THE RESPONSE EQUATION METHOD: A NEW ROLE FOR SIMULATION OF ENVIRONMENTAL SYSTEMS

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Management of complex environmental systems described by linear, or non-linear partial differential equations is typically accomplished by simulation of the response of the environmental system to alternative planning strategies. The equations describing the physical, chemical and/or hydrologic processes occurring within the environmental system are transformed using numerical techniques into systems of linear equations. Following verification of the historical state variable regime the equations may be solved routinely for given boundary and initial conditions and most importantly, given management decisions. That is the response of the system, i.e., the variation in the state variables of the system, is determined as a consequence of the assumed management decisions. For differing combinations of management alternatives, the simulation must be performed again. Clearly for a large number of alternative strategies, the efficacy of a particular strategy may be difficult to determine especially in view of the possible interactions between the state variables of the environmental system. Purely economic considerations often preclude the examination of all the possible combinations of planning alternatives.

In the past, some of these problems have been obviated by using a mixture of mathematical programming and simulation. In the planning and design of surface water systems, an optimization model is formulated to act as a preliminary screening model for selection of management alternatives which best meet the objectives defined within the optimization model. The solutions of the model, the optimal planning strategies, are then simulated to see if they do not represent, in a local sense, optimal management of the environmental system. In many cases however, the mathematical programming model is a simplified representation of the environmental system. The optimal planning strategies may or may not simulate the response of the system when other more complicating physical or hydrologic processes are considered.

A new technique, the response equation method, is presented to address these problems in the management of point and non-point sources of pollution in surface and groundwater systems. The technique begins with the partial differential equations describing the mass transport of contaminants within surface or groundwater systems. The equations are transformed using numerical techniques. The resulting system of equations is then imbedded in the constraint set of the management model: all of the assumed physical processes taking place within the system are implicit within the optimization model. The solution of the programming problem, the optimal management decisions, are then predicated upon the actual response of the environmental system. More importantly however is the fact that all the possible management decisions are considered within the optimization model, in contrast to strictly a simulation approach which at best can consider a limited number of management alternatives.

The Management Model

The management or planning problem for an environmental system is to maximize or minimize an objective function $f(\underline{u},\phi)$ whose value depends upon the management decisions, $\underline{u}$, and possibly the state variables of the system, ϕ. The function can represent benefits, costs, or purely physical objectives such as minimizing the deviations from desired states of the system. The decisions are limited by a constraint set, X, which defines the feasible ranges of the decision alternatives, environmental quality constraints, and possibly budgetary limitations. Mathematically the problem may be formulated as*

*We limit the discussion to single objective planning problems. The formulation for multiple objective optimization is conceptually similar.

$$\min_{\underline{u}\in X} f(\underline{u},\phi) \tag{1}$$

The relationship between the state, ϕ, and decision variables of the system is described in general by a system of partial differential equations, reflecting conservation of mass, energy, or momentum within the system. Considering the mass transport of constituents within surface and groundwaters the governing equation may be written,

$$L\,\{\phi\} = 0 \tag{2}$$

$$C\,(\phi) = 0 \text{ on } \delta$$

where we assume L is a linear, differential operator, δ is the boundary of the system on which C is satisfied, and ϕ is the dependent variable, the state variable of the system. In many management models, the system's partial differential equations are simplified to such an extent, that analytical solutions are often obtained expressing the state variables of the system as a function of the possible management decisions. Often however, such equations bare little semblance to the complex physical processes actually occurring within the environmental system.

The Response Equation Method

The response equation method begins with the partial differential equations characterizing the environmental system. The equations are transformed using finite differences, finite elements, or in absence of a variational principle, the method of weighted residuals (the Galerkin method). Restricting our attention to parabolic partial differential equations which describe contaminant transport in surface and groundwaters, the Galerkin procedure begins by assuming that a solution to equation (2) may be represented by

$$\phi \simeq \hat{\phi} = \sum_{i=1}^{n} N_i\,(x,y)\,\tilde{\phi}_i\,(t) \tag{3}$$

where N_i are Lagrangian shape, basis or coordinate functions which are assumed to be linearly independent and to satisfy the boundary conditions of the system. The $\tilde{\phi}_i$ are undetermined coefficients which are equal to the value of the dependent variable at selected node points within the system. Since we are approximating the solution of the equation by a finite series, there will be associated with the approximation a non-zero residual. The Galerkin method minimizes the residual by requiring the orthogonality of the basis functions and the differential operator L over the domain D

$$\int_D L\,\{\sum_{j=1}^{n} N_j\,\tilde{\phi}_j\}\,N_i dD = 0,\ \forall_i \tag{4}$$

