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Techniques of Water-Resources Investigations
of the United States Geological Survey

Chapter B4

REGRESSION MODELING OF GROUND-WATER FLOW

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Book 3
APPLICATIONS OF HYDRAULICS

For two parameters, b_1 and b_2, the relationships given by equation 3.3-27 are illustrated in figure 3.3-5. (Note the use of scaled parameters; see equation 3.3-17.)

If $\Theta=90°$, then, as discussed in section 3.3.1, no improvement in parameters is likely to result from application of the Gauss-Newton procedure. However, application of the Marquardt parameter, $\mu>0$, will result in $\Theta<90°$ (Marquardt, 1963) because vector $\underline{\delta}$ is shifted progressively toward $\underline{g}$ as μ increases. Thus, a viable scheme for choosing μ is to define a maximum value of Θ, $\Theta_{mx}<90°$, and compute μ so that Θ never exceeds Θ_{mx}. This can be accomplished rather simply. At the beginning of the regression set $\mu_0=0$. Then at each iteration r, check and recompute μ as necessary:

$$\left.\begin{aligned}&\mu_r=\mu_\ell\\&\text{if } \underline{\delta}_{r+1}^T\underline{g}_r\geq\cos\Theta_{mx}\sqrt{(\underline{\delta}_{r+1}^T\underline{\delta}_{r+1})(\underline{g}_r^T\underline{g}_r)} \text{ or}\\&\mu_{\ell+1}=\frac{3}{2}\mu_\ell+0.001\\&\text{if } \underline{\delta}_{r+1}^T\underline{g}_r<\cos\Theta_{mx}\sqrt{(\underline{\delta}_{r+1}^T\underline{\delta}_{r+1})(\underline{g}_r^T\underline{g}_r)}\end{aligned}\right\} \quad (3.3\text{-}28)$$

At the beginning of iteration r, $\ell=1$ and $\mu_\ell=\mu_{r-1}$. Then equation 3.3-20 is solved and equation 3.3-28 is applied. If the second part of equation 3.3-28 is employed, equation 3.3-20 is resolved using $\mu_{\ell+1}$, ℓ is incremented by one, and equation 3.3-28 is used again. This process is continued until the first part of equation 3.3-28 is used, at which point the appropriate value of μ for iteration r has been found. The formula for computing $\mu_{\ell+1}$ from μ_ℓ is empirical but gives what experience has shown to be a good range in values of μ. For each resolution of equation 3.3-20, $\underline{S}_r^T\underline{\omega}\,\underline{S}_r$ and $\underline{g}_r$ are not recomputed. Thus, the calculations are not extensive.

Computation of ρ is designed to prevent disastrous overshoot and to keep $\rho\underline{\delta}$ within the region R defined by equation 3.3-25. A simple but usually effective scheme is to estimate the maximum fraction that any of the parameters could change and still remain within R and then to prevent any parameter from changing any more than this amount over any iteration. Let t_{mx} be this maximum fractional change. Then at iteration r, ρ is calculated as follows:

$$t=\max_i|d_i^{r+1}/c| \quad (3.3\text{-}29)$$

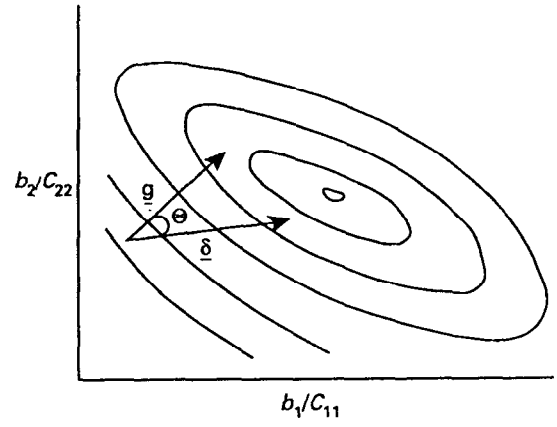

Figure 3.3-5

$$\left.\begin{aligned}&\rho=1 \text{ if } t\leq t_{mx} \text{ or}\\&\rho=t_{mx}/t \text{ if } t>t_{mx}\end{aligned}\right\} \quad (3.3\text{-}30)$$

where $c=b_i^r$ if $b_i^r\neq 0$ and $c=1$ if $b_i^r=0$.

3.4 Regression Including Prior Information

3.4.1 Model Structure

Recall that the standard nonlinear regression model including prior information on the parameters may be written in the form (equation 3.1-32)

$$\underline{Y}=\underline{f}(\underline{\xi},\underline{\beta})+\underline{\epsilon} \quad (3.4\text{-}1)$$

where

$$\underline{Y}=\begin{bmatrix}\underline{Y}_s\\ \underline{Y}_p\end{bmatrix} \quad (3.4\text{-}2)$$

$$\underline{f}(\underline{\xi},\underline{\beta})=\begin{bmatrix}\underline{f}_s(\underline{\xi},\underline{\beta})\\ \underline{f}_p(\underline{\xi},\underline{\beta})\end{bmatrix} \quad (3.4\text{-}3)$$

$$\underline{\epsilon}=\begin{bmatrix}\underline{\epsilon}_s\\ \underline{\epsilon}_p\end{bmatrix} \quad (3.4\text{-}4)$$

and subscripts s and p indicate sample and prior information, respectively. To correspond with the above partitions into sample and prior information, the sensitivity matrix should be written in the form

$$\underline{\underline{X}}=\begin{bmatrix}\underline{\underline{X}}_s\\ \underline{\underline{X}}_p\end{bmatrix} \tag{3.4-5}$$

where $\underline{\underline{X}}$ is a function of $\underline{\beta}$ for a nonlinear model. The transformation of $\underline{\underline{X}}$ to $\underline{\underline{S}}$ used to control round-off error is defined analogously. Finally, recall that the weight matrix is partitioned as

$$\underline{\underline{\omega}}=\begin{bmatrix}\underline{\underline{\omega}}_s & \underline{\underline{0}}\\ \underline{\underline{0}} & \underline{\underline{\omega}}_p\end{bmatrix} \tag{3.4-6}$$

where $\underline{\underline{\omega}}_s$ and $\underline{\underline{\omega}}_p$ correspond to sample and prior information, respectively.

Often partition $\underline{\underline{X}}_p$ will be obtained in a different manner than $\underline{\underline{X}}_s$. For example, the model for the sample information may be numerical of the type in equation 3.3-22, whereas the model for the prior information may be of the analytical linear or nonlinear form. Thus, $\underline{\underline{X}}_s$ would be obtained as described in section 3.3.2, and $\underline{\underline{X}}_p$ would be obtained as described in section 3.3.1. Other types of differences are handled in a similar fashion. Obviously, if sample and prior models are of the same type, then $\underline{\underline{X}}_s$ and $\underline{\underline{X}}_p$ are obtained in the same manner.

Despite the possibilities for combinations of linear, nonlinear, analytical, and numerical models, remember that all models have the general form of the incremental linear model when expanded in the Taylor series. Because all models resolve to the incremental linear form, for simplicity subsequent discussions in this section are based on this model only.

