UNITED STATES

DEPARTMENT OF THE INTERIOR

GEOLOGICAL SURVEY

A MODEL FOR THE SIMULATION OF FLOW OF VARIABLE-DENSITY GROUND WATER IN THREE DIMENSIONS UNDER STEADY-STATE CONDITIONS

By Emanuel Weiss

Open-File Report 82-352

Denver, Colorado

1982

UNITED STATES DEPARTMENT OF THE INTERIOR

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GEOLOGICAL SURVEY

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SYMBOLS AND DEFINITIONS

a	angle between the x-axis and α-axis.
b	angle between the y-axis and β-axis.
c	angle between the z-axis and γ-axis.
c_s	dissolved-solids concentration, in M/L^3.
c_p	pure-water concentration, in M/L^3.
$\overline{c}_p$	vertically averaged pure-water concentration of an aquifer, in M/L^3.
$\overline{c}^c_p$	vertically averaged pure-water concentration of a confining layer, in M/L^3.
g	acceleration of gravity, in L/T^2.
h_o	freshwater hydraulic head, in L.
$\overline{h}_o$	vertically averaged freshwater hydraulic head, in L.
h^a	a quasi-hydraulic head, in L.
$\overline{h}^a$	vertically averaged quasi-hydraulic head, in L.
h^a_u	quasi-hydraulic head at top of aquifer, in L.
h^a_L	quasi-hydraulic head at bottom of aquifer, in L.
$\hat{i}, \hat{j}, \hat{k}$	unit vector along the x-direction, y-direction, and z-direction.
$\vec{j}$	mass-flux density of pure water, in M/L^2T.
j_α, j_β	mass-flux density of pure water in the α-direction, and in the β-direction.

$\vec{\vec{k}}$, $\bar{\vec{k}}$ — permeability tensor and the vertically averaged permeability tensor, in L^2.

$\bar{k}_{xx}$ — vertically averaged xx-component of the permeability tensor, in L^2.

k^c_{zz} — zz-component of the confining-layer permeability tensor, in L^2.

K^c — vertical component of hybrid hyraulic conductivity for a layer, in L/T.

$\vec{\vec{K}}^c$ — hybrid hydraulic-conductivity tensor for a confining layer, in L/T.

$K^c_{\gamma\gamma}$ — $\gamma\gamma$-component of a hybrid hydraulic-conductivity tensor for a confining layer, in L/T.

$\vec{n}$ — outward-directed vector normal to top and bottom aquifer surface with magnitude equal to the secant of the angle between $\vec{n}$ and $\hat{\gamma}$.

p, $\bar{p}$ — pressure and vertically averaged pressure, in M/LT^2.

Q — source-sink term for pure water, in M/L^3T.

$\vec{q}$ — specific discharge of ground water, in L/T.

S — ground-water storage coefficient, dimensionless.

$d\vec{S}$ — differential surface element.

$T_{\alpha\alpha}$, $T_{\beta\beta}$ — $\alpha\alpha$-component and $\beta\beta$-component of hybrid transmissivity, in L^2/T.

dV — differential aquifer-volume element.

W — pure-water mass flux per unit of horizontal area--being recharged to or discharged from an aquifer, in M/L^2T.

$\overline{z}$	average aquifer elevation, $(z_u + z_L)/2$.
z_u	aquifer-top elevation, in L.
z_L	aquifer-bottom elevation, in L.
Δz	confining-layer thickness, in L.
dz	differential associated with z-coordinate.
α, β, γ	orthogonal curvilinear coordinates of the $\alpha\beta\gamma$-system.
$\hat{\alpha}$, $\hat{\beta}$, $\hat{\gamma}$	unit vectors along the α-direction, β-direction, and γ-direction; these are the principal directions of the permeability tensor.
$d\alpha$, $d\beta$, $d\gamma$	differentials associated with the α, β, and γ-coordinates.
γ_x, γ_y	projection of $\hat{\gamma}$ on the x and y axes.
μ	ground-water viscosity, in M/LT.
$\overline{\mu}$	vertically averaged ground-water viscosity, in M/LT.
ρ	ground-water density, in M/L^3.
$\overline{\rho}$	vertically averaged ground-water density, in M/L^3.
ρ_o	reference density, here taken as the density of pure water at 4° Celsius and 1 atmosphere pressure.
$\vec{\vec{\tau}}$	hybrid transmissivity tensor with geometric factors, in L^2/T.

A MODEL FOR THE SIMULATION OF FLOW OF VARIABLE-DENSITY GROUND WATER IN THREE DIMENSIONS UNDER STEADY-STATE CONDITIONS

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ABSTRACT

A computer program has been developed as part of the U.S. Geological Survey's national program of Regional Aquifer System Analysis (RASA) that generates input to ground-water flow models to enable them to simulate variable-density ground-water flow. Information required for the program's operation is: aquifer elevation, thickness, and ground-water density. Included in the report is a computer program for calculating ground-water density from aquifer depth, temperature, and dissolved solids concentration.

The 60-page report describes the theoretical development and documents two FORTRAN programs used to generate the necessary flow-model input. An example for a symmetrical basin is fully worked out.

INTRODUCTION

The Northern Great Plains of Montana, North Dakota, South Dakota, and Wyoming are underlain by an extensive (approximately 12 million square kilometers) Paleozoic aquifer system. In this system, water occurring at depths as much as 4,570 meters is subject to large pressures and temperatures and contains dissolved-solids concentrations as much as 350 grams per liter. These concentrations result from the dissolution of the many salt beds in the system. Consequently, ground-water density varies significantly throughout the system.

Because of the variable ground-water density, common modelling techniques that do not incorporate variable density could not be used. Therefore, the ground-water flow model described in this report was developed and used in the U.S. Geological Survey's Northern Great Plains Regional-Aquifer System Analysis.

A differential equation that describes the pure-water component of steady-state flow through a two-dimensional aquifer, and the leakage in and out of that aquifer, was developed from the principles of mass balance and Darcy's law. Some assumptions made in the development were:

1. Pure-water concentration and porosity do not change at any point in the ground-water system. This is the steady-state assumption.
2. For aquifers with anisotropic permeability distributions, there exists only gradual small-angle deviations of the principal axes from fixed axes alined with the vertical and horizontal. This assumption avoids terms that contain both a derivative with respect to x, and a derivative with respect to y, which is required in order to use most constant-density flow programs.
3. The mass-flux density of pure water is continuous and the first-order partial derivatives of its components are bounded and continuous. This assumption allows use of the divergence theorem and implies that no sharp density, pressure, viscosity, or permeability interfaces exist.
4. Necessary ground-water density data throughout the system are available. This allows the assignment of an average density to each node.

Although throughout the mathematical development, steady-state conditions are assumed, use of the model for transient simulations is discussed later in this report.

The equation for two-dimensional flow through an aquifer that is derived in this report is analogous to the equation for flow of constant-density ground water in two dimensions. Hence, an analogous finite-difference equation results, which means existing programs for flow of constant-density ground water can be used for simulations.

From the analogous equations, a correspondence is made between the constant-density parameters and the variable-density parameters. Where constant-density parameters were input, now variable-density parameters are input. The parameter that corresponds to aquifer transmissivity is a hybrid transmissivity consisting of the product of aquifer thickness and permeability, pure-water concentration, and the acceleration of gravity divided by ground-water viscosity. Similarly, the variable that corresponds to confining-bed leakance is a hybrid confining-bed leakance. Terms involving densities, hybrid hydraulic conductivities, and slopes that are generated in the variable-density development have no apparent counterpart in the constant-density equation. Because these terms can be calculated before each simulation, they are considered known, much like the sinks and sources in the constant-density equation are considered known. To make the analogy complete between the development here and the constant-density equation, these terms are called pseudosources. Pseudosources are input to the constant-density flow program as if they were recharge or discharge from wells. For a similar treatment of variable-density flow, see de Josselin de Jong (1960).

The theory and application outlined here has been verified for tilted, nonleaky aquifers with static ground-water systems having linear and quadratic density distributions. The application reproduced the results of coastal ground-water flow around a freshwater/salt-water interface, described by Bennett and Giusti (1971).

Readers desiring a quick overview of the paper or desiring to avoid mathematical detail may want to start with the sections entitled Nature of the Pseudosource Contributions and Variable-Density Modelling Scheme.

MATHEMATICAL DEVELOPMENT

Separation of Bedding-Plane Flow From Leakage

The density of the liquid in a ground-water system is the sum of the concentration of dissolved solids and concentration of pure water present:

$$\rho = c_s + c_p \quad . \tag{1}$$

Here, concentration of dissolved solids means the mass of dissolved solids divided by the volume of ground water containing those solids, and concentration of pure water means the mass of pure water divided by the volume of ground water. Each of these concentrations is affected by ambient temperature and pressure, and each has its own sinks and sources.