Using Green's theorem for evaluation of second-order and higher derivatives in order to avoid the imposition of continuity conditions between adjacent elements, the orthogonality conditions produces a set of first-order ordinary differential equations or

$$A\,\frac{d\tilde{\phi}}{dt} + B\tilde{\phi} + \underline{f} + \underline{g}\,(\underline{u}) = \underline{0} \tag{5}$$

The matrices A and B are dependent upon the parameters of the environmental system and the basis function (triangular, isoparametric, Hermitian). The components of the $\underline{f}$ vector contain the boundary conditions of the system. The $\underline{g}$ vector however depends implicitly upon the management decisions, $\underline{u}$. Generally the vector will contain the point and non-point sources of contaminants introduced to the system. The management problem is concerned with the control of the contaminant sources so as to maintain environmental quality standards from a public health, economic, or aesthetic point of view.

The response equations of the system, equation (5), may be directly imbedded within the constraint set of the mathematical model. If the problem is a steady-state management problem then we have

$$B \underline{\tilde{\phi}} + \underline{f} + \underline{g}(\underline{u}) = \underline{0} \tag{6}$$

which forms a set of linear equality constraints. In this case we may solve for the state variables in terms of the management decisions directly through performing the matrix inversion, $\underline{\tilde{\phi}} = -B^{-1}(\underline{f} + \underline{g}(\underline{u}))$. Or we may consider the state variables as an augmented set of decision variables which are determined as a by-product of the optimization procedure (1, 15, 16).

In the dynamic case, the response equations may be imbedded within the constraint equations by discretizing the time derivatives using fully implicit numerical techniques. The response equations, the equality constraints, are then written for each time step over the planning period. The mathematical programming problem that involves an optimization over all of the discrete planning intervals.**

However, it is also possible to obtain an analytical relationship between the state and decision variables of the system. The response equation, equation (5), is a linear system of first-order ordinary-differential equations. The general solution of the system is given by(3).

$$\underline{\phi}(t) = e^{Dt}\underline{\phi}_o + (D^{-1}e^{Dt} - D^{-1})(-A^{-1}\underline{f} - A^{-1})\underline{g}(\underline{u}) \tag{7}$$

where

$D = -A^{-1}B$

$\underline{\phi}_o$ = initial condition of ϕ

The exponential terms may be evaluated using the Cayley-Hamilton Theorem, or

$$\underline{\phi}(t) = M\lambda_t M^{-1}\underline{\phi}_o + (D^{-1}M\lambda_t M^{-1} - D^{-1})(-A^{-1}\underline{f} - A^{-1}\underline{g}(\underline{u})) \tag{8}$$

where the M matrix is composed of the eigenvectors of D and λ_t is a diagonal matrix with the elements $[e^{\lambda_k t}]$. The λ_k's are the eigenvalues of D.

Equation (8) expresses the temporal variation of the state variables of the system as a linear function of the management decisions, $\underline{u}$. When decisions are made over a sequence of planning periods, equation (8) may be used recursively to generate the relationships between the state variables of the system and any previous management decisions. For example, $\underline{\phi}_o$ is the initial state vector of the system. In each succeeding planning period, $\underline{\phi}_o$ depends upon the decisions made in the previous planning periods. Defining the length of a planning period as τ and $\underline{u}^\tau$ as the decisions made at the beginning of period τ, then we have at the end of any planning period

$$\underline{\phi}(\tau) = M\lambda_{t=\tau}M^{-1}\underline{\phi}(\underline{u}^{\tau-1},\ldots\underline{u}^{o}) + (D^{-1}M\lambda_{t=\tau}M^{-1} - D^{-1})\cdot$$

$$(-A^{-1}\underline{f} - A^{-1}\underline{g}(\underline{u}^\tau)) \tag{9}$$

$\underline{\phi}(\tau)$ becomes the initial conditions for the $\tau+1$ planning period.

A similar expression can be written for all τ up to T_{max}, the total length of the planning horizon. The equations may then be substituted directly into the management model to eliminate the model's explicit dependence upon the state variables, $\underline{\phi}$. Either approach leads to a management model predicated upon the response characteristics of the environmental system. The discretized approach however is the more general; for problems with complex objective functions the substitution of equation (8), may obviate the simplifications introduced by the analytical solution approach.

**Alternatively, the entire management problem may be reformulated as a problem in optimal control where the response equations now become the equations of motion of the system and the objective function becomes a functional whose value depends upon the state and decision variables (7).