3.4.2 Solution Procedures

Whenever $\underline{\underline{\omega}}_s$ and $\underline{\underline{\omega}}_p$ are both known, solution for both linear and nonlinear models is unaltered from that given in the previous sections. However, recall that, because of the block diagonal form of equation 3.4-6, $S(\underline{b})$ and, hence, the normal equations can be written in a special form. By applying the standard minimization technique to $S(\underline{b})$ as given by equation 3.1-42, which can be written in the form

$$S(\underline{b})=[\underline{e}_s^T,\underline{e}_p^T]\begin{bmatrix}\underline{\underline{\omega}}_s & \underline{\underline{0}}\\ \underline{\underline{0}} & \underline{\underline{\omega}}_p\end{bmatrix}\begin{bmatrix}\underline{e}_s\\ \underline{e}_p\end{bmatrix}, \tag{3.4-7}$$

the normal equations for the incremental linear model become

$$[\underline{\underline{X}}_s^T,\underline{\underline{X}}_p^T]\begin{bmatrix}\underline{\underline{\omega}}_s & \underline{\underline{0}}\\ \underline{\underline{0}} & \underline{\underline{\omega}}_p\end{bmatrix}\begin{bmatrix}\underline{\underline{X}}_s\\ \underline{\underline{X}}_p\end{bmatrix}(\hat{\underline{b}}-\underline{b})$$

$$=[\underline{\underline{X}}_s^T,\underline{\underline{X}}_p^T]\begin{bmatrix}\underline{\underline{\omega}}_s & \underline{\underline{0}}\\ \underline{\underline{0}} & \underline{\underline{\omega}}_p\end{bmatrix}\begin{bmatrix}\underline{Y}_s-\underline{f}_s(\underline{\xi},\underline{b})\\ \underline{Y}_p-\underline{f}_p(\underline{\xi},\underline{b})\end{bmatrix} \tag{3.4-8}$$

or

$$(\underline{\underline{X}}_s^T\underline{\underline{\omega}}_s\underline{\underline{X}}_s+\underline{\underline{X}}_p^T\underline{\underline{\omega}}_p\underline{\underline{X}}_p)(\hat{\underline{b}}-\underline{b})$$

$$=\underline{\underline{X}}_s^T\underline{\underline{\omega}}_s(\underline{Y}_s-\underline{f}_s(\underline{\xi},\underline{b}))+\underline{\underline{X}}_p^T\underline{\underline{\omega}}_p(\underline{Y}_p-\underline{f}_p(\underline{\xi},\underline{b})) \tag{3.4-9}$$

where $\underline{f}_s(\underline{\xi},\underline{b})$ and $\underline{f}_p(\underline{\xi},\underline{b})$ are for sample and prior information, respectively. Equation 3.4-9 is of the same form, and thus applies, as the equation for each iteration of solution of a nonlinear regression problem.

Frequently, the weight matrix is constructed from variance-covariance matrices for $\underline{\epsilon}_s$ and $\underline{\epsilon}_p$ that are given in the form

$$\mathrm{Var}(\underline{\epsilon}_s)=\underline{\underline{V}}_s\sigma^2 \tag{3.4-10}$$

$$\mathrm{Var}(\underline{\epsilon}_p)=\underline{\underline{U}} \tag{3.4-11}$$

where the usual form $\underline{\underline{V}}_p\sigma^2$ for equation 3.4-11 cannot be used because $\mathrm{Var}(\underline{\epsilon}_p)$ is not known as a function of σ^2. Thus, with $\underline{\underline{\omega}}$ defined as

$$\underline{\underline{\omega}}=\begin{bmatrix}[\mathrm{Var}(\underline{\epsilon}_s)]^{-1} & \underline{\underline{0}}\\ \underline{\underline{0}} & [\mathrm{Var}(\underline{\epsilon}_p)]^{-1}\end{bmatrix}\sigma^2$$

$$=\begin{bmatrix}\underline{\underline{V}}_s^{-1} & \underline{\underline{0}}\\ \underline{\underline{0}} & \underline{\underline{U}}^{-1}\sigma^2\end{bmatrix} \tag{3.4-12}$$

then equation 3.4-9 becomes

$$(\underline{X}_s^T\underline{V}_s^{-1}\underline{X}_s+\underline{X}_p^T\underline{U}^{-1}\underline{X}_p\sigma^2)(\hat{\underline{b}}-\underline{b})$$

$$=\underline{X}_s^T\underline{V}_s^{-1}(\underline{Y}_s-\underline{f}_s(\underline{\xi},\underline{b}))$$

$$+\underline{X}_p^T\underline{U}^{-1}\sigma^2(\underline{Y}_p-\underline{f}_p(\underline{\xi},\underline{b})). \qquad (3.4\text{-}13)$$

Hence, σ^2 apparently would have to be known to form the regression solution, whereas σ^2 is considered to be an unknown.

Theil (1963) showed that, for a linear model, σ^2 may be estimated for use in equation 3.4-13 by its ordinary least squares estimate (that is, the estimate obtained when prior information is not used). Bias produced by this estimate was shown by Theil (1963) to be of the order of $n_s^{-1/2}$. The procedure to be followed is to first solve the ordinary least squares problem by omitting all prior information; then find the estimate of σ^2 (to be given further on); finally use this estimate of σ^2 in the normal equations to solve the complete problem, including prior information.

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4 Numerical Nonlinear Regression Solution of General Steady-State Ground-Water Flow Problems

4.1 Assumed Model and Solution Procedure

A model to solve fairly general steady-state ground-water flow problems by using the regression procedures presented in section 3 is given in this section. A complete description of the method is given first. Documentation and listing of the computer program are given in the appendix, section 4.3.4.

4.1.1 Problem Specification

The equation assumed to govern ground-water flow for the class of problems to be analyzed is derived from equation 1.1-1 by letting $\partial h/\partial t \rightarrow 0$, which results in

$$\frac{\partial}{\partial x}(T_{xx}\frac{\partial h}{\partial x})+\frac{\partial}{\partial y}(T_{yy}\frac{\partial h}{\partial y})+R(H-h)+W$$

$$+\sum_{\ell=1}^{N}\delta(x-a_\ell)\delta(y-b_\ell)Q_\ell=0\ , \qquad (4.1\text{-}1)$$

where the symbols are defined the same as for equation 1.1-1.

Functions $T_{\xi\xi}$ (that is, T_{xx} and T_{yy}), R, and W are each formulated within the region being modeled as the product of a parameter and a given (or known) function. To provide for spatial variability of parameters, the region is subdivided into a number of discrete zones within each of which the parameters are assumed constant. Hence, known spatial variability (often, but not necessarily, smooth or continuous) is superimposed upon the discontinuous spatial variability dictated by the parameter zonation. As an example, hydraulic conductivity $K_{\xi\xi}$ may often be considered to be constant within particular rock types, each of which may be considered to be a discrete zone. Thus $K_{\xi\xi}$ may be considered to be a parameter. Thickness b may be known from measurements and may vary continuously. The function $T_{\xi\xi}$ is, of course, given as $K_{\xi\xi}b$. Finally, because the controls that dictate a particular zonation may vary from parameter to parameter, zones for one type of parameter (for example, the parameter contained in $T_{\xi\xi}$) do not necessarily correspond to zones for another type (for example, the parameter contained in W). An example of zonation is given in figure 4.1-1 where the given function is unity so that the parameters are $T_{\xi\xi}$ and W.

Internal boundary conditions applying at discontinuities in $T_{\xi\xi}$ are that the specific discharge normal to the boundary and the hydraulic head both remain unchanged as the boundary is crossed. External boundary conditions applying on the periphery of the region being modeled include specified specific discharge normal to the boundary, specified hydraulic head at the boundary, or a mixture of the two types along the boundary.

Specific discharge q_B normal to the boundary is assumed to vary along the boundary in a manner similar to that of $T_{\xi\xi}$. It may have discontinuities and may vary smoothly between discontinuities. Discontinuities in q_B might often be expected to correspond to discontinuities in $T_{\xi\xi}$.

Hydraulic head variation along a specified head boundary is a continuous function, h_B, although the boundary may be subdivided into segments within each of which head h_B may vary linearly or curvilinearly with distance.

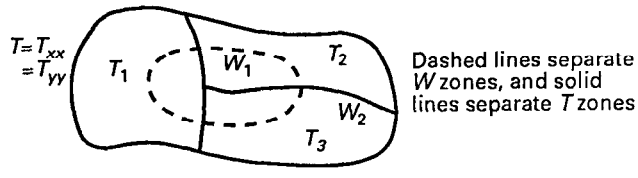


Figure 4.1-1

Subdivision into segments is often based on the causes of the known head conditions along various segments of the boundary.

Unknown quantities to be determined are $T_{\xi\xi}$, R, W, q_B, and h_B. Single values of T_{xx} or T_{yy}, R, and W (or multipliers such as K_{xx} or K_{yy}) are assumed to be parameters in each zone, although any of these parameters may be held constant (assumed known as exact prior information) in each zone. Separate zones (or segments) are specified for the values of q_B, and single multipliers for the fluxes in each flux zone are assumed to be parameters. Within each of the separate segments (zones) of a specified head boundary the heads are adjusted as a linear function of distance by the regression procedure so that the parameters are the values of head at each end of each segment. Even though the adjustment is linear, the actual shape of the head profile along the boundary may be curvilinear.