The continuity equation (or mass-balance equation) for the steady-state, pure-water constituent is:

$$\nabla \cdot \vec{j} + Q = 0 \tag{2}$$

where $\vec{j}$ is the mass-flux density of pure water, and Q is the source-sink term for pure water. Q is a negative value for a sink and a positive value for a source. The mass-flux density of pure water is the product of the pure-water concentration and the specific discharge of the ground water:

$$\vec{j} = c_p \vec{q} \quad . \tag{3}$$

In particular, the continuity equation applies to every point within the aquifer volume element shown in figure 1.

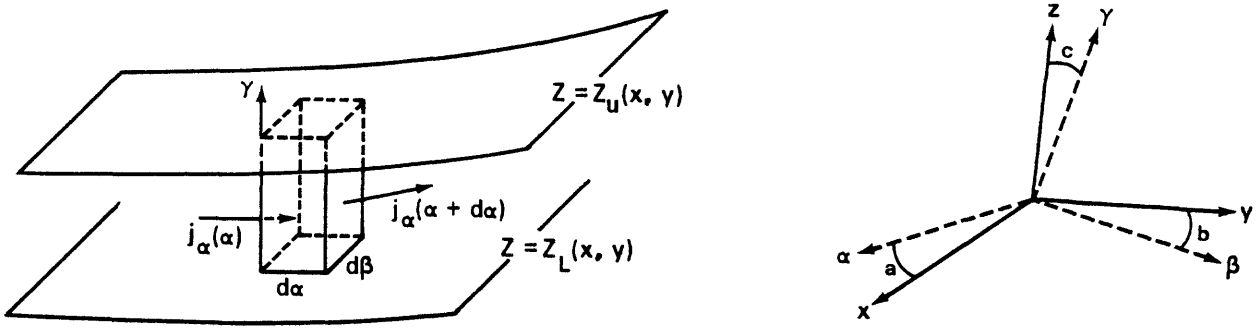

Figure 1.--The infinitesimal volume element extending from the bottom to the top of the aquifer with mass-flux density of pure water moving into one face and out the opposite face. Three coordinate systems are used here: the orthogonal xyz-system, the orthogonal $\alpha\beta\gamma$-system, and the nonorthogonal $\alpha\beta z$-system. The α-, β-, and γ-axes are the principal axes of the permeability tensor.

Here, the α and β axes are principal axes of the permeability tensor nearest the horizontal, and the z-axis is along the vertical (see the section entitled Coordinate Systems in the MATHEMATICAL SUPPLEMENT for details). The volume element, dV, extends along the γ-direction from the bottom of the aquifer to the top. The principal axes are assumed not to change direction along the vertical extent of the aquifer. The aquifer is bounded on the top and the bottom by beds of lesser permeability. Integrating the continuity equation over the volume element:

$$\int_{dV} \nabla \cdot \vec{j} + \int_{dV} Q = 0 \ . \tag{4}$$

Using the divergence theorem on the first integral results in:

$$\int_{S} \vec{j} \cdot d\vec{S} + \int_{dV} Q = 0 \ . \tag{5}$$

Where the integration over S is over the six faces of the infinitesimal volume element:

$$\int_S \vec{j}\cdot d\vec{S} = \int_{\text{sides}} \vec{j}\cdot d\vec{S} + \int_{\substack{\text{bottom}\\+\\\text{top}}} \vec{j}\cdot d\vec{S} \ . \qquad (6)$$

On the right-hand side of equation 6 the first integral sums flow into and out of the volume element in the $\alpha\beta$-plane; whereas, the last sums flow through the top and the bottom of dV. Flow within the aquifer now is separated from leakage.

In the $\alpha\beta\gamma$-system, the off-diagonal terms of the permeability tensor are zero. However, because the quasi-three-dimensional approach requires vertical averages of hydraulic conductivity, specific storage, and hydraulic head, integrations along the vertical need to be done. Hence, in the following development, vertical averages of the α- and β-components of the mass-flux density of pure water are introduced.

Consider now only flow through the sides of the volume element:

$$\begin{aligned}\int_{\text{sides}} \vec{j}\cdot d\vec{S} = &\int j_\alpha(\alpha+d\alpha)\cos a \cos b\, d\beta dz \\ &- \int j_\alpha(\alpha)\cos a \cos b\, d\beta dz + \int j_\beta(\beta+d\beta)\cos a \cos b\, d\alpha dz \\ &- \int j_\beta(\beta)\cos a \cos b\, d\alpha dz \ . \qquad (7)\end{aligned}$$

Specifically, the first two integrals represent net outflow from dV in the α-direction. The next two integrals represent net outflow from dV in the β-direction. The surface elements in the $\beta\gamma$-plane are cos a cos b $d\beta dz$ (see the section entitled Surface Elements in the Nonorthogonal $\alpha\beta z$-System in the MATHEMATICAL SUPPLEMENT for details). Because j_α is only infinitesimally dependent on β, the first two integrals of equation 7 become:

$$[\int j_\alpha(\alpha+d\alpha)\cos a \cos b\, dz - \int j_\alpha(\alpha)\cos a \cos b\, dz]\, d\beta \ . \qquad (8)$$

Dividing equation 8 by $d\alpha d\beta$ and letting $d\alpha d\beta$ approach zero results in:

$$\frac{\partial}{\partial \alpha} \int \cos a \cos b \, j_\alpha(z) dz = \frac{\partial}{\partial \alpha} (\cos a \cos b \int j_\alpha(z) dz) \ . \qquad (9)$$

A similar argument can be made for the last two terms in equation 7. The combined results contain vertical averages of the mass-flux densities of pure water, j_α and j_β.

Now consider flow through the top and bottom of the volume element. The last term of equation 6 can be written:

$$\vec{j}(z_u) \cdot d\vec{S}(z_u) + \vec{j}(z_L) \cdot d\vec{S}(z_L) = \int_{\substack{\text{bottom} \\ + \\ \text{top}}} \vec{j} \cdot d\vec{S} \ . \qquad (10)$$

After equation 10 is divided by $d\alpha d\beta$ and $d\alpha d\beta$ is made to approach zero, the result is:

$$\vec{j}(z_u) \cdot \vec{n}_u + \vec{j}(z_L) \cdot \vec{n}_L \ . \qquad (11)$$

Here, $\vec{n}_u$ is a vector normal to the surface $z = z_u(x, y)$ directed outward from dV and $\vec{n}_L$ is similarly defined:

$$\vec{n}_u = \nabla(z - z_u) \ , \ \vec{n}_L = \nabla(z_L - z) \ . \qquad (12)$$

Finally, consider the pure water that is pumped from or into the volume element. Treating the last term in equation 5 as previously:

$$\lim_{d\alpha d\beta \to 0} \left[\int_{dV} Q dz \, d\alpha d\beta \cos a \cos b / d\alpha d\beta \right.$$

$$\left. = \int_{dV} Q \cos a \cos b \, dz \right] \simeq \int Q dz \ . \qquad (13)$$

Combining equations 7, 11, and 13 results in:

$$0 = \frac{\partial}{\partial \alpha} \left(\cos a \cos b \int j_\alpha(z) dz \right) + \frac{\partial}{\partial \beta} \left(\cos a \cos b \int j_\beta(z) dz \right)$$

$$+ \vec{j}(z_u) \cdot \vec{n}_u + \vec{j}(z_L) \cdot \vec{n}_L + \int Q dz \ . \qquad (14)$$

Averaging the Mass-Flux Density of Pure Water in the Vertical Dimension

A parameterization of Darcy's law that contains pressure and density is (Scheidegger, 1974):

$$\vec{q} = -\frac{\vec{\vec{k}}}{\mu}\cdot(\nabla p - \rho\vec{g}) \quad . \tag{15}$$

However, a form that leads to a more accurate approximation in the following development utilizes the quasi hydraulic head, h^a, defined with a density that varies in the xy-plane

$$h^a = p/\,\bar{\rho}g + z \quad . \tag{16}$$

Where $\bar{\rho}$ is the vertically averaged ground-water density within the aquifer. With these definitions, it follows that:

$$\nabla h^a = \nabla p/\,\bar{\rho}g + \hat{k} + p/g\,\nabla\left(\frac{1}{\bar{\rho}}\right) \tag{17}$$

and that

$$\vec{q} = -\frac{\vec{\vec{k}}}{\mu}\,\bar{\rho}g\left(\nabla h^a + \left(\frac{\rho-\bar{\rho}}{\bar{\rho}}\right)\hat{k} - p/g\,\nabla\left(\frac{1}{\bar{\rho}}\right)\right) \quad . \tag{18}$$

