \beta_1^O N_1 - \alpha_6^O \beta_2^O N_2 \qquad \textbf{(III-35)}$$

where

O	=	the concentration of dissolved oxygen [mg/L]
O^*	=	the saturation concentration of dissolved oxygen at the local temperature and pressure [mb/L]
α_3^O	=	the rate of oxygen production per unit of algal photosynthesis [mg-O/mg-A]
α_4^O	=	the rate of oxygen uptake per unit of algae respired [mg-O/mg-A]
α_5^O	=	the rate of oxygen uptake per unit of ammonia nitrogen oxidation [mb-O/mg-N]
α_6^O	=	the rate of oxygen uptake per unit of nitrite nitrogen oxidation [mb-O/mg-N]
L^{BOD}	=	concentration of ultimate carbonaceous BOD [mg/L]
K_1^{BOD}	=	carbonaceous BOD deoxygenation rate, temperature dependent [day^{-1}]
K_2^O	=	the reaeration rate in accordance with the Fickian diffusion analogy [temperature dependent [day^{-1}]
K_4^O	=	sediment oxygen demand rate, temperature dependent [g/ft^2-day]
β_1^O	=	ammonia oxidation rate coefficient, temperature dependent [day^{-1}]
β_2^O	=	nitrite oxidation rate coefficient, temperature dependent [day^{-1}]
N_1	=	ammonia nitrogen concentration [mg-N/L]
N_2	=	nitrite nitrogen concentration [mg-N/L]

Other modelled processes directly involving DOX concentrations are:
- the solubility of DOX in water as a function of temperature, total dissolved solids (TDS), and atmospheric pressure (Bowie et al, 1985);
- reaeration from the atmosphere (St. John et al, 1984; Churchill et al, 1962; O'Connor and Dobbins, 1958; Owens et al, 1964; Thackston and Krenkel, 1969; Langbien and Durum,

1967; Tsivoglou and Wallace, 1972);

- reduction in reaeration from the atmosphere due to ice cover (TenEch, 1978); and
- reaeration due to flow past dams (Butts and Evans, 1983).

Coliform concentrations are estimated using first order decay functions (Bowie et al, 1985):

$$\frac{dE^{col}}{dt} = -K_5^{col} E^{col} \tag{III-36}$$

where

E^{col} = concentration of coliforms [colonies L^{-3}]

K^{col}_5 = coliform die-off rate, temperature dependent [T^{-1}].

A nonconservative consitutent (nonc) is modelled assuming first order decay and sources and sinks.

$$\frac{dc^{nonc}}{dt} = -K_6^{nonc} c^{nonc} - \sigma_6^{nonc} c^{nonc} + \frac{\sigma_7^{nonc}}{d} \tag{III-37}$$

where

c^{nonc} = concentration of the nonconservative constituent [m-nonc L^3];

K^{nonc}_6 = decay rate for the constituent, temperature dependent [T^{-1}];

σ^{nonc}_6 = rate coefficient for constituent settling, temperature dependent [T^{-1}; and

σ^{nonc}_7 = benthal source for constituent, temperature dependent [m-nonc $L^{-2}T$].

Temperature is modeled using a heat balance on each stream element (reach). The balance includes inputs and losses from all forcing functions and heat exchange between the atmosphere and the water surface. The water-air heat balance includes long and short wave radiation, convection and evaporation. The computed temperatures are used to correct rate coefficients in source/sink terms for other water quality variables.

Reaction coefficients utilized within the above equations include those for:

- Ratio of chlorophyll-a to algal biomass
- Fraction of algal biomass that is nitrogen
- Fraction of algal biomass that is phosphorus
- O_2 production per unit of algal growth
- O_2 uptake per unit of algae respired
- O_2 uptake per unit of NH_3 oxidation
- O_2 uptake per unit of NO_2 oxidation
- Maximum algal growth rate
- Algal respiration rate
- Michaelis-Menton half-saturation constant for light

- Michaelis-Menton half-saturation constant for nitrogen
- Michaelis-Menton half-saturation constant for phosphorus
- Non-algal light extinction coefficient
- Linear algal self-shading coefficient
- Nonlinear algal self-shading coefficient
- Algal preference factor for ammonia
- Algal settling rate
- Benthos source rate for dissolved phosphorus
- Benthos source rate for ammonia nitrogen
- Organic nitrogen settling rate
- Organic phosphorus settling rate
- Arbitrary non-conservative settling rate
- Benthal source rate for arbitraty non-conservative settling rate
- Carbonaceous deoxygeneration rate constant
- Reaeration rate constant
- Rate of loss of BOD due to settling
- Benthic oxygen uptake
- Coliform die-off rate
- Arbitrary non-conservative decay coefficient
- Rate constant for the biological oxidation of NH_3 to NH_2
- Rate constant for the biological oxidation of NH_2 to NH_3
- Rate constant for the hydrolysis of organic-N to ammonia
- Rate constant for the decay of organic-P to dissolved-P

III.8. Mass Balance Expressions for Alpha and Beta Canals

For alpha canals a simple approach is used to describe contaminant concentration changes in response to diversions and loadings. In these canals, we are mainly interested in conservative contaminants such as salt. For this purpose, the following expression is adequate for each reach:

$$c_{\hat{e},\acute{e}+1,k}^{1s} = \frac{\tilde{n}_{\hat{e},\acute{e},k}^{1s} - \tilde{n}_{\hat{e},\acute{e},k}^{1si} - \tilde{n}_{\hat{e},\acute{e},k}^{1so} - \tilde{n}_{\hat{e},\acute{e},1,k}^{2s}}{q_{\hat{e},\acute{e}+1,k}^{1s}} \qquad \text{(III-38)}$$

where
$\tilde{n}$ = mass flow rate (ie., flowrate times concentration) [MT^{-1}]; and

An analagous expression applies for beta canals:

$$c_{\hat{e},\acute{e},\check{e}+1,k}^{2s} = \frac{\tilde{n}_{\hat{e},\acute{e},\check{e},k}^{2s} - \tilde{n}_{\hat{e},\acute{e},\check{e},k}^{2si} - \tilde{n}_{\hat{e},\acute{e},\check{e},k}^{2so} - \tilde{n}_{\hat{e},\acute{e},\check{e},k}^{ca}}{q_{\hat{e},\acute{e}+1,k}^{2s}} \qquad \text{(III-39)}$$

The average concentration of the water delivered to M&I and UCA users in a stress period is:

$$c_{\ddot{y},k}^{mt} = \frac{\tilde{n}_{\ddot{y},k}^{m} + \tilde{n}_{\ddot{y},k}^{mg}}{q_{\ddot{y},k}^{mt}} \qquad \text{(III-40)}$$

$$c_{\hat{e},\acute{e},\check{e},k}^{cat} = \frac{\tilde{n}_{\hat{e},\acute{e},\check{e},k}^{ca} + \tilde{n}_{\hat{e},\acute{e},\check{e},k}^{cag}}{q_{\hat{e},\acute{e},\check{e},k}^{cat}} \qquad \text{(III-41)}$$

where
$c_{\ddot{y},k}^{mt}$ = average concentration of water delivered to M&I user $\ddot{y}$ during the stress period [M L^{-3}]; and

$c_{\hat{e},\acute{e},\check{e},k}^{cat}$ = average concentration of water delivered to UCA user $(\hat{e},\acute{e},\check{e})$ during the stress period [M L^{-3}].

To determine the average concentration of water delivered during a season, we must know how much water is delivered during the season:

$$V_{\ddot{y}}^{mto} = \sum_{k=1}^{K} q_{\ddot{y},k}^{mt} \, \Delta t_{k} \tag{III-42}$$

$$V_{\hat{e},\acute{e},\ddot{e}}^{cato} = \sum_{k=1}^{K} q_{\hat{e},\acute{e},\ddot{e},k}^{cat} \Delta t_{k} \tag{III-43}$$

The average concentrations of water delivered during the entire planning period to a city and a UCA are:

$$c_{\ddot{y}}^{mtavg} = \frac{\sum_{k=1}^{K} \Delta t_{k} (\tilde{n}_{\ddot{y},k}^{m} + \tilde{n}_{\ddot{y},k}^{mg})}{V_{\ddot{y}}^{mto}} \tag{III-44}$$

$$c_{\hat{e},\acute{e},\ddot{e}}^{catavg} = \frac{\sum_{k=1}^{K} \Delta t_{k} (\tilde{n}_{\hat{e},\acute{e},\ddot{e},k}^{ca} + \tilde{n}_{\hat{e},\acute{e},\ddot{e},k}^{cag})}{V_{\hat{e},\acute{e},\ddot{e}}^{cato}} \tag{III-45}$$

where

$c_{\ddot{y}}^{mtavg}$ = average concentration of water delivered to M&I user $\ddot{y}$ during the planning period $[M \ L^{-3}]$; and

$c_{\hat{e},\acute{e},\ddot{e}}^{catavg}$ = average concentration of water delivered to UCA user $(\hat{e},\acute{e},\ddot{e})$ during the planning period $[M \ L^{-3}]$.

III. 9. Salt Loading to Groundwater and Surface Water

Salinity loading to groundwater must be estimated to provide inputs for the groundwater simulation. Equations for salinity loading due to M&I and UCA users are directly analagous to each other. All can be modified to account for lag in the soil profile. Loading due to deep percolation from a UCA is:

$$C_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{dpca} = \frac{\left[q_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{cat} C_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{cat} - q_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{rfca} C_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{cat} - E_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{sac} q_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{cat} C_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{cat} \right]}{q_{\hat{\theta},\hat{\theta},\hat{\theta},k}^{dpca}} \tag{III-46}$$

where
$E^{sac}_{\hat{\theta},\hat{\theta},\hat{\theta}}$ = assumed proportion of the salt applied to the UCA that remains in the soil profile and does not leach to groundwater or runoff the land during stress period k.

Assumptions in the previous equation include:
- surface water runoff from the UCA has the same concentration as irrigation water applied to the UCA;
- the user assumes what proportion of the salt loading will remain in the soil profile;
- the mass of contaminant leaching to groundwater is the difference between the mass applied and that running off or increasing the salt in storage.

Salt loading from M&I and UCA users to canals are also analagous to each other, and merely involve changes in superscripts and subscripts from the above expression.

III.10. Crop Yield Response to Water and Salinity

Many expressions relating crop production to water availability have been reported in the literature (Hexem and Heady, 1978; Letey et al, 1985; Doorenbos and Kassam, 1979; Feddes et al, 1978; Hanks, 1983). Howell et al (1990) summarize some of these. Hoffman et al (1990) and Rhoades et al (1992) summarize work relating crop production to salinity and water availability. Because of the need to be suitable for S/O model optimization, and the relative ease of collecting the necessary data, PROMOD includes the relations listed below.

Assuming only a water deficiency can cause crop yield to be less than its maximum potential value, a simple approach for predicting crop yield involves the following piecewise linear expressions:

$$y_{\hat{e},\acute{e},\ddot{e}} = y^{pot}_{\hat{e},\acute{e},\ddot{e}} \qquad \text{for } w^{ymax}_{\hat{e},\acute{e},\ddot{e}} \leq V^{cato}_{\hat{e},\acute{e},\ddot{e}} \qquad\qquad \textbf{(III-47)}$$

$$y_{\hat{e},\acute{e},\ddot{e}} = y^{pot}_{\hat{e},\acute{e},\ddot{e}} \left[\frac{V^{cato}_{\hat{e},\acute{e},\ddot{e}} - w^{ymin}_{\hat{e},\acute{e},\ddot{e}}}{w^{ymax}_{\hat{e},\acute{e},\ddot{e}} - w^{ymin}_{\hat{e},\acute{e},\ddot{e}}} \right] \qquad \text{for } w^{ymin}_{\hat{e},\acute{e},\ddot{e}} \leq V^{cato}_{\hat{e},\acute{e},\ddot{e}} < w^{ymax}_{\hat{e},\acute{e},\ddot{e}} \qquad\qquad \textbf{(III-48)}$$

$$y_{\hat{e},\acute{e},\ddot{e}} = 0 \qquad \text{for } V^{cato}_{\hat{e},\acute{e},\ddot{e}} < w^{ymin}_{\hat{e},\acute{e},\ddot{e}} \qquad\qquad \textbf{(III-49)}$$

where

$y_{\hat{e},\acute{e},\ddot{e}}$ = crop yield in UCA (ê,é,ë) [M];

$y^{pot}_{\hat{e},\acute{e},\ddot{e}}$ = maximum potential crop yield in UCA (ê,é,ë) (assuming adequate water, fertility and trace elements and acceptable salinity) [M];

$w^{ymax}_{\hat{e},\acute{e},\ddot{e}}$ = water needed for delivery in the UCA in order to achieve maximum potential crop yield [L³]; and

$w^{ymin}_{\hat{e},\acute{e},\ddot{e}}$ = minimum water needed the UCA in order to obtain any crop yield at all [L³].

Those piecewise linear expressions can also be represented in another form that is useful within the optimization module of a S/O model:

$$y_{\hat{e},\acute{e},\ddot{e}} = \frac{y^{pot}_{\hat{e},\acute{e},\ddot{e}}}{w^{ymax}_{\hat{e},\acute{e},\ddot{e}} - w^{ymin}_{\hat{e},\acute{e},\ddot{e}}} \left[\min \left(w^{ymax}_{\hat{e},\acute{e},\ddot{e}}, V^{cato}_{\hat{e},\acute{e},\ddot{e}} \right) - \min \left(w^{ymin}_{\hat{e},\acute{e},\ddot{e}}, V^{cato}_{\hat{e},\acute{e},\ddot{e}} \right) \right] \qquad \textbf{(III-50)}$$

where

min(q,r) = an expression stating that the computer model will utilize the smaller of the two values: q and r.

The following piecewise linear expressions are applicable if salinity is the only factor which can reduce yield (i.e. if water is assumed adequate). For practicality in this S/O

model, we consider the salinity of the irrigation water rather than that of the root zone.

$$y_{\hat{e},\acute{e},\ddot{e}} = y^{pot}_{\hat{e},\acute{e},\ddot{e}} \qquad \text{for } EC^{catavg}_{\hat{e},\acute{e},\ddot{e}} \leq EC^{ymin}_{\hat{e},\acute{e},\ddot{e}} \qquad\qquad \text{(III-51)}$$

$$y_{\hat{e},\acute{e},\ddot{e}} = y^{pot}_{\hat{e},\acute{e},\ddot{e}} \left[1 - \frac{EC^{catavg}_{\hat{e},\acute{e},\ddot{e}} - EC^{ymin}_{\hat{e},\acute{e},\ddot{e}}}{EC^{ymax}_{\hat{e},\acute{e},\ddot{e}} - EC^{ymin}_{\hat{e},\acute{e},\ddot{e}}} \right] \qquad \text{for } EC^{ymin}_{\hat{e},\acute{e},\ddot{e}} < EC^{catavg}_{\hat{e},\acute{e},\ddot{e}} < EC^{ymax}_{\hat{e},\acute{e},\ddot{e}} \qquad \text{(III-52)}$$

$$y_{\hat{e},\acute{e},\ddot{e}} = 0 \qquad \text{for } EC^{ymax}_{\hat{e},\acute{e},\ddot{e}} \leq EC^{catavg}_{\hat{e},\acute{e},\ddot{e}} \qquad\qquad \text{(III-53)}$$

where

$EC^{catavg}_{\hat{e},\acute{e},\ddot{e}}$ = average electrical conductivity value of the irrigation water delivered to the UCA during the planning period [dSm^{-1}];

$EC^{ymax}_{\hat{e},\acute{e},\ddot{e}}$ = average electrical conductivity value of the irrigation water above which there will be no crop yield in the UCA [dSm^{-1}]; and

$EC^{min}_{\hat{e},\acute{e},\ddot{e}}$ = lowest average electrical conductivity value of the irrigation water which will not cause crop yield reduction in the UCA [dSm^{-1}].

Those piecewise linear expressions can be represented in a single expression useful within a S/O model:

$$y_{\hat{e},\acute{e},\ddot{e}} = y^{pot}_{\hat{e},\acute{e},\ddot{e}} \left[1 - \frac{\min\left(EC^{ymax}_{\hat{e},\acute{e},\ddot{e}}, EC^{catavg}_{\hat{e},\acute{e},\ddot{e}}\right) - \min\left(EC^{catavg}_{\hat{e},\acute{e},\ddot{e}}, EC^{ymin}_{\hat{e},\acute{e},\ddot{e}}\right)}{EC^{ymax}_{\hat{e},\acute{e},\ddot{e}} - EC^{ymin}_{\hat{e},\acute{e},\ddot{e}}} \right] \qquad \text{(III-54)}$$

To use the above approach the modeler must assume apriori which yield reduction expression is most appropriate for each UCA. For UCAs where both water shortage and high salinity of irrigation water exist, the modeler will need to pick one of the expressions and change the appropriate threshold values ($w^{ymax}_{\hat{e},\acute{e},\ddot{e}}$, $w^{ymax}_{\hat{e},\acute{e},\ddot{e}}$, $EC^{min}_{\hat{e},\acute{e},\ddot{e}}$, $EC^{ymax}_{\hat{e},\acute{e},\ddot{e}}$) to permit simultaneous consideration of both yield reduction causes. Musharrafieh et al (1993) and Peralta et al (1994) show the utility of other piecewise linear expressions for optimal crop water management.

An alternative yield expression lets us use different effects of water shortage depending upon when during the irrigation season the shortage occurs. We assume that water availability is the only resource that might prevent achieving maximum crop yield.

$$y_{\hat{e},\acute{e},\ddot{e}} = y^{p}_{\hat{e},\acute{e},\ddot{e}} \left[1 - \sum_{k=1}^{n} \frac{C^{crw}_{\hat{e},\acute{e},\ddot{e},k} u_{\hat{e},\acute{e},\ddot{e},k}}{W_{(\hat{e},\acute{e},\ddot{e},k)}} \right] \qquad \text{(III-55)}$$

where

$u_{\hat{e},\acute{e},\ddot{e}}$ = the volume of unsatisfied water needs in a UCA during stress period k [L^3];

$W_{\hat{e},\acute{e},\ddot{e}}$ = water (including irrigation and effective precipitation) required in stress

period k in order to produce the maximum potential yield, known, $[L^3]$;

$c^{crw}_{\hat{e},\acute{e},\ddot{e}}$ = a dimensionless crop loss coefficient. It equals the proportional reduction in the annual potential yield that results from a proportional lack of adequate irrigation water in time step k, known by site-specific studies; and

$u_{\hat{e},\acute{e},\ddot{e}} / w_{\hat{e},\acute{e},\ddot{e}}$ = the proportion of water needs in time step k that are unsatisfied.

IV. S/O Module Simulation Abilities: Approach Selection and Simplified Simulation Expressions

IV.1. Introduction and Literature Review

An optimization problem formulated by the user will consist of an objective function, and desirable constraints and bounds. The objective function is an equation, the value of which will be maximized (or minimized) in order to best achieve user objectives. The model will calculate the optimal water management strategy for that objective, subject to restrictions that the user places on the strategy or consequences of implementing the strategy. These consequences must be represented by simulation equations within the S/O module.

S/O module constraint equations must describe how a state variable will respond to decision variables. There are several approaches for doing this, each having particular strengths and weaknesses. Here we discuss the more common, proven, approaches that can be used within linear, quadratic or nonlinear optimization models. These three approaches are: embedding, response matrix, and regression methods. The purpose of this section is to describe the advantages and weaknesses of the three most appropriate approaches.

In the embedding (EM) method, a numerical equation (usually finite difference or finite element) is included directly as a constraint (Willis and Yeh, 1987). In the response matrix (RM) approach influence coefficients are first created using a simulation model or equation. The influence coefficients are used in superposition expressions, which are included as constraints within the S/O model (Gorelick, 1983).

More recently the regression (RE) approach has been used to describe changes in state variables that cannot be well described using influence coefficients. Again, a preliminary simulation model is used. In this approach, many preliminary runs are made to develop a data base of system response to stimuli (pumping or diversion). Then regression expressions are computed. One regression expression is developed to describe how each particular state variable will respond to all decision variables. Finally, the regression expressions are included as constraints within the S/O model.

EM and RM methods are ideally suited for linear systems (confined aquifers), but must be adapted to address significantly nonlinear aquifers (unconfined aquifers where the change in head significantly affects transmissivity or flow equations). EM and RM methods generally assume that aquifer transmissivity does not change significantly during the planning horizon, i.e. they assume that internal groundwater flow is linear. The RE method might or might not assume that the system is linear, depending on the model that is used during the pre-optimization simulation.

Many researchers have applied cyclical approaches to correct the error caused by treating a nonlinear system as if it were linear, or have shown that the error was acceptable (Heidari, 1983; Danskin and Gorelick, 1985; Peralta and Killian, 1985; Willis and Finney, 1985; Jones et al., 1987; Lall and Santini, 1989; Willis and Jones, 1987; Willis and Yeh, 1987).

Cycling is commonly part of the process for adapting to the nonlinearity of unconfined aquifers. Cycling involves:

1) assuming aquifer saturated thicknesses based on assumedly appropriate aquifer heads;

2) computing transmissivities (EM method) or transmissivities and influence coefficients based on those saturated thicknesses (RM method);

3) computing an optimal strategy using those transmissivities or influence coefficients;

4) comparing the system responses to the optimal strategy computed by the S/O model with theose computed by a normal, more-detailed, simulation model (using the optimal strategy as input); and

5) stopping or returning to step 1for the next cycle.

Below is a summary of characteristics of the EM, RM and RE approaches. Cited papers utilize linear, quadratic or nonlinear optimization.

The EM approach:

■ has been widely used for both surface and groundwater systems management.

■ requires, in its constraint set, one equation per stress period per cell or reach.

■ is commonly used in surface water S/O models to maintain continuity and volume balance in stream or reservoir reaches (OMara and Duloy, 1984; Martin, 1986; Peralta et al. 1990, and many others).

■ is used to manage reservoir-river systems (Dorfman, 1962; Palmer et al., 1982; Randall et al., 1990; Ford et al, 1981; HEC, 1991; and many others)

■ has been used to constrain BOD and O_2 in a stream resulting from loadings (Thomann and Sobel, 1964; Sobel, 1965; Loucks et al., 1967; ReVelle et al., 1968), Shih, 1970; Lohani and Tanh, 1978; Simonovic and Orlob, 1984; Burn, 1989; and Cardwell and Ellis, 1993). We consider this an embedding application even if the equation is used without multiple cells or stress periods.

■ maintains continuity and volume balance in aquifer cells and layers when applied to groundwater problems. The number of constraint equations can become large if there are many cells or stress periods (Tung and Kolterman, 1985).

■ has been used for some transient groundwater flow problems (Yazcigil and Rasheeduddin, 1987; Willis et al., 1989).

■ is not recommended for most transient groundwater flow problems.

■ is most useful for steady state groundwater planning (Peralta and Killian, 1987) which can often be interpreted as sustained groundwater yield planning (Knapp and Fienerman, 1985).

■ can require significantly less computer memory and processing time than the RM approach for steady-state problems, if many of the study area cells contain pumping as a decision variable and head must be constrained at many cells (Peralta et al, 1992; Takahashi and Peralta, 1992).

■ will require more computer memory and processing time than a RM model for a steady-state problem if there are comparatively few pumping values being optimized and heads being constrained (Peralta et al, 1991).

■ has been applied to some groundwater contamination problems (Willis, 1979).

■ can be appropriate for managing dispersed groundwater contamination, when spatial discretization is coarse, cells are large, and a high degree of accuracy is not critical (Gharbi and Peralta, 1994).

■ is not very practical for managing point-source groundwater contaminant plumes. Individuals seeking to simulate and control point-source contaminant plumes usually

try to reduce cell size (increasing the number of cells) to improve modelling and management accuracy. This tendency to use many cells makes the EM approach inefficient.

The RM approach:

■ is widely used for groundwater management.

■ requires, in its constraint set, one superposition equation per location and period for each state variable being constrained. The superposition equation might require one influence coefficient per decision variable/state variable pair, per stress period.

■ requires one pre-optimization simulation per stimulus (decision variable) location

■ is perfectly applicable for steady and transient management of linear systems. These include confined aquifers, and streams having linear stage-discharge relations. Usually the stage-discharge relation is only assumed linear over a particular range of interest. Otherwise, a piecewise linear relation can be used.

■ is readily adaptable for steady and transient management of unconfined aquifers (see above discussion on cycling).

■ might or might not be preferred to an EM approach for steady-state problems, depending on the proportion of pumping decision variables and locations where head must be constrained (see above EM approach discussion).

■ is adaptable for steady and transient management of stream-aquifer systems (Morel-Seytoux, 1975; Morel-Seytoux et al, 1980; Danskin and Gorelick, 1985; Reichard, 1987; Peralta et al, 1988; Mueller and Male, 1993; Morel-Seytoux, 1994). When utilized stage-discharge relations are not linear, they are sometimes linearized.

■ is useful to control groundwater contaminant movement by controlling hydraulic gradients or velocities (Molz and Bell, 1977; Colarullo et al., 1984; Atwood and Gorelick, 1985; Lefkoff and Gorelick, 1986; and Peralta and Ward, 1991).

■ is not useful for explicitly constraining the groundwater or surface water contaminant concentration that will result from management.

The RE approach:

■ requires, in its constraint set, one equation per location and period per state variable being addressed with that approach.

■ requires significant pre-optimization simulations (how much depends on the number of decision variables affecting the state variables and how many stress periods there are in the planning horizon).

■ is useful for managing a wide range of reactive and conservative surface water contaminant concentrations, including BOD and O_2 (Ejaz and Peralta, 1994)

■ is very useful for managing groundwater contaminant concentrations (Alley, 1986; Lefkoff and Gorelick, 1990)

■ is not needed to manage water table heads because they can be readily addressed using the easier EM or RM methods.

■ can be used to manage heads or volumes of nonaqueous liquids (Cooper et al, 1994).

IV.2. Rationale and Selection of Simulation Approaches for S/O Module

PROMOD is designed to best utilize each of the three approaches to the extent appropriate for a particular management problem. As a result of the above observations, PROMOD utilizes:

■ EM method to provide Muskingum routing in streams or reservoir when reservoirs exist and lag times are important.

■ RM method to provide Manning equation-style routing in streams when reservoirs do not exist and lag times are unimportant.

■ EM method to maintain a volume balance for canals. In the ISM, C/AI interflow is determined via continuity expression and is unaffected by aquifer or surface water heads. Generally, there is at least one variable (q^{2s} or q^{ca}) needing to be constrained per canal section. For this situation, both EM and RM approaches require one constraint equation per section. However, since the RM approach requires pre-optimization simulation, the EM approach is preferred.

■ RM method to describe aquifer head response to pumping, stream diversion, reservoir release, deep percolation, and discharge from drains, springs, or flowing wells.

■ RM method to describe streamflow response to pumping, stream diversion, reservoir release, deep percolation, and discharge from drains, springs, or flowing wells.

■ RE method to describe groundwater or surface water mass flow rates, concentrations or nonaqueous phase liquid heads.

To employ the RM and RE methods, PROMOD's S/O module includes some simulation expressions formulated differently than those of the previous chapter. These alternative superposition or regression (respectively) expressions represent (within the SSM and the S/O) the same processes modelled by the ISM. They are used to make it easier for the S/O model to compute an optimal strategy. They are more simple in nature than the original numerical expressions, and take up less computer memory. To the extent possible, they assume system linearity. The simplified simulation expressions are developed using pre-optimization simulation runs. The rest of this chapter discusses these simplified expressions.

IV.3. Simplified Expressions for System Head and Streamflow Response to Hydraulic Stresses, and Expression Development

IV.3.1 Groundwater head and flow response equations

The S/O model employs the response matrix method to represent some system responses to stimuli. This means that those processes of the physical system are assumed to be addressable using linear systems theory via superposition (Bear, 1987; Reilley et al, 1987). For example, confined aquifer head response to pumping is a linear process. (Addressing nonlinear aquifer systems is discussed previously. Frequently, errors resulting from assuming system linearity are small, or can be addressed by cycling (Peralta and Kowalski, 1985; Reichard, 1987).