4.1.2 Matrix Form of Regression Model

For most field problems, equation 4.1-1 with its attendant boundary conditions cannot be solved analytically. Thus, the regression solution must be based on a numerical solution of equation 4.1-1, which is expressed as a matrix equation. The particular numerical solution method is given in the appendix, section 4.3.1.

The matrix equation comprising the numerical solution is given as

$$\underline{D}\underline{h}=\underline{q} \qquad (4.1\text{-}2)$$

where

$\underline{D}$=the square coefficient matrix of order m, the number of nodes used to discretize the modeled region;
$\underline{h}$=the hydraulic head vector of order m; and
$\underline{q}$=the known vector of order m.

Matrix $\underline{D}$ contains parameters for $T_{\xi\xi}$ and R, whereas vector $\underline{q}$ can contain all parameter types. To express any specified head value, say $h_j=h_{Bj}$,

$$D_{jj}=1 \qquad D_{ji}=D_{ij}=0,\ i\neq j \qquad (4.1\text{-}3)$$

$$q_j=h_{Bj} \qquad (4.1\text{-}4)$$

where D_{jj}, D_{ij}, and D_{ji} are components of $\underline{D}$, and q_j is a component of $\underline{q}$. To accomplish the condition that $D_{ij}=0$ in equation i, $i\neq j$, the term $D_{ij}h_{Bj}$ is transferred to the right-hand side of equation i so that q_i contains the term $-D_{ij}h_{Bj}$. Then D_{ij} in $\underline{D}$ is set to zero.

The known head value is computed from

$$h_{Bj}=\frac{h^0_{Bj}[L_jH_t+(1-L_j)H_s]}{L_jH^0_t+(1-L_j)H^0_s} \qquad (4.1\text{-}5)$$

where

s=node at one end of the boundary segment within which node j lies;
t=node at the other end;
H_s=head (parameter) at node s;
H_t=head (parameter) at node t;
L_j=ratio of distance along the boundary from node s to node j, to distance along the boundary from node s to node t; and
superscript 0= an initial or reference value.

Indices s and t can be equal so that $j=s=t$ for the case where only one specified head is present. Also, H_s and H_t can represent the same parameter, so that the entire specified head boundary behaves as a unit.

Because equation 4.1-2 is a linear matrix equation, the modified Gauss-Newton procedure is employed to solve the regression problem. Equation 4.1-2 is the same as equation 3.3-21, except that in equation 4.1-2 the coefficient matrix $\underline{D}$ and right-side vector $\underline{q}$ are not functions of dependent variable vector $\underline{h}$. Hence, sensitivities may be calculated using equation 3.3-24.

Prior information is assumed to be given (if available) on each parameter individually so that

$$\underline{X}_p=[\underline{I}_{n_p},\underline{0}]_{(n_p\times p)} \qquad (4.1\text{-}6)$$

where $\underline{I}_{n_p}$ is the identity matrix of order n_p. Thus, in equation 4.1-6, direct prior information is assumed to be given on the first n_p parameters. Placement of these parameters first in the vector $\underline{\beta}$ simplifies theoretical statement of equation 4.1-6 but is not necessary in practice.

The linearized regression model assumed, then, is of the form of equation 3.3-7 partitioned as suggested by equations 3.4-2 through 3.4-5:

$$\left.\begin{aligned} \underline{Y}_s &= \underline{f}_s(\underline{\xi},\underline{b}_r)+\underline{X}_s^r(\underline{b}_{r+1}-\underline{b}_r)+\underline{e}_s \\ \underline{Y}_p &= \underline{f}_p(\underline{\xi},\underline{b}_r)+\underline{X}_p^r(\underline{b}_{r+1}-\underline{b}_r)+\underline{e}_p, \end{aligned}\right\} \quad (4.1\text{-}7)$$

where $\underline{Y}_s$ is the vector of heads at observation points, $\underline{f}_s(\underline{\xi},\underline{b}_r)$ is the vector of computed heads at observation points for iteration r, $\underline{Y}_p$ is the vector of prior estimates of the first n_p parameters, $\underline{f}_p(\underline{\xi},\underline{b}_r)$ is the vector of the first n_p elements of the computed parameter vector (on which there is prior information) for iteration r, and, from equation 4.1-6, $\underline{X}_p^r=[\underline{I}_{n_p},\underline{0}]$.

No correlation or other coupling is assumed to exist among components of either $\underline{\epsilon}_s$ or $\underline{\epsilon}_p$. Matrix $\underline{\omega}$ is assumed to be of the form

$$\underline{\omega}=\begin{bmatrix} \underline{V}_s^{-1} & \underline{0} \\ \underline{0} & \underline{U}^{-1}\sigma^2 \end{bmatrix} \quad (4.1\text{-}8)$$

where

$$\underline{V}_s^{-1}=[\mathrm{Var}(\underline{\epsilon}_s)]^{-1}\sigma^2 \quad (4.1\text{-}9)$$

$$\underline{U}^{-1}\sigma^2=[\mathrm{Var}(\underline{\epsilon}_p)]^{-1}\sigma^2 \quad (4.1\text{-}10)$$

and both $\underline{V}_s^{-1}$ and $\underline{U}^{-1}$ are diagonal.

4.1.3 Nonlinear Regression Solution

Nonlinear-regression solution for the model given in section 4.1.2 is accomplished by using the algorithm at the end of section 3.3.1. Nodal sensitivities are calculated as illustrated in the appendix, section 4.3.2. We assume that observation points may be located anywhere within the flow region, so that computed heads, $\underline{f}_s(\underline{\xi},\underline{b}_r)$ and sensitivities, $\underline{X}_s^r$, at observation points in general must be obtained by interpolation from surrounding nodal values. Standard bilinear interpolation using the four adjacent nodes surrounding an observation is used as the interpolation method (Wang and Anderson, 1982, p. 153-155).

The normal equations used are equation 3.3-20, as modified to include prior information also (see equation 3.4-13):

$$\begin{aligned} &[(\underline{S}_s^r)^T\underline{V}_s^{-1}\underline{S}_s^r+(\underline{S}_p^r)^T\underline{U}^{-1}\underline{S}_p^r s^2 \\ &+\mu\underline{I}]\underline{\delta}_{r+1}=(\underline{S}_s^r)^T\underline{V}_s^{-1}(\underline{Y}_s-\underline{f}_s(\underline{\xi},\underline{b}_r)) \\ &+(\underline{S}_p^r)^T\underline{U}_s^{-1}s^2(\underline{Y}_p-\underline{f}_p(\underline{\xi},b_r)) \end{aligned} \quad (4.1\text{-}11)$$

where subscripts s and p refer to sample and prior information, respectively;

$\underline{S}_p^r$ = the matrix $[\underline{I}_{n_p},\underline{0}]$ from equation 4.1-6, transformed using equation 3.3-16;

$\underline{f}_p(\underline{\xi},\underline{b}_r)$ = a vector composed of the rth estimate of those parameters on which there is prior information; and

s^2 = the ordinary least-squares estimate of σ^2 (to be developed later).

4.2 Singularity and Conditioning

Singularity of the least-squares coefficient matrix can occur whenever (1) no measured flow rates (such as well or spring discharges) are in the model and (2) an attempt is made to compute all parameters. To understand how this occurs, consider first the case where there are no specified head parameters and no prior information, but all other parameters are to be computed. Also, assume for simplicity that all observation points correspond to node points. In this case it can be shown (appendix, section 4.3.3) that

$$\underline{J}\underline{b}=\underline{0} \quad (4.2\text{-}1)$$

where subscripts r were omitted to simplify nomenclature, and $\underline{J}=\{\underline{J}_j\}=\{\partial\underline{q}/\partial b_j-(\partial\underline{D}/\partial b_j)\underline{h}\}$. By using equation 3.3-23,

$$\underline{J}_j=\frac{\partial\underline{q}}{\partial b_j}-\frac{\partial\underline{D}}{\partial b_j}\underline{h}=\underline{D}\,\frac{\partial\underline{h}}{\partial b_j} \quad (4.2\text{-}2)$$

so that

$$\underline{J}\underline{b}=\sum_{j=1}^{p}\underline{J}_j b_j=\underline{D}\sum_{j=1}^{p}\frac{\partial\underline{h}}{\partial b_j}b_j \quad . \quad (4.2\text{-}3)$$

Because $\underline{D}$ is nonsingular,

$$\underline{D}^{-1}\underline{D}\sum_{j=1}^{p}\frac{\partial \underline{h}}{\partial b_j}b_j=\underline{0}$$

or, by eliminating those nodes not corresponding to observation points from $\partial \underline{h}/\partial b_j$,

$$\sum_{j=1}^{p}\underline{X}_{sj}b_j=\underline{0}\ . \qquad (4.2\text{-}4)$$

Equation 4.2-4 can also be written in the form

$$\underline{X}_s\underline{c}=\underline{0} \qquad (4.2\text{-}5)$$

where

$$\underline{c}=\underline{b}=[b_1,b_2,...,b_p]^T\ . \qquad (4.2\text{-}6)$$

Recall that equation 4.2-5 implies that the least-squares coefficient matrix is singular.