Continuing with the integrations indicated in the first term of equation 14:

$$\int j_\alpha dz = -\int c_p\bar{\rho}g/\mu\left(\vec{\vec{k}}\cdot\left\{\nabla h^a + \frac{\rho-\bar{\rho}}{\bar{\rho}}\,\hat{k} - p/g\,\nabla\left(\frac{1}{\bar{\rho}}\right)\right\}\right)_\alpha dz \quad . \tag{19}$$

The factor $\rho_p\vec{\vec{k}}\,\bar{\rho}g/\mu$ can be taken outside the integral by use of the Mean Value Theorem. According to this theorem, once outside the integral, the factor can be assigned some value that it would assume along the path of integration such that an equality results with the expression where it is inside the integral. It is assumed here that the value of this factor needed for equality is approximately equal to the product of factors outside the integral in equation 20:

$$\int j_\alpha dz \simeq - \bar{c}_p \bar{\rho} g / \bar{\mu}\, \hat{\alpha}\cdot\vec{\bar{k}} \cdot \int \left(\nabla h^a + \frac{\rho-\bar{\rho}}{\bar{\rho}} \hat{k} - p/g\, \nabla\frac{1}{\bar{\rho}} \right) dz \ . \qquad (20)$$

The last integral of equation 20 can be done immediately:

$$- \int p/g\, \nabla\left(\frac{1}{\bar{\rho}}\right) dz = - \frac{1}{g} \nabla\left(\frac{1}{\bar{\rho}}\right) \int p dz = - \bar{p}/g\, (z_u - z_L)\, \nabla\frac{1}{\bar{\rho}} \ . \qquad (21)$$

Using Leibnitz' rule for the first integral of equation 20:

$$\begin{aligned} \int_{z_L}^{z_u} \nabla h^a\, dz &= \nabla \int_{z_L}^{z_u} h^a\, dz - h_u^a\, \nabla(z_u - z) + h_L^a\, \nabla(z_L - z) \\ &= \nabla \left\{ (z_u - z_L)\bar{h}^a \right\} - h_u^a\, \nabla(z_u - z) + h_L^a\, \nabla(z_L - z) \\ &= (z_u - z_L)\nabla\bar{h}^a + \bar{h}^a\, \nabla(z_u - z_L) - h_u^a \nabla(z_u - z) + h_L^a\, \nabla(z_L - z) \ . \end{aligned} \qquad (22)$$

Inserting the definitions of $\vec{n}_u$ and $\vec{n}_L$ provided in equation 12, and multiplying by $\hat{\alpha}\cdot\vec{\bar{k}}$, equation 22 becomes:

$$\begin{aligned} \hat{\alpha}\cdot\vec{\bar{k}} \int_{z_L}^{z_u} \nabla h^a\, dz &= (z_u - z_L)\, \hat{\alpha}\cdot\vec{\bar{k}}\cdot\nabla\bar{h}^a - (\bar{h}^a - h_L^a)\, \hat{\alpha}\cdot\vec{\bar{k}}\cdot\vec{n}_L \\ &\quad - (\bar{h}^a - h_u^a)\, \hat{\alpha}\cdot\vec{\bar{k}}\cdot\vec{n}_u \ . \end{aligned} \qquad (23)$$

If $\vec{n}_u$ and $\vec{n}_L$ are parallel to the γ-axis or have no component along the α-axis, then the last two terms of equation 23 are zero. Commonly the uncertainty of the position of the aquifer/confining-layer interface allows the interface position to be defined so that $\vec{n}_u$ and $\vec{n}_L$ are parallel to the γ-prinicipal direction. Here the last two terms of equation 23 are neglected. Whether or not they are negligible for a particular model study needs to be considered before the theory outlined here can be applied.

The factors $(h_u^a - \bar{h}^a)$ and $(h_L^a - \bar{h}^a)$ are both zero for aquifers containing uniform water with no vertical flow. Under the same conditions, similar

factors for a derivation using hydraulic head would not be zero. Thus, the use of quasi hydraulic head seems to increase modelling accuracy under the condition that the last two terms of equation 22 are neglected.

Combining the results in equations 21 and 23, it follows that equation 20 becomes:

$$\int j_\alpha dz \simeq - \bar{c}_p \bar{\rho} g / \bar{\mu} \, (z_u - z_L) \, \hat{\alpha} \cdot \vec{\bar{k}} \cdot \left(\nabla \bar{h}^a - \bar{p} / g \, \nabla \frac{1}{\bar{\rho}} \right) . \tag{24}$$

Defining the vertically averaged hydraulic head as:

$$\bar{h}_o = \bar{p} / \rho_o g + \bar{z} \tag{25}$$

where ρ_o is a reference density. The last factor in equation 24 can be written in terms of this traditional hydrologic variable:

$$\nabla \bar{h}^a - \bar{p} / g \, \nabla \left(\frac{1}{\bar{\rho}} \right) = \frac{1}{\bar{\rho} g} \nabla \bar{p} + \nabla \bar{z} = \rho_o / \bar{\rho} \left(\nabla \bar{h}_o + \Delta \bar{\rho} / \rho_o \, \nabla \bar{z} \right) . \tag{26}$$

Combining equations 14, 24, and 26:

$$\frac{\partial}{\partial \alpha} \left(\bar{c}_p \, \hat{\alpha} \cdot \vec{\tau} \cdot \nabla \bar{h}_o \right) + \frac{\partial}{\partial \beta} \left(\bar{c}_p \, \hat{\beta} \cdot \vec{\tau} \cdot \nabla \bar{h}_o \right) = \vec{j}(z_u) \cdot \vec{n}_u + \vec{j}(z_L) \cdot \vec{n}_L + W$$
$$- \frac{\partial}{\partial \alpha} \left(\bar{c}_p \Delta \bar{\rho} \, \hat{\alpha} \cdot \vec{\tau} \cdot \nabla \bar{z} \right) - \frac{\partial}{\partial \beta} \left(\bar{c}_p \Delta \bar{\rho} \, \hat{\beta} \cdot \vec{\tau} \cdot \nabla \bar{z} \right) \tag{27}$$

where

$$\Delta \bar{\rho} = \bar{\rho} - \rho_o \text{ , and}$$

$$\vec{\tau} = \cos a \cos b \, \vec{\bar{k}} \, \rho_o g \, (z_u - z_L) / \bar{\mu} .$$

If the approximation leading to equation 24 had been developed with hydraulic head instead of quasi-hydraulic head, then $\vec{\tau}$ would contain $\bar{\rho}$ instead of ρ_o. Note that $\nabla \bar{h}_o$ and $\nabla \bar{z}$ are in the horizontal.

Here,

$\vec{\vec{\tau}}$ is the product of a hybrid transmissivity tensor and a geometrical factor. (See the section entitled Small-Angle Approximations for Aquifer Flow in the MATHEMATICAL SUPPLEMENT.),

W is the pure-water mass flux per unit horizontal area that is being recharged (if negative) or discharged (if positive) to the aquifer, and

$\vec{j}(z)\cdot\vec{n}$ is the mass flux leaking out of (if positive) or into (if negative) the aquifer's upper surface if subscript u, or lower surface if subscript L.

The first two and last two terms of equation 27 describe flow in the $\alpha\beta$-plane; the third and fourth describe flow through the top and the bottom of the aquifer.

Although the vertical integrations have been done, the hybrid transmissivity tensor in equation 27 has to be expressed in a specific coordinate system before calculations can begin. In the section entitled Small-Angle Approximations for Aquifer Flow, this tensor is expressed in the $\alpha\beta\gamma$-system; and the resulting derivatives with respect to α and β are expressed in terms of x, y, and z. Then the restriction that the angles between the α- and x-axes and the β- and y-axes be small is used. Thus, terms containing derivatives with respect to both x and y are small compared to other terms. These terms then are neglected in order to select terms usable in constant-density algorithms. The third and fourth terms of equation 27, the leakage terms, are treated similarly.