Employing superposition means that model constraint equations include summations of products of influence coefficients and decision variables. When all constraint equations are represented together in vector form, a matrix of influence coefficients results. This is termed a response matrix (Willis and Yeh, 1987).

The S/O model uses summation constraint equations to describe the effect of pumping and diversion on aquifer head, stream stage, stream flow, and river-aquifer interflow. How these constraints are formulated is discussed below. The S/O model also includes expressions describing the effect on other state conditions that are functions of head. These are described later.

The following summation expression is used to define head at a location ô and future time n (Peralta and Aly, 1993). It is similar to other superposition expressions used by Illangasekare and Morel-Seytoux (1982), Morel-Seytoux (1975b) and many others.

$$h(\hat{o},n) = h^{non}(\hat{o},n) + \sum_{k=1}^{n} \left[\sum_{\hat{a}=1}^{M^{pb}} \delta^h(\hat{o},\hat{a},n-k+1) \frac{g(\hat{a},k)}{g^{ut}(\hat{a})} + \sum_{\hat{e}=1}^{M^{dvf}} \beta^h(\hat{o},\hat{e},n-k+1) \frac{z(\hat{e},k)}{z^{ut}(\hat{e})} \right] \text{(IV-1)}$$

where

h = aquifer potentiometric surface elevation (head) [L];

ô = index denoting an observation location, at which system response is being evaluated;

n = number of the stress period for which system response is being computed;

h^{non} = potentiometric surface elevation that results without implementing the optimal strategy, (nonoptimal head) [L];

k = index for stress period;

M^{pb} = M^p + M^b total number of cells at which water can vertically recharge or discharge from the aquifer via optimal pumping, deep percolation that can directly result from water application or use (a decision variable), or canal

losses that can result from optimal water management[1];

M^p = total number of cells at which groundwater pumping will be optimized.

M^b = total number of cells at which vertical fluxes other than pumping can occur from of to the aquifer.

â = index denoting a potential pumping cell.

$\delta^h(\hat{o},\hat{a},n-k+1)$ = influence coefficient describing effect of groundwater pumping at cell â in stress period k, on potentiometric surface elevation at cell ô by the end of period n [L];

$g(\hat{a},k) = p(\hat{a},k) + b(\hat{a},k)$ = difference between the nonoptimal and optimal vertical discharge or recharge rate at cell â during stress period k [L³/T];

$p(\hat{a},k)$ = difference between the nonoptimal and optimal groundwater pumping (extraction, - ; injection, +) rate at cell â during stress period k [L³/T];

$b(\hat{a},k)$ = sum of all changes in deep percolation or canal/aquifer interflow that result at cell â during stress period k, from the computed optimal management strategy [L³/T];

$g^{ut}(\hat{a})$ = magnitude of 'unit' discharge or recharge stimulus in cell â [L³/T]. This does not necessarily have a magnitude of one;

M^{dvf} = $M^d + M^v + M^f$;

M^d = total number of reaches at which surface water diversion from a stream can be optimized;

M^v = total number of locations at which reservoir release can be optimized;

M^f = total number of locations at which changes in canal flow to a stream, (resulting from optimal water management) can occur;

ê = index denoting a potential river water diversion reach;

$\beta^h(\hat{o},\hat{e},n-k+1)$ = influence coefficient describing effect of river water diversion or inflow at reach ê or reservoir release at location ê in stress period k, on potentiometric surface elevation at cell ô by the end of period n [L];

$z(\hat{e},k) = d(\hat{e},k) + v(\hat{e},k)$ = difference between nonoptimal and optimal diversion, reservoir release or other management decision directly adding water to or removing water from the stream (indirect effects felt through the aquifer are not included) [L³/T];

$d(\hat{e},k)$ = difference between nonoptimal and optimal diversion or reservoir release [L³/T];

$v(\hat{e},k)$ = a decision variable describing some difference in flow from or to a stream between nonoptimal and optimal water management, other than those caused by diversion, reservoir release, or flow from an aquifer [L³/T].

$z^{ut}(\hat{e})$ = magnitude of 'unit' diversion, reservoir release, or direct discharge or source at location ê [L³/T]. This does not necessarily have a magnitude of one.

The S/O model can use polygon (cell), point (node), or line influence coefficients in Equation IV-1. PROMOD has the option to compute the head at a well located in the center of a cell. One way is to replace cell influence coefficients with

---

[1]Cells where pumping or diversion are permitted occur in the optimal strategy. Whether they pump or divert or neither is determined by the optimization algorithm of the S/O model.

well influence coefficients using analytical or numerical procedures reported previously (Prickett, 1967; Trescott et al, 1976; Verdin et al, 1981).

An analogous expression to Eq. IV-1 exists for linearly estimating streamflow. Here, Equation IV-2 differs from Equation IV-1 only in the substitution of q^s for h, δ^s for δ^h, and β^s for β^h.

$$q^s(\hat{u},n) = q^{snon}(\hat{u},n) + \sum_{k=1}^{n} \left[\sum_{\hat{a}=1}^{M^{pb}} \delta^s(\hat{u},\hat{a},n-k+1) \frac{g(\hat{a},k)}{g^{ut}(\hat{a})} + \sum_{\hat{e}=1}^{M^{dvf}} \beta^s(\hat{u},\hat{e},n-k+1) \frac{z(\hat{e},k)}{z^{ut}(\hat{e})} \right] \quad \text{(IV-2)}$$

where

q^s = stream flow rate [L^3/T];

$\hat{u}$ = index denoting a stream flow observation or control reach;

q^{snon} = stream flow rate that results without implementing the optimal strategy (nonoptimal stream flow) [L^3/T];

$\delta^s(\hat{u},\hat{a},n-k+1)$ = influence coefficient describing effect of groundwater stimulus at cell $\hat{a}$ in stress period k, on stream flow at reach $\hat{u}$ by the end of period n [L];

$\beta^s(\hat{u},\hat{e},n-k+1)$ = influence coefficient describing effect of river water diversion or inflow at reach $\hat{e}$ or reservoir release at location $\hat{e}$ in stress period k, on stream flow rate at reach $\hat{u}$ by the end of period n [L];

Stream or aquifer interflow is defined via (Belaineh and Peralta, 1993; Peralta and Aly (1993):

$$q^{sri}(\ddot{u},n) = q^{snon}(\ddot{u},n) +$$

$$\sum_{k=1}^{n} \left[\sum_{\hat{a}=1}^{M^{pb}} \delta^{sri}(\ddot{u},\hat{a},n-k+1) \frac{g(\hat{a},k)}{g^{ut}(\hat{a})} + \sum_{\hat{e}=1}^{M^{dvf}} \beta^{sri}(\ddot{u},\hat{e},n-k+1) \frac{z(\hat{e},k)}{z^{ut}(\hat{e})} \right] \quad \text{(IV-3)}$$

where

$\ddot{u}$ = index denoting a stream/aquifer interflow observation or control reach;

$\delta^{sri}(\ddot{u},\hat{a},n-k+1)$ = influence coefficient describing effect of groundwater stimulus at cell $\hat{a}$ in stress period k, on stream flow at reach $\ddot{u}$ by the end of period n [L];

$\beta^{sri}(\ddot{u},\hat{e},n-k+1)$ = influence coefficient describing effect of river water diversion or inflow at reach $\hat{e}$ or reservoir release at location $\hat{e}$ in stress period k, on stream flow rate at reach $\ddot{u}$ by the end of period n [L];

An expression for stream stage comparable to Equation IV-3 involves

substituting σ for h, σ^{non} for h^{non}, δ^{σ} for δ^{sri}, and β^{σ} for β^{sri}. The stream stage constraint needs to be used with care, especially if the stage-discharge relation is not well approximated by a linear expression near the discharge of interest.

IV.3.2 Development of groundwater head and stream flow response equations

The δ^h influence coefficients above are calculated automatically by S/O model in the following manner. First, the model computes a nonoptimal potentiometric surface (h^{non}). This consists of steady state or transient heads that result from assumed pumping. This is generally the result of a no-change-in-management strategy. Next, the model computes the surface that will result from a specified unit groundwater stimulus, $g^{ut}(\hat{a})$, occuring at a cell $\hat{a}$. For steady-state conditions, the difference between the two surfaces at cell $\hat{o}$ is the influence coefficient $\delta^h(\hat{o},\hat{a},1)$.

When developing the coefficients for transient conditions, the unit pumping is performed only in the first stress period (all stress periods must be of the same duration). Thus, k is 1 and the resulting coefficients have the indexing of $\delta^h(\hat{o},\hat{a},n)$, where n is the number of the stress period at which the influence is being observed.

The δ^s, δ^{sri}, and δ^{σ} coefficients are developed at the same time as the δ^h coefficients, and in a similar fashion. They represent changes in stream stage, streamflow and stream/aquifer or river/aquifer interflow. Of these flow processes, stream stage is probably the most nonlinear.

The β^h, β^s, β^{sri} and β^{σ} coefficients are developed in a similar manner, but using diversion, release or surface water return flow of $z^{ut}(\hat{e})$ as the unit stimulus for each potential location $\hat{e}$.

There are other interesting state responses in addition to the four state variables described above. These include: head difference between two locations, hydraulic gradient, groundwater velocity, and contaminant velocity. Since all of these are functions of head, they can all be derived from the above expressions. Thus, the model computes and uses the resulting head difference, gradient and velocity influence coefficients.

IV.4. Simplified expressions for groundwater response to advective-dispersive transport, and expression development

IV.4.1 Groundwater contaminant concentration response equations

Alley (1986) and Lefkoff and Gorelick (1990) demonstrated that saturated zone solute transport can be represented using regression equations, after sufficient simulations are systematically performed to develop those expressions. Regression-developed expressions most likely to be useful are shown below. Using one of these expressions for concentrations within an S/O model is much more simple, and yields solutions more easily, than embedding the transport and reaction equations within the model directly.

A polynomial expression has been successfully applied to predict groundwater contamination concentration for specified locations. It has also been applied for LNAPL (lighter-than-water non-aqueous phase liquid) management (Cooper et al, 1994). Peralta and Aly (1994) maximized the mass of groundwater contaminant removal using the same form of expression.

$$
WW(\ddot{o},k) = \sum_{ii=1}^{II} \sum_{\hat{a}=1}^{M^{pb}} \sum_{k=1}^{n} AA(ii,\hat{a},k) \ [g(\hat{a},k)]^{BB(ii,\hat{a},k)}
$$

$$
+ \ \sum_{ii=1}^{II} \sum_{\hat{e}=1}^{M^{dvf}} \sum_{k=1}^{n} AA\,'(ii,\hat{e},k) \ [z(\hat{e},k)]^{BB\,'(ii,\hat{e},k)} \tag{IV-4}
$$

where
ww(x,k)	= a nonlinear state variable; examples include: groundwater contaminant concentration, head of an aqueous or nonaqueous phase liquid within an aquifer, area of nonaqueous lens floating on groundwater, volumes of nonaqueous phase liquid as free product, residual within the aquifer, or captured by pumping;
II	= a the number of terms in the polynomial expression;
AA, BB, AA' and BB'	= regression coefficients.

An exponential expression is (undocumented feature of Peralta and Aly, 1993):

$$WW(\ddot{o},k) = \sum_{jj=1}^{JJ} \sum_{\hat{a}=1}^{M^{pb}} \sum_{k=1}^{n} CC(jj,\hat{a},k) \; exp\left(DD(jj,\hat{a},k)[g(\hat{a},k)]^{EE(jj,\hat{a},k)}\right)$$

$$+ \sum_{jj=1}^{JJ} \sum_{\hat{e}=1}^{M^{dvf}} \sum_{k=1}^{n} CC'(jj,\hat{e},k) \; exp\left(DD'(jj,\hat{e},k)[z(\hat{e},k)]^{EE(jj,\hat{e},k)}\right)$$

(IV-5)

where

JJ = the number of terms in the exponential polynomial;

CC, DD, CC' and DD' = regression coefficients.

A logarithmic expression is (personal communication, Aly, A.H., 1993):

$$WW(\ddot{o},k) = \sum_{\hat{a}=1}^{M^{pb}} \sum_{k=1}^{n} FF(\hat{a},k) \; log(g(\hat{a},k))$$

$$+ \sum_{\hat{e}=1}^{M^{dvf}} \sum_{k=1}^{n} FF'(\hat{e},k) \; log(z(\hat{e},k))$$

(IV-6)

where

FF and FF' = regression coefficients.

IV.4.2 Development of groundwater contaminant concentration response equations

Figure IV-1 shows a flow chart of the steps involved in developing polynomial expressions suitable for predicting contaminant concentration that results in groundwater as a result of hydraulically stimulating the aquifer. Within PROMOD this process is automated and data files are transferred automatically.

The process involves systematically making many simulations and then fitting regression expressions to the results of the simulations. These pre-regression analysis simulations can take a lot of time. They are usually performed overnight, or when the computer is not needed. For efficiency, no more simulations than necessary are performed. The first step is to determine the duration of the planning period. There is no need to simulate for longer than the planning period. The range of physically, legally or socially feasible groundwater pumping or recharge rates is determined, as is the number of stress periods within the planning period. A matrix of simulations to be performed is determined, and these are run.

Simulation results are summarized and analyzed statistically, to develop coefficients suitable for the above equations. The degree to which the expressions can predict system response in some selected simulations is evaluated. If error is unacceptably great, some additional simulations are performed. These simulations are selected to provide additional data within the solution space region where error is unacceptable.

Once the regression expressions perform adequately for the performed simulations, they are included within the S/O model as constraints. An optimal water management strategy is computed. Then the optimal strategy is input to the simulation model and system response is calculated. If the simulation model predicts the same response as the S/O model, for significant state variables, the optimal strategy is acceptable.

If the simulation model predicts a significantly different system response for a state variable that is tightly constrained in the optimal strategy, the regression expression must be improved. Some more simulations are performed, using data from the optimal strategy as input. The results are included when performed a new expanded regression analysis. A new regression expression is developed, and included within the S/O model. A new optimal strategy is computed. This cycling process continues until post-optimization simulation indicates that implementing the optimal strategy in the field would yield acceptable system responses (at least according to the assumedly calibrated simulation model).
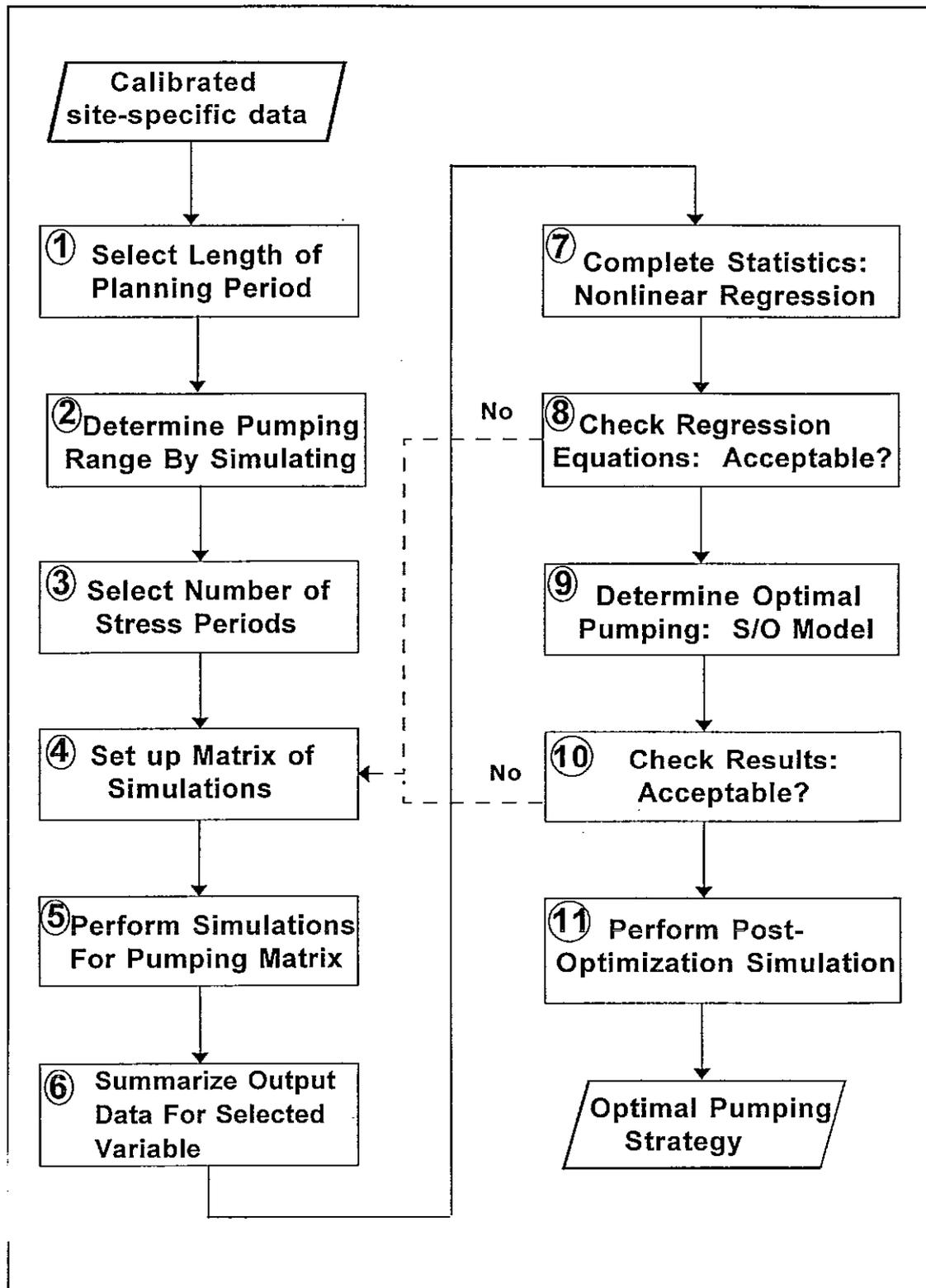
Figure IV-1 Developing polynomial expression for groundwater concentration: flow chart

IV.5. Simplified Expressions for Stream Water Quality Response to Loading and Expression Development

IV.5.1 Stream contaminant concentration response equations

Ejaz and Peralta (1994) demonstrated simplified expressions suitable for describing stream water quality resulting from stream loadings due to point and diffuse sources. They developed these to emulate the detailed simulation modelling of QUAL2E (Brown and Barnwell, 1987). The following form was tested for a hypothetical system having steady flow, one point source, several upstream sources, and several diffuse sources. It was accurate within several percent for BOD_5, organic nitrogen, nitrogen as ammonia, nitrite and nitrate ($N-NH_3$, $N-NO_2$, and $N-NO_3$, respectively), total nitrogen, organic phosphorus, dissolved phosphorus, total phosphorus, and chlorophyl A in a stream section:

$$\tilde{n}(\hat{u},j) = \beta^d(j) \sum_{\tilde{u}=1}^{M^{sri}} \tilde{n}^{sri}(\tilde{u},j) +$$

$$\beta^{ov}(j) \sum_{i=1}^{M^{ov}} \tilde{n}^{ov}(i,j) + \beta^P(j) \tilde{n}^P(\hat{e},j) \tag{IV-7}$$

such that $\tilde{n}^d(\tilde{u},j)$, $\tilde{n}^P(\hat{e},j)$ are stream inflows

where

$^{sri}, ^{ov}, ^P$ = designate stream/aquifer interflow, overland or source flow, and point source, respectively. Stream/aquifer interflow and point sources are treated as decision variables. Source or overland flows are assumed known;

$\tilde{n}^x(i,j)$ = mass flow rate of the jth constituent in the ith reach of the xth source or control location [M/T];

$\beta^x(j)$ = regression coefficient describing the contribution of specific mass flow rate to $\tilde{n}^x(i,j)$.

The concentration at a stream reach of interest is determined by:

$$c^x(i,j) = \tilde{n}^x(i,j) / q^x(i) \tag{IV-8}$$

where

$c^x(i,j)$ = concentration of the jth constituent in the ith reach of the xth source/control location [M/L^3];

$q^x(i)$ = flow rate in the ith reach of the xth source or control location [L^3/T].

Ejaz and Peralta (1994) showed the following to be appropriate for defining dissolved oxygen (DOX) in a stream:

$$\tilde{n}(\hat{u},DOX) = \beta^o(DOX) + \beta^d(DOX) \sum_{\hat{u}=1}^{M^{sri}} \tilde{n}^{sri}(\ddot{u},DOX)$$

$$+ \beta^{ov}(DOX) \sum_{i=1}^{M^{ov}} \tilde{n}^{ov}(i,DOX) + \beta^p(DOX) \tilde{n}^p(\hat{e},DOX) \qquad \text{(IV-9)}$$

$$+ \beta(BOD) \tilde{n}(\hat{u},BOD) + \beta(TON) \tilde{n}(\hat{u},TON)$$

$$+ \beta(CHA) \tilde{n}(\hat{u},CHA)$$

where
$\beta^o(DOX)$ = regression coefficient describing the contribution of the background concentration of dissolved oxygen to the DOX mass flow rate at reach $\hat{u}$, [M/T].

Again, concentration is determined by simple division.

IV.5.2 Development of stream contaminant concentration response equations

Ejaz (1994) addressed the Figure IV-2 area when developing optimal mass loading rates. He used a cyclical procedure (Figure IV-3) for developing regression equations and an optimal loading strategy for one scenario. (A 'scenario' is a unique management problem being solved.) For the stream concentration problem, the seven-step procedure of Figure IV-3 is termed a cycle.

1)   Assume three values for flow rate and concentration for each constituent in upstream, point, and non-point sources based on historical stream data and expected treatment efficiencies of STP and OLF systems.

2)   Run QUAL2E for every unique combination of flow rates and concentrations in upstream, point, and non-point sources. For instance, the concentrations of all the constituents in diffused sources (C_j^d) were changed simultaneously and three values were assumed when all other variables were held constant. They made 729 (3^6) runs in this step;

3)   Note results (flow rate and concentration of each constituent) at the control site for each simulation;

4)   Perform multiple regression analysis on the results for each constituent. (Many forms of regression expressions were tested. Of these the mass flow rate regression equation 3 was the best for predicting concentration of all constituents except dissolved oxygen. Regression equation 4 was best for dissolved oxygen);

5)   Assemble the S/O model using appropriate coefficients and computing the optimal solution.

6)   Simulate system response (concentrations of constituents at control site) to the optimal strategy using the QUAL2E model and compare results with those predicted by the S/O model; and

7)   Halt if S/O model prediction is acceptably close to that of the QUAL2E model, otherwise, return to (1) and repeat the steps.