If a known flow rate Q_i is at node i, then equation 4.2-1 becomes

$$\underline{J}\underline{b}=\underline{Q} \qquad (4.2\text{-}7)$$

where

$$\underline{Q}=[0,0,...,Q_i,...,0]^T_{(m)} \qquad (4.2\text{-}8)$$

so that, all other things being equal,

$$\underline{X}_s\underline{c}\neq\underline{0}\ . \qquad (4.2\text{-}9)$$

In the case where at least one parameter j is fixed, then $\underline{J}\underline{b}$ has column j of $\underline{J}$ and element j of $\underline{b}$ deleted. Thus, equation 4.2-1 no longer holds, so that equation 4.2-9 will hold, if no other source of singularity exists.

Whenever there are specified head parameters, $\underline{J}$ and $\underline{X}_s$ both contain columns resulting from these parameters, and $\underline{J}\underline{b}\neq\underline{0}$. However, for those columns not involving the specified head parameters, $\sum_j \underline{J}_j b_j=\underline{0}$, where j denotes all parameters except specified head parameters. If $c_j=0$ for those columns resulting from specified head parameters and $c_j=b_j$ for the remaining columns, then equation 4.2-5 holds for the entire sensitivity matrix, which indicates that the problem is again singular. Because addition of specified head parameters has no influence on this type of singularity, it is assumed for simplicity for the remainder of this section that there are no specified head parameters.

Singularity caused by attempting to find all parameters in the absence of known flow rates can be rectified by using prior information. For the case of prior information, equation 4.2-5 can be written

$$\begin{bmatrix}\underline{X}_s\\ \underline{X}_p\end{bmatrix}\underline{c}=\underline{0}\ . \qquad (4.2\text{-}10)$$

The only way for equation 4.2-10 to hold is if $\underline{X}_s\underline{c}=\underline{0}$ and $\underline{X}_p\underline{c}=\underline{0}$. If the only cause of the singularity is given by equation 4.2-1, then $\underline{c}=\underline{b}$ is the only linearly independent solution of equation 4.2-10, and, if $\underline{X}_p$ is derived from equation 4.1-6, $X_{pii}=0$ $(i=1,2,...,p)$ is the only way that equation 4.2-10 can hold. Hence, prior information on any parameter can theoretically condition the problem so that all parameters can be found.

The maximum number of parameters that can be found for any problem can also be obtained through nondimensionalization (or partial nondimensionalization) to find the smallest number of independent groups. In addition, nondimensionalization also illustrates the idea that solution is actually often best expressed in terms of ratios of the parameters. As an example, consider the case where a region is composed of two zones where T_1, T_2, W_1, and W_2 are parameters. Then the flow equations for each zone are

$$\left.\begin{aligned}T_1\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\right)+W_1=0\\ T_2\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\right)+W_2=0\end{aligned}\right\} \qquad (4.2\text{-}11)$$

and the boundary conditions between zones are

$$\left.\begin{aligned} T_1\left|\frac{\partial h}{\partial n}\right|_1 &= T_2\left|\frac{\partial h}{\partial n}\right|_2 \\ (h)_1 &= (h)_2 \end{aligned}\right\} \qquad (4.2\text{-}12)$$

where the notation $(\cdot)_1$ indicates that the quantity in parentheses is evaluated just within the 1 side of the boundary and similarly for $(\cdot)_2$. If equations 4.2-11 and 4.2-12 are written in the alternative forms

$$\left.\begin{aligned} \frac{T_1}{T_2}\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\right)+\frac{W_1}{T_2}&=0 \\ \frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{W_2}{T_2}&=0 \end{aligned}\right\} \qquad (4.2\text{-}13)$$

$$\left.\begin{aligned} \frac{T_1}{T_2}\left|\frac{\partial h}{\partial n}\right|_1 &= \left|\frac{\partial h}{\partial n}\right|_2 \\ (h)_1 &= (h)_2\,, \end{aligned}\right\} \qquad (4.2\text{-}14)$$

instead of four independent parameters, there are only three written as ratios: $W_1/T_2, W_2/T_2, T_1/T_2$. A known flow rate in zone 1, Q_1, would add the term Q_1/T_2 to the first part of equation 4.1-13. In this case W_1/T_2, W_2/T_2, T_1/T_2, and Q_1/T_2 could all be considered parameters. Knowing Q_1 (either exactly or with uncertainty) would provide unique estimates of the four original parameters. Another approach would be to find T_1, T_2, W_1, W_2 as parameters, knowing that the problem is not singular because there are four independent ratios for the problem.

Another common way for singularity to occur is if a column of $\underline{\underline{X}}_s$ is zero: $\underline{X}_{sj}=\underline{0}$. This results if measurements are taken at points where there is no sensitivity to the parameter, b_j, corresponding to the column. If this is the only source of singularity, then $\underline{c}=[0,0,\ldots,b_j,0,\ldots,0]^T$ is the only linearly independent solution of equation 4.2-5. In this case if $\underline{\underline{X}}_p$ is derived from equation 4.1-6 and there is prior information on b_j, then $\underline{\underline{X}}_p\underline{c}\neq\underline{0}$, so that the prior information solves the singularity problem. Addition of prior information on any other parameter alone obviously will not help.

Two sources of singularity result if $\underline{\underline{X}}_{sj}=\underline{0}$ and $\underline{\underline{J}}\underline{b}=\underline{0}$. In this case one solution of equation 4.2-5 is, as before, given by equation 4.2-6. However, because $\underline{\underline{X}}_{sj}=\underline{0}$, c_j can be any arbitrary value less than infinity and so can be set to zero. Hence, $\underline{c}=[b_1,b_2,\ldots,0,b_{j+1},\ldots,b_p]^T$, where the zero appears in row j of $\underline{c}$, is another solution to equation 4.2-5. Addition of prior information on parameter j alone does not solve the singularity problem because, even though X_{pjj} does not equal zero, c_j and X_{pii}, $i\neq j$, do equal zero so that $\underline{\underline{X}}_p\underline{c}=\underline{0}$. A third solution of equation 4.2-5 is $\underline{c}=[0,0,\ldots,b_j,0,\ldots,0]^T$. In this instance addition of prior information on any or all parameters except parameter j yields $\underline{\underline{X}}_p\underline{c}=\underline{0}$. Thus, if $\underline{\underline{X}}_{sj}=\underline{0}$ and $\underline{\underline{J}}\underline{b}=\underline{0}$, then the problem is singular unless prior information is added on parameter j and at least one other parameter.

If the columns of $\underline{\underline{X}}_s$ are almost linearly dependent, then the problem is ill-conditioned. Thus, if either Q_i in equation 4.2-8 is almost zero or $\underline{\underline{X}}_{sj}\cong\underline{0}$, then an ill-conditioned problem can result. However, ill-conditioning can occur in a number of ways. The techniques given in section 3.2.3 can be used to detect conditioning problems.

Problem 4.2-1

Solve problem 3.2-1 with the regression computer program (appendix 4.3.4). Assume that the stream tube is one foot wide and that transmissivities are unity. Place a row of nodes along each side of the stream tube, but specify observed heads only along one row or down the center of the tube (number of observed heads should be the same as in problem 3.2-1). Allow two iterations. What would happen if you were to attempt to estimate both W and T?

Problem 4.2-2

Figure 1 gives the zone map for a steady-state ground-water flow system in a hypothetical region. The finite difference mesh and types of boundary conditions also are shown on the map. Use the regression program (appendix 4.3.4) to construct a regression flow model for the region.