Leakage Description

Because the quasi-three-dimensional formulation does not allow nodes within the confining bed, there is no way to formulate standard finite-difference equations for movement of variable-density liquid through a confining bed within the quasi-three-dimensional context. The approach here is to assume that an average ground-water density ($\overline{\rho}^c$) is driving an average pure-water concentration ($\overline{c}_p^c$) through the confining layer. These average densities are the sum of their respective densities above and below the confining bed divided by two. With this assumption and the conservation of pure-water mass constraint, the flow of pure water through the confining layer can be approximated using the third and fourth terms of equation 27, as:

$$\vec{j}(z_L)\cdot\vec{n}_L + \vec{j}(z_u)\cdot\vec{n}_u \simeq \rho_o K_{\gamma\gamma}^c \left(\frac{\partial h_o}{\partial z} + \Delta\overline{\rho}^c/\rho_o \right) \Bigg]_L - \rho_o K_{\gamma\gamma}^c \left(\frac{\partial h_o}{\partial z} + \Delta\overline{\rho}^c/\rho_o \right) \Bigg]_u \quad (28)$$

Here,

$\Delta\overline{\rho}^c$ is the difference between the average ground-water density ($\overline{\rho}^c$) in the confining layer and the reference density (ρ_o), and

$K_{\gamma\gamma}^c$ is the $\gamma\gamma$-component of the hybrid hydraulic conductivity for a confining bed. Specifically,

$$K_{\gamma\gamma}^c = \overline{k}_{\gamma\gamma}^c \, \overline{c}_p^c g / \overline{\mu}$$

where

$\overline{k}_{\gamma\gamma}^c$ is the $\gamma\gamma$-component of the confining-layer permeability tensor.

For details of the derivation see the section entitled Calculating Leakage Terms in the MATHEMATICAL SUPPLEMENT.

Combining equations 27 and 28 and the results of the section entitled Small-Angle Approximations for Aquifer Flow yields:

$$\frac{\partial}{\partial x}\left(T_{\alpha\alpha}\frac{\partial \bar{h}_o}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{\beta\beta}\frac{\partial \bar{h}_o}{\partial y}\right) = \left(K'_{\gamma\gamma}\frac{\partial \bar{h}_o}{\partial z}\right)_L - \left(K'_{\gamma\gamma}\frac{\partial \bar{h}_o}{\partial z}\right)_u + W/\rho_o$$

$$- \frac{\partial}{\partial \alpha}\left(T_{\alpha\alpha}\,\Delta\bar{\rho}/\rho_o\,\frac{\partial \bar{z}}{\partial \alpha}\right) - \frac{\partial}{\partial \beta}\left(T_{\beta\beta}\,\Delta\bar{\rho}/\rho_o\,\frac{\partial \bar{z}}{\partial \beta}\right)$$

$$+ \left(K'_{\gamma\gamma}\,\Delta\bar{\rho}/\rho_o\right)_L - \left(K'_{\gamma\gamma}\frac{\Delta\bar{\rho}^c}{\rho_o}\right)_u . \qquad (29)$$

Here

$T_{\alpha\alpha}$ and $T_{\beta\beta}$ are the components of a hybrid transmissivity tensor corresponding to the α- and β-directions. For example,

$$T_{\alpha\alpha} = \bar{k}_{\alpha\alpha}\,\bar{c}_p g\,(z_u - z_L)/\,\bar{\mu} .$$

The first five terms of equation 29 are completely analogous to the terms in the steady-state constant-density flow equation. The last four terms of equation 29 are new terms caused by the variable density of the ground water. If the density of ground water is the reference density, then each of these terms is zero. To carry the analogy further, the last four terms can be thought of as sources or sinks and grouped with $\frac{W}{\rho_o}$ into a new variable $\frac{W'}{\rho_o}$. Hence, within the quasi-three-dimensional context, the flow of the pure-water component through a fixed variable-density distribution is analogous to a constant-density liquid flowing through an aquifer with a hybrid transmissivity, with a new source distribution, and with surrounding confining beds of hybrid vertical hydraulic conductivities.

VARIABLE-DENSITY MODELLING AND PARAMETERS

Transient Approximations

Although the basic assumption of the development above is that the system be in the steady state, transient approximations can be made with pseudosources. What this involves is allowing pressure distribution to change with time, but ignoring the effects of this change on the viscosity or density distributions. This is done routinely in most transient simulations of constant-density liquids. Hence, if the transient effects in a pseudosource simulation are restricted to an area of constant density or approximately constant density, then the resulting simulation should be as good as most transient simulations of constant-density liquids.

Furthermore, if one is interested primarily in simulating pressure changes and not interested in the effects those pressure changes have on the density distribution, then a short transient simulation with pseudosources should be a good first approximation to actual pressure changes. This is reasonable, because although density changes coincidentally with pressure, pressure-induced density changes commonly are small relative to both changes induced by fluctuations in temperature and dissolved-solids content. Density changes that occur due to thermal and dissolved-solids transport are much slower than those that occur due to pressure changes. Hence, if transient pseudosource simulations are terminated before significant thermal and dissolved-solids transport can occur, then such simulations are in approximate agreement with the assumption of a fixed-density distribution. Judicious termination makes such pseudosource simulations good approximations.

To affect such simulations one needs only to add the term:

$$\frac{\bar{c}_p}{\bar{\rho}} S \frac{\partial \bar{h}_o}{\partial t}$$

to the right-hand side of equation 29, and complete the analogy with the constant-density case. Here, S is the (dimensionless) storage coefficient for ground water.

Nature of the Pseudosource Contributions

A pseudosource is simply a source or sink of pure water applied to any aquifer element to supplement the net inflow or outflow of pure water obtained by calculating flow using only a hydraulic-head gradient. Consider the hydraulic-head parameterization of Darcy's law:

$$\vec{q} = - \vec{\vec{k}} \rho_o g/\mu \cdot (\nabla h_o + \Delta\rho/\rho_o \hat{k}) \quad . \tag{30}$$

Equation 30 follows from the definition of hydraulic head for the reference density and the pressure-density parameterization of Darcy's law in equation 15. The pseudosource contribution to an aquifer element results solely from the second term on the right-hand side of equation 30. Each pseudosource strength is the sum of six contributions corresponding to flows through each of the six faces of the aquifer element or nodal block.

The preceding development shows a division of each pseudosource into bedding-plane contributions and contributions associated with flow through the bottom and top faces of the aquifer element. The sixth and seventh terms of equation 29 are the $\alpha\beta$-plane contributions and the eighth and ninth terms are the bottom and top contributions.

The sixth and seventh terms in equation 29 are the pseudosource contributions resulting from liquid-density differences within an aquifer, or the aquifer pseudosource contributions. For each aquifer, the sum of these terms is zero. This fact follows immediately from the application of the two-dimensional divergence theorem, wherein the surface integrals over regions where the ground-water density is different from the reference density are transformed to line integrals around those regions. The line integrals are zero, because they are in a region where the density is the reference density.

The eighth and ninth terms in equation 29 are the pseudosource contributions resulting from liquid-density differences within confining layers, or the confining-layer pseudosource contributions. From equation 29, it is seen that for each confining-layer pseudosource contribution added to an aquifer below the confining layer, exactly the same contribution is subtracted from the aquifer above the confining layer. Hence, confining-layer contributions can be thought of as transfer contributions. The confining-layer pseudosource contribution to any aquifer represents a correction to the reference-density leakage. For good confining layers, this contribution within any nodal area usually is much smaller than the aquifer pseudosource contribution. However, the net confining-layer pseudosource contribution to any aquifer is not necessarily zero; it is zero for any multi-aquifer system.

The mass balance of any constant-density model will not be substantially affected by the addition of pseudosources. The pseudosources' main effect, when added to a constant-density model, is to alter the calculated hydraulic-head distribution in areas where the density differs from the

reference density. The amount by which the calculated hydraulic-head distribution is altered is a direct physical consequence of density differences. That is, it may happen that the field distribution of hydraulic heads in a variable-density problem can be matched with a constant-density model without pseudosources by adjusting certain model parameters; however, such an adjustment is not representative of the aquifers or hydrology.

Variable-Density Modelling Scheme

To simulate a variable-density flow problem, the last four terms of equation 29 need to be calculated for each node. The calculated values are used as well-input to the constant-density model. The variable-density modelling scheme is summarized in figure 2.

Note that initially no accurate calculation of pure-water concentration need be made. Estimates for the hybrid transmissivity and for hybrid leakance can be used for calibration. Once a final calibration is attained, then values of permeability and viscosity can be extracted from hybrid transmissivities and leakances, using pure-water concentration. On the other hand, ground-water density needs to be known before any calculation of pseudosource strengths can begin.

MATHEMATICAL SUPPLEMENT*

Coordinate Systems

There are three coordinate systems used in this report. One is alined with the horizontal and vertical, the orthogonal xyz-system; another is alined

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*Equations numbered M1 through M21 are in this MATHEMATICAL SUPPLEMENT section.