By applying the above process for multiple scenarios, Ejaz (1994) was able to address a multiobjective problem and formulate a pareto optimum (Figure IV-4). Conflicting goals (subject to downstream water quality criteria), are to maximize the populations of humans and dairy cattle, while disposing of their treated wastewater to the stream. Human wastewater is treated by municipal facility and discharged to stream as a point source. Dairy wastewater is treated by overland flow and discharged as a nonpoint source.
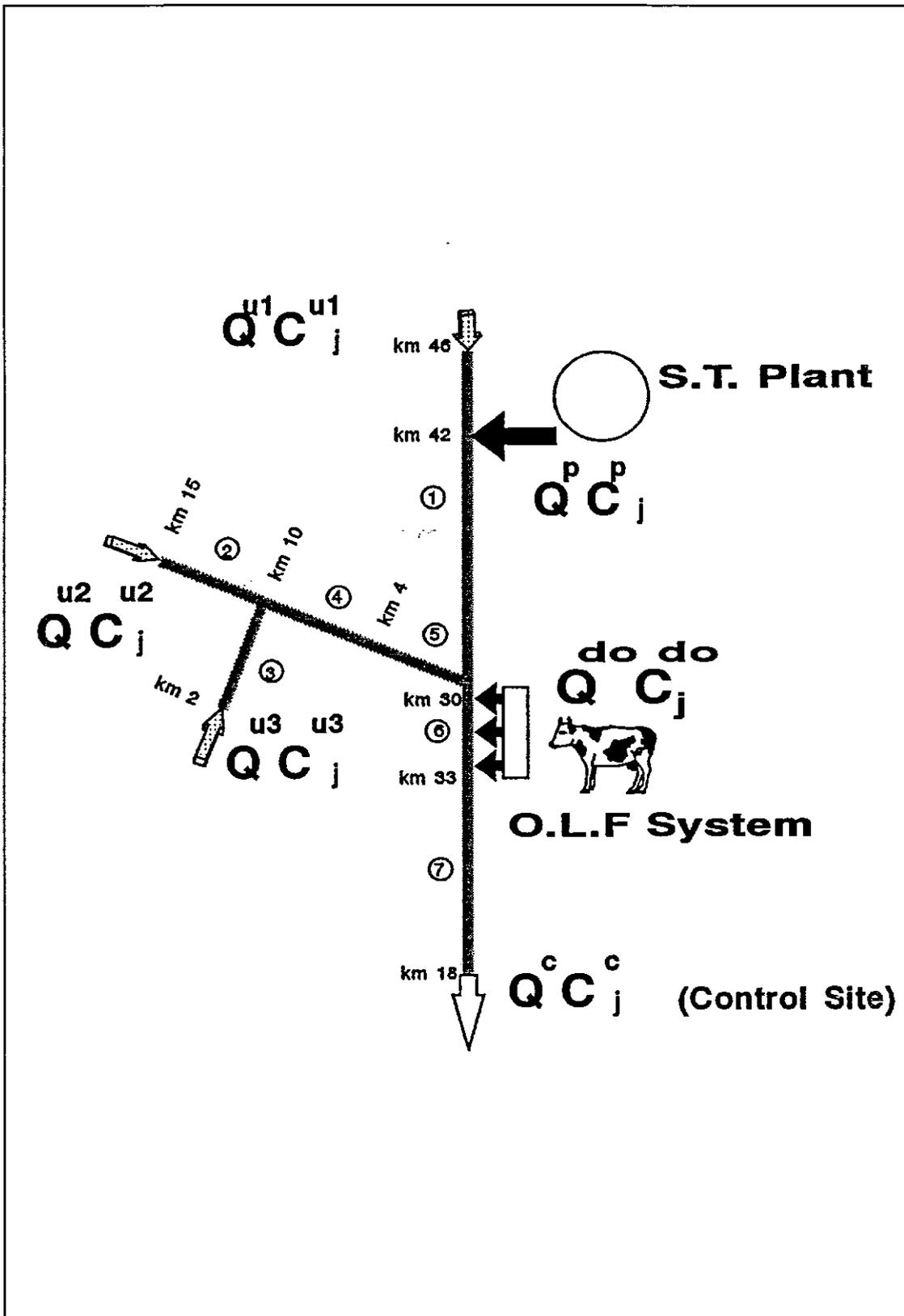
Figure IV-2 Maximizing contaminant loading to streams: study area (Ejaz, 1994)
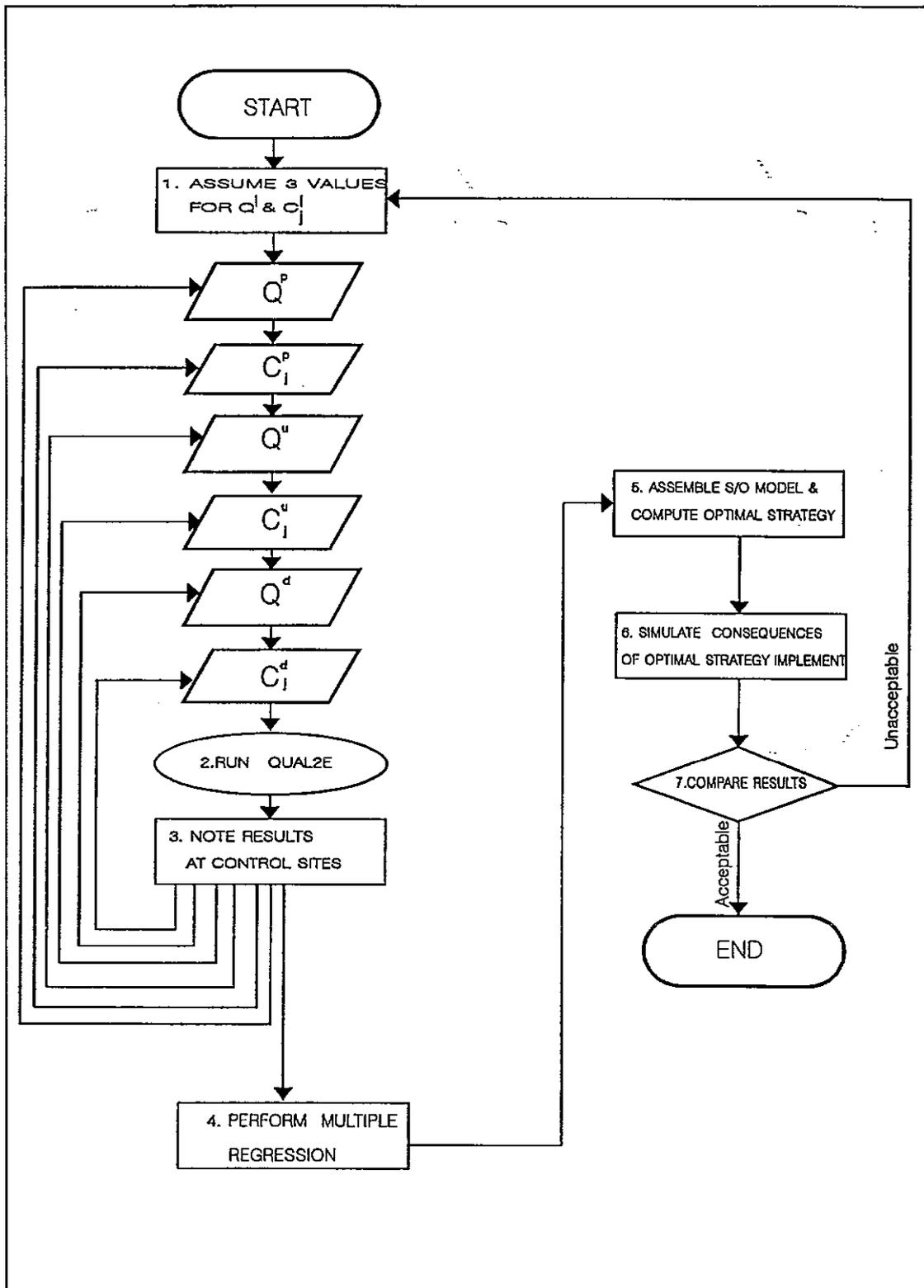
Figure IV-3 Developing regression expression for surface water concentration: flow chart (Ejaz and Peralta, 1994)
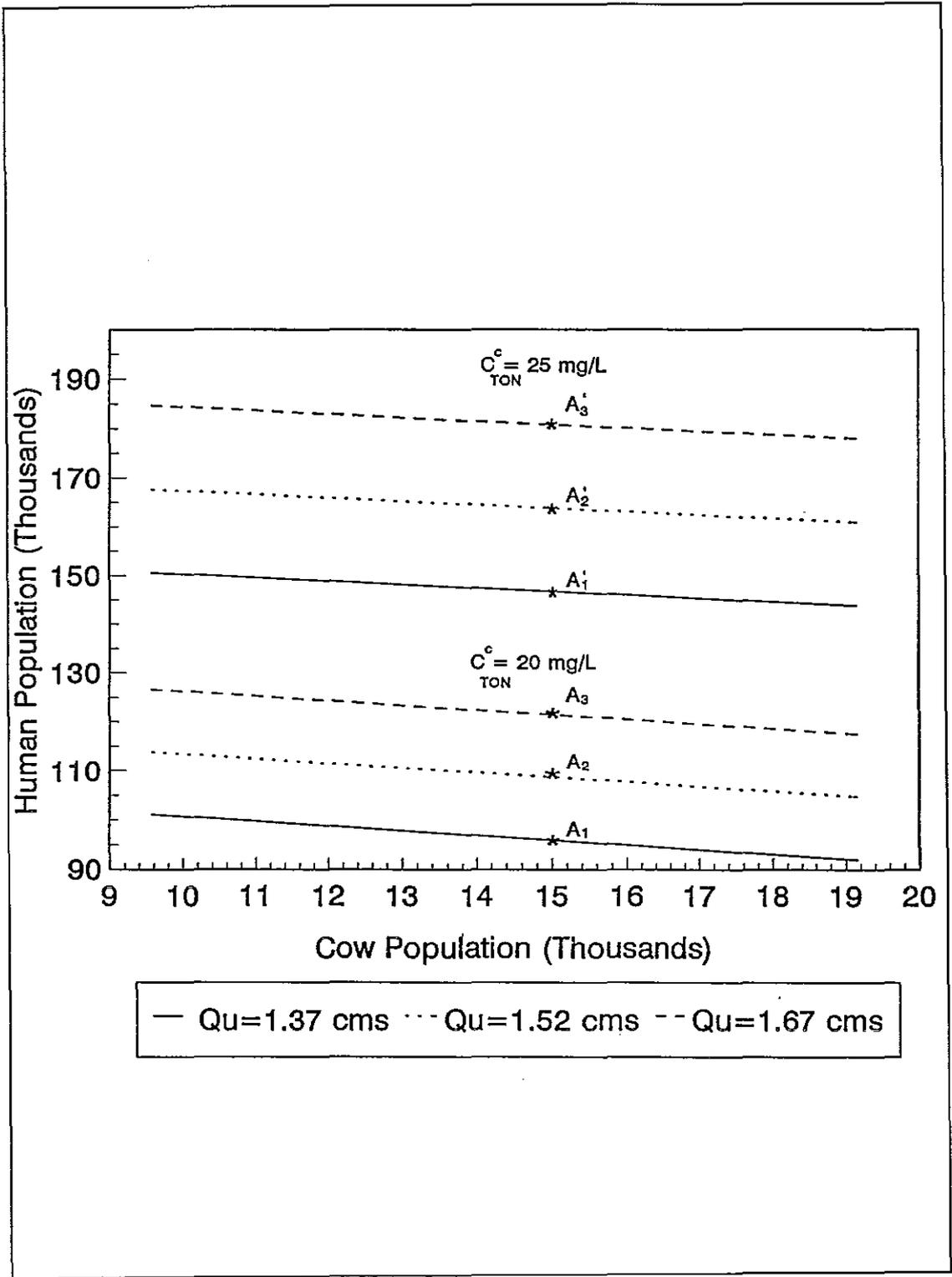
Figure IV-4 Pareto optima (human versus dairy cow populations) as functions of upstream inflow rate and upper bound on total nitrogen permitted at a stream control point (Ejaz, 1994)

IV.6. Simplified Expressions for Other Contaminant Related Processes

Probably, contaminant leaching beneath the root zone can also be described using a regression approach (current research is testing this hypothesis). Peralta et al (1994) demonstrate a S/O model that maximizes irrigated crop yield, subject to constraints on how much pesticide is permitted to reach an underlying ground water table. Musharrafieh et al (1994) demonstrate a goal-programming S/O model that determines optimal irrigation application rates subject to constraints on salt build-up within the root zone, or contaminant leaching. Daza (1994) demonstrates a S/O model for regional conjunctive use planning that includes furrow irrigation system design so as to prevent unacceptable deep percolation or surface water runoff.

V. Options of the Simulation/Optimization Module (S/O)

V.1. Introduction

The PROMOD S/O module can compute optimal water management strategies for a wide range of posed management problems (scenarios). As stated previously, a 'strategy' is a spatially and/or temporally, distributed set of values of groundwater pumping, surface water diversion, reservoir release, or water delivery to users. A management problem or scenario is defined by the objective function and the bounds and constraints that are selected. Changing coefficients or weights within these expressions changes the scenario.

In this chapter we discuss the objective functions and bounds and constraints that can be employed within the S/O module. We change the notation slightly from that used previously—replacing subscripts with arguments within parentheses. Subscripts were used in the chapter on functional relations to keep the equations as short as possible. However, in this chapter we add constraints that would require use of subscripts on subscripts.

We avoid this difficulty by using arguments instead of subscripts. For example, we use $q^m(\ddot{y},k)$ instead of $q^m_{\ddot{y},k}$. Another reason for using arguments now is because that is how the proposed PROMOD output will appear. DOS-based computers do not directly print superscripts or subscripts. DOS will print $q^m_{\ddot{y},k}$ as qmÿ,k. We prefer that it print qm(ÿ,k), and assume that we can easily interpret a superscript printed on the same line as the base variable. Therefore, we use $q^m(\ddot{y},k)$ here, which is not too dissimilar from the qm(ÿ,k) the printer will print.

Please bear in mind that when we show a state variable in this section, the value of that variable is computed within the S/O module using either simplified or detailed expression (Chapter IV or III, respectively). For example, when head at period k is bounded via a constraint equation, recall that it is represented in the model via a Chapter IV superposition expression.

Before proceeding, we should give perspective to how PROMOD will use the objective and constraint equation information presented. Refer to Figure I-1, a flow chart of PROMOD processes. Six data sets (DS a-f) are shown across the top of that figure. The results from step 1 are sufficient information to appropriately apply a simulation model to the study area. Step 2 utilizes the calibrated study area data, computes the system response to nonoptimal management, and computes system response to different sets of potential stimuli (DS b). Thus, step 2 requires as possible locations of potential stimulus (pumping, diversion, etc.) to develop the influence coefficients.

Step 3 requires as input knowledge of the stimuli locations (DS b), as well as all potential locations at which system response will need to be constrained (DS c). Step 3 computes influence coefficients and regression expressions linking the stimuli and response locations.

Step 4 requires input of DS b-d. Data set d identifies which objective function will be chosen, the weights with which decision variables are considered in the objective function, and which state variables will actually be considered in a particular optimization scenario. Thus, the actual optimization problem being solved is specified in DS d.

Step 5 is performed to analyze the consecuences of implementing a computed strategy under conditions than those initially assumed, or to analyze how changes in assumptions would change the optimal strategy that is computed. Actions can return from step 5 to step 2, and cycle. Once analysis is complete step 6 can be accomplished.

The subsequent discussion explains the options for posing a management scenario for which you wish to compute an optimal strategy. In the equations, cells are identified by the same index number that they would be identified by in data sets. DS b and c contain the information needed to cross reference an index number to a cell at a particular (row, column, layer). Different index numbers are used to identify cells, reaches, or groups thereof as location(s) of: potential pumping, potential diversion, aquifer head control, HGV (head difference, hydraulic gradient, groundwater velocity, or contaminant velocity), stream flow control, stream stage control, river-aquifer interflow control, contaminant mass flow rate, unit command areas, and other processes.

Selected names and index numbers for cells, cell pairs, reaches and groups for the constraint equations are summarized in Tables V-1 and V-2. These same names and indices should be used in discussing input and output file formats in a future PROMOD manual. These alphanumeric values are chosen because they can be printed out by most word procesors as well as DOS, and so can appear the same everywhere.

It is helpful to explain the rationale for some of the terminology in the equations. For example, superscripted M parameters refer to the number: (1) of cells or reaches of specific types, (2) cells or reaches in groups of specific types, or (3) groups of specific types. For the first two categories (which refer to cells or reaches), the superscript is in lower case. For the last category (which refers to groups), the superscript is in upper case.

A ^{G} superscript on a variable indicates that the term is the sum of that variable for a particular group.

	Decision Variables											
Variable Description	Pumping (cell) [1]	Diversion (reach)	ΣPumping (sum of cells) [2]	ΣDiversion (sum of reaches)	Σ(Pumping+Diversion) (sum of cells and reaches) [3]	Reservoir Release	Surface water flow to UCA	ΣSurface water to group of UCAs (sum of sw to UCAs)	Surface water flow to M&I user	ΣSurface water flow to group of M&I users (sum of sw to M&I users)	ΣGround water & surface water flow to group of UCAs (sum of gw + sw to group of UCAs)	ΣGround water & surface water flow to group of M&I users (sum of gw + sw for group of M&Is)
Symbol	p	d	p^G	d^G	pd^G	d	q_l^{ca}	q^{casG}	q^m	q^{msG}	q_l^{catG}	q^{mtG}
No. of cells or reaches	M^p	M^d				M^v	M^{ca}		M^m			
Index	â	ê				ê	(ê,é,ë),T		ÿ			
No. of groups			M^{pG}	M^{dG}	M^{pdG}	M^{vG}		M^{casG}		M^{msG}	M^{catG}	M^{mtG}
Group name and index			pg(à)	dg(è)	pdg(á) psg(á) dsg(á)	vg(æ)		casg(ê,é)		msg(âÿ)	catg(ä) catgg(ä) catsg(ä)	mtg(ý)
No. cells or reaches in group			M^{pg}(à)	M^{dg}(è)	M^{psg}(á) M^{dsg}(á)	M^{vg}(æ)		M^{casg}(ê,é)		M^{msg}(âÿ)	M^{catgg}(ä) M^{catsg}(ä)	M^{mtg}(ý)

[1]   g = extraction (-), d = diversion (+), reservoir release (-).

[2]   A pumping group pg(à) might include the same pumping cells as a group catgg(ä) or mtg(ý).

[3]   To properly constrain the sum of extraction(-) and diversion(+), pumpings are automatically subtracted from diversion. Injection is not normally included.

Table V-1. Selected indexing and numbers in sets related to decision variables. (enhanced from Peralta and Aly, 1993)

Variable Description	Aquifer Head (cell)	HGV (pair of cells)	River-Aquifer or Stream-Aquifer Interflow (cell or reach) [3]	ΣRiver-Aquifer or ΣStream-Aquifer Interflow (sum of cells or reaches) [3]	Stream Reach Outflow (reach) [4]	Stream or Reser-voir Stage (reach) [4]	Reser-voir Storage	Hydro-power	Mass flow rate	Stream Water Con-centra-tion	Groundwater Con-centra-tion	Concentration of water delivered to M&I user in stress period	Avg. Concentration of water delivered to M&I user in planning period	Concentration of water delivered to UCA in stress period	Avg. Concentration of water delivered to UCA in stress period	Total Crop yield	Subsurface Drainage Water (group of cells)
																State Variables	
Symbol	h	Ω	q^{ar}	q^{SR}	q^{r}	σ	ST	P	$\tilde{n}$	c	ww	c^{mi}	c^{miavg}	c^{ca}	c^{caavg}	Y	q^{bd}
No. of cells or reaches	M^{h}		M^{ar}		M^{r}	M^{r}	M^{vs}	M^{hp}	M^{mi}	M^{c}	M^{ww}	M^{m}	M^{m}	M^{ca}	M^{ca}	M^{cac}	M^{bd}
Index	$\grave{o}$		$\hat{\imath}$		$\hat{u}$	$\acute{u}$	$\hat{e}$	$\hat{e}$	$\ddot{u}$	$\hat{u}$	$\ddot{o}$	$\hat{y}$	$\hat{y}$	Υ	Υ	$(\hat{e},\acute{e},\hat{e}\hat{e})$	$(\hat{u},\acute{o},\ddot{o})$
No. of groups		M^{HGV}		M^{SRG}			M^{vsg}	1								M^{CACG}	
Group name and index		hgv(ð)		srg(î)			vsg(æs)	vg(æ)								cacg(î)	
No. cells or reaches in group		2		M^{srg}(î)			M^{vsg}(æs)	M^{vg}(æ)									

Table V-2. Selected indexing and numbers in sets related to selected state variables.

V.2. Objective Function Options

V.2.1. A simple objective function and its interpretation

PROMOD is capable of optimizing steady-state or transient problems having a wide range of objectives and constraints. For easy application, over 50 are canned and easily available to the user. Objective functions that are hard-coded are listed in a subsequent subsection.

The most basic objective function is linear. As is explained later, because groundwater extraction is negative, if C^p is positive, minimizing the value of Z is the same as maximizing groundwater pumping. The linear objective function for maximizing or minizing the sum of groundwater extraction and surface water diversion is of a general form. Either option can be selected. Unless stated otherwise, here we will use the minimize version here:

$$\min Z = \sum_{k=1}^{K} \left[\sum_{\hat{a}=1}^{M^p} C^p(\hat{a},k)\ p(\hat{a},k) + \sum_{\hat{e}=1}^{M^d} C^d(\hat{e},k)\ d(\hat{e},k) \right] \qquad \text{(V-1)}$$

where

Z	= objective function value;
K	= total number of stress periods within the optimization (planning) period;
$C^p(\hat{a},k)$	= cost or weighting coefficient for managed pumping in cell $\hat{a}$ during stress period k [\$ per L^3/T] or [dimensionless];
$C^d(\hat{e},k)$	= cost or weighting coefficient for managed diversion in cell $\hat{e}$ during stress period k [\$ per L^3/T] or [dimensionless];

The weighting coefficients provide flexibility to perform linear economic optimization or to convert a minimization effort to maximization. For example, if each C coefficient represents the present value of the cost of providing water, Equation V-1 would minimize the total present value of provided water.

It is helpful to discuss the relations between maximization, minimization, and the inherent sign of optimized variables (Table V-3). These are based on the fact that the process of minimizing the sum of negative variables is equivalent to maximizing the sum of the same variables if they are positive in sign.

For example, if you want to develop a pumping strategy that extracts as much groundwater from the aquifer as possible, you want to obtain a large absolute value for the sum of groundwater extractions. In this case, you will use a positive coefficient for groundwater extraction and choose to minimize the sum.

If you want to develop a pumping strategy that minimizes the total rates of extraction and injection needed to contain a contaminant plume, you will use a negative C^p for extraction and a positive C^p for injection.

If you wish to maximize the total rates of water delivered by extracting groundwater and diverting river water, you will use a positive C^p for pumping and a negative C^p for diversion. (See the eight-stress period conjunctive management example in the Applications section.)

Table V-3. Signs of weighting coefficients needed to achieve specified management goals (for objective functions which minimize). (Peralta and Aly, 1993).

	DECISION VARIABLES AND THEIR SIGN CONVENTIONS		
	Extraction, g or p (-)	Injection, b or p (+)	Diversion, d (+)
To obtain a large absolute value.	$C^p = (+)$	$C^p = (-)$	$C^d = (-)$
To obtain a small absolute value.	$C^p = (-)$	$C^p = (+)$	$C^d = (+)$

Thus, PROMOD can minimize or maximize as desired by the user. The model calculates optimal values for the decision variables shown above (groundwater extraction and injection and surface water diversion) while satisfying the other equations (constraints and bounds) discussed subsequently. As mentioned previously, those constraint equations addressing heads, flows or gradients utilize superposition and influence coefficients. Other constraints include regression, volume and mass balance equations.

Appendix B shows how you can address a multiobjective optimization problem. That representative multiobjective optimization problem is to simultaneously try to minimize the industrial pumping needed to control a contaminant plume while maximizing the municipal pumping needed for water supply.

V.2.2. PROMOD hard-coded objective functions

Below are listed objective functions that can be used by selecting their respective option identification number (options 2-49 are from draft revisions for the US/REMAX vs 2.7 user's manual; internal memo, A.H.Aly). For brevity, only a few of these are explained. The rest are analagous, but involve different decision or state variables, or sums thereof. Either maximization or minimization can be performed for any objective function.

1) Sum of groundwater pumping and diversion (See equation V-1 above.)
2) Sum of linear and quadratic terms of groundwater pumping and diversion. Generally, the goal is to maximize this sum. As described previously, to achieve this, weighting coefficients of the proper sign should be chosen.

$$Z = \sum_{k=1}^{K} \sum_{\hat{a}=1}^{M} [p \; C^{p1}(\hat{a},k) \; p(\hat{a},k) + C^{p2}(\hat{a},k) \; p(\hat{a},k) \; h^{1p}(\hat{a},k)]$$

$$+ \sum_{k=1}^{K} \sum_{\hat{e}=1}^{M^d} [\; C^{d1}(\hat{e},k) \; d(\hat{e},k) \; C^{d2}(\hat{e},k) \; d(\hat{e},k) \; h^{1d}(\hat{e},k)]$$

(V-2)

where

$C^{p1}(\hat{a},k), C^{p2}(\hat{a},k)$ = respectively, linear and quadratic cost or weighting coefficients for managed pumping [$ per L^3/T; $ per L^4/T] or [dimensionless];

$C^{d1}(\hat{e},k), C^{d2}(\hat{e},k)$ = respectively, linear and quadratic cost or weighting coefficient for managed diversion [$ per L^3/T; $ per L^4/T] or [dimensionless]; and

h^{1p}, h^{1d} = the head that needs to be overcome for the pumped or diverted (respectively) water to be used. For pumping, the head can be the total dynamic lift. For the diversion, it might be the head needed to push the diverted water to the user [L].

3) goal programming for the pumping values (sum of the absolute deviations). This objective function is the sum of all goal programming over-achievement and underachievement-variables for groundwater pumping. As is explained for objective function option 13, in goal programming, a target value of decision or state variable is used. The model appropriate for this objective function includes an equation linking target (desired) pumping rates and the rates computed by the s/o model. The model computes a pumping strategy that is as close to the target rates as possible, without violating any constraints or bounds. The objective function is the sum of the absolute values of the differences between the target pumping rates and the rates computed by the s/o model. An example goal programming objective function is presented for heads, below.

4) goal programming for the pumping values (square deviations). This objective function is the sum of the squared values of all differences between the target pumping rates and the rates computed by the s/o model. It attempts to minimize 'outriders'.

5) goal programming for the diversion values (absolute deviations)
6) goal programming for the diversion values (square deviations)

7) goal programming for the pumping values from a group of pumping cells (absolute deviations). This objective function attempts to assure that the target pumping rate for

a group (possibly a subgroup of all pumping rates being optimized) is achieved as closely as possible.

8) goal programming for the pumping values from a group of pumping cells (square deviations)

9) goal programming for the diversion values from a group of diversion cells (absolute deviations)

10) goal programming for the diversion values from a group of diversion cells (square deviations)

11) goal programming for the pumping and diversion values from a group of pumping+diversion (absolute deviations)

12) goal programming for the pumping and diversion values from a group of pumping+diversion (square deviations)

13) goal programming for the head values in the head control cells (absolute deviations). This permits one to attempt to achieve target heads at specified (control) locations to the extent possible, subject to other constraints. For example, this can be used to develop a sustained groundwater yield pumping strategy that will maintain target groundwater levels as much as possible (Yazdanian and Peralta, 1986).

$$Z = \sum_{k=1}^{n} \sum_{\hat{o}=1}^{M^h} [C^{+h}(\hat{o},k) \ h^+(\hat{o},k) + C^{-h}(\hat{o},k)h^-(\hat{o},k)] \tag{V-3}$$

where

$C^{+h}(\hat{o},k)$, $C^{-h}(\hat{o},k)$ = weights assigned to groundwater head over-achievement and under-achievement variables, respectively [dimensionless, or $\$L^{-1}$];

$h^+(\hat{o},k)$, $h^-(\hat{o},k)$ = groundwater head over-achievement and under-achievement, respectively [h]. Both must be positive, and only one can be nonzero at one stress period for a particular location.

Over- and under-achievement heads are defined as:

$$h(\hat{o},k) = h^+(\hat{o},k) + h^-(\hat{o},k) = h^t(\hat{o},k) \tag{V-4}$$

where
$h^t(\hat{o},k)$ = target head (i.e. the head we are trying to achieve)[L].

14) goal programming for the head values in the head control cells (square deviations)

15) goal programming for the gradient values in the HGV control pairs (absolute deviations)

16) goal programming for the gradient values in the HGV control pairs (square

deviations)

17) goal programming for the outflow values in the stream flow control cells (absolute deviations)
18) goal programming for the outflow values in the stream flow control cells (square deviations)

19) goal programming for the stage values in the stream stage control cells (absolute deviations)
20) goal programming for the stage values in the stream stage control cells (square deviations)

21) goal programming for the (river or stream/aquifer) interflow values in the interflow control cells (absolute deviations)
22) goal programming for the interflow values in the head control cells (square deviations)

23) goal programming for the interflow values in the groups of interflow control cells (absolute deviations)
24) goal programming for the interflow values in the groups of interflow control cells (square deviations)

25) goal programming for the nonlinear variables values (absolute deviations). This can be used to cause the model to attempt to achieve target groundwater or surface water concentrations. (Gharbi and Peralta, 1984).
26) goal programming for the nonlinear variables values (square deviations).

26) Maxmin objective function for individual pumping locations. This maximizes the smallest pumping rate among all of those considered within the objective function, subject to other constraints.
27) Maxmin objective function for individual diversion locations.
28) Maxmin objective function for group of pumping locations.
29) Maxmin objective function for group of diversion locations.
30) Maxmin objective function for group of pumping + diversion locations.
31) Maxmin objective function for head control locations.
32) Maxmin objective function for gradient control pairs.
33) Maxmin objective function for stream flow control locations.
34) Maxmin objective function for stream stage control locations.
35) Maxmin objective function for river (or stream)/aquifer interflow control locations.
36) Maxmin objective function for groups of river (or stream)/aquifer interflow control locations.
37) Maxmin objective function for nonlinear variables control locations.
38) Minmax objective function for individual pumping locations.
39) Minmax objective function for individual diversion locations.

40) Minmax objective function for group of pumping locations.
41) Minmax objective function for group of diversion locations.
42) Minmax objective function for group of pumping+diversion locations.
43) Minmax objective function for head control locations.
44) Minmax objective function for gradient control pairs.
45) Minmax objective function for stream flow control locations.
46) Minmax objective function for stream stage control locations.
47) Minmax objective function for river (or stream)/aquifer interflow control locations.
48) Minmax objective function for groups of river (or stream)/aquifer interflow control locations.
49) Minmax objective function for nonlinear variables at control locations.

50) Integer programming objective function. This permits one to use both an on/off switch and a rate for selected decision variables. For example, assigning an integer variable (and its weighting or cost coefficient) to a pumping well means that the user can consider both the cost of well installation and the cost of pumping within the objective function:

$$Z = \sum_{k=1}^{K} \sum_{\hat{a}=1}^{M^P} [\ C^P(\hat{a},k)\ p(\hat{a},k)\ +\ C^{ip}(\hat{a})\ I^P(\hat{a})]$$

$$+ \sum_{k=1}^{K} \sum_{\hat{e}=1}^{M^d} [\ C^d(\hat{e},k)\ d(\hat{e},k)\ \ C^{id}(\hat{e})\ I^d(\hat{e})\ ]$$

(V-5)

where
$C^{ip}(\hat{a})$, $C^{id}(\hat{e})$ = respectively, cost of installing a well or diversion structure at locations $\hat{a}$ and $\hat{e}$, respectively [$]; and
$I^P(\hat{a})$, $I^P(\hat{e})$ = respectively, integer variables indicating a well or diversion structure.

51) Sum of mass flow rates being injected into the aquifer or discharged to streams (without exceeding specified downstream limits on contaminant concentrations).

52) Mass of contaminant removed from an aquifer:

$$\sum_{\hat{a}=1}^{M^P} \sum_{k=1}^{K} C^P\ p(\hat{a},t)\ ww(\hat{a},t)$$

(V-6)

53) Sum of surface water and/or groundwater delivered to the cities and unit command areas. Of course, the weighting coefficient assigned to each flow can serve to emphasize or deemphasize that flow. For example, putting a zero weight before one flow means that the s/o model does not include that flow with those that it is maximizing.

54) Crop production and crop production benefits. That objective function includes crop yield, y, which can be defined via any of several expressions of Chapter III. Multiplication of the yield by a weight permits the gross return of the crop to be optimized:

$$\text{Weighted Crop Yield} = \sum_{(\Upsilon \,\in\, cacg(1))}^{M^{cacG}} C^{cr} \, y(\Upsilon) \qquad\qquad \text{(V-7)}$$

where
M^{cacG} = number of cells in all agricultural command areas (UCAs);
cacg(1) = set of all cells belonging in UCAs;
Υ = index referring to a particular UCA. This is an alternative notation to $(\hat{e}, \acute{e}, \ddot{e})$;
$C^{cr}(\Upsilon)$ = weight assigned to UCA Υ. This can be the economic benefit per unit of crop yield. It can also be a cost per unit crop yield, depending on user intent [M^{-1}].