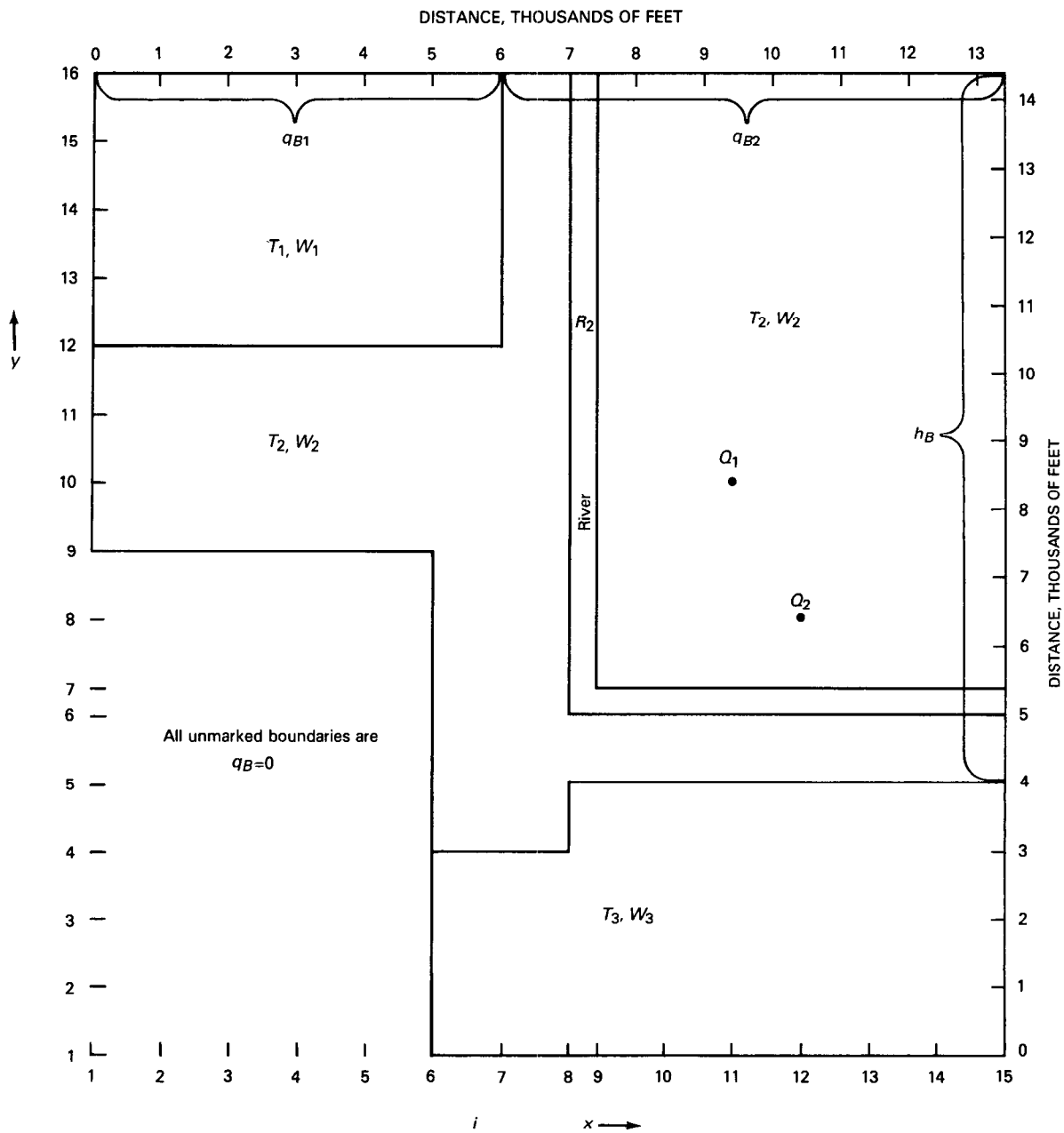

DISTANCE, THOUSANDS OF FEET
0 1 2 3 4 5 6 7 8 9 10 11 12 13
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
q_{B1}
q_{B2}
T_1, W_1
T_2, W_2
R_2
T_2, W_2
h_B
Q_1
River
Q_2
All unmarked boundaries are
q_B=0
T_3, W_3
y
i
x
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
DISTANCE, THOUSANDS OF FEET

Figure 1

Prior information exists on the following parameters:

		standard deviation
T_2=420 ft^2/d		=84
W_1=0.0004 ft/d		0.00012
W_3=0.00017 ft/d		0.000051
R_2=0.08 d^{-1}		0.008
Q_1=-97,000 ft^3/d		1940
Q_2=-51,000 ft^3/d		1020
h_B at (15,16)=10.4 ft		1.04
h_B at (15,7)=4.8 ft	one parameter	0.48
h_B at (15,6)=4.8 ft	one parameter	0.48
h_B at (15,5)=5.4 ft		0.54

Assume that h_B varies linearly between the estimated values. For one reason or another, the estimates of h_B at the four nodes are not observations. (They may have been interpolated from a contour map, for example.)

There is no prior information on the remaining parameters, but probable limits of variation for these parameters are

$$30 \le T_1 \le 80$$
$$10 \le T_3 \le 40$$
$$-0.0003 \le W_2 \le -0.00005$$
$$0.2 \le q_{B1} \le 0.8$$
$$0.15 \le q_{B2} \le 0.4$$

From these ranges, initial estimates of the parameters may be determined.

The observed head data in table 1 were collected. They are of uniform reliability.

Table 1.

Node	Value (ft)	Node	Value (ft)
(8,2)	60.70	(7,11)	6.68
(14,2)	75.64	(13,11)	-15.32
(12,3)	60.27	(3,12)	16.88
(10,4)	29.67	(5,12)	15.87
(7,5)	4.22	(9,12)	4.48
(11,5)	4.37	(11,12)	-18.34
(13,5)	6.07	(13,13)	-2.47
(15,5)	5.81	(15,13)	8.10
(10,7)	4.57	(3,14)	54.12
(8,8)	5.21	(5,14)	38.27
(12,8)	-44.89	(10,14)	0.053
(15,8)	7.01	(12,14)	-2.92
(7,9)	6.95	(7,15)	8.30
(4,10)	12.21	(14,15)	4.54
(9,10)	4.04	(2,16)	85.82
(11,10)	-89.36	(11,16)	2.26

The river stage is about 4.5 ft everywhere.

Assuming that $\sigma^2=1$, find all possible parameters for the model. First, however, determine how many parameters you can find!

Examine the sensitivity maps. Are there data in relatively high sensitivity areas for all parameters? Do you think that there are places where new data points would improve the results?

4.3 Appendices

4.3.1 Integrated Finite Difference Model

The numerical solution of equation 4.1-1 is obtained by using integrated finite difference methods. A rectangular grid of nodes is assumed as indicated in figure 4.3-1. Each node point is enclosed by a subdomain, which is a rectangular region bounded by sides located half way between adjacent node points.

The coordinates of a typical node (i,j) are given as (x_i,y_j). With the nomenclature shown in figure 4.3-1, equation 4.1-1 can be integrated over a subdomain enclosing node (i,j) to produce

$$\int_{\Delta y_j} \left(T_{xx}\frac{\partial h}{\partial x}\right)_{i+\frac{1}{2}} dy - \int_{\Delta y_j} \left(T_{xx}\frac{\partial h}{\partial x}\right)_{i-\frac{1}{2}} dy$$

$$+\int_{\Delta x_i} \left(T_{yy}\frac{\partial h}{\partial y}\right)_{j+\frac{1}{2}} dx - \int_{\Delta x_i} \left(T_{yy}\frac{\partial h}{\partial y}\right)_{j-\frac{1}{2}} dx$$

$$+\int_{\Delta x_i}\int_{\Delta y_j} R(H-h)\,dx\,dy$$

$$+\int_{\Delta x_i}\int_{\Delta y_j} W\,dx\,dy + \sum_{p=1}^{N_{i,j}} Q_p = 0 \qquad (4.3\text{-}1)$$

where

$$\left.\begin{aligned} \Delta x_i &= \tfrac{1}{2}(\Delta x_{i+\frac{1}{2}} + \Delta x_{i-\frac{1}{2}}) \\ \Delta y_j &= \tfrac{1}{2}(\Delta y_{j+\frac{1}{2}} + \Delta y_{j-\frac{1}{2}}) \end{aligned}\right\} \qquad (4.3\text{-}2)$$

and $N_{i,j}$ is the number of pumping wells in subdomain $\Delta x_i \Delta y_j$.