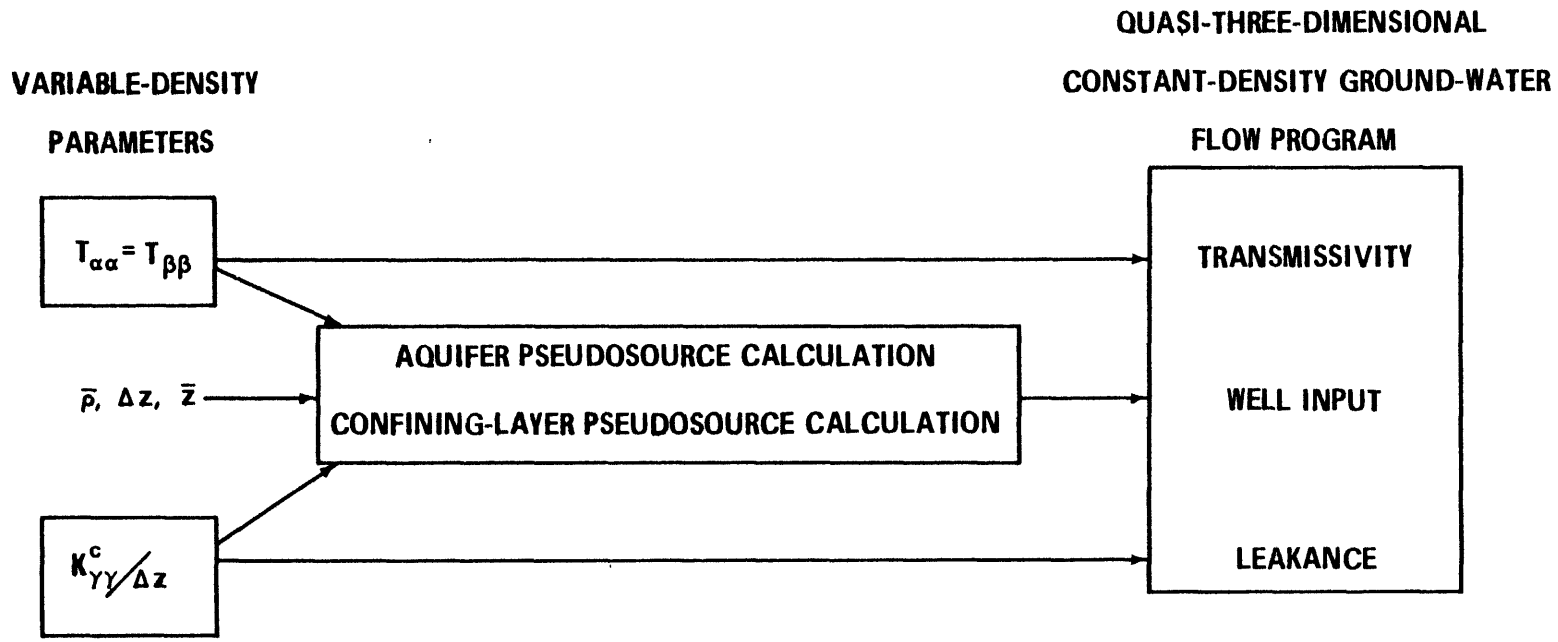

Figure 2.--Flow diagram for input to pseudosource calculation and flow program for constant-density ground water. The hybrid transmissivities and leakances (containing the concentration of pure water) are inputted to both the pseudosource calculation and the ground-water flow program. The vertically averaged ground-water densities, confining-bed thicknesses, and average aquifer elevation are inputted only to the pseudosource calculation.

with the principal axes of the permeability tensor, the orthogonal αβγ-system; and the third is the nonorthogonal αβz-system (fig. 3).

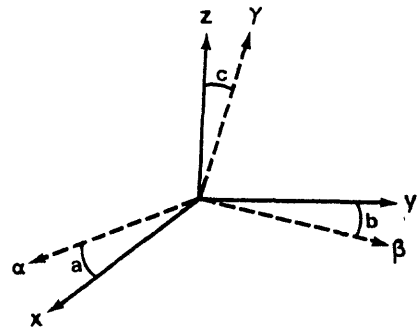

Figure 3.--The three coordinate systems used in discussion.

A restriction on the αβγ-system is that the α-axis lies in xz-plane. This restriction simplifies the relationship among coordinate systems, but may generate off-diagonal permeability components in the αβγ-system because the α-axis may no longer be able to be alined with a principal axis.

Expressing the unit vectors $\hat{\alpha}$, $\hat{\beta}$, and $\hat{\gamma}$ in the xyz-system:

$$\hat{\alpha} = (\cos a,\ 0,\ \sin a), \text{ and} \tag{M1}$$

$$\hat{\beta} = (-\sin a \sin b,\ \cos b,\ \cos a \sin b) \tag{M2}$$

where a is positive when α lies above the xy-plane, and b is positive when β lies above the xy-plane. Then:

$$\hat{\alpha} \times \hat{\beta} = \hat{\gamma}\ , \text{ and} \tag{M3}$$

$$(\hat{\alpha} \times \hat{\beta})_z = \hat{\gamma} \cdot \hat{k} = \cos a \cos b = \frac{\partial \gamma}{\partial z}\ . \tag{M4}$$

Similarly:

$$\gamma_x = (\hat{\alpha} \times \hat{\beta})_x = -\sin a \cos b = \frac{\partial \gamma}{\partial x}\ , \text{ and} \tag{M5}$$

$$\gamma_y = (\hat{\alpha} \times \hat{\beta})_y = -\sin b = \frac{\partial \gamma}{\partial y}\ . \tag{M6}$$

Equation M4 is used in the discussion below and follows from equations M1, M2, and M3. Here $\hat{\alpha}$ is the unit vector along the α-axis, and $\hat{\beta}$, $\hat{z}$, and $\hat{\gamma}$ are unit vectors along their respective axes.

Surface Elements in the Nonorthogonal $\alpha\beta z$-System

In equation 7 the transformation of the surface integral from the $\alpha\beta\gamma$-system to the nonorthogonal $\alpha\beta z$-system is accomplished using Jacobian transformation theory and equation M4 in the following:

$$\hat{\alpha}\cdot d\vec{S} = d\beta d\gamma = \frac{\partial(\beta,\gamma)}{\partial(\beta,z)}\, d\beta dz = \frac{\partial\gamma}{\partial z}\, d\beta dz = \cos a \cos b\, d\beta dz \ . \qquad (M7)$$

Calculating Leakage Terms

The third and fourth terms of equation 27 now can be shown to lead to the corresponding terms of equation 28. The assumptions made are:

1. The density of the water in the confining layer can be represented by the average density.
2. The dip of the interfaces between the aquifer and confining-layer, relative to the $\alpha\beta$-plane, is small.
3. The α- and β-components of the mass-flux densities of pure water at the aquifer confining-layer interfaces are approximately equal to or smaller than the γ-components.
4. The principal directions of the confining layer are the same as those of the aquifer.

Using definition of $\vec{n}_u$ of equation 12 in the third term of equation 27 and applying assumptions 2 and 3 above, then:

$$\vec{j}(z_u)\cdot\vec{n}_u = j_\gamma(z_u) - j_\beta(z_u)\frac{\partial z_u}{\partial\beta} - j_\alpha(z_u)\frac{\partial z_u}{\partial\alpha} \simeq j_\gamma(z_u) \ . \qquad (M8)$$

Substituting the head parameterization of Darcy's law from equation 30 into equation M8 and applying assumption 4 above results in:

$$j_\gamma = \rho_o \hat{\gamma}\cdot\left(\vec{\vec{K}}^c\cdot\left(\nabla h_o + \Delta\overline{\rho}^c/\rho_o \hat{k}\right)\right) = \rho_o K^c_{\gamma\gamma}\left(\frac{\partial h_o}{\partial\gamma} + \Delta\overline{\rho}^c/\rho_o \cos a \cos b\right). \quad (M9)$$

Here

$K^c_{\gamma\gamma}$ is the $\gamma\gamma$-component of the hybrid hydraulic conductivity (containing the concentration of pure water ($\overline{c}^c_p$) of the confining layer), and

$\Delta\overline{\rho}^c$ is the difference between the average ground-water density in the confining layer ($\overline{\rho}^c$) and the reference density (ρ_o).

From equations M4, M5, and M6:

$$\frac{\partial}{\partial\gamma} = \hat{\gamma}\cdot\nabla = -\sin a \cos b \frac{\partial}{\partial x} - \sin b \frac{\partial}{\partial y} + \cos a \cos b \frac{\partial}{\partial z}. \quad (M10)$$

Because angles a and b are small, equation M10 reduces to:

$$\frac{\partial}{\partial\gamma} \simeq \cos a \cos b \frac{\partial}{\partial z}. \quad (M11)$$

Using equation M11 in equation M9 yields:

$$j_\gamma \simeq \rho_o K^c_{\gamma\gamma} \cos a \cos b\left(\frac{\partial h_o}{\partial z} + \Delta\overline{\rho}^c/\rho_o\right) \simeq \rho_o K^c_{\gamma\gamma}\left(\frac{\partial h_o}{\partial z} + \Delta\overline{\rho}^c/\rho_o\right). \quad (M12)$$

Note that the term in equation M12 that contains factor $\frac{\partial h_o}{\partial z}$ is analogous to the leakage terms of a constant-density model.