Following the discretized approach, the management problem may then be rewritten as

$$\min \sum_{\tau=1}^{T_{max}} f_\tau(\underline{u}^\tau, \underline{\phi}^k) \tag{10a}$$

$$A\left\{\frac{\underline{\tilde{\phi}}^k - \underline{\tilde{\phi}}^{k-1}}{\Delta t}\right\} + B\underline{\tilde{\phi}}^k + \underline{f} + \underline{g}(\underline{u}^\tau) = \underline{0}\ ,\ k=1,\ldots\tau,\ \tau=1,\ T_{max} \tag{10b}$$

$$\tilde{\phi}_j^{\,k} \in \chi\ ,\ \forall k \tag{10c}$$

$$\underline{\phi}^k,\ \underline{u}^\tau \geq 0\ ,\ \forall k,\ \tau \tag{10d}$$

where τ is the length of each planning period, and T_{max} is the length of planning horizon, and Δt is the discretized time step within each planning period, and f_τ is the system objective for each planning period. The constraint set is defined by response equations, the non-negativity of the state and decision variables, and the set χ, representing all points within the system where environmental quality standards are to be maintained.

Equations (10a-10d) define the mathematical programming problem for optimal management or control of the environmental system subject to point and non-point contaminant loadings. Note that the constraint equation encompasses all of the physical, biochemical relationships present in the governing system equation (for example dispersion, molecular diffusion, biochemical reations).

An Example

Consider the management problem of optimal control of groundwater quality in an unconfined aquifer. Municipal wastewaters are to be injected to the zone of saturation of the aquifer following pre-treatment. The groundwater aquifer is to conjunctively serve as a waste disposal sink for the municipal wastewaters and as a potential source of water supply. The planning problem is one of defining the effluent discharge standards for the groundwater basin to prevent excessive deterioration of the quality of the native groundwater. That is water quality constraints are maintained throughout the aquifer system.

Assuming that the fluid within the aquifer is homogeneous, i.e., of constant density and viscosity, and that the vertical flows within the aquifer are insignificant, the flow and mass transport equations characterizing the groundwater system are (4, 8)

$$\nabla \cdot T\,\nabla h - \sum_{i\in\Omega} Q_i\,\delta(\underline{x}-\underline{x}_i) = S\frac{\partial h}{\partial t} \tag{11a}$$

$$\nabla \cdot \underline{D}\,\nabla c^\rho - \nabla \cdot c^\rho\underline{q} - \sum_{i\in\Omega} Q_i c^{*\rho}_i\,\delta(\underline{x}-\underline{x}_i) - k_s^{\,\rho}c^\rho - (1-n)k_a^{\,\rho}A^\rho = \frac{\partial}{\partial t}(nc^\rho + (1-n)A^\rho) \tag{11b}$$

where

T is the transmissivity tensor, L^2/T
h is the hydraulic head (L)
$\underline{D}$ is the dispersion tensor (L^2/T)
S is the storage coefficient (L^0)
$\underline{q}$ is the mass average velocity $[L/T]$
Q_i is the injection rate $[L^3/T]$
$c^{*\rho}$ is the concentration of constituent ρ injected at site i $[M/L^3]$
n is the porosity (L^0)
Ω is the set of all injection sites within the basin
δ is the Dirac delta function
c^ρ is the concentration of constituent ρ $(\frac{M}{L^3})$
A^ρ is the concentration of constituent ρ in the adsorbed phase $(\frac{M}{L^3})$
$k^\rho_{s,a}$ are the reaction coefficients in the solution and adsorbed phases (1/T).

The assumptions are made that biochemical degradation is represented by a first-order reaction (5, 10, 11), and that adsorption follows the linear equilibrium adsorption isotherm.

Assuming that the injection rates and locations have been determined in a prior groundwater screening model, the flow equations may be solved using the Galerkin procedure (13). From Darcy's law, the mass average velocity may be determined to calculate the convective mass transport and the magnitude of hydrodynamic dispersion occuring within the system (2). Again performing the method of weighted residual, the covective-dispersion equation becomes,

$$E\,\underline{c}^{\rho} + F\frac{d\underline{c}^{\rho}}{dt} + \underline{R} + \underline{M} = 0 \quad \rho\epsilon\Gamma \tag{12a}$$