If $T_{\xi\xi}$, R, and W are assumed to be constant in each cell (A,B,C,D) adjacent to node (i,j), then a valid numerical approximation of equation 4.3-1 is

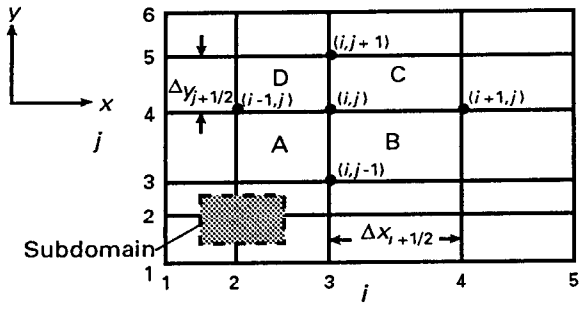


Figure 4.3-1

$$T_{xxi+½j}\Delta y_j\frac{h_{i+1j}-h_{i,j}}{\Delta x_{i+½}}$$

$$-T_{xxi-½j}\Delta y_j\frac{h_{i,j}-h_{i-1j}}{\Delta x_{i-½}}$$

$$+T_{yyi,j+½}\Delta x_i\frac{h_{i,j+1}-h_{i,j}}{\Delta y_{j+½}}$$

$$-T_{yyi,j-½}\Delta x_i\frac{h_{i,j}-h_{i,j-1}}{\Delta y_{j-½}}$$

$$+R_{i,j}\Delta x_i\Delta y_j(H_{i,j}-h_{i,j})$$

$$+W_{i,j}\Delta x_i\Delta y_j+Q_{i,j}=0 \qquad (4.3\text{-}3)$$

where

$$T_{xxi+½j}=\frac{\Delta y_{j-½}T_{xxB}+\Delta y_{j+½}T_{xxC}}{2\Delta y_j} \qquad (4.3\text{-}4)$$

$$T_{xxi-½j}=\frac{\Delta y_{j-½}T_{xxA}+\Delta y_{j+½}T_{xxD}}{2\Delta y_j} \qquad (4.3\text{-}5)$$

$$T_{yyi,j+½}=\frac{\Delta x_{i-½}T_{yyD}+\Delta x_{i+½}T_{yyC}}{2\Delta x_i} \qquad (4.3\text{-}6)$$

$$T_{yyi,j-½}=\frac{\Delta x_{i-½}T_{yyA}+\Delta x_{i+½}T_{yyB}}{2\Delta x_i} \qquad (4.3\text{-}7)$$

$$R_{i,j}=\frac{\Delta x_{i-½}\Delta y_{j-½}R_A+\Delta x_{i+½}\Delta y_{j-½}R_B+\Delta x_{i+½}\Delta y_{j+½}R_C+\Delta x_{i-½}\Delta y_{j+½}R_D}{4\Delta x_i\Delta y_j} \qquad (4.3\text{-}8)$$

$$W_{i,j}=\frac{\Delta x_{i-½}\Delta y_{j-½}W_A+\Delta x_{i+½}\Delta y_{j-½}W_B+\Delta x_{i+½}\Delta y_{j+½}W_C+\Delta x_{i-½}\Delta y_{j+½}W_D}{4\Delta x_i\Delta y_j} \qquad (4.3\text{-}9)$$

$$Q_{i,j}=\sum_{p=1}^{N_{i,j}}Q_p \ . \qquad (4.3\text{-}10)$$

Because of the way that the cells are designated, all zone boundaries are assumed to pass through node points; for example, see figure 4.3-2.

If the node points in equation 4.3-3 are designated as

$$k=i+NC\cdot(j-1) \qquad (4.3\text{-}11)$$

where NC is the number of columns (in the i direction), then the grid is renumbered as in figure 4.3-3. Equation 4.3-3 then becomes

$$T_{xxk,3}\Delta y_j\frac{h_{k+1}-h_k}{\Delta x_{i+½}}-T_{xxk,1}\Delta y_j\frac{h_k-h_{k-1}}{\Delta x_{i-½}}$$

$$+T_{yyk,4}\Delta x_i\frac{h_{k+NC}-h_k}{\Delta y_{j+½}}-T_{yyk,2}\Delta x_i\frac{h_k-h_{k-NC}}{\Delta y_{j-½}}$$

$$+R_k\Delta x_i\Delta y_j(H_k-h_k)+W_k\Delta x_i\Delta y_j+Q_k=0 \qquad (4.3\text{-}12)$$

where

$$T_{xxk,1}=T_{xxi-½j},\ T_{yyk,2}=T_{yyi,j-½},$$

$$T_{xxk,3}=T_{xxi+½j}\ ,\ \text{and}$$

$$T_{yyk,4}=T_{yyi,j+½}\ .$$

In matrix form the numerical solution is

$$\underline{\underline{D}}\underline{h}=\underline{q} \qquad (4.3\text{-}13)$$

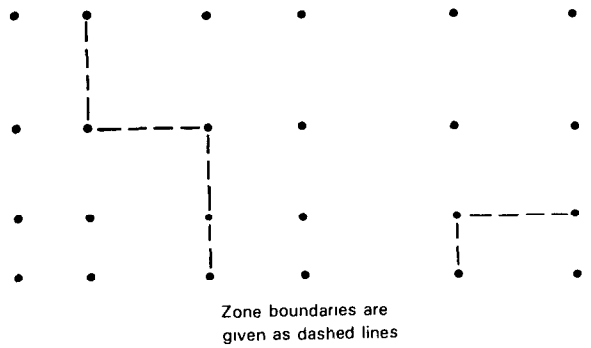


Figure 4.3-2

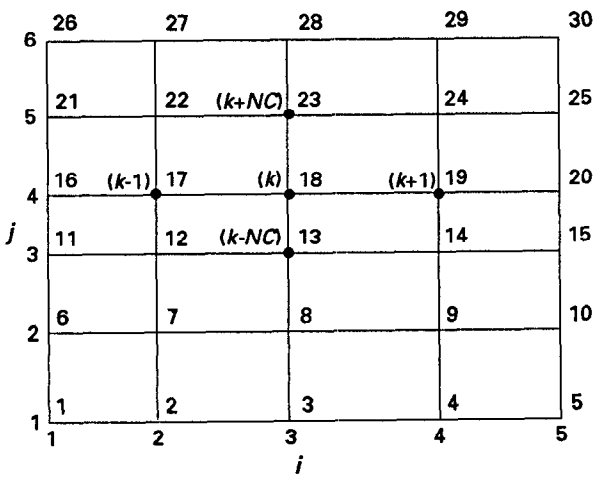


Figure 4.3-3

where, from equation 4.3-12 for node k not on a specified head boundary,

$$D_{k,k-NC}=-T_{yyk,2}\frac{\Delta x_i}{\Delta y_{j-\frac{1}{2}}}\ , \qquad (4.3\text{-}14)$$

$$D_{k,k-1}=-T_{xxk,1}\frac{\Delta y_j}{\Delta x_{i-\frac{1}{2}}}\ , \qquad (4.3\text{-}15)$$

$$D_{k,k}=T_{xxk,3}\frac{\Delta y_j}{\Delta x_{i+\frac{1}{2}}}+T_{yyk,4}\frac{\Delta x_i}{\Delta y_{j+\frac{1}{2}}}+T_{xxk,1}\frac{\Delta y_j}{\Delta x_{i-\frac{1}{2}}}+T_{yyk,2}\frac{\Delta x_i}{\Delta y_{j-\frac{1}{2}}}+R_k\Delta x_i\Delta y_j\ , \qquad (4.3\text{-}16)$$

$$D_{k,k+1}=-T_{xxk,3}\frac{\Delta y_j}{\Delta x_{i+\frac{1}{2}}}\ , \qquad (4.3\text{-}17)$$

$$D_{k,k+NC}=-T_{yyk,4}\frac{\Delta x_i}{\Delta y_{j+\frac{1}{2}}}\ , \qquad (4.3\text{-}18)$$

$$q_k=R_k\Delta x_i\Delta y_j H_k+W_k\Delta x_i\Delta y_j+Q_k\ . \qquad (4.3\text{-}19)$$

For node k on a specified head boundary, $D_{k,k-NC}=D_{k,k-1}=D_{k,k+1}=D_{k,k+NC}=0$, $D_{k,k}=1$, and $q_k=h_{Bk}$, the specified head. All remaining $D_{k,\ell}=0$ for equation k in both cases. To preserve symmetry of $\underline{D}$, equations ℓ, $\ell\neq k$, are modified as indicated just after equation 4.1-4.