55) Multiobjective optimization (E-constraint method) (Cohon and Marks, 1975). This permits the user to select one of the above objective functions as the principal objective, and to select up to 3 other objective functions to be used as constraints. This is an application of the E-constraint method of multiobjective optimization. (See Appendix B for a brief discussion of the E-constraint method).

56) Multiobjective optimization (Weighting method) (Major, 1977; Loucks et al., 1981). This permits the user to formulate a composite objective function equaling the sum of up to 5 other objective functions. (See Appendix B for a brief discussion of the weighting method.)

One application is to maximize the positive valued sum of groundwater pumping and the negative of groundwater contaminant concentration over-achievement variables. That can be used to maximize regional sustained groundwater yield planning, while preventing concentrations for exceeding target values too much. It can be preferable to include the concentrations within the objective function as a sort of 'soft constraint' rather than restricting concentrations with a firm bound. The soft constraint approach permits the solution to be feasible while a hard bound might not. Another application permits one to maximize the net economic return of implementing a particular management strategy. In this example one would sum one Objective Function (2), and two Objective Functions (54). Use Objective Function (2) to determine the water related costs of a management strategy. Use coefficients in one implementation of Objective Function 54 so as to reflect only the fixed costs of production in all UCAs (ignoring yield entirely). Use coefficients in another implementation of Objective Function 54 to reflect the gross return of the crop. The sum of all three objective functions is the net economic return. Cost coefficients can be selected to reflect the present value of this return for the entire planning horizon.

V.3. Overview of Possible Constraints and Bounds and PROMOD Processing

Constraints are equations defining what decision variable values or system responses to those values are acceptable to management and nature. Upper or lower limits on individual decision or state variables are also termed bounds. The most important constraints are listed below. Detailed formulation of the constraints are presented in subsequent sections.

- ■ decision variables
    - ■ groundwater pumping (withdrawal or recharge) rates
    - ■ surface water diversion rates
    - ■ reservoir release rates
    - ■ groundwater pumped for M&I use
    - ■ groundwater pumped for UCA use
    - ■ surface water delivered for M&I use
    - ■ surface water delivered to UCA
- ■ sums of decision variables, and relations between decision variables and their sums
    - ■ group sums of groundwater extraction rates, diversion rates, extraction plus diversion
    - ■ relative change in decision variable values with time (monotonicity)
    - ■ relation between total extraction and total injection.
    - ■ total surface water delivered for M&I use
    - ■ total surface water delivered for UCA use
    - ■ total groundwater + surface water delivered for M&I use
    - ■ total groundwater + surface water delivered for UCA use
    - ■ reservoir release
- ■ aquifer state variables and conditions
    - ■ potentiometric surface elevation
    - ■ potentiometric surface head difference, hydraulic gradient, groundwater velocity or contaminant transport velocity between a pair of locations (any two points located in any two layers) (These are termed HGV constraints.)
    - ■ groundwater contaminant concentration, or nonlinear state variables
- ■ river, reservoir or stream state variables[1]
    - ■ river-aquifer interflow
    - ■ sum of river-aquifer, stream-aquifer, and/or reservoir-aquifer interflows (for specified groups of cells)
    - ■ stream flow rate
    - ■ stream or reservoir stage
    - ■ reservoir storage
    - ■ surface water contaminant mass flow rate or concentration

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[1] The term 'river' is used when MODFLOW's river package is utilized to develop influence coefficients. The term 'stream' is used when the STR package or other code is utilized to develop influence coefficients. Diversion can be considered only when the STR package is used.

- other variables interesting to management
  - hydropower
  - proportion of canal section inflow that must be diverted to a smaller canal
  - crop yield
  - average concentration of water delivered to M&I or UCA users
  - concentration of water leaving M&I or UCA users

V.4. Bounds on Individual Decision Variables

These bounds are upper and lower limits on variables about which managers commonly must make decisions. Such limits can be expressed by superscripting the variable with L or U to denote lower or upper limits respectively. Numerical values of the bounds can vary with cell, group and time. (Bounds on pumping and diversion are from Peralta and Aly 1993)

Upper limits might be placed on groundwater extraction for several reasons:
- it might be impractical to export to another location any groundwater that cannot be used in the cell from which it is pumped;
- law might prohibit pumping more than a specified amount or rate, or more than can be beneficially utilized; and
- it might be impossible to install new wells, resulting in existing well capacity serving as an upper bound.

$$p^L(\hat{a},k) \leq p(\hat{a},k) \leq p^U(\hat{a},k) \quad \text{for } \hat{a} = 1..M^P, k = 1..K \qquad \textbf{(V-8)}$$

When formulating the above bounds, note that groundwater extraction is negative in sign, groundwater recharge and river water diversion are positive. Thus, sample lower and upper bounds on groundwater extraction might be -10 and 0, respectively. Lower and upper bounds on injection at a cell might be 0 and 15, respectively.

Limits on river water diversion or reservoir release can be imposed as:

$$d^L(\hat{e},k) \leq d(\hat{e},k) \leq d^U(\hat{e},k) \quad \text{for } \hat{e} = 1..M^d, k = 1..K \qquad \textbf{(V-9)}$$

Bounds on diversion might be 0 and 1000, respectively.

Bounds can be imposed on surface water delivered to individual M&I and UCA users:

$$q^{mL}(\ddot{y},k) \leq q^m(\ddot{y},k) \leq q^{mU}(\ddot{y},k) \quad \text{for } \ddot{y} = 1..M^m, k = 1..K \qquad \textbf{(V-10)}$$

$$q^{caL}(\Upsilon,k) \leq q^{ca}(\Upsilon,k) \leq q^{caU}(\Upsilon,k) \quad \text{for } \Upsilon = 1..M^{ca}, k = 1..K \qquad \textbf{(V-11)}$$

Bounds can be imposed on the rate of groundwater plus surface water delivered to individual M&I and UCA users during a stress period. A limit might reflect the crop water need plus the water expected to be lost due to inefficiencies.

$$q^{mtL}(\ddot{y},k) \leq q^{mt}(\ddot{y},k) \leq q^{mtU}(\ddot{y},k) \quad \text{for } \ddot{y} = 1..M^m, \, k = 1..K \tag{V-12}$$

$$q^{catL}(\Upsilon,k) \leq q^{cat}(\Upsilon,k) \leq q^{catU}(\Upsilon,k) \quad \text{for } \Upsilon = 1..M^{ca}, \, k = 1..K \tag{V-13}$$

Bounds can be imposed on the total water volume delivered to individual M&I and UCA users during the entire planning period:

$$V^{mtoL}(\ddot{y},k) \leq V^{mto}(\ddot{y},k) \leq V^{mtoU}(\ddot{y},k) \quad \text{for } \ddot{y} = 1..M^m, \, k = 1..K \tag{V-14}$$

$$V^{catoL}(\Upsilon,k) \leq V^{cato}(\Upsilon,k) \leq V^{catoU}(\Upsilon,k) \quad \text{for } \Upsilon = 1..M^{ca}, \, k = 1..K \tag{V-15}$$

V.5. Constraints on Sums of Decision Variables, Relations between Decision Variables, and Relations between Sums of Decision Variables

Lower and upper bounds can be placed on the sums of pumping, diversion or pumping plus diversion in specified groups of cells, in each time step. If such a bound represents the minimum total rate of water that must be provided, it might be termed a demand constraint (and be based on current or historic water demand). If a bound represents the maximum total rate of water that can be provided, it might be termed a capacity constraint (and be based upon the maximum water that can feasibly be used, conveyed or distributed).

$$p^{GL}(\grave{a},k) \le p^{G}(\grave{a},k) = \left[\sum_{\hat{a} \in pg(\grave{a})} p(\hat{a},k) \right] \le p^{GU}(\grave{a},k) \text{ for } \grave{a}=1..M^{PG}, k=1..K \qquad (V-16)$$

$$d^{GL}(\grave{e},k) \le d^{G}(\grave{e},k) = \left[\sum_{\hat{e} \in dg(\grave{e})} d(\hat{e},k) \right] \le d^{GU}(\grave{e},k) \text{ for } \grave{e} = 1..M^{DG}, k=1..K \qquad (V-17)$$

$$pd^{GL}(\acute{a},k) \le pd^{G}(\acute{a},k) = \left[\sum_{\hat{e} \in dsg(\acute{a})} d(\hat{e},k) - \sum_{\hat{a} \in psg(\acute{a})} p(\hat{a},k) \right] \le pd^{GU}(\acute{a},k)$$

$$\text{for } \acute{a} = 1..MPDG, \ k = 1..K \qquad (V-18)$$

where,

$p^{G}(\grave{a},k)$	= sum of pumping in pumping group à in stress period k, $[L^3/T]$;
$pg(\grave{a})$	= set identifying each cell, $pc(\hat{a})$, belonging to pumping group à. There are $M^{pg}(\grave{a})$ such cells;
M^{PG}	= the number of groups of pumping cells considered. A group should have either extraction or injection cells in it, but not both;
$d^{G}(\grave{e},k)$	= sum of diversion in diversion group è in stress period k, $[L^3/T]$. There are $M^{dg}(\grave{e})$ such cells;
$dg(\grave{e})$	= set identifying each cell, $dc(\grave{e})$, belonging to diversion group è;
M^{DG}	= the number of groups of diversion reaches considered
$pd^{G}(\acute{a},k)$	= sum of pumping and diversion in pumping-diversion group á in stress period k, $[L^3/T]$. This is the sum of pumping and diversion in groups $psg(\acute{a})$ and $dsg(\acute{a})$, respectively, $[L^3/T]$;
$dsg(\acute{a})$	= set identifying each diversion cell, $dc(\hat{a})$, belonging to pumping-diversion group $pdg(\acute{a})$. There are $M^{dsg}(\acute{a})$ such reaches;
$M^{dsg}(\acute{a})$	= number of diversion reaches in pumping-diversion group $pdg(\acute{a})$.
$psg(\acute{a})$	= set identifying each pumping cell, $pc(\hat{a})$, belonging to pumping-diversion group $pdg(\acute{a})$. There are $M^{psg}(\acute{a})$ such cells;

M^{PDG} = number of pumping-diversion groups considered;

pdg(á) = set including all pumping cells of psg(á) and all diversion reaches of dsg(á).

When considering Equation V-16, remember that groundwater extraction is a negative quantity (in keeping with MODFLOW convention). Thus, lower and upper bounds of -4,000 and -1,000, respectively, might represent capacity and demand constraints.

When considering Equation V-17, realize that diversion is a positive value to be in harmony with STR convention. You would not usually include injection cells in a combined pumping-diversion group such as is shown in Equation V-18. There, the effect of subtracting pumping extraction (-) is to sum diversion and extraction.

Long term planners and water users sometimes wish to assure that future pumping does not change erratically with time. In other words, that legally permitted pumping does not increase in one stress period (consisting of several years) and decrease in the next period. Thus, they might wish to assure that pumping is never less in one period than in a previous period. This goal can be achieved through monotonicity constraints, applicable to pumping or diversion. Depending on user preference, pumping and/or diversion can be forced to monotonically increase or decrease with stress period. Alternatively, pumping or diversion can be permitted to change freely with stress period (Peralta and Aly, 1993).

$$p(\hat{a}, k-1) \leq p(\hat{a}, k) \qquad \text{for } k = 2..K \qquad \qquad \text{(V-19)}$$

OR

$$p(\hat{a}, k) \text{ is not monotonically restricted for } k = 1..K) \qquad \text{(V-20)}$$

OR

$$p(\hat{a}, k-1) \geq p(\hat{a}, k) \qquad \text{for } k = 2..K \qquad \qquad \text{(V-21)}$$

AND/OR

$$d(\hat{e}, k-1) \leq d(\hat{e}, k) \qquad \text{for } k = 2..K \qquad \qquad \text{(V-22)}$$

OR

$$d(\hat{e}, k) \text{ is not monotonically restricted for } k = 1..K \qquad \text{(V-23)}$$

OR

$$d(\hat{e},k-1) \geq d(\hat{e},k) \qquad \text{for } k = 2..K \tag{V-24}$$

The equations below can be used to control the ratio between total groundwater withdrawal and total artificial recharge by pumping during stress period k. You can select none or only one of the four options. The first insures that total extraction equals total injection. The second insures that total extraction is not less than total injection. The third insures that total injection is not less than total extraction (since extraction is negative in size and injection is positive, their sum will equal zero if using this option). The last option is to not impose any such constraint. If one of these four equations is utilized, it will be effective for each stress period. You do not need to specify any groups to use the below expression. If this constraint option is selected, PROMOD automatically considers all groundwater pumping cells.

$$\left[\sum_{\hat{a}=1}^{M^P} p(\hat{a},k) = 0 \right] \qquad \text{for } k = 1..K \tag{V-25}$$

OR

$$\left[\sum_{\hat{a}=1}^{M^P} p(\hat{a},k) \leq 0 \right] \qquad \text{for } k = 1..K \tag{V-26}$$

OR

$$\left[\sum_{\hat{a}=1}^{M^P} p(\hat{a},k) \geq 0 \right] \qquad \text{for } k = 1..K \tag{V-27}$$

OR

$$\sum_{\hat{a}=1}^{M^P} p(\hat{a},k) \quad \text{not restricted} \qquad \text{for } k = 1..K \tag{V-28}$$

V.6. Bounds on Water Delivered to Groups of Users (UCAs and M&I Users).

Lower and upper bounds can be placed on how much total surface water and the sum of surface water and groundwater is delivered to groups of M&I or UCA users. Bounds on groundwater pumped from a specified group of locations was specified previously (p^G). As mentioned for sums of pumping and diversion rates, these bounds can represent demand or capacity constraints.

Bounds on total surface water delivered to groups of M&I users are:

$$q^{msGL}(\ddot{Y},k) \leq q^{msG}(\ddot{Y},k) = \left[\sum_{\ddot{y} \, \in \, msg(\ddot{Y})} q^{mt}(\ddot{y},k) \right] \leq q^{msGU}(\ddot{Y},k) \text{ for } M^{MSG} \text{ groups, } k=1..K \qquad (V-29)$$

where,

$q^{msG}(\ddot{Y},k)$ = sum of surface water delivered to M&I group $\ddot{Y}$ in stress period k, [L^3/T];

$msg(\ddot{Y})$ = set identifying each surface flow providing water to M&I group $\ddot{Y}$. There are $M^{msg}(\ddot{Y})$ such flows; and

M^{MSG} = the number of groups of M&I users considered.

Bounds on total surface water delivered to groups of UCAs are:

$$q^{casGL}(\acute{e},k) \leq q^{casG}(\acute{e},k) = \left[\sum_{\Upsilon \, \in \, casg(\acute{e})} q^{ca}(\Upsilon,k) \right] \leq q^{casGU}(\acute{e},k) \text{ for } M^{CASG} \text{ groups, } k=1..K \qquad (V-30)$$

where

$q^{casG}(\acute{e},k)$ = sum of surface waters delivered to UCA group $\acute{e}$ in stress period k, [L^3/T]. There are $M^{casg}(\grave{e})$ such flows within that group;

$casG(\acute{e})$ = set identifying all q^{ca} flows within UCA group $\acute{e}$; and

M^{CASG} = the number of groups of UCA surface water inflows considered.

Total flowrate of water delivered to different groups of M&I users is bounded as:

$$q^{mtGL}(\acute{y},k) \leq q^{mtG}(\acute{y},k) = \left[\sum_{\ddot{y} \, \in \, mtsg(\acute{y})} q^{m}(\ddot{y},k) + \sum_{\hat{a} \, \in \, mtgg(\acute{y})} p(\hat{a},k) \right] \leq q^{mtGU}(\acute{y},k) \qquad (V-31)$$

for M^{MTG} groups of municipal/industrial users ,k=1..K

where

$q^{mtG}(\acute{y},k)$ = sum of groundwater and surface waters delivered to M&I group $\acute{y}$ in stress period k, [L^3/T]. This is the sum of groundwater pumping and q^m in groups $mtgg(\acute{y})$ and $mtsg(\acute{y})$, respectively, [L^3/T]. Note that group $mtgg(\acute{y})$ is

	equivalent to one group pg(à);
mtsg(ŷ)	= subset (subgroup) identifying each q^m providing any surface water to M&I group mtg(ŷ). There are $M^{mtsg}(ŷ)$ such flows;
$M^{mtsg}(ŷ)$	= number of surface flows (q^m) providing water to M&I users in M&I group mtsg(ŷ);
mtgg(ŷ)	= subset (subgroup) identifying each pumping cell, pc(â), providing groundwater to M&I group mtg(ŷ). There are $M^{mtgg}(ŷ)$ such cells;
$M^{mtgg}(ŷ)$	= number of pumping cells providing groundwater to M&I group mtg(ŷ), which is the same number providing groundwater to M&I subroup mtgg(ŷ);
$M^{MTG}(ŷ)$	= number of M&I groups to which total water provided in any stress period is bounded; and
mtg(ŷ)	= set including all pumping cells of mtgg(ŷ) and all surface flows of mtsg(ŷ).

Total flowrate of water delivered to different groups of UCAs is bounded as:

$$q^{catGL}(ä,k) \leq q^{catG}(ä,k) = \left[\sum_{\Upsilon \in catsg(ä)} q^{ca}(\Upsilon,k) + \sum_{â \in catgg(ä)} p(â,k) \right] \leq q^{catGU}(ä,k) \qquad \text{(V-32)}$$

for M^{CATG} groups of UCAs, k=1..K

where

$q^{catG}(ä,k)$	= sum of groundwater and surface waters delivered to UCA group ä in stress period k, $[L^3/T]$. This is the sum of groundwater pumping and q^{ca} in groups catgg(ä) and catsg(ä), respectively, $[L^3/T]$. Note that group catgg(ä) is equivalent to one group pg(à);
catsg(ä)	= subset (subgroup) identifying each q^{ca} providing any surface water to UCA group catg(ä). There are $M^{catsg}(ä)$ such flows;
$M^{catsg}(ä)$	= number of surface flows (q^{ca}) providing water to UCAs in UCA group catsg(ä);
catgg(ä)	= subset (subgroup) identifying each pumping cell, pc(â), providing groundwater to UCA group catg(ä). There are $M^{catgg}(ä)$ such cells;
$M^{catgg}(ä)$	= number of pumping cells providing groundwater to UCA group catg(ä), which is the same number providing groundwater to UCA subroup catgg(ä);
$M^{CATG}(ä)$	= number of UCA groups to which total water provided in any stress period is bounded; and
catg(ä)	= set including all pumping cells of catgg(ä) and all surface flows of catsg(ä).

V.7. Bounds on Aquifer State Variables

These constraints establish limits on the maximum or minimum aquifer potentiometric heads that are allowed or desired at control points:

$$h^L(\hat{o},k) \leq h(\hat{o},k) \leq h^U(\hat{o},k) \quad \text{for } \hat{o} = 1..M^h, k = 1..K \tag{V-33}$$

where
$h(\hat{o},k) =$ groundwater potentiometric surface elevation at head control cell $\hat{o}$ by the end of stress period k [L]. This equals the nonoptimal (unmanaged) head $h^{non}(\hat{o},k)$ minus the drawdown resulting from the optimal pumping strategy by the end of the time step.

The following constraints limit the head difference, gradient, seepage velocity, or contaminant velocity that can occur between two control locations. It is positive if head decreases from a point 1 to a point 2 in the same or different layers. All four types of constraints can be represented by:

$$\Omega^L(\grave{o},k) \leq \Omega(\grave{o},k) \leq \Omega^U(\grave{o},k) \quad \text{for } \grave{o} = 1..M^{HGV}, k = 1..K \tag{V-34}$$

$$\Omega(\grave{o},k) = \left[h(\hat{o}_{\grave{o},1},k) - h(\hat{o}_{\grave{o},2},k) \right] / C^{HGV}(\grave{o}) \tag{V-35}$$

where

$h(\hat{o}_{\grave{o},1},k)$	= potentiometric surface head at point 1 (some cell $\hat{o}$) of HGV pair $\grave{o}$ at end of period k, [L];
$h(\hat{o}_{\grave{o},2},k)$	= potentiometric surface head at point 2 (a second cell $\hat{o}$) of HGV pair $\grave{o}$ at end of period k, [L];
$C^{HGV}(\grave{o})$	= 1, to control head difference;
	= $L^{\grave{o}}$, to control hydraulic gradient;
	= $(L^{\grave{o}} \theta) / J$, to control seepage velocity;
	= $(L^{\grave{o}} \theta R_f) / J$, to control contaminant velocity;
$L^{\grave{o}}$	= distance between pair of control locations, $\hat{o}_{\grave{o},1}$ and $\hat{o}_{\grave{o},2}$ [L];
J	= average hydraulic conductivity between control pair locations [L/T];

Any of the four definitions for $C^{HGV}(\grave{o})$ can be used to control water or contaminant movement between the two points comprising control pair $\grave{o}$. For example, below are four equivalent sets of bounds. To develop these, assume that locations $\hat{o}_{\grave{o},1}$ and $\hat{o}_{\grave{o},2}$ are 10 m apart, $\theta = 0.1$, $J = 10$ m/day, and $R_f = 1.25$. Naturally, you would only use one definition of $C^{HGV}(\grave{o})$ for a particular $\grave{o}$.

$$0.01 \ \le \ \text{potentiometric head difference} \ \le \ 1000 \qquad \textbf{(V-36)}$$

$$0.001 \ \le \ \text{hydraulic gradient} \ \le \ 100 \qquad \textbf{(V-37)}$$

$$0.1 \ \le \ \text{seepage velocity} \ \le \ 10,000 \qquad \textbf{(V-38)}$$

$$0.08 \ \le \ \text{contaminant velocity} \ \le \ 8,000 \qquad \textbf{(V-39)}$$

The following can be used to restrict groundwater contaminant concentrations, or state variables described by polynomial, exponential or logarithmic expression:

$$ww^L(\delta,k) \ \le \ ww(\delta,k) \ \le \ ww^U(\delta,k) \qquad \text{for } \delta = 1..M^\delta, \ k = 1..K \qquad \textbf{(V-40)}$$

V.8. Bounds on River, Stream and Reservoir State Variables and Conditions

The types of constraints that can be imposed on river- or stream-related flows and conditions depends on what data packages and simulation modules are used when simulating to compute influence coefficients. For example, either (but not both) river-aquifer or stream-aquifer interflow (r/ai and s/ai, respectively) can be constrained for user-specified cells or groups of cells:

$$q^{srL}(\hat{\imath},k) \leq q^{sr}(\hat{\imath},k) \leq q^{srU}(\hat{\imath},k) \quad \text{for } \hat{\imath} = 1..M^{sr}, \, k = 1..K \tag{V-41}$$

$$q^{SRL}(\grave{\imath},k) \leq q^{SR}(\grave{\imath},k) = \left[\sum_{\hat{\imath} \, \in \, rg(\grave{\imath})} q^{sr}(\hat{\imath},k) \right] \leq q^{SRU}(\grave{\imath},k) \quad \text{for } \grave{\imath} = 1...M^{SRG}, k = 1..K \tag{V-42}$$

where

$q^{sr}(\grave{\imath},k)$	= rate of r/ai or s/ai at cell ì by end of stress period k (negative for flow from aquifer to stream or river) $[L^3/T]$;
M^{sr}	= number of cells at which r/ai or s/ai can be constrained;
$q^{SR}(\grave{\imath},k)$	= net r/ai or s/ai in grouping ì and time k $[L^3/T]$;
$srg(\grave{\imath})$	= set identifying all r/ai or s/ai interflow cells, î , belonging to grouping ì. There are $M^{rg}(\grave{\imath})$ such cells;
M^{SRG}	= total number of groups of stream or river cells at which total r/ai or s/ai can be constrained.

If the upper bound on r/ai or s/ai is zero and the lower bound is a negative number, we are trying to force the aquifer to provide flow to the surface water body. This might be a tight bound if you are trying to maximize pumping from the aquifer.

Stream flow can be constrained at specific cells.

$$q^{sL}(\hat{u},k) \leq q^{s}(\hat{u},k) \leq q^{sU}(\hat{u},k) \quad \text{for } \hat{u} = 1..M^{s}, \, k = 1..K \tag{V-43}$$

where

M^{s} = number of cells at which stream flow can be constrained.

Bounds on streamflow should not be negative. A positive flow, q^{s}, denotes water flowing downstream.

Stream and reservoir stage are bounded using:

$$\sigma^{L}(\acute{u},k) \leq \sigma(\acute{u},k) \leq \sigma^{U}(\acute{u},k) \quad \text{for } \acute{u} = 1..M^{\sigma}, \, k = 1..K \tag{V-44}$$

where

M^{σ} = number of cells at which stream or reservoir stage can be constrained.

The stream stage constraint should be used only with caution and generally only for a range of stages at which the reach stage-discharge relation is nearly linear.

Reservoir storage is constrained using:

$$ST^L(\hat{e},k) \leq ST(\hat{e},k) \leq ST^U(\hat{e},k) \quad \text{for } \hat{e} = 1 \ M^{vsg} , \ k = 1..K \tag{V-45}$$

where

M^{vsg} = number of reservoir reaches in a particular grouping (there might be more than one reach in one reservoir).

Bounds can be imposed on what proportion of water entering a canal section is diverted to a smaller canal:

$$v^{2sL}(\hat{e},\acute{e},1,k) \leq v^{2s}(\hat{e},\acute{e},1,k) \leq v^{2sU}(\hat{e},\acute{e},1,k) \tag{V-46}$$

$$v^{caL}(\hat{e},\acute{e},\ddot{e},k) \leq v^{ca}(\hat{e},\acute{e},\ddot{e},k) \leq v^{caU}(\hat{e},\acute{e},\ddot{e},k) \tag{V-47}$$

Bounds on surface water mass flow rate and concentration can be bounded using:

$$\tilde{n}^L(\ddot{u},k) \leq \tilde{n}(\ddot{u},k) \leq \tilde{n}^U(\ddot{u},k) \quad \text{for } \ddot{u} = 1..M^{mf}, \ k = 1..K \tag{V-48}$$

$$c^L(\ddot{u},k) \leq c(\ddot{u},k) \leq c^U(\ddot{u},k) \quad \text{for } \ddot{u} = 1..M^c, \ k = 1..K \tag{V-49}$$

where

M^{mf} = the number of reaches at which mass flow rate is constrained.
M^c = the number of reaches at which streamflow concentration is constrained.

V.9. Other Types of Bounds and Constraints

The quality of the groundwater and surface water delivered to all M&I and UCA users in period k after mixing can be bounded via:

$$c^{mtL}(\ddot{y},k) \leq c^{mt}(\ddot{y},k) \leq c^{mtU}(\ddot{y},k) \quad \text{for } \ddot{y} = 1..M^m, \ k = 1..K \tag{V-50}$$

$$c^{catL}(\Upsilon,k) \leq c^{cat}(\Upsilon,k) \leq c^{catU}(\Upsilon,k) \quad \text{for } \Upsilon = 1..M^{ca}, \ k = 1..K \tag{V-51}$$

The average quality of the groundwater and surface water delivered to all M&I and UCA users after mixing during the planning period can be bounded via:

$$c^{mtavgL}(\ddot{y}) \leq c^{mtavg}(\ddot{y}) \leq c^{mtavgU}(\ddot{y}) \quad \text{for } \ddot{y} = 1..M^m \tag{V-52}$$

$$c^{catavgL}(\Upsilon) \leq c^{catavg}(\Upsilon) \leq c^{catavgU}(\Upsilon) \quad \text{for } \Upsilon = 1..M^{ca} \tag{V-53}$$

Alternatively, the average concentration for some portion of the total planning period can be bounded.