Small-Angle Approximations for Aquifer Flow

Because the α- and β-axes are oriented along principal axes the τ-dyadic is diagonal in the $\alpha\beta\gamma$-system; that is:

$$\vec{\vec{\tau}} = \tau_{\alpha\alpha}\hat{\alpha}\hat{\alpha} + \tau_{\beta\beta}\hat{\beta}\hat{\beta} + \tau_{\gamma\gamma}\hat{\gamma}\hat{\gamma}. \quad (M14)$$

Equation M14 establishes the notation for what follows. Consider one component of a mixed dyadic: The subscript α corresponds to the $\alpha\beta\gamma$-system, and the subscript x, y, or z corresponds to the xyz-system. Then:

$$\hat{\alpha}\cdot\vec{\tau}\cdot\hat{i} = \tau_{\alpha x} = \tau_{\alpha\alpha}(\hat{\alpha}\cdot\hat{i}) = \tau_{\alpha\alpha}\cos a \ , \tag{M15}$$

$$\tau_{\alpha y} = 0 \ , \tag{M16}$$

$$\tau_{\alpha z} = \tau_{\alpha\alpha}\sin a \ . \tag{M17}$$

Equation M16 follows from the restriction that the α-axis lies in the xz-plane. The last three equations relate some of the components of a mixed dyadic to the principal component $\tau_{\alpha\alpha}$ in the $\alpha\beta\gamma$-system. The relationship is made through the geometry that relates the $\alpha\beta\gamma$-system to the xyz-system.

The first term of equation 27 now can be expanded:

$$\frac{\partial}{\partial\alpha}\left(\bar{c}_p\ \hat{\alpha}\cdot\vec{\tau}\cdot\nabla\bar{h}_o\right) = \frac{\partial}{\partial\alpha}\bar{c}_p\left(\tau_{\alpha x}\frac{\partial}{\partial x} + \tau_{\alpha z}\frac{\partial}{\partial z}\right)\bar{h}_o$$

$$= \frac{\partial}{\partial\alpha}\left(\bar{c}_p\ \tau_{\alpha x}\frac{\partial\bar{h}_o}{\partial x}\right) . \tag{M18}$$

In equation M18, equation M16 and the fact that $\bar{h}_o$ is independent of z were used. Using equations M1, M16, and M18 and the assumption that a is small leads to the following:

$$\left(\frac{\partial}{\partial\alpha} = \hat{\alpha}\cdot\nabla = \cos a\frac{\partial}{\partial x} + \sin a\frac{\partial}{\partial z}\right)\left(\bar{c}_p\ \tau_{\alpha\alpha}\cos a\frac{\partial\bar{h}_o}{\partial x}\right)$$

$$\simeq \cos a\frac{\partial}{\partial x}\left(\bar{c}_p\ \tau_{\alpha\alpha}\cos a\frac{\partial\bar{h}_o}{\partial x}\right) . \tag{M19}$$

A similar deduction can be made for the second term of equation 27 namely:

$$\left(\frac{\partial}{\partial\beta}\ \bar{c}_p\ \hat{\beta}\cdot\vec{\tau}\cdot\nabla\bar{h}_o\right) \simeq \cos b\frac{\partial}{\partial y}\left(\bar{c}_p\ \tau_{\beta\beta}\cos b\frac{\partial\bar{h}_o}{\partial y}\right) . \tag{M20}$$

Unless a small-angle approximation is made, terms containing both the derivative with respect to x and the derivative with respect to y are needed to describe flow along the aquifer bedding plane. This is true only for anisotropic aquifers. For small angles a and b that change gradually, it is a very good approximation to write:

$$\left(\frac{\partial}{\partial\alpha}\ \bar{c}_p\ \hat{\alpha}\cdot\vec{\tau}\cdot\nabla\bar{h}_o\right) + \frac{\partial}{\partial\beta}\left(\bar{c}_p\ \hat{\beta}\cdot\vec{\tau}\cdot\nabla\bar{h}_o\right) \simeq \frac{\partial}{\partial x}\left(\rho_o\ T_{\alpha\alpha}\ \frac{\partial\bar{h}_o}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho_o\ T_{\beta\beta}\ \frac{\partial\bar{h}_o}{\partial y}\right) \qquad \text{(M21)}$$

for combined results of equations M19 and M20. Here

$$T_{\alpha\alpha} = \bar{k}_{\alpha\alpha}\ \bar{c}_p g\ (z_u - z_L)/\ \bar{\mu}\ ,$$

and $T_{\beta\beta}$ is similarly defined. They are components of a hybrid transmissivity tensor. Results similar to those obtained above hold for the last two pseudosource terms of equation 27. Both are used to obtain equation 29.

COMPUTER CODE TO CALCULATE PSEUDOSOURCE STRENGTHS

The last four terms in equation 29 are the pseudosource terms. Each term need to be calculated to implement the scheme in figure 2. The following two paragraphs describe how these terms can be calculated in the $\alpha\beta\gamma$-system.

The factors in the confining-layer pseudosource contributions can be assigned an average value at each node. Once this is done, the confining-layer term can be multiplied by the nodal area $\Delta\alpha\ \Delta\beta$ to determine the confining-layer pseudosource contribution at each node.

The derivatives in the aquifer pseudosource contributions need to be converted to finite-difference equations. This is done for the α-term below:

$$- \frac{\partial}{\partial \alpha} \left(T_{\alpha\alpha} \, \overline{\Delta\rho}/\rho_o \, \frac{\partial z}{\partial \alpha} \right) \simeq - \frac{1}{\Delta\alpha_j} \left[\left(T_{\alpha\alpha} \, \overline{\Delta\rho}/\rho_o \right)_{j+\frac{1}{2}} \left(\frac{\overline{z}_{j+1} - \overline{z}_j}{\Delta\alpha_{j+\frac{1}{2}}} \right) \right.$$

$$\left. - \left(T_{\alpha\alpha} \, \overline{\Delta\rho}/\rho_o \right)_{j-\frac{1}{2}} \left(\frac{\overline{z}_j - \overline{z}_{j-1}}{\Delta\alpha_{j-\frac{1}{2}}} \right) \right] . \qquad (31)$$

Here $(T_{\alpha\alpha})_{j+\frac{1}{2}}$ is the harmonic mean of the hybrid transmissivity between node j and j+1; along the α-direction. The harmonic mean needs to be used for proper calculation at boundaries. The factor $(\overline{\Delta\rho}/\rho_o)_{j+\frac{1}{2}}$ is a weighted average and $\Delta\alpha_{j+\frac{1}{2}}$ is a simple average of their values at nodes j and j+1. After all the factors in equation 31 are calculated, the result is multiplied by the nodal area $\Delta\alpha \, \Delta\beta$ to determine the aquifer pseudosource contribution. The α-term is combined with a β-term and upper and lower confining-layer terms to determine a total pseudosource contribution for each node. The total pseudosource contribution is used as well-input to the simulation. For use in the U.S. Geological Survey's constant-density ground-water flow model (Trescott, 1976), each pseudosource term in equation 29 needs to be multiplied by the nodal area $\Delta x \, \Delta y$ instead of $\Delta\alpha \, \Delta\beta$, because all well-input in that model is divided by $\Delta x \, \Delta y$ before being used in model calculations.

Because the first four terms and the last two terms of equation 29 originate from small-angle approximations, a calculation of the sixth and seventh terms in the $\alpha\beta\gamma$-system may not lead to the best approximation of variable-density flow. Aquifer pseudosources were calculated as described above; they were calculated with $(T_{\alpha\alpha})_{j+\frac{1}{2}}$ as the harmonic mean of $T_{\alpha\alpha}$ along the x-direction between nodes j and j+1; and they were calculated with Δx in place of $\Delta\alpha$ in equation 31, with $(T_{\alpha\alpha})_{j+\frac{1}{2}}$ as the harmonic mean of $T_{\alpha\alpha}$ along

the x-direction between nodes j and j+1. The result of each calculation was input to the U.S. Geological Survey's model to simulate a tilted, nonleaky, isotropic aquifer with a static, linear-density distribution. At 5 degrees tilt, the pseudosource simulations started to show deviations from the analytically derived hydraulic-head distribution. The worst error occurred using the first method. At the aquifer bottom, where ground-water density was 1.17 grams per cubic centimeter, the error was -0.13 meter in 38.4 meters of hydraulic head. The total hydraulic head was caused by the linear increase in density with depth. The error monotonically went to zero as the density approached 1. The simulation that showed the best agreement with the analytic hydraulic-head distribution used pseudosources calculated by the last described method. Here the maximum error was 0.012 meter, but the error went to zero much more slowly than in the first method. This is the pseudosource calculation documented in the following pages.