The flow across specified flow boundaries is incorporated by using the Q_k term, so that the total flow crossing the specified flow boundary of the subdomain around node k is added into Q_k. If $Q_k=0$ on a boundary node and the head at the node is not specified, then the boundary for the node is automatically a no-flow type. When computing the total flow to add into a specified flow node, remember that nodes are on boundaries so that subdomains for boundary nodes are only fractions of the full subdomains. For example, see figure 4.3-4.

4.3.2 Computation of Nodal Sensitivities for the Integrated Finite Difference Model

Partial derivatives $\underline{J}_\ell$, defined by

$$\underline{J}_\ell=\frac{\partial \underline{q}}{\partial b_\ell}-\frac{\partial \underline{D}}{\partial b_\ell}\underline{h},\ \ell=1, 2,...,p \qquad (4.3\text{-}20)$$

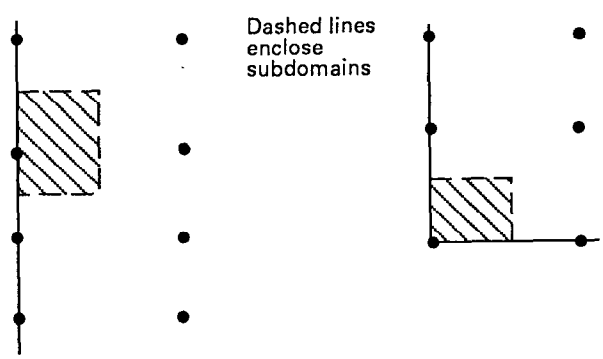


Figure 4.3-4

are employed in equation 3.3-24 to compute sensitivities for the nonlinear regression solution of the numerical model given in section 4.3.1. Using the definitions of the elements of $\underline{D}$ and $\underline{q}$ given in section 4.3.1, partial derivatives for the various parameters are computed as follows:

1. $b_\ell = T_{xxA}$ at node k

$$\frac{\partial D_{k,k-NC}}{\partial b_\ell} = 0 \qquad (4.3\text{-}21)$$

$$\frac{\partial D_{k,k-1}}{\partial b_\ell} = -\frac{\Delta y_j}{\Delta x_{i-\frac{1}{2}}} \frac{\partial}{\partial T_{xxA}} \cdot \left(\frac{\Delta y_{j-\frac{1}{2}} T_{xxA} + \Delta y_{j+\frac{1}{2}} T_{xxD}}{2\Delta y_j} \right) = -\frac{\Delta y_{j-\frac{1}{2}}}{2\Delta x_{i-\frac{1}{2}}} \qquad (4.3\text{-}22)$$

$$\frac{\partial D_{k,k}}{\partial b_\ell} = \frac{\Delta y_{j-\frac{1}{2}}}{2\Delta x_{i-\frac{1}{2}}} \qquad (4.3\text{-}23)$$

$$\frac{\partial D_{k,k+1}}{\partial b_\ell} = 0 \qquad (4.3\text{-}24)$$

$$\frac{\partial D_{k,k+NC}}{\partial b_\ell} = 0 . \qquad (4.3\text{-}25)$$

Similar expressions result for $b_\ell = T_{xxB}, T_{xxC}$, and T_{xxD}. If more than one of the cells $A, \ldots, D$ lie in the same zone, then derivatives for the individual expressions are summed to form the final value. For example, if $b_\ell = T_{yyA} = T_{yyB} = T_{yyC} = T_{yyD}$, then

$$\frac{\partial D_{k,k-NC}}{\partial b_\ell} = \frac{\partial D_{k,k-NC}}{\partial T_{yyA}} + \frac{\partial D_{k,k-NC}}{\partial T_{yyB}} + \frac{\partial D_{k,k-NC}}{\partial T_{yyC}} + \frac{\partial D_{k,k-NC}}{\partial T_{yyD}}$$

$$= -\frac{\Delta x_i}{\Delta y_{j-\frac{1}{2}}} \left(\frac{\Delta x_{i-\frac{1}{2}}}{2\Delta x_i} + \frac{\Delta x_{i+\frac{1}{2}}}{2\Delta x_i} + 0 + 0 \right)$$

$$= -\frac{\Delta x_i}{\Delta y_{j-\frac{1}{2}}} . \qquad (4.3\text{-}26)$$

Derivatives for any configuration of zone boundary are handled by combinations of the form of equations 4.3-21 through 4.3-26.

An example of application of equations 4.3-21 through 4.3-26 for an irregular zone boundary is given in figure 4.3-5. Let $T_{xx} = T_{yy} = T$ for simplicity. Then, for a two-zone problem, the two transmissivities are T_1 and T_2.

For node 7:

$$\frac{\partial D_{7,2}}{\partial T_1} = -\frac{\Delta x_2}{\Delta y_{1\frac{1}{2}}}, \frac{\partial D_{7,6}}{\partial T_1} = -\frac{\Delta y_2}{\Delta x_{1\frac{1}{2}}}, \frac{\partial D_{7,7}}{\partial T_1} = \frac{\Delta y_2}{\Delta x_{2\frac{1}{2}}} + \frac{\Delta x_2}{\Delta y_{2\frac{1}{2}}} + \frac{\Delta y_2}{\Delta x_{1\frac{1}{2}}} + \frac{\Delta x_2}{\Delta y_{1\frac{1}{2}}},$$

$$\frac{\partial D_{7,8}}{\partial T_1} = -\frac{\Delta y_2}{\Delta x_{2\frac{1}{2}}}, \frac{\partial D_{7,12}}{\partial T_1} = -\frac{\Delta x_2}{\Delta y_{2\frac{1}{2}}} .$$

For node 7 the derivatives of the D_{ij}'s with respect to T_2 are all zero because T_2 does not appear in any of the D_{ij}'s. For node 8:

$$\frac{\partial D_{8,3}}{\partial T_1} = -\frac{\Delta x_3}{\Delta y_{1\frac{1}{2}}}, \frac{\partial D_{8,7}}{\partial T_1} = -\frac{\Delta y_2}{\Delta x_{2\frac{1}{2}}}, \frac{\partial D_{8,8}}{\partial T_1} = \frac{\Delta y_{1\frac{1}{2}}}{2\Delta x_{3\frac{1}{2}}} + \frac{\Delta x_{2\frac{1}{2}}}{2\Delta y_{2\frac{1}{2}}} + \frac{\Delta y_2}{\Delta x_{2\frac{1}{2}}} + \frac{\Delta x_3}{\Delta y_{1\frac{1}{2}}},$$

$$\frac{\partial D_{8,9}}{\partial T_1} = -\frac{\Delta y_{1\frac{1}{2}}}{2\Delta x_{3\frac{1}{2}}}, \frac{\partial D_{8,13}}{\partial T_1} = -\frac{\Delta x_{2\frac{1}{2}}}{2\Delta y_{2\frac{1}{2}}}$$

$$\frac{\partial D_{8,3}}{\partial T_2} = \frac{\partial D_{8,7}}{\partial T_2} = 0, \frac{\partial D_{8,8}}{\partial T_2} = \frac{\Delta y_{2\frac{1}{2}}}{2\Delta x_{3\frac{1}{2}}} + \frac{\Delta x_{3\frac{1}{2}}}{2\Delta y_{2\frac{1}{2}}}$$

$$\frac{\partial D_{8,9}}{\partial T_2} = -\frac{\Delta y_{2\frac{1}{2}}}{2\Delta x_{3\frac{1}{2}}}, \frac{\partial D_{8,13}}{\partial T_2} = -\frac{\Delta x_{3\frac{1}{2}}}{2\Delta y_{2\frac{1}{2}}}$$