Distinct bounds on hydropower and crop yield do not need to be expressed here. Both of these are objective functions. The sum of all hydropower production or crop yield can be restricted through the E-constraint method of multiobjective optimization (discussed previously).

V.10. Review and Summary

PROMOD allows you to select the objective function, constraints and bounds needed to pose a particular management problem. Via three data sets (DC) b and c (Fig I-1), you select all locations for decision variable and state variable control that you might want to consider in your optimization (or series of optimizations). Via DC d you can choose to use all those previous selections, or only some of them in one particular optimization.

Absolutely required data includes that needed for the objective function. Other equations will also be used since without some bounds and constraints, the problem is meaningless. You generally will bound or constrain state variables or conditions and will frequently bound decision variables or combinations thereof.

VI. SAMPLE APPLICATIONS

VI.1. Introduction

PROMOD is applicable to a wide range of management problems. We illustrate three potential applications here. Although the example studies were performed using other codes, PROMOD will make it easier and faster to perform such studies. That will help bring S/O modelling into everyday practice. The examples are:

1. Maximizing allocation of groundwater and surface water in a dynamic stream aquifer system. This example illustrates how a different management scenarios can be posed for a particular study area. It discusses the error of assuming that a slightly nonlinear system is linear.) It explains how 'marginals' can be used to refine an optimal strategy (see also Appendix A). This example is from Appendix F (G. Belaineh et al) of Peralta and Aly (1993).

2. Maximizing conjunctive use while maximizing contaminant loading to a stream. Increasing groundwater pumping reduces flow from aquifer to stream, and contaminant dilution.

3. Maximizing sustained groundwater yield from a complex multilayer aquifer. There is a tradeoff between groundwater pumping and discharge from springs.

VI.2. Conjunctive Water Management and Allocation

VI.2.1. Study area and problem description

This example illustrates optimization of the conjunctive use of surface and ground water. The S/O model is applied to a small hypothetical model area designed with a minimal number of cells to run quickly for instructional purposes (adapted from Peralta and Aly, 1993). (Accuracy of computations due to discretization is not an issue and is not addressed here.) The area has a single layer aquifer and a stream, (Figure VI-1).

For illustration, the area is discretized into 26 cells, of which 9 have a uniform size of 10 km length and 0.2 km width. The remaining 17 are boundary cells or thin internal cells with one of their side dimensions being 1 m (3 ft), defined to facilitate computations. The 0.2 km cell width is a function of the 10 m river width (cell width $\approx$ 20 * river width).

The stream is in excellent hydraulic connection with the aquifer and has an average width of 10 m (30 ft) and an average depth of 3 m (9 ft). Reach transmissivity varies from 8 to 80,000 m²/day (24 to 240,000 ft²/week) for reach length of 1 m and 10,000 m respectively. In two of the very small downstream river cells, reach transmissivity is set to zero, so that they will experience no streamflow depletion. The value of hydraulic conductivity is 4.5 m/day (14.0 ft/day), saturated thickness is 53 m (160 ft), and specific yield is 0.2 for all cells. No-flow boundary conditions exist along all sides of the aquifer. Initially, the water table is flat and level, with initial head of 3 m (9 ft) above the river bottom. Initially the stream level is equal to the water table elevation. The river bottom elevation is 50 m (150 ft) above a horizontal datum.

The time horizon for this unsteady optimization problem is 8 weeks (Table VI-1).

Water is diverted for irrigation use from two diversion points (cells 8 and 18). Surface water diversion is supplemented by pumping from wells located in cells 7 and 24.

The objective is to maximize total water provided by diverting surface water and pumping groundwater. Solution is subject to constraints on head in the pumping cells, bounds on downstream flow, and bounds on pumping and/or diversion in groups of cells. Solutions are provided for seven different scenarios. The mathematical formulation and symbol notations are shown later in the section.

Table VI-1. Stream inflow data used for the specified planning period.

Week	1	2	3	4	5	6	7	8
Mean inflow at stream entrance $(10^6 \ m^3/d)$	0.285	1.140	0.571	0.500	0.430	0.371	0.314	0.285

V.2.2. Problem formulation:

In the following we have substituted the actual parameter values used in the problem where possible. No substitution was performed for parameters having more than one value. An equation number such as V-1^s indicates that this is a form of Equation V-1 in which numerical values are substituted.

Objective function:

$$MINIMIZE \quad Z \quad = \quad \sum_{k=1}^{8} \left[\sum_{\hat{a}=1}^{2} (1) \, p(\hat{a},k) + \sum_{\hat{e}=1}^{2} (-1) \, d(\hat{e},k) \right] \tag{V-1^s}$$

subject to:

$$-0.4 \; 10^6 \; \leq \; p(\hat{a},k) \; \leq \; 0 \qquad \text{for } \hat{a} = 1...2, \; k = 1...8 \tag{V-8^s}$$

$$0 \; \leq \; d(\hat{e},k) \; \leq \; d^U(\hat{e},k) \qquad \text{for } \hat{e} = 1...2, \; k = 1...8 \tag{V-9^s}$$

$$-0.2 \; 10^6 \; \leq \; p^G(1,k) \; = \; \left[\sum_{\hat{a}=1}^{2} p(\hat{a},k) \right] \leq 0 \quad \text{for } k=1...8 \; (\text{Scenario 5a}) \tag{V-16^s}$$

$$0 \; \leq \; d^G(1,k) \; = \; \left[\sum_{\hat{e}=1}^{2} d(\hat{e},k) \right] \leq 1.0 \; 10^6 \qquad \text{for } k=1...8 \; (\text{Scenario 5b}) \tag{V-17^s}$$

$$0 \; \leq pd^G(1,k) = \left[\sum_{\hat{e}=1)}^{2} d(\hat{e},k) - \sum_{\hat{a}=1}^{2} p(\hat{a},k) \right] \leq 0.4 \; 10^6 \; \text{for } k=1...8 \; (\text{Scenario 5c}) \tag{V-18^s}$$

$$h^L(\hat{o},n) \; \leq \; h(\hat{o},n) \; \leq \; 55 \qquad \text{for } \hat{o}=1...2, \; k=1...8 \tag{V-33^s}$$

$$q^{sL}(\hat{u},n) \; \leq \; q^s(\hat{u},n) \; \leq \; 9.99 \; 10^6 \qquad \text{for } \hat{u}=1...2, \; k=1...2 \tag{V-41^s}$$

Not to scale

Key:
- ◇ Pumping and head control location
- ◆ Surface water diversion location
- ↔ Stream flow control location
- ▨ Impermeable material
- ▬ No flow boundary
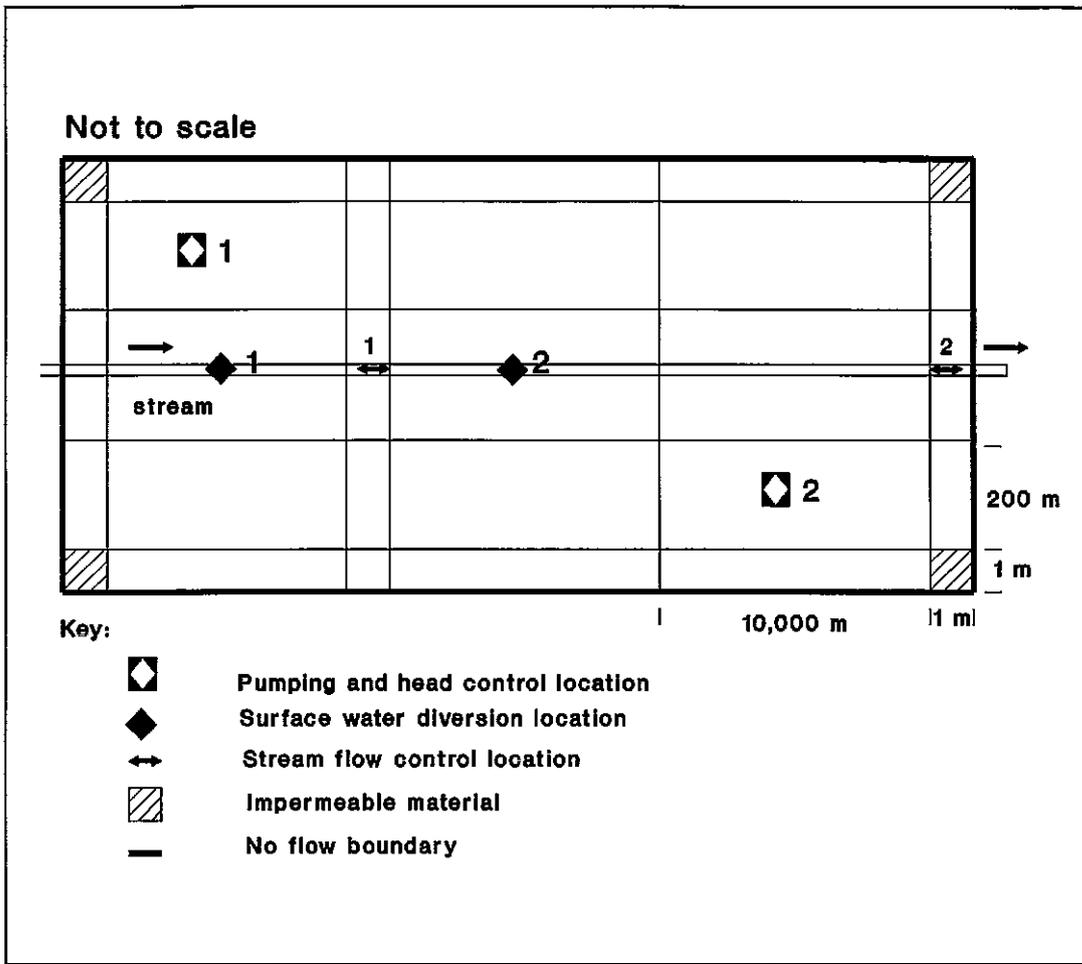
Figure VI-1. Map of study area for conjunctive use problem.
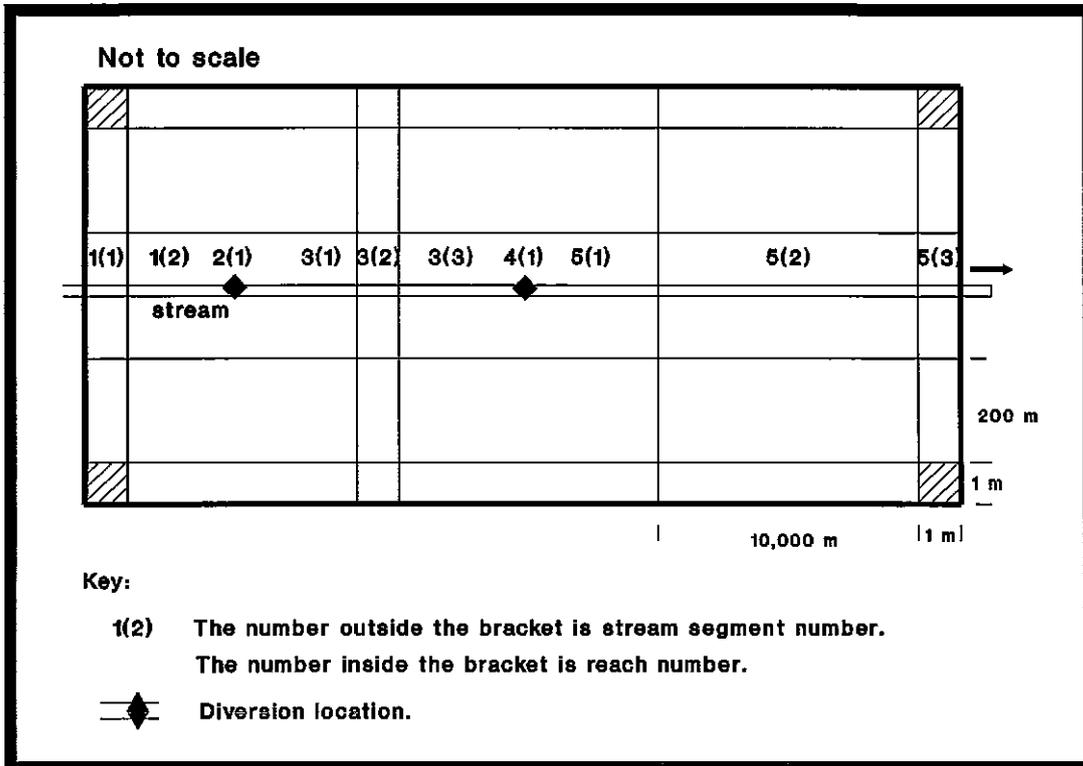
Figure VI-2. Distorted map of study area for conjunctive use problem, showing the stream segments and reaches utilized.

V.2.3. Application and results

The management objective is to maximize water delivered by diversions from two points and by withdrawing groundwater (pumping) from two cells. Time varying optimal strategies are obtained using the S/O model for seven different scenarios (Table VI-2).

The scenarios differ in the utilized constraints and bounds. These imposed criteria are displayed in the first 10 columns. Scenarios 1 through 4 differ from one another on the basis of the variations of the bounds on the state and decision variables. Scenarios 5a through 5c demonstrate applications of constraining groups of decision variables. Groups of groundwater pumping cells and surface diversion reaches are constrained in Scenarios 5a and 5b, respectively. In Scenario 5c pumping and diversion are grouped together.

Table VI-2 The summary of the scenarios.

		UTILIZED BOUNDS AND CONSTRAINTS									OPTIMAL STRATEGIES		
1	2	3	4	5	6	7	8	9	10	11	12	13
scenario	bound	q^{sl} (10^6 m^3/d)	q^{sl} (10^6 m^3/d)	h (m)	g (10^6 m^3/d) per pump cell	d (10^6 m^3/d) per div. cell	Σg (10^6 m^3/d) per pair of pump cell	Σd (10^6 m^3/d) per pair of div. cell	$\Sigma(g{+}d)$ (10^6 m^3/d) per each of four cells	g (10^6 m^3/d) time avg. per pump cell	d (10^6 m^3/d) time avg. per div. cell	$\Sigma(g{+}d)$ (10^6 m^3/d) time avg. per all cells
1	upp low	0.15*	0.10*	55.00 46.00*	0.40* 0.00	0.50* 0.00				0.096	0.206	0.603
2	upp low	0.15*	0.10*	55.00* 50.00	0.40 0.00	0.50* 0.00				0.027	0.237	0.528
3	upp low	0.15*	0.10*	55.00* 50.00	0.40 0.00	1.00* 0.00				0.026	0.252	0.556
4	upp low	0.25*	0.20*	55.00* 51.00	0.40* 0.00	1.00 0.00				0.003	0.215	0.436
5a	upp low	0.15*	0.10*	55.00* 49.00	0.40* 0.00	0.50* 0.00	0.20* 0.00			0.040	0.231	0.542
5b	upp low	0.25*	0.20*	55.00* 51.00	0.40* 0.00	1.00* 0.00		1.00* 0.00		0.004	0.204	0.416
5c	upp low	0.07*	0.05*	55.00* 50.00	0.40* 0.00	1.00 0.00*			0.40* 0.00	0.010	0.190	0.400

* This constraint is tight for at least one cell for at least one stress period.
Note: Here, groundwater pumping, p, equals groundwater extraction,g. Here it is presented as a positive value. Copies of computed output are shown in subsequent pages. In this example there is only one reach per cell. Also, diversion "cells" are more properly termed "reaches".

The last three columns of Table VI-2 summarize the time average rates computed to be optimal for the 8 week period. Values in column 11 are obtained by summing the pumping for both cells and all stress periods and dividing by 16. Values in column 12 are comparable for diversion.

Column 13 contains time average daily delivery rates. Such a value is determined by adding the column 11 value multiplied by the number of pumping cells to the column 12 value multiplied by the number of diversion points. To compute the total volume of water delivered during eight weeks one multiplies the column 13 value by 56, (7 days/week * 8 weeks).

Results show the effect of tightening or relaxing constraints. The greatest water can be delivered under Scenario 1 (col. 13). That optimal strategy is tight (prevented from further improvement) by the lower bounds on flow (q_{sL}),and h (h^L) and upper bounds on g (g^U) and d (d^U)(see asterisk in Table VI-2). The tight bound of zero for pumping means that the model would like to inject water (recharge the aquifer) to improve total system performance. However, it does not consider where that injected water might have come from.

Raising the lower bound on h in Scenario 2 causes the objective function to decrease. Subsequently raising the upper bound on diversion (column 7) in scenario 3 permits a slight increase in average total delivery rate to $0.556*10^6 m^3/d$ (col. 13). Raising the lower bound on streamflow (col. 3 and 4) and on h (column 5) in Scenario 4 causes a reduction in diversion (col. 12) and total delivery (col. 13).

Scenario 5a differs from Scenario 2 in that a little more drawdown is permitted at pumping cells (col. 5). However, there is a new restriction on the total groundwater pumping rate (col. 8). Both the lower bound on aquifer head and the upper bound on group pumping become tight. Average total delivered water increases to 0.542 from $0.528*10^6 m^3/d$ per cell.

When compared with Scenario 3, Scenario 5b shows the effect of simultaneously raising the lower bounds on streamflow (cols. 3 and 4), and imposing an upper limit on the sum of diversions (col. 9). Each of these constraints is tight in scenario 5b. Total delivery is less for Scenario 5b than for Scenario 3.

Compared with Scenario 5b, Scenario 5c shows the effect of relaxing the lower bounds on streamflow (cols. 3 and 4), removing the constraint on total diversion (col. 9), and imposing an upper bound on total water delivered in any stress period (col. 10). The average total delivery rate decreases (col. 13).

S/O model output for all scenarios is found on subsequent pages. Output includes values of decision and state variables, groups of variables, bounds and constraints and marginals.

No cycling is employed in most of these scenarios. Although developed for an unconfined aquifer, the optimal strategies are adequately accurate without that effort. After each optimal strategy is computed, it is used as input in a nonlinear MODFLOW simulation. System response calculated by MODFLOW is compared with that predicted by the S/O model for control locations. The greatest error in aquifer head is 0.11 m. This corresponds to an error of less than 1 percent, in terms of predicting change in head. The greatest error in streamflow is $0.254 \ 10^5 \ m^3/d$. This is less than 3 percent error, in terms of predicting change in flow. The error in streamflow is negligible after 2 cycles.

V.2.4. Interpreting S/O model output (scenario 1) and use of marginals

Figure VI-3 shows representative S/O model output (derived from Peralta and Aly, 1993). Immediately the reader notes that the S/O model computed an optimal solution, and the value of the objective function. The optimal pumping and diversion variables are shown next. The â index of pumping excitation cell PE(â) corresponds to what is seen in the equations of Chapter V. DOS cannot print superscripts, so they are shown on the same line as the variable name itself. Thus, pL(â,k) is the lower bound on pumping in cell â in period k. The optimal value is shown next, followed by the upper bound and the marginal (explained below). Other parts of the data reveal optimal diversion rates, the optimal heads and streamflows that will result, and the sums of pumping, diversion and pumping plus diversion rates.

The marginal shown in the last column of the output files specifies the rate of change in the value of the objective function per unit change in the bound of the corresponding variable. The marginal can be used to predict the value of the objective function that will result from changing tight bounds. Let Z_{old} be the old value of objective function and Δ var be the change in variable bound. The new objective function (Z_{new}) resulting from the change in the bound can be predicted using the following relationship (as long as the variable changes to become tight at the new bound values, and as long as no other decision variable changes in value).

$$Z_{new} = Z_{old} + (\partial Z/\partial var)*(\Delta\ var) \tag{VI-1}$$

Table VI-3 compares objective values calculated using equation F-1 with values computed by S/O model. Two comparisons are made. The first is made by changing the pumping bound of Scenario 1 for pumping cell 1 in stress period 2. The second involves changing the bound on diversion in diversion reach 1 in the same period.

For example, the objective function value for Scenario 1 (here called run 1a) is -4,824,090. The $\partial Z/\partial p(1,2)$ is 0.0393. Changing the lower bound on p(1,1) to -400,100 should cause (0.0627)(-100) change in Z, resulting in

$$Z_{new} = -4,824,090 + (0.0393)(-100)$$
$$= -4,824,094.$$

Actually, when the S/O model was rerun with the new bound (run 1b) Z_{new} was -4,824,090. The slight error is due to the round off. A similar effect is noted when comparing the results of run 1c with those of 1a.

Figure VI-3. S/O model output for Scenario 1.

```
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^

Model status:  OPTIMAL SOLUTION FOUND
Objective value (Z):-3.20000E+6

SOLVER USED IS  MINOS


========================================================================

OPTIMAL GROUNDWATER PUMPING RATES p(â,k), EXTRACTION(-) AND INJECTION(+),
[L^3/T]
```

CELL PE(â)	STRESS PERIOD k	L.BOUND pL(â,k)	OPTIMAL p(â,k)	U.BOUND pU(â,k)	MARGINAL ∆Z / ∆p(â,k)
1	1	-4.0000E+5	0.0000	0.0000	0.0000
1	2	-4.0000E+5	0.0000	0.0000	0.0000
1	3	-4.0000E+5	0.0000	0.0000	0.0000
1	4	-4.0000E+5	0.0000	0.0000	0.0000
1	5	-4.0000E+5	0.0000	0.0000	0.0000
1	6	-4.0000E+5	0.0000	0.0000	0.0000
1	7	-4.0000E+5	-5.3484E+4	0.0000	0.0000
1	8	-4.0000E+5	-4.0191E+4	0.0000	0.0000
2	1	-4.0000E+5	0.0000	0.0000	0.0000
2	2	-4.0000E+5	0.0000	0.0000	0.0000
2	3	-4.0000E+5	0.0000	0.0000	0.0000
2	4	-4.0000E+5	0.0000	0.0000	0.0000
2	5	-4.0000E+5	0.0000	0.0000	0.0000
2	6	-4.0000E+5	0.0000	0.0000	0.0000
2	7	-4.0010E+5	0.0000	0.0000	0.0000
2	8	-4.0000E+5	-7.0323E+4	0.0000	0.0000

```
========================================================================
OPTIMAL DIVERSION RATES, d(ê,k),  [L^3/T]
```

CELL DE(ê)	STRESS PERIOD k	L.BOUND dL(ê,k)	OPTIMAL d(ê,k)	U.BOUND dU(ê,k)	MARGINAL ∆Z / ∆d(ê,k)
1	1	0.0000	3.28939E+5	1.00000E+6	0.0000
1	2	0.0000	0.0000	1.00000E+6	0.0000
1	3	0.0000	0.0000	1.00000E+6	0.0000
1	4	0.0000	25582.1338	1.00000E+6	0.0000
1	5	0.0000	0.0000	1.00000E+6	0.0000
1	6	0.0000	3.36546E+5	1.00000E+6	0.0000
1	7	0.0000	2.71183E+5	1.00000E+6	0.0000
1	8	0.0000	2.29032E+5	1.00000E+6	0.0000
2	1	0.0000	71061.1197	1.00000E+6	0.0000
2	2	0.0000	4.00000E+5	1.00000E+6	0.0000
2	3	0.0000	4.00000E+5	1.00000E+6	0.0000
2	4	0.0000	3.74418E+5	1.00000E+6	0.0000
2	5	0.0000	4.00000E+5	1.00000E+6	0.0000
2	6	0.0000	63454.1210	1.00000E+6	0.0000
2	7	0.0000	75332.6387	1.00000E+6	0.0000
2	8	0.0000	60453.7656	1.00000E+6	0.0000

```
========================================================================
```

OPTIMAL CONJUNCTIVE STREAM DIVERSION RATES+PUMPING RATES, pdG(á,k), [L^3/T]
FOR GROUPS OF DIVERSION AND PUMPING LOCATIONS

GROUP pdg(á)	STRESS PERIOD k	L.BOUND pdGL(á,k)	OPTIMAL pdG(á,k)	U.BOUND pdGU(á,k)	MARGINAL $\triangle Z$ / $\triangle$pdG(á,k)
1	1	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	2	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	3	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	4	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	5	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	6	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	7	0.0000	4.00000E+5	4.00000E+5	-1.0000
1	8	0.0000	4.00000E+5	4.00000E+5	-1.0000

==
OPTIMAL HYDRAULIC HEADS, h(ô,k), [L]

CELL HC(ô)	STRESS PERIOD k	L.BOUND hL(ô,k)	OPTIMAL h(ô,k)	U.BOUND hU(ô,k)	MARGINAL $\triangle Z$ / $\triangle$h(ô,k)
1	1	50.0000	52.7488	55.0000	0.0000
1	2	50.0000	52.5059	55.0000	0.0000
1	3	50.0000	52.2587	55.0000	0.0000
1	4	50.0000	52.0263	55.0000	0.0000
1	5	50.0000	51.8157	55.0000	0.0000
1	6	50.0000	51.6078	55.0000	0.0000
1	7	50.0000	50.6353	55.0000	0.0000
1	8	50.0000	50.0000	55.0000	0.0000
2	1	50.0000	52.7376	55.0000	0.0000
2	2	50.0000	52.4523	55.0000	0.0000
2	3	50.0000	52.1581	55.0000	0.0000
2	4	50.0000	51.8818	55.0000	0.0000
2	5	50.0000	51.6301	55.0000	0.0000
2	6	50.0000	51.4043	55.0000	0.0000
2	7	50.0000	51.2045	55.0000	0.0000
2	8	50.0000	50.0000	55.0000	0.0000

==
AVERAGE OPTIMAL HYDRAULIC HEADS [L]

CELL	TIME AVERAGE OPTIMAL HEAD
1	51.6998
2	51.6836

==
OPTIMAL OUTFLOW FROM STREAM REACHES, qs(û,k), [L^3/T]

REACH SC(û)	STRESS PERIOD k	L.BOUND qsL(û,k)	OPTIMAL qs(û,k)	U.BOUND qsU(û,k)	MARGINAL $\triangle Z$ / $\triangle$qs(û,k)
1	1	70000.0000	70000.0000	0.99900E+7	0.0000
1	2	70000.0000	1.21915E+6	0.99900E+7	0.0000
1	3	70000.0000	6.14655E+5	0.99900E+7	0.0000
1	4	70000.0000	5.10237E+5	0.99900E+7	0.0000
1	5	70000.0000	4.60035E+5	0.99900E+7	0.0000
1	6	70000.0000	70000.0000	0.99900E+7	0.0000
1	7	70000.0000	70000.0000	0.99900E+7	0.0000
1	8	70000.0000	70000.0000	0.99900E+7	0.0000
2	1	50000.0000	2.40098E+5	0.99900E+7	0.0000
2	2	50000.0000	9.27784E+5	0.99900E+7	0.0000
2	3	50000.0000	3.20556E+5	0.99900E+7	0.0000
2	4	50000.0000	2.20807E+5	0.99900E+7	0.0000
2	5	50000.0000	1.32618E+5	0.99900E+7	0.0000
2	6	50000.0000	72371.5028	0.99900E+7	0.0000
2	7	50000.0000	50000.0000	0.99900E+7	0.0000
2	8	50000.0000	50000.0000	0.99900E+7	0.0000

```
AVERAGE OPTIMAL OUTFLOW FROM STREAM REACHES  [L^3/T]

   REACH      TIME AVERAGE STREAM OUTFLOW
     1                3.85509E+5
     2                2.51779E+5


=====================================================================
SUMMARY OF OPTIMAL PUMPING RATES  [L^3/T]

STRESS PERIOD      SUM OF PUMPING RATES      SUM OF ABS. PUMPING RATES
     1                  0.0000                      0.0000
     2                  0.0000                      0.0000
     3                  0.0000                      0.0000
     4                  0.0000                      0.0000
     5                  0.0000                      0.0000
     6                  0.0000                      0.0000
     7               -5.3484E+4                  53484.2378
     8               -1.1051E+5                   1.10515E+5


=====================================================================
AVERAGE OPTIMAL PUMPING RATES   [L^3/T]

PUMPING CELL      TIME AVERAGE PUMPING RTAE
     1                -1.1709E+4
     2                -8790.4068


=====================================================================
SUMMARY OF OPTIMAL DIVERSION  RATES   [L^3/T]

STRESS PERIOD      SUM OF DIVERSION RATES
     1                4.00000E+5
     2                4.00000E+5
     3                4.00000E+5
     4                4.00000E+5
     5                4.00000E+5
     6                4.00000E+5
     7                3.46516E+5
     8                2.89485E+5


=====================================================================
AVERAGE OPTIMAL DIVERSION RATES [L^3/T]

DIVERSION LOCATION      TIME AVERAGE DIVERSION RATE
     1                     1.48910E+5
     2                     2.30590E+5


=====================================================================
SUMMARY OF OPTIMAL PUMPING + DIVERSION  RATES [L^3/T]

STRESS PERIOD      SUM OF ABS. PUMPING  +  DIVERSION  RATES
     1                     4.00000E+5
     2                     4.00000E+5
     3                     4.00000E+5
     4                     4.00000E+5
     5                     4.00000E+5
     6                     4.00000E+5
     7                     4.00000E+5
     8                     4.00000E+5


=====================================================================
AVERAGE OPTIMAL DIVERSION + ABSOLUTE PUMPING RATES  [L^3/T] = 4.00000E+5
```

Table VI-3. Comparison between objective functions: predicted and computed by S/O model and predicted using marginal value from previous optimization run.

run	lower bound on pumping	marginal	computed obj. function	predicted obj. function
1a	-400,000	0.0393	-4,824,090	
1b	-400,100	0.0393	-4,824,090	-4,824,094

run	lower bound on diversion	marginal	computed obj. function	predicted obj. function
1a	500,000	-0.9298	-4,824,090	
1c	500,100	-0.9298	-4,824,180	-4,824,182

VI.3. Coordinating Waste Loading and Conjunctive Use

VI.3.1. Study area and problem description (modified from Ejaz, 1994)

A community is discharging non-industrial wastewater, after treatment by a sewage treatment plant (STP) to a stream. The stream obtains most of its water from upstream inflow and flow from an underlying aquifer (Figure VI-4). The stream and aquifer are very well connected. Treated water released to the stream is diluted by the streamflow.