Data-Deck Instructions

The following lists the data required for this program and their corresponding formats:

CARD	COLUMN	FORMAT	VARIABLE	DEFINITION
1	10	F10.6	PSLL	Print options of intermediate terms.
2	1-10	I10	IØ	Number of rows.
	11-20	I10	JØ	Number of columns.
	21-30	I10	KK	Layer number.

All the following data require a parameter card either preceding an array or as the sole value for that array:

Every parameter card	COLUMN	FORMAT	VARIABLE	DEFINITION
	1-10	G10.0	FAC	If IVAR = 0, FAC is the value assigned to every element of the matrix for this layer. If IVAR = 1, FAC is the multiplication factor for the following set of data cards for this layer.
	11-20	G10.0	IVAR	0--If no data cards are to be read in for this layer. 1--If data cards for this layer follow.
	21-30	G10.0	IPRN	0--If data for this layer are to be printed. 1--If data for this layer are not to be printed.

When data sets are included, start each row on a new card as follows:

DATA SET	COLUMN	FORMAT	VARIABLE	DEFINITION
1	1-80	20F4.0	DENL	Density array of lower aquifer.
2	1-80	20F4.0	DENU	Density array of upper aquifer.
3	1-80	20F4.0	THKL	Thickness of lower confining bed.
4	1-80	20F4.0	THKU	Thickness of upper confining bed.
5	1-80	20F4.0	TKL	Hybrid leakance of lower confining bed.
6	1-80	20F4.0	TKU	Hybrid leakance of upper confining bed.
7	1-80	20F4.0	T	Hybrid-transmissivity array--Inactive nodes need to have transmissivity set to zero, otherwise pseudosource calculation will be wrong.
8	1-80	20F4.0	DEN	Aquifer-density array data.
9	1-80	20F4.0	ELEV	Aquifer-elevation array data.
10	1-80	20F4.0	THCK	Aquifer-thickness array data.
11	1-80	8G10.0	DELX(J)	Grid spacing in x-direction.
12	1-80	8G10.0	DELY(I)	Grid spacing in y-direction.

Example of a Pseudosource Calculation

It is the purpose of this example to illustrate the data input (fig. 4) and results of a pseudosource calculation for a hypothetical symmetrical basin. It is assumed that the aquifer is bounded above and below by impermeable confining layers. The hybrid transmissivity is constant throughout the aquifer and is set to zero where the nodes are inactive. The symmetrical basin is described by the density and elevation arrays; that is, the elevation decreases and the density increases toward the center of the basin.

It can be seen from the output (fig. 5) that the sum of the aquifer pseudosource terms is approximately zero; this should hold true for every pseudosource calculation. Furthermore, each term can be introduced directly as well-input to Group IV data set 1 of Trescott (1976); terms with negative values correspond to a discharge well, and terms with positive values correspond to a recharge well. Pseudosource program variables are defined in table 1.

Column numbers on computer card	4	8	10	12	16	20	24	28	30	32
PSLL			0							
IØ,JØ,KK			7			7			1	
DENL			1.0							
DENU			1.0							
THKL			1.0							
THKU			1.0							
TKL			0.0							
TKU			0.0							
		115.4				1				
T	0	0	0	0	0	0	0	0		
	0	1	1	1	1	1	1	0		
	0	1	1	1	1	1	1	0		
	0	1	1	1	1	1	1	0		
	0	1	1	1	1	1	1	0		
	0	1	1	1	1	1	1	0		
	0	0	0	0	0	0	0	0		
		1.E-3				1				
DEN	1000	1000	1000	1000	1000	1000	1000	1000		
	1000	1000	1000	1000	1000	1000	1000	1000		
	1000	1000	1010	1010	1010	1010	1000	1000		
	1000	1000	1010	1020	1010	1010	1000	1000		
	1000	1000	1010	1010	1010	1010	1000	1000		
	1000	1000	1000	1000	1000	1000	1000	1000		
	1000	1000	1000	1000	1000	1000	1000	1000		
			-5			1				
ELEV	0	0	0	0	0	0	0	0		
	0	0	0	0	0	0	0	0		
	0	0	1	1	1	0	0			
	0	0	1	2	1	0	0			
	0	0	1	1	1	0	0			
	0	0	0	0	0	0	0			
	0	0	0	0	0	0	0			
THCK			1							
DELX		1000								
DELY		1000								
	/*									
	//									

Figure 4.--Data for a symmetrical basin example

```
LOWER DENSITY DATA        =   1.000000      FOR LAYER   1
UPPER DENSITY DATA        =   1.000000      FOR LAYER   1
LOWER C.B. THKNESS        =   1.000000      FOR LAYER   1
UPPER C.B. THKNESS        =   1.000000      FOR LAYER   1
LOWER C.B. LEAKANCE       =   0.0           FOR LAYER   1
UPPER C.B. LEAKANCE       =   0.0           FOR LAYER   1
```

TRANSMISSIVITY DATA MATRIX, LAYER 1

1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.0
3	0.0	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.0
4	0.0	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.0
5	0.0	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.0
6	0.0	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.115E 03	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0

DENSITY DATA MATRIX, LAYER 1

1	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01
2	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01
3	0.100E 01	0.100E 01	0.101E 01	0.101E 01	0.101E 01	0.100E 01	0.100E 01
4	0.100E 01	0.100E 01	0.101E 01	0.102E 01	0.101E 01	0.100E 01	0.100E 01
5	0.100E 01	0.100E 01	0.101E 01	0.101E 01	0.101E 01	0.100E 01	0.100E 01
6	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01
7	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01	0.100E 01

Figure 5.--Output for symmetrical basin example

ELEVATION DATA MATRIX, LAYER 1

1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	-0.500E 01	-0.500E 01	-0.500E 01	0.0	0.0
4	0.0	0.0	-0.500E 01	-0.100E 02	-0.500E 01	0.0	0.0
5	0.0	0.0	-0.500E 01	-0.500E 01	-0.500E 01	0.0	0.0
6	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	0.0	0.0	0.0	0.0	0.0	0.0

THICKNESS DATA = 1.000000 FOR LAYER 1

DELX = 1000.000

DELY = 1000.000

PSEUDOSOURCE TOTAL CONTRIBUTION

0.0	-2.885	-2.885	-2.885	0.0
-2.885	5.770	-5.770	5.770	-2.885
-2.885	-5.770	34.62	-5.770	-2.885
-2.885	5.770	-5.770	5.770	-2.885
0.0	-2.885	-2.885	-2.885	0.0

Figure 5.--Output for symmetrical basin example--Continued

```
                                    PS VERTICAL CONTRIBUTION

 0.0          0.0          0.0          0.0          0.0
 0.0          0.0          0.0          0.0          0.0
 0.0          0.0          0.0          0.0          0.0
 0.0          0.0          0.0          0.0          0.0
 0.0          0.0          0.0          0.0          0.0
      1            2            3     -2.880.0          2.885     0.0
      1            2            4     -2.880.0          2.885     0.0
      1            2            5     -2.880.0          2.885     0.0
      1            3            2     -2.88 2.885       0.0       0.0
      1            3            3      5.77-2.885      -2.885     0.0
      1            3            4     -5.770.0           5.770     0.0
      1            3            5      5.77-2.885      -2.885     0.0
      1            3            6     -2.88 2.885       0.0       0.0
      1            4            2     -2.88 2.885       0.0       0.0
      1            4            3     -5.77 5.770       0.0       0.0
      1            4            4     34.62-17.31      -17.31     0.0
      1            4            5     -5.77 5.770       0.0       0.0
      1            4            6     -2.88 2.885       0.0       0.0
      1            5            2     -2.88 2.885       0.0       0.0
      1            5            3      5.77-2.885      -2.885     0.0
      1            5            4     -5.770.0           5.770     0.0
      1            5            5      5.77-2.885      -2.885     0.0
      1            5            6     -2.88 2.885       0.0       0.0
      1            6            3     -2.880.0           2.885     0.0
      1            6            4     -2.880.0           2.885     0.0
      1            6            5     -2.880.0           2.885     0.0

                                    SUM OF P.S. TERMS
                                   ******************

 TOTAL PSA =     0.0          TOTAL PSB =     0.0          TOTAL PS3 =     0.0          TOTAL PS  =          0.0

 NORMAL END OF PROCESSING PROGRAM JDB3
 PROGRAMMED BY DOUG LOW  --RASA PROJECTS DENVER
 PROGRAM VERSION NUMBER 6SJ7
```

Figure 5.--Output for symmetrical basin example--Continued

Table 1.--*Definition of some pseudosource program variables*

Variable	Definition
COSA, COSB	Cosines of the angles between the bedding plane and the x- and y-axes.
DA, DB	Hypotenuse of the right triangle formed by the grid spacing and the bedding plane in the x- and y-directions.
DAP, DAM	Values of the total differential of alpha in the plus x-direction and minus x-direction from node (I,J).
DELX, DELY	The grid spacing in the x- and y-directions.
DEN	Average ground-water density for each nodal area.
DENL, DENU	Average ground-water density for each nodal area in the aquifer below and above the aquifer for which pseudo-sources are calculated.
DZA, DZB	Elevation change from node (I,J-1) to node (I,J+1) divided by two, and elevation change from node (I-1,J) to node (I+1,J) divided by two.
ELEV	Elevation array for the aquifer for which pseudosources are calculated.
IO, JO	Number of nodes in the x- and y-directions.