The transformed equation holds for each constituent within the aquifer, $\rho\epsilon\Gamma$, where Γ is the set of all constituents. The matrix elements are defined as

$$E_{ij} = \int_A \{D^*_{k\ell}\frac{\partial N_i}{\partial x_k}\frac{\partial N_j}{\partial x_\ell} + q_k N_i \frac{\partial N_j}{\partial x_k} + N_i N_j \frac{\partial q_k}{\partial x_k} - k^{*\rho} N_i\}\, dA \tag{12b}$$

$$F_{ij} = \int_A \hat{n}\, N_i\, N_j\, dA \tag{12c}$$

$$R_i = -\int_\delta N_i\, D_{k\ell}\frac{\partial}{\partial x_\ell}\left(\sum_{m=1}^{n} c^{\rho}_m N_m\right)\ell_k d\delta \tag{12d}$$

$$M_i = \int_\Omega N_i \sum_{j\epsilon\Omega} Q_j\, c^*{}_j^{\rho}\, \delta(\underline{x}-\underline{x}_i)\, dA \tag{12e}$$

where ℓ_k are the direction cosines associated with boundary δ.

The k, ℓ notation indicates variation in the x and y variables. $\hat{n}$ and k^* are lumped parameter values reflecting the effects of adsorption and the kinetic reactions (16). Note that the components of $\underline{M}$, M_i depends explicitly upon the source concentrations entering the groundwater system.

Defining $\epsilon^{\rho}{}_{\tau}$ as the percentage removal efficiency of constituent ρ (the effluent standards), in planning period τ then we can write

$$c^*{}_j^{\rho}\,(1-\epsilon^{\rho}{}_{\tau}) \tag{13}$$

as the concentration of constituent ρ entering the groundwater system. Let C^{ρ} be the cost of obtaining the effluent standards $\epsilon^{\rho}{}_{\tau}$. Defining χ as the set of control points within the aquifer where water quality constraints are to be maintained, i.e., the groundwater quality is constrained to less than or equal to the prevailing groundwater quality standards, $\tilde{c}^{*\rho}$, then the planning model may be written as

$$\min \sum_{\tau=1}^{T_{max}} \frac{\sum_{\rho\epsilon\Gamma} C_{\rho}\,(\epsilon_{\tau}{}^{\rho})}{(1+\rho)^{\tau}} \tag{14a}$$

$$E\underline{c}^{\rho} + F\underline{c}^{\rho}{}_k - F\underline{c}^{\rho}{}_{k-1} + \underline{R} + \underline{M}\,(\underline{\epsilon}^{\tau}) = 0 \quad \rho\epsilon\Gamma,\ k=1,\ldots\tau,$$

$$\tau=1,\ldots T_{max} \tag{14b}$$

$$c^{\rho}{}_j \leq \tilde{c}^{*\rho},\ j\epsilon\chi,\ \rho\epsilon\Gamma \tag{14c}$$

$$0 \leq \epsilon^{\rho}{}_{\tau} \leq 1,\ \rho\epsilon\Gamma,\ \forall\tau \tag{14d}$$

$$\underline{c}^{\rho}{}_k,\ \epsilon^{\rho}{}_{\tau} \geq 0,\ \rho\epsilon\Gamma,\ \forall k,\ \tau \tag{14e}$$

The planning model minimizes the sum of the discounted costs over the entire planning horizon, $\tau=1,\ldots T_{max}$ (ρ is the assumed discount rate). The response equations, equation (14b), are written over a Δt increment within each planning period. For example, if the length of a planning period is τ, then there are $\tau/\Delta t$ response equations for each constituent. Equation (10c) ensures that the groundwater quality does not degrade to the extent that the water supply becomes degraded. Again the state variables, the constituent concentrations are considered as an augmented set of decision variables. The solution of the mathematical programming problem gives the optimal effluent standards, $\epsilon^{\rho}{}_{\tau}$, to prevent degradation of the subsurface environment (the results are discussed in 16, 17).

Final Comments

The response equation method is a practical tool for the management of surface and groundwater quality systems. The technique has been extended to include conjunctive ground and surface wastewater treatment and to delineate the effects on the groundwater environment of the land application of municipal wastewaters (15, 16, 17).

The important point however is that in using the response equation method, the decision variables enter linearly into the response equations. By considering the concentrations of the various constituents as an augmented set of decision variables, the constraint set becomes separable, and convex. The implications of this should be quite clear, for there are numerous algorithms for solution of mathematical programming problems with convex constraint sets. Depending upon the form of the objective function, i.e., whether the function is concave or convex, algorithms such as the Frank-Wolfe algorithm(16), Tui's method (14) or piece-wise separable convex programming may be applicable. The response equation method increases the number of variables for a management problem: a consequence of considering the state variables as psuedo decision variables. However, the structure of the model permits efficient solution of the management problem. Of primary importance, however, is that the management problem encompasses all of the physical processes originally defined in a pure simulation of the problem. The optimal management decisions are then based upon the actual response of the environmental system.

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