The single layer alluvial aquifer is unconfined. It has constant inflow boundaries running parallel to the stream. Rainfall percolates to the aquifer, providing another source of recharge.

Management goals are:

1) The regional water resources agency wishes to increase water supply by installing pumping wells and diverting water from the stream. They wish to consider pumping in 20 cells near the river, and diverting water in two locations. Figure VI-4 shows 3 diversion locations. Of these, the most upstream location is actually the location of the STP discharge. It is an augmentation (a negative diversion, a source to the stream rather than a sink).

2) The municipality expects to grow. It wishes to be able to discharge as much treated wastewater as possible to the stream.

3) Diverted water and water flowing to downstream users must satisfy specified quality standards. Increased groundwater pumping or wastewater discharge should not cause concentrations at a monitoring (control) location to exceed the legal standards. During even the dry season, standards should be satisfied for BOD_5, dissolved oxygen (DOX), organic nitrogen (OGN), nitrogen as ammonia (NH_3), nitrite nitrogen (NO_2), nitrate nitrogen (NO_3), organic phosphorus (OGP), dissolved phosphorus (DSP), chlorophyll-a (CHA), and total dissolved solids (TDS).

This is a multiobjective management problem. Goals of the regional agency and the municipality conflict with each other and with environmental restrictions. Increasing groundwater pumping decreases flow from aquifer to stream, decreasing stream dilution and increasing downstream concentrations, even if wastewater discharge is unchanged.
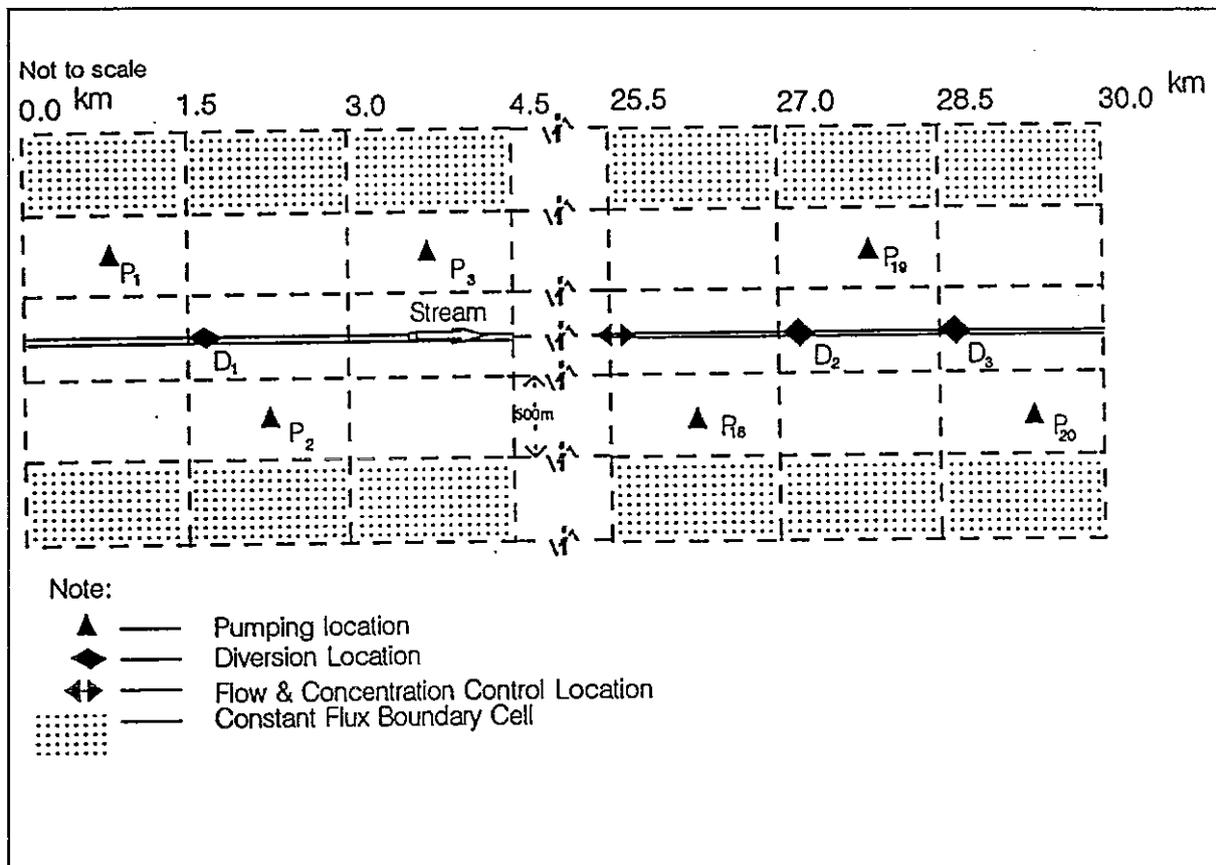
Figure VI-4 Study area for multiobjective problem: maximizing conjunctive use versus maximizing waste load (Ejaz, 1994).

VI.3.2. S/O model application and results

The applied S/O model utilizes equations mentioned previously:
- The objective function is to maximize the sum of groundwater pumped and stream water diverted. (Eq V-1)
- Bounds are imposed on individual groundwater pumping and surface water diversion rates, aquifer head at pumping locations, and streamflow and concentration of 10 constituents at one stream monitoring location. (Equations V-8, 9, 33, 49)
- The second objective, maximizing loading, is imposed as a constraint. To do this we use the E-constraint method, objective option 55 (Chapter V).

Because this is a multiobjective problem, developing a pareto optimum (tradeoff curve) for one set of assumptions and input data is more appropriate than computing a single optimal strategy. Upstream inflow is a significant input parameter. Upstream inflow (inflow from above the wastewater discharge) affects how much water can be conjunctively used and how much wastewater can be discharged. Thus, we assume a range of upstream inflow rates, and compute a tradeoff curve for each using the E-constraint method (Figure VI-5).

Figure VI-5 shows pareto optima for upstream inflow rates of 1.4, 1.5 and 1.6 m^3s^{-1}. The median upstream inflow rate corresponds to the seven day average minimum flow in the stream occurring once in ten years (7Q10).

For all optimizations, the restrictive (tight) constraints are contaminant concentrations. A tight constraint is one which prevents the objective function from being any better. Here, at least one concentration is at its upper bound at the monitoring location for each optimization. This tightness prevents more water allocation and more wastewater discharge.

Note the slope of the pareto optima. Increasing the water conjunctively supplied causes a decreasing population for which waste water can be treated and discharged. The slope verifies that the first two objectives conflict.

To illustrate figure interpretation, assume that the water agency can accept a compromise total water supply (sum of diversion and pumping) of 1500 lps (34 MGD) (points A_1, A_2, and A_3). For that value, the STP can discharge treated wastewater generated by populations of 228,00, 238,000 and 248,000 for upstream inflows of 1.4, 1.5, and 1.5 m^3s^{-1}. For these populations, STP discharges are 15.96, 16.66 and 17.36 MGD, respectively (assuming per capita wastewater production of 270 l or 70 gallons per day).

Accuracy of S/O model results are tested. Post-optimization simulation with QUAL2E confirms that concentrations computed by S/O model are acceptably accurate. If downstream flowrates are tight constraints, post-optimization simulation with MODFLOW +STR is used to confirm S/O model accuracy.

Sensitivity analysis is performed by testing how much the optimal strategy changes in response to changes in input assumptions. Developing a family of pareto optima (for different assumed upstream inflow rates) is one form of sensitivity analysis. Other analyses show that relaxing tight bounds on concentrations permits an increase in population creating the wasteload.
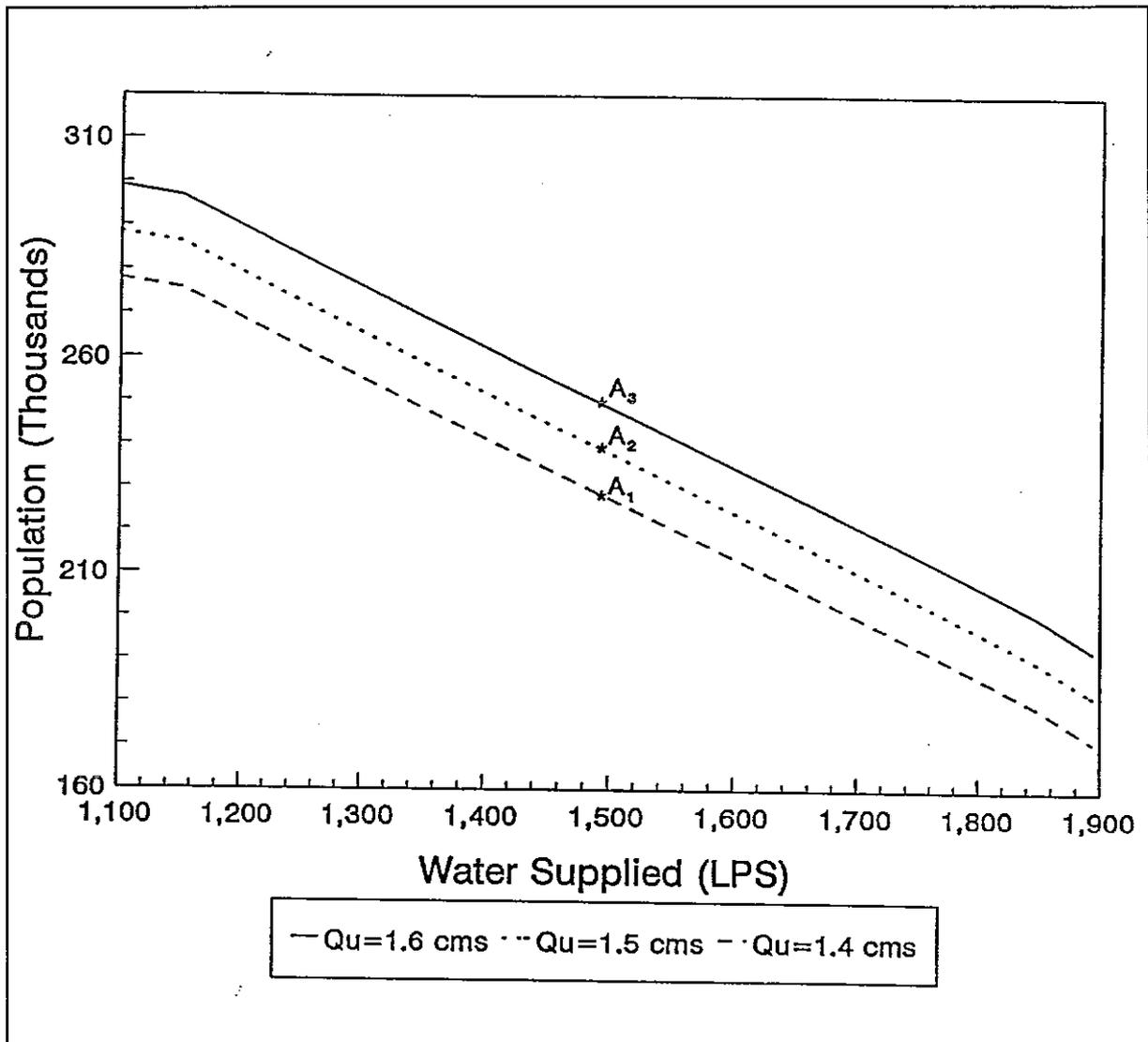
Figure VI-5 Pareto optima for multiobjective problem: maximizing conjunctive use versus maximizing waste load (Ejaz, 1994).

VI.4. Sustained Groundwater Yield Planning

VI.4.1. Study area and management problem

The eastern shore of Utah's Great Salt Lake is increasingly urbanized. The shore area is underlain by multilayer aquifers which are recharged primarily from the mountains (Figure VI-6). In the 450 square mile area of interest here, the aquifers discharge primarily via pumping, springs and flowing wells. Currently over 50 % of their discharge is by springs, flowing artesian wells, evapotranspiration, and flow to the Great Salt Lake. The springs and flowing wells provide much water for agriculture, wildlife and the natural ecology.

Municipalities want to increase groundwater pumping. Consequences will be declining aquifer head and a reduction in discharge from springs and flowing wells. We want to know, how much can pumping increase without causing more than 20 feet of drawdown? What is the tradeoff between groundwater pumping and discharge from springs and artesian wells?

VI.4.2. S/O model application and results

The applied S/O model utilizes equations mentioned previously:
- The objective function is to maximize the sum of groundwater pumping (i.e. minimize the sum of groundwater pumping having a negative sign).
- Bounds are imposed on individual groundwater pumping and aquifer head.
- An objective of maximizing flow from springs and artesian wells is employed as a constraint using objective option 55.

Takahashi (1992) developed optimal sustained groundwater yield pumping strategies using steady-state influence coefficients. He optimized pumping beyond current pumping by assuming 61 potential pumping cells in the area shown in Figure VI-7. (He used the same grid and aquifer input parameters as Clark et al, 1990.) He shows that sustainable groundwater pumping can increase 50 % without causing more than 20 feet of drawdown. Later, using an enhanced S/O model and more potential pumping locations, he determined that the tradeoff is about 1 unit of flowing discharge lost per two units of groundwater pumping gained.
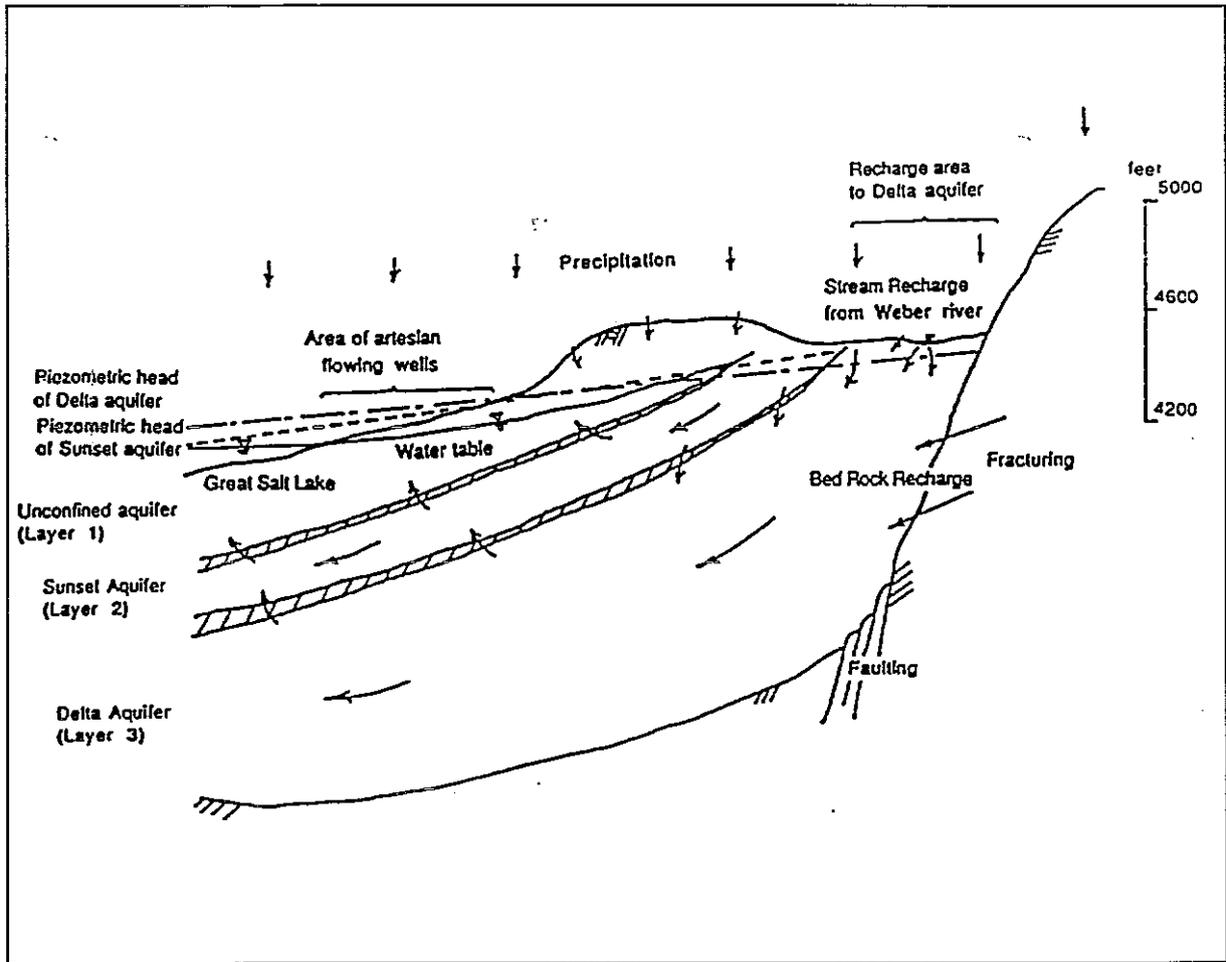
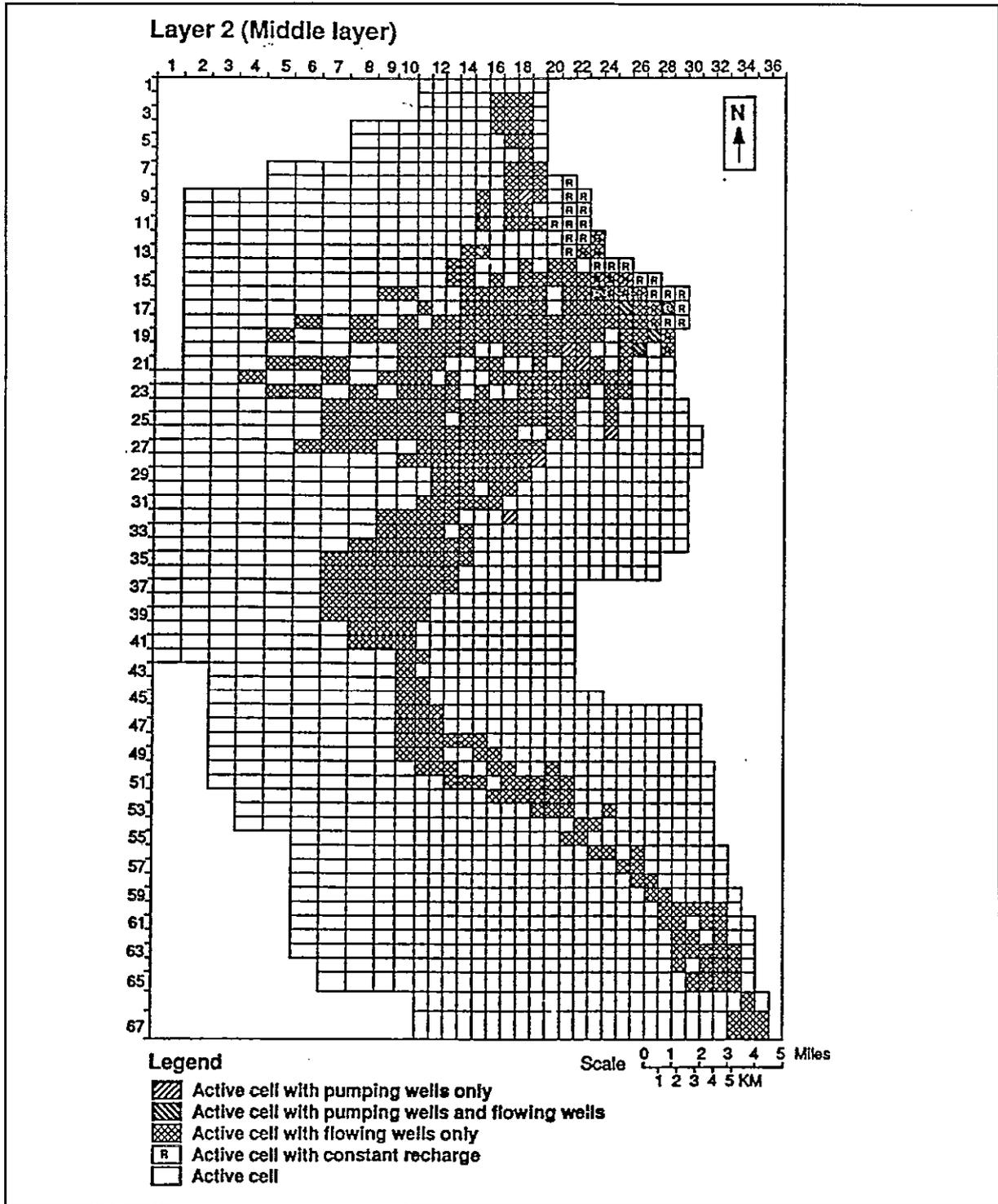Figure VI-6 Generalized profile of the East Shore Area aquifer system (Clark et al, 1990)

Figure VI-7 Discretization of layer 2 of the finite difference model applied to the East Shore Aquifer System (Clark et al, 1990)

VII. Other PROMOD Modules and Processes, and Related Topics

VII.1. Other PROMOD Modules and Processes

VII.1.1. Introduction

So far, we have discussed steps 2,3, and 4 of the PROMOD flow chart (Fig I-1). These include the:
■ integrated simulation module (ISM, chapter III), which computes system response to management;
■ simplified simulation module (SSM, chapter IV), which prepares for optimization by calculating influence coefficients and regression expressions; and
■ simulation/optimization module (S/O, chapter V), which computes optimal water management strategies.

In this section we discuss other PROMOD activities listed in Figure I-1. These include model calibration, uncertainty analysis, and tools to enhance reporting of PROMOD results.

VII.1.2. Calibration optimization module (COM)

Model calibration is critically important for successful model use. Calibration must precede using the ISM, SSO or S/O modules for prediction or optimization. We cannot truly optimize management of a complex system unless we can predict, with acceptable accuracy, how the system will respond to our management. Simulation (ISM and SSO) and S/O modules must be reasonable representations of the physical system for management purposes. For any of these modules to be appropriate for management, the ISM must first be accurately calibrated.

During a calibration process, the modeller attempts to cause a simulation model to compute the same system responses (heads, for example) to known stimuli (groundwater pumping, for example) as are observed in the physical system during some 'calibration period'. When the model can do this with acceptable accuracy, the model is considered calibrated.

We can improve and speed calibration by using computer models which solve the 'inverse' problem (Anderson and Woessner, 1992). A normal simulation model solves for heads (after we provide it with system physical parameters, boundary and initial conditions, and system stimuli). An inverse model solves for physical parameters, and some boundary conditions and stimuli (after we provide it with some boundary conditions, initial conditions, heads, and some stimuli).

Inverse models use optimization algorithms to compute the system parameters that cause computed system responses to best match field values. Usually a least squares criterion is used to determine how well the matching is accomplished. The set of physical system parameters (for example, spatially distributed transmissivity, storativity and deep percolation

rates) that cause the smallest sum of squares of differences between observed and computed heads, is the best estimate of the system parameters (tempered by professional judgement).

Inverse models are becoming more commonly used (Cooley, 1977; Carrera et al, 1984; Carrera and Neuman, 1986; Cooley and Naff, 1990; Faust et al., 1990). There are both public domain and commercial inverse models available.

To aid most beneficial use of PROMOD, the COM module includes:

■ MODFLOWP (Hill, 1990), an inverse model for aquifers that is compatible with MODFLOW. Like MODFLOW, MODFLOWP is public domain, supported by the U.S. Geological Survey, and easily obtained by anyone worldwide.

■ inverse models to calibrate parameters for stream, reservoir and canal distribution system parameters.

■ inverse models to calibrate the most significant QUAL2E parameters.

The COM module will make it easier to use PROMOD than it would be otherwise. It will help assure that results are more accurate, increasing PROMOD use worldwide.

VII.1.3. Post-optimization simulation and uncertainty analysis module (SUA)

VII.1.3.1. Post-optimization simulation.

The SUA automates the following post-optimization simulation activities:

■ transmitting an optimal strategy (computed by the S/O module) to the ISM for simulation.

■ comparing system responses computed by S/O module with those computed to result (from the optimal strategy) by the ISM.

■ cycling until strategy convergence is obtained (as described previously and below).

The SUA also makes it easy to perform sensitivity and uncertainty analyses. We discuss the need for these activities in the next section.

We use simulation immediately after computing an optimal strategy to verify that the ISO computes the same system responses to the optimal strategy as does the S/O. This is most important for cells, reaches and times at which state variables are near their bounds. An example of a possible future situation is illustrative.

Assume that a management goal is to assure that streamflow at reach 30 never drops below 100 L^3T^{-1}. In the S/O module, this value is used as a lower bound on streamflow at that location. In other words, $q^{sL}(30,k) = 100$.

After computing an optimal strategy, assume the S/O module prints out that the streamflow at reach 30 resulting from the strategy is precisely 100 L^3T^{-1} [$q^s(30,k) = q^{sL}(30,k) = 100$]. Within the S/O module, $q^{sL}(30,k)$ is tight at its lower bound.

We know that the S/O module uses a simplified simulation expression to compute q^s (Equation IV-2). This equation is subject to error if stage is not linearly proportional to streamflow. Since the error can be over 10 % for the first optimization, we want to check and see how much error exists. We especially want to make sure that actual streamflow in the field (the real world) will not be less than 100 L^3T^{-1}.

We check the accuracy of the results by inputting the optimal strategy into the ISM, simulating, and comparing the results of the ISM and the S/O. The ISM is potentially more

accurate at predicting system response than the S/O.

If the ISM predicts more than 100 L^3T^{-1}, the optimal strategy will not cause too low a streamflow in the field (assuming a well calibrated model). If we want more accuracy we might assume new magnitudes of unit stimuli, compute new influence coefficients, compute a new optimal strategy, and compare anew.

If the ISM predicts less than 100 L^3T^{-1}, the optimal strategy will cause too low a streamflow in the field. We must cycle until post-optimization simulation indicates that the optimal strategy will cause acceptable consequences (flows not less than 100 L^3T^{-1}). Usually 2-4 cycles are needed for strategy convergence. A strategy has converged when decision and state variable values no longer change with cycle.