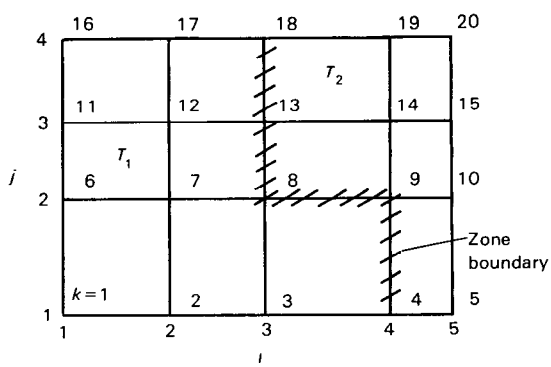


Figure 4.3-5

2. $b_\ell = R_A$ at node k

$$\frac{\partial D_{k,k-NC}}{\partial b_\ell} = \frac{\partial D_{k,k-1}}{\partial b_\ell} = \frac{\partial D_{k,k+1}}{\partial b_\ell}$$

$$= \frac{\partial D_{k,k+NC}}{\partial b_\lambda} = 0 \qquad (4.3\text{-}27)$$

$$\frac{\partial D_{k,k}}{\partial b_\ell} = \Delta x_i \Delta y_j \left| \frac{\Delta x_{i-\frac{1}{2}} \Delta y_{j-\frac{1}{2}}}{4 \Delta x_i \Delta y_j} \right| = \frac{1}{4} \Delta x_{i-\frac{1}{2}} \Delta y_{j-\frac{1}{2}} \qquad (4.3\text{-}28)$$

$$\frac{\partial q_k}{\partial b_\ell} = \frac{1}{4} \Delta x_{i-\frac{1}{2}} \Delta y_{j-\frac{1}{2}} H_k \,. \qquad (4.3\text{-}29)$$

Derivatives for R_B, R_C, and R_D are similar.

3. $b_\ell = W_A$ at node k

$$\frac{\partial q_k}{\partial b_\ell} = \frac{1}{4} \Delta x_{i-\frac{1}{2}} \Delta y_{j-\frac{1}{2}} \,. \qquad (4.3\text{-}30)$$

All derivatives of D_{ij} are zero.

4. $b_\ell = q_{B1}$, boundary flux 1 in Q_k, where, for example, $Q_k = q_{B2} \cdot \frac{1}{2} \Delta y_{j-\frac{1}{2}} + q_{B1} \cdot \frac{1}{2} \Delta y_{j+\frac{1}{2}}$ (see figure 4.3-6).

$$\frac{\partial q_k}{\partial b_\ell} = \frac{1}{2} \Delta y_{j+\frac{1}{2}} \,. \qquad (4.3\text{-}31)$$

A similar expression results for $b_\ell = q_{B2}$, and if $q_{B1} = q_{B2}$, the derivative is the sum of two parts, of equation 4.3-31 and its analog for q_{B2}.

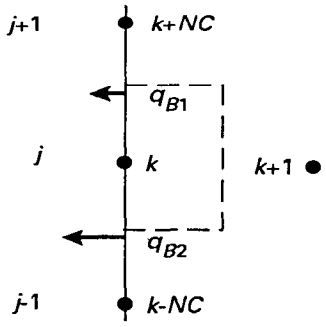
5. $b_\ell = H_s$ or H_t

The specified head at any node k along a specified head boundary is given as

$$h_{Bk} = A_k [L_k H_t + (1 - L_k) H_s] \qquad (4.3\text{-}32)$$

where

$$A_k = \frac{h^0_{Bk}}{L_k H^0_t + (1 - L_k) H^0_s} \qquad (4.3\text{-}33)$$



Dashed line encloses the subdomain for node k

Figure 4.3-6

and the meanings of the symbols are defined after equation 4.1-5.

If node m (here only m indicates an arbitrary node number) is adjacent to a boundary segment bounded by nodes s and t, and node k lies in the segment so that it appears in equation m, then for $b_\ell = H_s$,

$$\frac{\partial q_m}{\partial b_\ell} = -D_{m,k} \frac{\partial h_{Bk}}{\partial H_s} = -D_{m,k} A_k (1 - L_k) \,. \qquad (4.3\text{-}34)$$

Similarly, for $b_\ell = H_t$,

$$\frac{\partial q_m}{\partial b_\ell} = -D_{m,k} \frac{\partial h_{Bk}}{\partial H_t} = -D_{m,k} A_k L_k \,. \qquad (4.3\text{-}35)$$

If node k lies on the boundary, then the equation for node k in equation 4.3-13 becomes

$$h_k = h_{Bk}$$

$$= A_k [L_k H_t + (1 - L_k) H_s] \qquad (4.3\text{-}36)$$

and, for $b_\ell = H_s$,

$$\frac{\partial q_k}{\partial b_\ell} = A_k (1 - L_k) \qquad (4.3\text{-}37)$$

and similarly for $b_\ell = H_t$.

4.3.3 Derivation of Equation 4.2-1

By careful examination of equations 4.3-12 through 4.3-19 it can be seen that, if there are

no specified head parameters, $\underline{q}-\underline{\underline{D}}\underline{h}=\underline{0}$ can be written in the form

$$a_{i1}b_1+a_{i2}b_2+\ldots+a_{ip}b_p-Q_i=0, \quad i=1, 2,\ldots,m \qquad (4.3\text{-}38)$$

where

a_{ij}=coefficient containing Δx, Δy, and head differences;
b_j=any parameter except a specified head parameter; and
Q_i=term not containing parameters in $\underline{b}$.

Define

$$\underline{J}_j=\frac{\partial \underline{q}}{\partial b_j}-\frac{\partial \underline{\underline{D}}}{\partial b_j}\underline{h}. \qquad (4.3\text{-}39)$$

Then, by carrying out the differentiations indicated in equation 4.3-39 and comparing the result with equation 4.3-38 it can be seen that

$$J_{ij}b_j=a_{ij}b_j \qquad (4.3\text{-}40)$$

so that

$$\sum_{j=1}^{p} J_{ij}b_j=\sum_{j=1}^{p} a_{ij}b_j=Q_i \; . \qquad (4.3\text{-}41)$$

If $\underline{b}$ contains all possible parameters (except specified head parameters) and there are no known fluxes, then $Q_i=0$ and

$$\sum_{j=1}^{p} J_{ij}b_j=0 \qquad (4.3\text{-}42)$$

or

$$\underline{\underline{J}}\underline{b}=\underline{0} \; . \qquad (4.3\text{-}43)$$

4.3.4 Documentation of Program for Nonlinear Regression Solution of Steady-State Ground-Water Flow Problems

Introduction.—This program is designed to obtain a nonlinear regression solution to the finite-difference model of steady-state ground-water flow given in section 4.3.1. Basic calculation methods are given in sections 4.1 and 4.3.2.

The program was developed using the Microsoft[1] Fortran Compiler, Version 3.3, with the DOS[1] 2.0 operating system on an IBM[1] PC/XT computer with the IBM[1] 8088 Math Coprocessor and 256 KB memory. Except for the OPEN statements near the beginning of the code, Fortran 66 was used throughout to make the code as machine independent as possible. The source code is contained in files INVFD.FOR and INVSUB.FOR in the 5¼ in. diskette accompanying this report. These two files must be linked or compiled together.

The computer program is composed of a main program and eight subroutines. The main program controls input-output and performs all computations that cannot be accomplished more effectively with subroutines. The eight subroutines (D4SOLV, COEF, LSTSQ, PRTOT, ORDER, ARRAY, ARRAYI, HOBS) perform the following specialized tasks:

D4SOLV Obtains an LDU factorization solution of the set of linear algebraic equations resulting from application of the finite difference methods, assuming the equations are ordered in an alternating diagonal fashion (Price and Coats, 1974).

COEF Computes coefficients necessary for the determination of sensitivities and heads.

LSTSQ Computes the coefficients of the normal equations and solves the system of equations to determine the vectors of parameter changes and parameters.

PRTOT Prints matrices or vectors in a column configuration.

ORDER Computes equation numbers at grid points corresponding to the alternating diagonal ordering scheme.

ARRAY Reads and (or) prints 1- and 2-dimensional real array variables.

ARRAYI Reads and (or) prints 1- and 2-dimensional integer array variables.

[1]Use of the trade names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.