VII.1.3.2. Uncertainty analysis

Common types of uncertainty analyses are sensitivity analysis, first order error analysis and Monte Carlo analysis. The SUA addresses uncertainty analysis to different degrees for groundwater and surface water components. This reflects the differences in the the data that is generally available, and the amount of computer processing time that is needed to perform the analysis.

The SUA automates sensitivity analysis for all flow and transport processes simulated by the ISM. To illustrate sensitivity analysis, assume that after computing a converged optimal pumping strategy, we want to know:

■ what will happen in the field if we use (implement) the optimal strategy, but physical system parameters are actually somewhat different than we assumed in developing the strategy; and

■ how the optimal strategy will differ if we assume different physical parameters.
Both of these questions are aspects of sensitivity analysis.

After user-input, the SUA automates the process of answering the first question. It systematically makes many simulations (calling the ISM). All of these simulations employ the same optimal strategy, but each uses a different set of assumed physical parameters. Usually only one parameter differs from its best calibrated value per simulation. The parameters are varied $\pm$ some proportion from the best calibrated value. The results of these simulations show us the range of possible consequences we might expect in the field, from implementing the optimal strategy.

After user-input, the SUA automates answering the second question by systematically making many converged optimizations using the S/O. Each optimization differs in the physical parameters that are assumed. Assumed parameters are usually varied as discussed above. The results of these optimizations show us how robust the optimal strategy or parts of the strategy are. For example, if a computed optimal diversion rate $d(3,5)$ is the same for all optimizations, it is considered robust. Usually groundwater pumping rates are fairly robust.

The SUA automates the Monte Carlo evaluation process to evaluate optimal strategy response to different system inflow or mass loading rates. Assuming one knows the probability distribution function of such an inflow, SUA automates use of implicitly stochastic optimization to develop optimal conjunctive use strategies. The statistical

characteristics of the inflow or loading can become characteristics of the optimal strategy developed for that inflow (Peralta et al, 1988), if information from one optimization is transmitted and utilized within a subsequent optimization. (This requires assuming that all other parameters are adequately described deterministically).

For surface water quality problems, the SUA performs sensitivity analysis, first order error analysis and Monte Carlo simulation. The SUA incorporates QUAL2E-UNCAS (Brown and Barnwell, 1987) and suggested ranges of parameter values for testing. (Walker, 1982; Koenig, 1986; NCASI, 1982a,b; McCutcheon, 1985).

VII.1.4. Graphical and summary module (GSM)

PROMOD makes it easy for users demonstrate to others the consequences and benefits of optimal water management. After user selection of options, the GSM automatically prepares contour plots, flow pathline drawings, cross-sections, 3-dimensional (3-D) surface drawings, and bar and pie charts in 2-D and 3-D. The GSM also summarizes results, such as those seen in section VI.2. into standard tables.

The GSM interfaces with computer-aided design and drafting (CAD) software. It allows the user to overlay GSM-produced drawings upon CAD drawings. The GSM includes a library of standardized symbols recommended to identify the locations of PROMOD decision and state variables in drawings (Figure VII-1).

Instructions provided with the GSM permit the user to prepare drawings that can be output as: colored or monochrome 35 mm slides, paper hardcopy, or transparencies of the same size. Prepared files are importable into many popular commercial wordprocessors. Once a drawing file is prepared, it can easily become either a presentation graphic or a figure in a report.

VII.1.5. PROMOD processing environment and design features

1) The PROMOD program will function within a WINDOWS environment. Experience worldwide has shown that this environment is very beneficial for computer management models (Merkley, 1993). It:
- speeds user learning.
- facilitates training.
- facilitates input data entry and output review.
- enhances transfer of data between modules.
- enhances the ability to review inputs or outputs using computer graphics at any time during model operation.
2) The PROMOD program will function on personal computers.
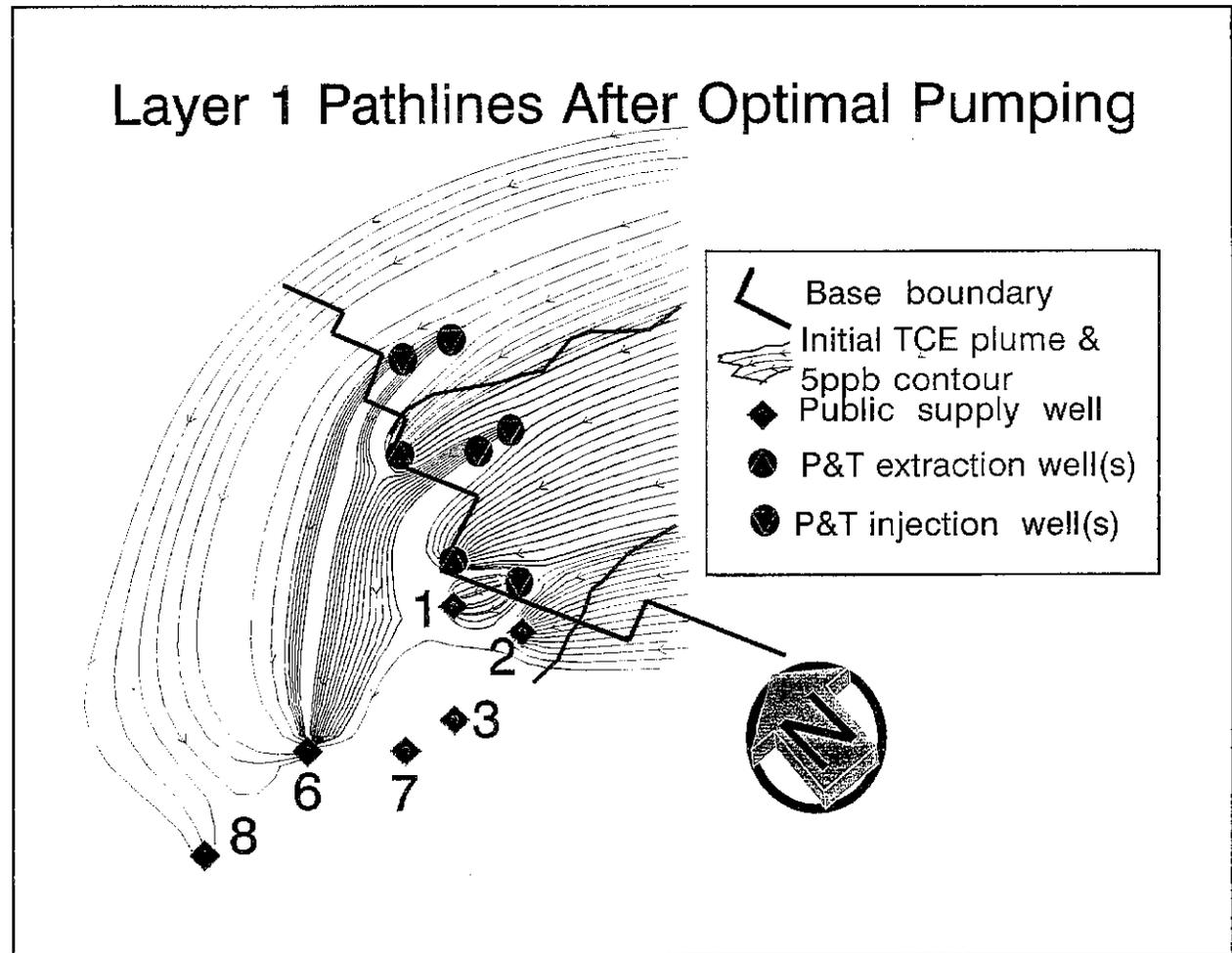3) The PROMOD program will be written modularly to ease upgrading.

Figure VII-1 Sample graphics output: pathlines of clean water, contaminated water, and treated and reinjected water (Peralta and Aly, 1994).

VII.2. Limitations and other considerations

All models should be used with care, keeping in mind their inherent assumptions. Some considerations for the PROMOD model are:

1)   We cannot optimize management of a system (using computers) until we can adequately simulate that system.

2)   Processes that PROMOD does not simulate are listed in the Introduction. However, capabilities can be augmented as needed.

3)   The type of optimality achieved by a PROMOD optimization depends upon the S/O model formulation that is used[1]. PROMOD will inform the user of the type, based upon the following:

■ If the objective function and all constraints are linear, a computed strategy is globally optimal.

■ If the objective function is quadratic and all constraints are linear there is a good probability that a computed strategy is globally optimal. PROMOD will determine whether global optimality has been achieved, using the method of principal minors.

■ If the objective function is nonlinear (other than quadratic) or if any of the constraint equations is nonlinear, the computed optimal strategy is locally optimal. One cannot theoretically prove global optimality of such a strategy. In such a case, PROMOD empirically attempts to get as close to global optimality as possible. To do so, it semi-automatically and systematically makes a number of optimizations. In each optimization it inputs a different set of initial guesses for decision variable values. In each case, the optimization algorithm begins its search for a optimal solution beginning with the provided initial guess. At the end of this systematic evaluation, PROMOD reports the best solution.

The inability to know for certain that PROMOD has computed a globally

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[1] Global versus Local Optimality

As explained in Appendix A, a set of bounds and constraints define a region of feasible solutions (a solution space). The optimal solution lies on the outer boundary of that solution space. If the solution space is convex (shaped like a bowl that will hold water against gravity), an optimization algorithm is absolutely guaranteed to find the best value of the objective function. This occurs because the algorithm changes variables with internal iteration in such a way that the objective function value always improves. Thus the algorithm moves along the outer surface of the decision space in the direction of improving objective function value. The algorithm stops when no further change in decision variables will cause the objective function to improve.

If the objective function and constraints are all linear, the solution space is convex, and the computed strategy is always globally optimal.

If the objective function and/or constraints are nonlinear, the solution space might have dimples or waves in it. In its search for an optimal solution, the optimization algorithm might get stuck in one of the dimples or troughs. It will stop there because it cannot improve the value of the objective function by any incremental move in any direction. Such a solution is termed locally optimal. It might or might not be the absolutely best solution possible. We cannot theoretically prove it either way.
Locally optimal

optimal solution is not of much concern. Experience with optimizing sustained groundwater yield pumping strategies for one study area showed that two different models (one using fully nonlinear groundwater equations and the other using linear surrogates of those equations) converge to the same solution (Takahashi, 1992). In addition, remember that all computed strategies satisfy all imposed constraints. The computed strategy does fulfill all management and physical restrictions, and, for complex problems, will probably be better than any strategy that can be devised otherwise.

4)   To compute optimal strategies for the range of discussed problems, PROMOD's S/O module must access powerful linear, mixed integer and nonlinear optimization algorithms (solvers). No public domain solver has been found that is robust enough to address the spectrum of management problems PROMOD must tackle. Developing any one of these rigorous solvers is be a multi-year, expensive process. For this reason, PROMOD utilizes existing commercial solver packages, as US/REMAX does (Peralta and Aly, 1993).

For training and small optimization problems, special training versions of PROMOD can use Demonstration versions of commercial solvers. The demo-solvers are generally available for minimal charge, but are limited in the size of the management problems they can address.[2]

For application to large optimization problems, normal versions of the commercial solvers will need to be used within PROMOD. PROMOD will do the linking automatically.

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[2]   Size of management problem is a function of the numbers of decision and state variables and the numbers and/or complexity of the equations that interrelate them. Management problem size has no relation to the size of the study area or the number of nonoptimally managed pumping cells or diversion points. Thus, even a demonstration solver could develop an optimal pumping strategy for a 10,000 cell study area, if the number of pumping and diversion rates being optimized was relatively small.

VIII. Summary and Recommendation

Simulation/Optimization models are being used increasingly to improve management of water resource systems. S/O models compute water management strategies that best satisfy user-specified objectives and goals. Personal experience has shown that modellers using S/O models can achieve management objectives 10-40% better than modellers using normal simulation (S) models alone.

As management problem complexity increases, the benefit of using a S/O versus S model increases. S/O models can and have been applied to a wide range of management problems. Selected examples are:

■ maximizing the sum of groundwater extracted plus surface water diverted from streams, without causing ecological problems or violating others' water rights.

■ maximizing the sum of groundwater and surface water delivered to water users. This differs from the previous goal in that it considers conveyance losses and return flows between the stream diversion point and the water user.

■ maximizing conjunctive water use while constraining how much treated or untreated wastewater the surface waters should remove from the area;

■ determining the mix of source and nonsource pollutant stream loadings that maximizes use of a stream-aquifer system without causing unacceptable water quality;

■ maximizing safe sustainable groundwater yield from an aquifer;

■ minimizing the pumping needed to prevent industrially contaminated groundwater from reaching public supply wells.

In all these situations, user selected constraints prevent the computed water management strategy from causing unacceptable consequences to the physical system. For example, constraints can be used to ensure that: water surface or water table elevations are adequate for wetlands, wildlife, navigation, irrigation, or public water supply; and that water quality values are acceptable for designated uses.

We propose coding of a computer program patterned after the methodology presented here. This will facilitate widespread use of S/O modelling techniques and will improve management abilities. The resulting model will be able to:

■ address water quantity and quality management in physical systems containing hydraulically connected aquifer, reservoir, stream and canal systems.

■ reflect the effect of water use efficiencies of agricultural, municipal and industrial water users on return flow and mass loading to surface water and groundwater.

■ consider the effect of irrigation water quantity and quality on crop yield.

■ compute optimal strategies for multiobjective problems, simultaneously addressing a wide range of goals (food and water supply, economic benefit, ecological preservation, drought protection, and others) and

■ run on personal computers.

The model will include:

■ calibration module enhanced by inverse problem optimization.

■ simulation module that includes several proven public domain codes as submodules, plus other software.

■ simulation/optimization module that incorporates the following in order to address a wide range of management problems:

      - over 50 basic objective function options plus any combination of those 50.

      - over 45 types of constraint and bound options.

      - robust solvers for linear, quadratic, nonlinear and mixed integer problems.

■ graphical summary module to help the manager present modelling results in a clear and compelling fashion.

      In summary, the proposed approach can provide a practical, user-friendly tool that will help managers know how best to solve many of their water resources problems.

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Appendix A
Why Use a Simulation/Optimization (S/O) Model:
Background, Illustrative Example and Comparison With Normal Simulation Models
(modified from Peralta and Aly, 1993)

A.1. Introduction and simple application of linear systems theory in groundwater management

Simulation/optimization (S/O) models can be used to greatly speed the process of computing desirable groundwater pumping strategies for plume management. They make the process of computing optimal strategies fairly straight-forward and can help minimize the labor and cost of groundwater contaminant clean-up.

To help illustrate what optimization is, a manual solution of a simple steady-state groundwater optimization problem is presented here. This graphically shows the problem an optimization algorithm addresses in calculating an optimal pumping and/or diversion strategy. After the example, the difference between using an S/O models and the simulation (S) models currently used by over 98 % of practitioners is discussed.

Response matrix (RM) S/O models utilize the multiplicative and additive properties of linear systems. The additive property permits superimposing the drawdowns due to pumping at different wells to compute the drawdown resulting at an observation well. This is commonly taught with image well theory in introductory groundwater classes. The multiplicative property means that the effect of doubling a pumping rate is a doubling of drawdown (examination of the Theis Equation shows that drawdown is linearly proportional to pumping). RM models use influence coefficients that describe system response (in head, gradient, etc.) to a 'unit' pumping rate. Application to nonlinear systems is discussed later.

The following equation illustrates use of the multiplicative property in groundwater head computation. Here we assume that the initial water table is horizontal and at equilibrium. Groundwater is extracted at a single well, index number â.

$$\Delta h(\hat{o}) = \delta^h(\hat{o}, \hat{a}) \frac{p(\hat{a})}{p^{ut}(\hat{a})} \tag{A-1}$$

where

$\Delta h(\hat{o})$ = change in steady-state aquifer potentiometric surface elevation at observation location ô [L];

$\delta^h(\hat{o}, \hat{a})$ = influence coefficient describing effect of steady groundwater pumping at location â on steady-state potentiometric surface elevation at location ô [L];

$p(\hat{a})$ = pumping rate at location â $[L^3/T]^1$;

$p^{ut}(\hat{a})$ = magnitude of steady 'unit' pumping stimulus in location â used to generate

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[1] For clarity and ease of explaining this example, pumping to extract groundwater is treated as positive in sign, and the δ^h influence coefficients are negative. In US/REMAX those signs are reversed to be consistent with MODFLOW.

the influence coefficient $[L^3/T]$. This does not necessarily equal 1.

Assume that a 'unit' steady pumping extraction rate of 1 m³/min at well â causes a drawdown of 1 m at observation point ô. In that case, $\delta^h(\hat{o},\hat{a})$ equals (-1) and $p^{ut}(\hat{a}) = 1$. Equation 1 shows that if $\delta^h(\hat{o},\hat{a})$ and $p^{ut}(\hat{a})$ are known, the change in head caused by any pumping rate can be easily computed. If pumping, p(â), equals 2 m³/min, head change will equal (-1)(2)/(1) or -2. This linear response is typical of confined aquifers (or approximates behavior of unconfined aquifers where the change in transmissivity due to pumping is small by comparison with the original transmissivity).

Similarly, the effect caused by a unit pumping at location â on the final difference in potentiometric surface elevation between locations, 1 and 2, of a pair of locations, ò, can be expressed as:

$$\delta^{\Delta h}(\hat{o},\hat{a}) = \delta^h(\hat{o}_{\hat{o},1},\hat{a}) - \delta^h(\hat{o}_{\hat{o},2},\hat{a}) \tag{A-2}$$

where

$\hat{o}_{\hat{o},1}$ = index referring to point 1 of pair of locations ò;
$\hat{o}_{\hat{o},2}$ = index referring to point 2 of pair of locations ò;

For example, if $\delta^h(\hat{o}_{1,x},\hat{a})$ for locations x=1 and x=2 of pair 1 are (-1) and (-1.02), respectively, $\delta^{\Delta h}(\hat{o},\hat{a})$ equals 0.02.

Assume that pumpings at M^P locations affect head at location ô. The cumulative effect at ô is simply the result of adding the effect of M^P pumping rates. The following summation expression illustrates this application of the additive property, with the same assumptions as above.

$$\Delta h(\hat{o}) = \sum_{\hat{a}=1}^{M^P} \delta^h(\hat{o},\hat{a}) \frac{p(\hat{a})}{p^{ut}(\hat{a})} \tag{A-3}$$

where
M^P = total number of locations at which water is being pumped from the aquifer.

Similarly, the additive property can be used to describe the effect on head difference due to pumping at M^P locations. The following expression is used in the subsequent example.

$$\Delta\Omega(\hat{o}) = \sum_{\hat{a}=1}^{M^P} \delta^{\Delta h}(\hat{o},\hat{a}) \frac{p(\hat{a})}{p^{ut}(\hat{a})} \tag{A-4}$$

where

$\Omega(\delta)$ = the difference in potentiometric surface elevation between locations 1 and 2 of pair δ, [L]. Here, since the initial steady-state potentiometric surface is horizontal, $\Omega(\delta)$ also equals the change in the difference due to pumping, $\Delta\Omega(\delta)$.

A.2. A simple manually solved groundwater optimization problem

Both additive and multiplicative properties are illustrated in this manually solved optimization problem. Assume the study area (top right of Fig. A-1) containing 2 pumping wells and 2 head-difference control locations (each such location consists of a pair of observation wells). The aquifer is at steady state and the initial potentiometric surface is horizontal.

The problem statement is to compute the minimum extraction needed to cause: head difference 1, ($\delta = 1$), to be at least 0.2 L and head difference 2 to be at least 0.15 L (towards the pumping wells), while assuring that the sum of pumping from both wells is at least 15 L^3/T. Such a situation might occur if you want to assure particular speeds of contaminant movement towards the extraction wells and want to treat a pumped water flowrate of at least 15 L^3/T.

The 4 parts of the problem statement are represented by the first 4 equations a-e, respectively, of Figure 1. The top (unnumbered) equation is the 'objective function', the value of which we wish to minimize. This contains 'decision variables' p(1) and p(2), pumping at wells P1 and P2, respectively. Coefficients multiplying these values are weights (sometimes these weights represent costs). Here the weights indicate that pumping at well 2 is less desirable than pumping at well 1.

Equations a-c are termed 'constraints'. Because it is an $\geq$ constraint, all points in the graph to the right of Line (a) satisfy that equation (Fig. A-1). All points to the right of Lines (b) and (c) satisfy Equations b and c, respectively.

Equations a and b are applications of Equation 4 above. In Equation a, both $p^{ut}(1)$ and $p^{ut}(2)$ equal 1.0. Also, $\delta^{\Delta h}(1,1)$ and $\delta^{\Delta h}(1,2)$ are 0.02 and 0.01, respectively. The 0.02 coefficient describes the effect of pumping p(1) on the difference in head between the two observation wells at control location 1. Each unit of p(1) will cause a 0.02 increase in head difference between the two observation points of control pair 1 (i.e., an increase in gradient toward pumping well 1). Each unit of p(2) will cause a 0.01 increase in head difference toward well 1 at the same location.

Equation b is similar to Equation a. It describes the effect of pumping on head difference across control pair 2.

Below the constraint equations are 'bound' Equations d and e. These prevent decision variables p(1) and p(2) from being negative (i.e. representing injection). Thus, only positive values of p(1) and p(2) are acceptable. This further defines the region of possible solutions.

Only points to the right or above all five of the constraint or bound lines satisfy all 5 equations. These points constitute the feasible 'solution space'. The optimization problem goal is to find the smallest combination of p(1) + 1.5*p(2) in the solution space. That

optimal combination will lie on the boundary between the feasible solution region and the infeasible region. In fact, it will be at a point where two or more lines intersect (a vertex of the solution space). For this simple problem of only 2 decision variables, a graphical or manual solution (evaluating Z at the intersections of the lines) is simple--the minimum value of Z is 18.75. p(1) and p(2) both equal 7.5.[2]
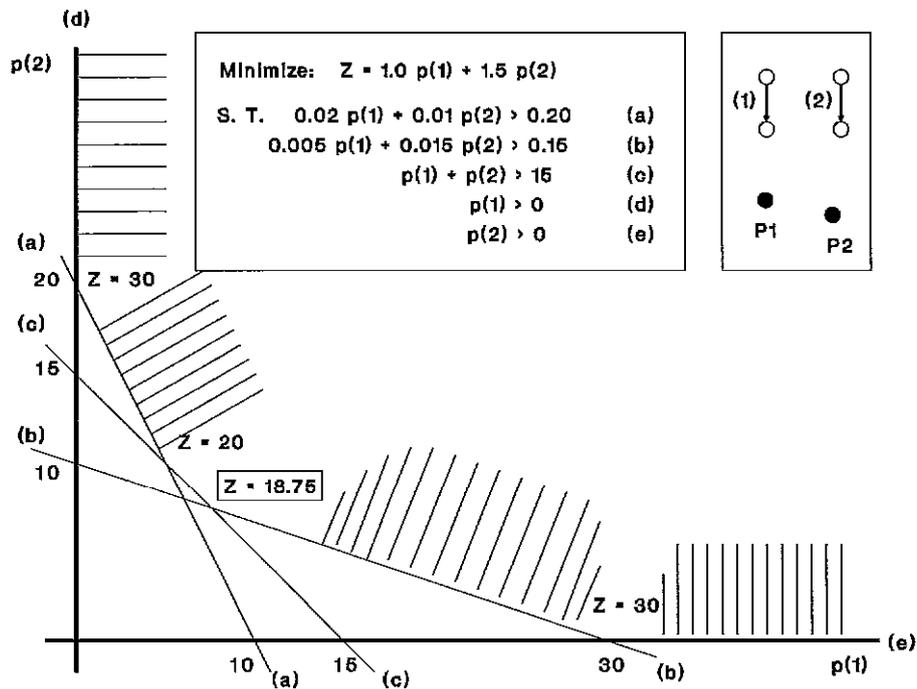
FIGURE A-1.   Graphical representation of simple pumping
                   optimization problem.

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[2] Note that if Equation 3 were p(1) + p(2) $\leq$ 15, the feasible solution space would be the small centrally located triangle. In that case the minimum objective function value would be Z = 18, (6 + 1.5*8), and the optimal pumping rate would be 6 + 8 = 14.

Also note that if, in a modification of the original problem, the weights in the objective function were both 1, there would be multiple optimal solutions of equal validity. The two points having original Z values of 18.75 and 20 would both have Z values of 15, as would all intermediate points on Line (c). However, generally this is not the case.

Optimization problems can become complex. For example, if we want to optimize 3 pumping rates in the above problem, we must solve the problem within 3-space (ie. 3 dimensions, one for each optimizable pumping rate). Problems can rapidly become difficult or impossible to solve manually.

Formal optimization algorithms can be used to calculate optimal solutions for optimization problems having virtually unlimited dimensions (number of pumping rates) and constraint equations. These algorithms systematically search the boundaries of the feasible solution space and rapidly find the optimal solution. Generic optimization algorithms have been developed and applied to a wide range of optimization problems, including those of groundwater management. US/REMAX contains such algorithms and makes formulation and solution of groundwater optimization problems fast and easy.

An S/O model has another advantage. It will quantify for you the effect[3] of each management goal (as implemented through a constraint or bound) on your objective function value. In effect, it tells you how much a constraint is consting you in terms of OF value. This shows which constraints you might want to consider changing to best improve the overall strategy.

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[3]   This value, termed the marginal, equals the rate of improvement in the objective function, (OF), per unit change in the constraint or bound. In the original sample problem, suppose that you would like to use even less pumping than the optimal strategy indicates is necessary. Is there a reasonable way to achieve this?

You know that the optimal solution is at the intersection of Lines (b) and (c), (Fig. A-1). Relaxing either constraint Equation b or c (i.e. moving their lines downward) will improve the OF value. Assume that you think you can live with relaxing Equation c, i. e. changing the 0.15 head difference constraint to 0.14. (Probably that head difference will still be adequate for our management goals.) For this problem, US/REMAX will tell us that the marginal of Equation c, $\partial Z/\partial\Omega$, equals (50). This means that the OF value will decrease in value 50 times as fast as you relax Equation c by decreasing the bound (for some finite amount of change). Proof of this value is shown below. Assume that if the right-hand side (RHS) of Eq. b is changed to 0.14, the new optimal solution will lie at the new intersection of Lines b and c. Solving for p(1) and p(2) at that point first requires rearranging Equation c.

p(1) = 15 - p(2)

Substituting for p(1) in the new Eq. b yields:

0.005   {15-p(2)} + 0.015 p(2) = 0.14
0.075 - 0.005 p(2) + 0.015 p(2) = 0.14
                    0.01   p(2) = 0.065
                           p(2) = 6.5

Substituting for p(2) in Eq. c yields:

p(1) = 15 - 6.5 = 8.5

The new value of the objective function is:

Z = 8.5 + 1.5{6.5} = 18.25

The change in the objective function value is:

ΔZ = 18.25 - 18.75 = -0.5

The rate of change in Z with respect to change in the restriction (i.e. RHS) of Eq. b is:

$\partial Z/\partial\Omega$ = -0.5/-0.01 = 50

Thus, US/REMAX automatically tells you how you can best modify your management. It tells you how much objective enhancement you can expect for small changes in constraints or bounds.

A brief comparison between using common simulation models and S/O models

If you cannot solve a posed groundwater management optimization problem manually, and you have only a standard simulation (S) model available, your approach is probably as follows.

■1) You specify what you want the pumping strategy to achieve (ie. what system responses-- heads, gradients, etc.) are acceptable.

■2) You assume a reasonable pumping strategy that you think might achieve those goals.

■3) You simulate system response to the pumping strategy using the simulation model.

■4) You evaluate acceptability of the strategy and its consequences.

■5) Based on the evaluation of step 4) you repeat steps 2-4) until you feel you should stop.

When using an S model, the process of assuming, predicting and checking might have to be repeated many times. As the numbers of possible pumping sites and system response requirements increase, the likelihood that you have assumed an acceptable strategy decreases. Assuming an optimal strategy becomes impractical or impossible as problem complexity increases.

On the other hand, a groundwater simulation/optimization (S/O) model directly computes the pumping strategy that best satisfies your goals. It contains both simulation equations and an operations research optimization algorithm. The simulation equations permit the model to appropriately represent aquifer response to hydraulic stimuli and boundary conditions (US/REMAX uses simulation equations similar to numbers 1-4 above, plus many others). The optimization algorithm permits the specified management objective to serve as the function driving the search for an optimal strategy.

Both S and S/O models require data describing the physical system. However, other inputs differ because of their different capabilities (Table I-1).

The normal S models compute aquifer responses to assumed boundary conditions and pumping values. The boundary conditions and pumping values are all used as data inputs. System response is the output.

On the other hand, S/O models directly calculate the best pumping strategies for the specified management goals. The goals and restrictions are specified via the objective function, constraint equations and bounds. Data needed to formulate these goals represent additional input required by S/O models (Table I-1). Outputs include optimal pumping rates and the resulting system responses.

Although S/O models require additional data, that is only the data needed to make sure that the computed strategy indeed satisfies all your management goals. For example, upper or lower bounds of pumping rates, heads or gradients reflect the range of values which you consider acceptable. The model automatically considers those bounds while calculating optimal pumping strategies. You might impose lower bounds on head, at a specific distance below current water levels or above the base of the aquifer. Upper bounds on head might be the ground surface or a specified distance below the ground surface.

In summary, the most important difference is that you must input a pumping strategy to an S model, while an S/O model computes it for you.

Appendix B
Case History
(Multiobjective Optimization: Maximizing Municipal Pumping,
While Controlling a Plume and Preventing Unacceptable River Dewatering.)
and Pareto Optimum Development.
(modified from Peralta and Aly, 1993)

B.1. Description

B.1.1. Introduction

Below we discuss a case history that combines concern about groundwater quality, public water supply and river depletion. It involves use of the Utah State Model for Optimizing Management of Stream/Aquifer Systems Using the Response Matrix Method US/REMAX (Peralta and Aly, 1993). First, the study area and problem are described. Second, the steady-state pumping strategy developed by a consultant using MODFLOW is presented. Third, the problem is posed for solution via optimization, US/REMAX is applied, an optimal strategy is computed and the improvement is noted. Then, the system response to implementing the optimal strategy is verified using MODFLOW. Finally, variations in the management goals are assumed and new optimal strategies are developed. Computed optimal strategies are compared.

B.1.2. Study area description and situation

The study area, consisting primarily of glacial outwash, is about 1.9 by 1.8 miles in size and is discretized into 36 rows and 34 columns (Fig B-1). The length of the cells ranges from 78.2 ft to 1980.2 ft. The width of the cells ranges from 138.4 ft to 1138.5 ft. The area is bounded on the west and east by impermeable material. There is fixed inflow from the north. The hydraulic gradient generally runs from north to south, paralleling flow in a river. The southern boundary consists of river cells.

Aquifer parameters were calibrated by a consultant. The unconfined aquifer is represented by three layers. Near the plume and the wells, the horizontal hydraulic conductivity is 600 ft/day for layers 1-3 (layer 1 is uppermost). Layer saturated thicknesses are about 22, 40 and 160 ft, respectively. Recharge due to rainfall is 0.027 ft/d.

A contaminant plume exists in the vicinity of an industrial facility. Unless influenced by groundwater pumping, the plume would migrate southward. Using 3 wells (referred to as industrial wells), that facility pumps and uses the underlying contaminated water. A municipality to the northeast of the facility also pumps from three wells. The municipal wells pump at rates of (113,100), (161,800), and (40,500) ft^3/d in cells (row,column,layer), (12,19,3), (13,21,3) and (13,21,2) respectively. Municipal pumping causes the contaminated water to flow toward the northeast, unless the industrial wells pump significantly.

Before US/REMAX was available, a consultant was asked to determine how much contaminated water must be pumped to keep the plume from reaching the public supply

wells. The consultant developed a pumping strategy through repeated uses of MODFLOW. For the next few years, the facility pumped at the recommended rate. Although it was not a consideration initially, a water supply agency then expressed concern about river flow depletion caused by the pumping. Another consideration is that the municipality might wish to increase pumping for public use--which will also cause river depletion. Accordingly, the consultant wanted to determine how the pumping strategy could be revised to satisfy the disparate and conflicting goals. To do so, he used US/REMAX.

Below are presented (Table B-1) and discussed the initial consultant solution (Scenario 1^{non}), the optimal solution to the same situation (Scenario 1), and optimal solutions to alternative management scenarios.

FIGURE B-1.(a)Finite-difference grid for the area, (b)well locations and locations of head difference constraints imposed in Scenarios 1-3.
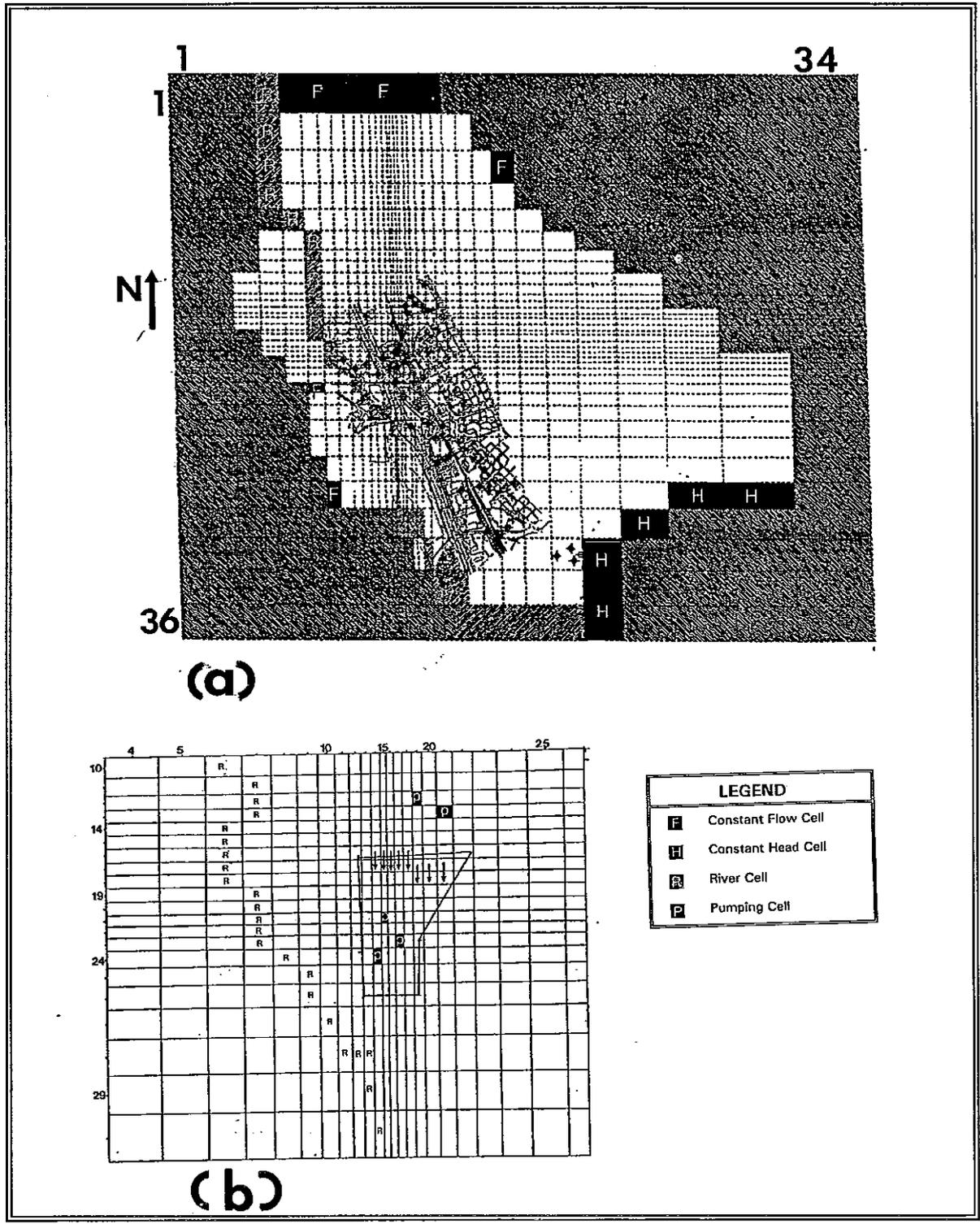
B.2. Developing Pumping Strategies

B.2.1. Developing a pumping strategy for the initial situation via common practice (Scenario 1^{non})

After calibrating MODFLOW, the consultant tested different combinations of pumping at the three industrial facility wells. Since the facility uses 267,380 ft^3/d (2 mgd) in its processing, the consultant tried to develop a pumping strategy that would require as little excess pumping as possible, while making sure that there would be a ground water divide between the plume and the municipality. This strategy, developed via repetitive simulation runs of MODFLOW, included pumping rates of 174,200, 108,100 and 192,000 ft^3/d) in cells (21,15,2), (23,17,2), and (24,14,2) respectively. Total industrial pumping is shown in Table B-1. Resulting flow from river to aquifer totaled 139,332 ft^3/d for the 30 river cells immediately downstream of (10,6). Achieved head differences in layer 1 are at least 0.2 for cell pairs ($\delta = 1..5$) (16,14)-(17,14); (16,15)-(17,15); (16,16)-(17,16); (16,17)-(17,17); and (16,18) -(17,18). The head difference is at least 0.15 for cell pairs ($\delta = 1..5$) (17,19)-(18,19); (17,20)-(18,20) and (17,21) - (18,21).

TABLE B-1. Scenario results.

Scenario	Lower Bound on Total Industrial Pumping	Upper Bound on Flow from River to Aquifer	Total Industrial Pumping	Total Municipal Pumping	Total Flow from River to Aquifer
1^{non}			474,296	315,350	139,332
1	267,380*		267,380	315,350	75,123
2			249,086	315,350	68,740
3		139,332*	369,100	416,460	139,332

Units are ft^3/day. Extraction is shown as positive for convenience, although it is a negative value in US/REMAX

* Tight bound or constraint. For Scenario 2, a head difference constraint is tight.

B.2.2. Developing, computing and verifying optimal pumping strategy for the initial situation via US/REMAX (Scenario 1)

The optimization problem objective is to minimize the value of Equation V-1^s, subject to the below restrictions. (Bounds on individual heads and pumping rates are used in US/REMAX, but are insignificant and not shown below.) The ^{s} superscript indicates that values for parameters are substituted into Equation V-1. Locations at which head difference constraints are imposed (to assure appropriate gradients) are mentioned above, shown in

Figure B-1(b), and defined via Equations V-34[s] and V-35[s]. Arrows in the figure indicate the direction of flow that will result from any computed optimal strategy.

$$\text{MINIMIZE:} \quad \sum_{\hat{a}=1}^{3} \left((-1)\ p(\hat{a},1) \right) \qquad\qquad \text{(V-1}^s\text{)}$$

subject to:

$$\sum_{\hat{a}=1}^{\bar{}} p(\hat{a},1) \leq -267{,}380 \qquad\qquad \text{(V-16)}^s$$

$$0.2 \ \leq \ \Omega(\grave{o},1) \quad \text{for } \grave{o} = 1 \ .. \ 5 \qquad\qquad \text{(V-34)}^s$$

$$0.15 \ \leq \ \Omega(\grave{o},1) \quad \text{for } \grave{o} = 6 \ .. \ 8 \qquad\qquad \text{(V-34)}^s$$

$$\Omega(\grave{o},1) = [h(\hat{o}_{\grave{o},1},1) - h(\hat{o}_{\grave{o},2},1)] \quad \text{for } \grave{o} = 1 \ .. \ 8 \qquad \text{(V-35)}^s$$

where

$p(\hat{a},1) =$	Steady-state groundwater pumping at location $\hat{a}$; $[L^3T^{-1}]$;
$h(\hat{o}_{\grave{o},1},1)$	= steady-state potentiometric surface elevation at point 1 (a location $\hat{o}$) of location-pair $\grave{o}$, $[L]$;
$h(\hat{o}_{\grave{o},2},1)$	= steady-state potentiometric surface elevation at point 2 (a second location $\hat{o}$) of location-pair $\grave{o}$, $[L]$;
$\grave{o} \quad =$	Index denoting a pair of locations at which a head difference constraint is imposed.

Optimization results are summarized in Table B-1 and shown as model output in Figure B-2. The optimal strategy computed for Scenario 1 is much less than that developed without optimization (Scenario 1[non]). It will prevent migration toward the municipal wells. The lower bound on the sum of industrial pumping is a tight constraint. Tight constraints are those which are satisfied exactly, and prevent the objective function value from improving further. None of the head-difference constraints is tight. They are 'loose'. In other words, there is more than 0.2 or 0.15 ft (depending on the pair) difference between the heads at each two cells coupled by an arrow in Figure B-1(b).

It is appropriate to verify that the computed strategy accomplishes its goal of plume capture, despite application of the linear US/REMAX model to a nonlinear unconfined aquifer. This is done by using the optimal strategy as input to MODFLOW, simulating system response and checking the resulting gradients. Because the system is unconfined there

is a very slight error (about 0.01 percent). The error is eliminated by cycling once.

B.2.3. **Developing optimal pumping strategy without placing a lower bound on industrial pumping (Scenario 2)**

Scenario 2 differs from Scenario 1 because it does not use a lower bound on total industrial pumping (Equation V-16^s). Results in Table B-1 show that 7 percent less than Scenario 1 pumping is actually needed to prevent the plume from moving toward the municipality. The 0.2 head difference constraint between cells (16,18) and (17,18) becomes tight. That constraint prevents pumping from being even lower.

B.2.4. **Developing optimal pumping strategy which maximizes municipal pumping while minimizing industrial pumping needed to control plume migration and preventing unacceptable river dewatering (Scenario 3)**

Scenario 3 illustrates how the conflicting objectives involving river dewatering, municipal pumping and plume control can be considered. Assume the consultant wants a strategy that will: (1) maximize total municipal pumping while minimizing total industrial pumping required to satisfy the gradient constraints, (2) have at least as much pumping from each individual municipal well as occurred in Scenario 1^{non}, and (3) not cause the river to lose more water to the aquifer than Scenario 1^{non},

To accomplish this: (1) M^P in the objective function is increased to 6; -1 is used for the C^P coefficient for each industrial well and +1 is used for each municipal well; (2) individual municipal well pumping rates of Scenario 1^{non} are used as lower bounds on the absolute value of pumping in those respective wells (the upper limit on negative pumping rates); and (3) a constraint on flow from river to aquifer is used. The problem formulation is as follows,

$$\text{MINIMIZE:} \quad \sum_{\hat{a}=1}^{\bar{} } ((-1) \ p(\hat{a},1)) + \sum_{\hat{a}=4}^{\bar{}} ((1) \ p(\hat{a},1)) \qquad \text{(V-1}^s\text{)}$$

subject to:

$$p(4,1) \leq -113{,}100 \ \text{ft}^3/\text{d} \qquad \text{(V-8}^s\text{)}$$
$$p(5,1) \leq -161{,}800 \ \text{ft}^3/\text{d(V-8}^s\text{)} \qquad \text{(V-8}^2\text{)}$$

$$p(6,1) \leq -40{,}500 \ \text{ft}^3/\text{d} \qquad \text{(V-8}^s\text{)}$$

$$0.2 \ \leq \ \Omega(\hat{o},1) \quad \text{for } \hat{o} = 1 \ .. \ 5 \qquad \text{(V-34}^s\text{)}$$

$$0.15 \ \leq \ \Omega(\hat{o},1) \quad \text{for } \hat{o} = 6 \ .. \ 8 \qquad \text{(V-34}^s\text{)}$$

$$\Omega(\hat{o},1) = [h(\hat{o}_{\hat{o},1},1) - h(\hat{o}_{\hat{o},2},1)] \quad \text{for } \hat{o} = 1 \ .. \ 8 \qquad \text{(V-35}^s\text{)}$$

$$q^{SR} = \left(\sum_{\hat{u}=1}^{30} q^{sr}(\hat{u}) \right) \leq 139{,}332 \qquad \text{(V-41}^s\text{)}$$

where

q^{SR} = total flow from river to aquifer in the 30 river cells (L^3/T);

$q^{sr}(\hat{u})$ = flow from river to aquifer in river cell $\hat{u}$ (L^3/T).

Table B-1 shows the results. The river-aquifer interflow constraint becomes the tight restriction. The model directly computes municipal and industrial pumping rates that achieve the gradient constraints and avoid excessive river dewatering.

B.2.5.   Developing alternative optimal strategies

The strategy for Scenario 3 actually represents one of a set of optimal strategies for what can be considered a multiobjective optimization problem. It is multiobjective because maximizing municipal pumping and minimizing industrial pumping are two distinct and conflicting objectives. They conflict because as municipal pumping increases, industrial pumping must also increase to keep the control gradients pointed away from the municipal wells.

Alternative optimal strategies belonging to the Pareto Optimum (set of optimal strategies) are shown in the curve of Figure B-3. Each point on the curve represents one optimal strategy that satisfies the gradient constraints. Here these are developed using the E-constraint method. (The lower bound on total pumping from industrial wells is relaxed in these other optimizations.) This technique is explained in Section B.3. Here, the objective function is: maximize municipal pumping. The constraints include bounds on hydraulic gradient and a bound on the sum of industrial pumping. (A lower bound is used because pumping extraction is negative, thus this functions as an upper bound on the absolute value of industrial pumping.)

This pareto optimum helps involved parties understand the tradeoffs between municipal pumping, industrial pumping, and river-aquifer interflow. A compromise strategy acceptable for all users can be selected from this curve.

FIGURE B-2. Optimal pumping strategy for Scenario 1, Cycle 2.

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    US/REMAX: Response Matrix Model For Conjunctive Groundwater Management
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Model status:  OPTIMAL SOLUTION FOUND
Objective value (Z): 267380.0


SOLVER USED IS  BDMLP
=============================================================================
OPTIMAL GROUNDWATER PUMPING RATES p(â,k), EXTRACTION(-) AND INJECTION(+),
[L^3/T]

CELL    STRESS PERIOD    L.BOUND      OPTIMAL      U.BOUND      MARGINAL
PE(â)        k           pL(â,k)      p(â,k)       pU(â,k)      ₐZ / ₐp(â,k)


  1          1         -1.0000E+8    -2.6738E+5    0.0000       0.0000
  2          1         -1.0000E+8     0.0000       0.0000       0.0000
  3          1         -1.0000E+8     0.0000       0.0000       0.0000
=============================================================================
OPTIMAL PUMPING RATES FOR GROUPS OF CELLS, pG(à,k), [L^3/T]

GROUP   STRESS PERIOD    L.BOUND      OPTIMAL      U.BOUND      MARGINAL
pg(à)        k           pGL(à,k)     pG(à,k)      pGU(à,k)     ₐZ / ₐpG(à,k)

  1          1         -1.000E+10    -2.6738E+5   -2.6738E+5    -1.0000
=============================================================================
OPTIMAL HYDRAULIC HEADS, h(ô,k), [L]

CELL    STRESS PERIOD    L.BOUND      OPTIMAL      U.BOUND      MARGINAL
HC(ô)        k           hL(ô,k)      h(ô,k)       hU(ô,k)      ₐZ / ₐh(ô,k)

  1          1         800.0000      870.3059     1000.0000     0.0000
  2          1         800.0000      870.2161     1000.0000     0.0000
  3          1         800.0000      870.1369     1000.0000     0.0000
  4          1         800.0000      870.0479     1000.0000     0.0000
  5          1         800.0000      869.9536     1000.0000     0.0000
  6          1         800.0000      869.6714     1000.0000     0.0000
  7          1         800.0000      869.5876     1000.0000     0.0000
  8          1         800.0000      869.5002     1000.0000     0.0000
  9          1         800.0000      870.0615     1000.0000     0.0000
 10          1         800.0000      869.9766     1000.0000     0.0000
 11          1         800.0000      869.9045     1000.0000     0.0000
 12          1         800.0000      869.8273     1000.0000     0.0000
 13          1         800.0000      869.7491     1000.0000     0.0000
 14          1         800.0000      869.4786     1000.0000     0.0000
 15          1         800.0000      869.4148     1000.0000     0.0000
 16          1         800.0000      869.3426     1000.0000     0.0000
=============================================================================
OPTIMAL HYDRAULIC HEAD DIFFERENCE / GRADIENT / VELOCITY, Ω(ô,k),
[L, L/L, or L/T]

PAIR    FROM   TO   STRESS PERIOD  L.BOUND    OPTIMAL    U.BOUND    MARGINAL
HGV(ò)  ô(ò,1)  ô(ò,2)      k      ΩL(ò,k)    Ω(ò,k)     ΩU(ò,k)    ₐZ / ₐΩ(ò,k)
  1      1  ->  9          1       0.2000     0.2444     0.272      0.0000
  2      2  ->  10         1       0.2000     0.2395     0.267      0.0000
  3      3  ->  11         1       0.2000     0.2324     0.260      0.0000
  4      4  ->  12         1       0.2000     0.2206     0.249      0.0000
  5      5  ->  13         1       0.2000     0.2045     0.233      0.0000
  6      6  ->  14         1       0.1500     0.1929     0.270      0.0000
  7      7  ->  15         1       0.1500     0.1729     0.180      0.0000
  8      8  ->  16         1       0.1500     0.1576     0.270      0.0000
=============================================================================
SUMMARY OF OPTIMAL PUMPING RATES  [L^3/T]

STRESS PERIOD       SUM OF PUMPING RATES      SUM OF ABS. PUMPING RATES
      1                 -2.6738E+5                  2.67380E+5
```
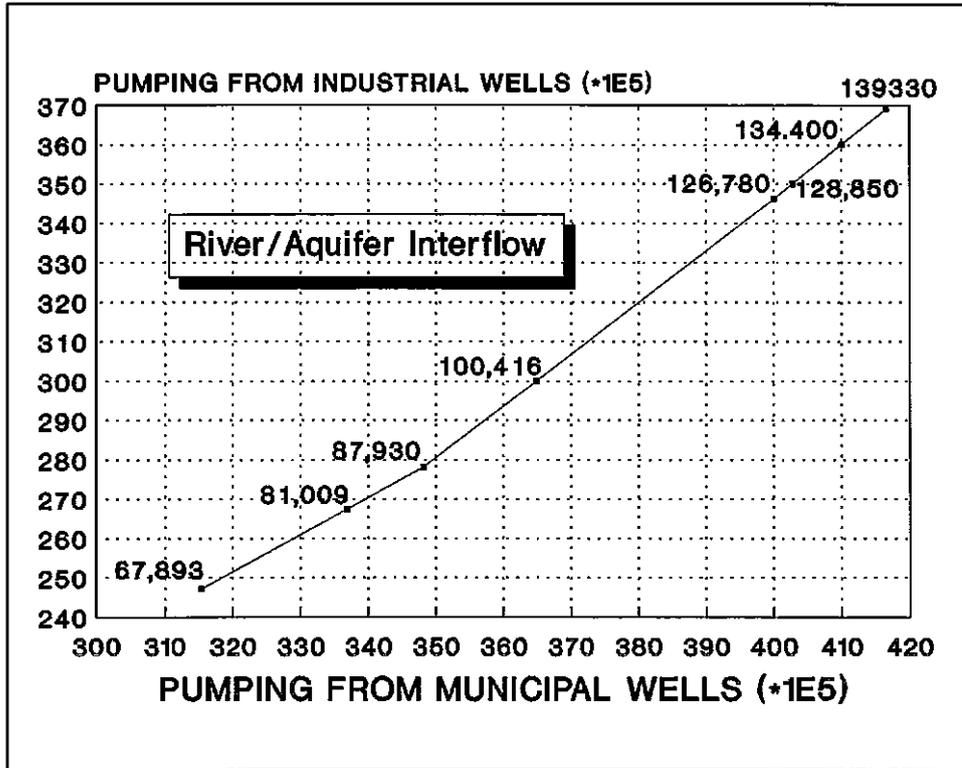
FIGURE B-3. Relation between total pumping from municipal wells and total pumping from industrial wells

B.3. Two Techniques of Pareto Optimum Development
in Multiobjective Optimization

B.3.1 Introduction

Two of the basic methods for addressing multiobjective optimization problems are presented here. Assume a situation in which the cost of using groundwater can become prohibitive. As one extracts more groundwater, water levels drop, pumping cost increases, and net return decreases. This situation will be addressed using two methods.

Assumed will be the conflicting objectives of maximizing total groundwater pumping (extraction) and maximizing total net return. The range of total pumping or net return in which these objectives conflict is termed the pareto optimum (noninferior solution set, set of nondominated solutions). For this problem, the pareto optimum can be drawn, as a 2-dimensional curve, having total pumping and total net return as the two axes. One cannot move in any direction on the pareto optimum without "hurting" one objective, although the other objective might be improved. In other words, on the pareto optimum, one cannot improve one objective function without hurting the other(s).

B.3.2. Weighting approach :

B.3.2.1 Model

Objective Function: Maximize W_1(sum of pumping) + W_2(net return)
Subject to: Equations describing the sytem and involving the two objectives.

B.3.2.2 Procedure for developing the Pareto Optimum

-Perform different optimizations using different values of W_1 and W_2.
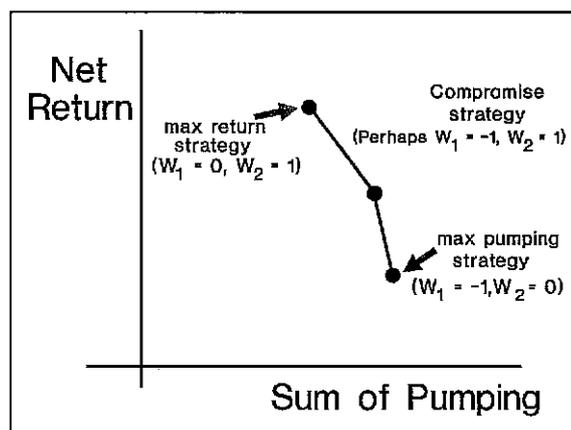-Plot the results on a graph in which the axes represent the conflicting objectives.

Figure B-4. Weighting method

B.3.3. E-Constraint method :

B.3.3.1 Models

Model 1
Objective Function: Maximize sum of pumping (set $W_2=0$)
Subject to: Equations describing the system and involving the two objectives.
Calculate net return for the resulting optimal strategy.

Model 2
Objective Function: Maximize net return
Subject to: Equations describing the system and involving the two objectives.
Sum of pumping $\geq$ X.

B.3.3.2 Procedure for developing the Pareto Optimum:

-Apply Model 1 to determine maximum pumping possible.
-Apply Model 2 without considering total pumping (X = 0)
-Apply Model 2 with different X values. X should range from 0 to the value
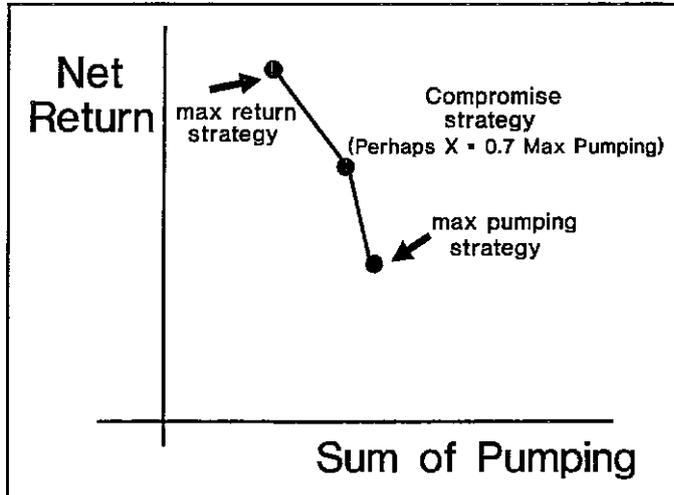calculated in the first step.
-Plot net return versus sum of pumping for each optimal strategy developed.

Figure B-5. E-Constraint method