Table 1.--*Definition of some pseudosource program variables*--Continued

Variable	Definition
PSA, PSB	The alpha- and beta-terms of the aquifer pseudosource contributions at each node.
PS3	Confining-layer pseudosource contributions for each node.
PST	Total pseudosource contribution for each node.
PSLL	A lower limit for each total nodal pseudosource contribution. If PST is less than PSLL the results of some calculations preliminary to PST will not be printed out.
SUMPST, SUMPSA	PST summed for all nodes, and PSA summed for all nodes.
T	Hybrid transmissivity.
TAP, TAM	Harmonic mean of the hybrid transmissivity between nodes (I,J+1) and (I,J), and between the nodes (I,J) and (I,J-1).
THKL, THKU	Thickness of lower and upper confining layer.
TKL, TKU	Hybrid leakance of lower and upper confining layer.
TPSA, TPSB, TPS3	Total aquifer pseudosource contributions, and total confining-layer pseudosource contributions.

Pseudosource FORTRAN Program

The following FORTRAN program (table 2) for calculating pseudosource contributions was written for a specific model study and for compatibility with the U.S. Geological Survey's ground-water flow model (Trescott, 1976). It contains code peculiar to that study and that compatibility. Some of these peculiarities are:

1. The elevation used as input is the elevation of the top of the aquifer. Aquifer thickness is used to calculate the elevation of the aquifer midpoint or average aquifer elevation.
2. No provision is made for calculating with aquifer anisotropy.
3. The aquifer pseudosources are calculated with Δx replacing $\Delta\alpha$ in equation 31, and with $(T_{\alpha\alpha})_{j+1}$ calculated as the harmonic mean of $T_{\alpha\alpha}$ along the x-direction between nodes j and j+1. The aquifer pseudosources from the β-principal directions are calculated similarly. Alternatives to the harmonic mean are discussed in Appel (1976).
4. Total pseudosource contributions are punched out in a format suited for immediate input to the model described in Trescott (1976).
5. The reference density is assumed to be equal to 1.

None of these peculiarities are difficult to change to suit an individual study.

The program was run on the U.S. Geological Survey's Amdahl 470 V/7* computer in Reston, Virginia, with an IBM System 360/370, FORTRAN IV, H-extended compiler. Typical central-processing unit time is 1 second.

---

*Any use of trade names is for descriptive purposes only and does not imply endorsement by the U.S. Geological Survey.

Table 2.--*FORTRAN program to calculate pseudosource terms*

```
     ----- FORTRAN PROGRAM TO CALCULA PSEUDOSOURCE TERMS FROM FIELD DATA & M

C----- FORTRAN PROGRAM TO CALCULA PSEUDOSOURCE TERMS FROM FIELD DATA & M  A  10
C-----   DATA  TESTED ON 16JUNE80                                         A  20
C*****                                                                    A  30
C*****30 MAY 1980                                                         A  40
      INTEGER BLK                                                         A  50
      DIMENSION T(21,26), DEN(21,26), ELEV(21,26), THCK(21,26), DELX(26)  A  60
     1, DELY(21), INFT(2,2), IOFT(9,4), IN(6), TF(3), DUM(3), PST(21,26)  A  70
     2, PSA(21,26), PSB(21,26), PS3(21,26), DENU(21,26), DENL(21,26), TK  A  80
     3L(21,26), TKU(21,26), THKL(21,26), THKU(21,26)                      A  90
      COMMON /MISC/ I0,J0,K0                                              A 100
      DATA BLK/' '/                                                       A 110
      DATA INFT/4H(20F,4H4.0),4H(8F1,4H0.4)/                              A 120
      DATA IOFT/'(1H0',',I2,',I2X,2',',0F6.',',1/(5',',X,20',',F6.1',',))  ',  A 130
     1'    ',',(1H0',',I5,',14F9',',5/(',6X,1',',4F9.',',5)) ',',    ',',  A 140
     2  ',',(1H0',',I5,',10E1',',2.5/',',(6X,',',10E1',',2.5)',',)   ',',    A 150
     3,',(1H0',',I5,',10E1',',1.3/',',(6X,',',10E1',',1.3)',',)   ',',    */  A 160
C********                                                                 A 170
C-----I0=21 THIS VARIABLE IS NOW READ IN                                  A 180
C-----J0=26  "      "    "    "    "    "                                 A 190
      K0=3                                                                A 200
      IRN=1                                                               A 210
      DO 110 I=1,6                                                        A 220
  110 IN(I)=BLK                                                           A 230
C-------READ IN PRINT OPTION OF INTERMEDIATE TERMS                       A 240
      READ (5,230) KCHK                                                   A 250
C-----READ          IN MATRIX SIZE AND                                    A 260
C-----READ IN LAYER NUMBER STARTING AT BOTTOM WITH ONE                    A 270
      READ (5,240) I0,J0,KK                                               A 280
C----    READ       IN LOWER DENSITY ARRAY                               A 290
      CALL ARRAY(DENL,INFT(1,1),IOFT(1,4),'LOWER DENSITY DATA    ',IRN,D  A 300
     1UM)                                                                 A 310
C---- READ IN UPPER DENSITY ARRAY                                         A 320
      CALL ARRAY(DENU,INFT(1,1),IOFT(1,4),'UPPER DENSITY DATA    ',IRN,D  A 330
     1UM)                                                                 A 340
C---- READ IN LOWER CONFINING BED THICKNESS ARRAY                         A 350
      CALL ARRAY(THKL,INFT(1,1),IOFT(1,1),'LOWER C.B. THKNESS      ',IR   A 360
     1N,DUM)                                                              A 370
C---- READ IN UPPER CONFINING BED THICKNESS ARRAY                         A 380
      CALL ARRAY(THKU,INFT(1,1),IOFT(1,1),'UPPER C.B. THKNESS    ',IRN,D  A 390
     1UM)                                                                 A 400
C---- READ IN LOWER CONFINING BED LEAKANCE                                A 410
      CALL ARRAY(TKL,INFT(1,1),IOFT(1,4),'LOWER C.B. LEAKANCE   ',IRN,DU   A 420
     1M)                                                                  A 430
C---- READ IN UPPER CONFINING BED LEAKANCE                                A 440
      CALL ARRAY(TKU,INFT(1,1),IOFT(1,4),'UPPER C.B. LEAKANCE   ',IRN,DU   A 450
     1M)                                                                  A 460
C---- READ IN HYBRID TRANSMISSIVITY ARRAY DATA                            A 470
C     INACTVE NODES MUST HAVE TRANSMISSIVITY SET TO ZERO                *  A 480
C     OTHERWISE PSEUDOSOURCE CALCULATION WILL BE WRONG                  *  A 490
C-----**********************************************************************  A 500
```

Table 2.--*FORTRAN program to calculate pseudosource terms*--Continued

```
      CALL ARRAY(T,INFT(1,1),IOFT(1,4),'TRANSMISSIVITY DATA      ',IRN,DU  A 510
     1M)                                                                  A 520
C---- READ IN DENSITY ARRAY DATA                                          A 530
      CALL ARRAY(DEN,INFT(1,1),IOFT(1,4),'DENSITY DATA           ',IRN,D  A 540
     1UM)                                                                 A 550
C---- READ IN ELEVATION ARRAY DATA                                        A 560
      CALL ARRAY(ELEV,INFT(1,1),IOFT(1,4),'ELEVATION DATA        ',IRN,   A 570
     1DUM)                                                                A 580
C---- READ IN THICKNESS ARRAY DATA                                        A 590
      CALL ARRAY(THCK,INFT(1,1),IOFT(1,4),'THICKNESS DATA        ',IRN    A 600
     1,DUM)                                                               A 610
C---- READ IN DELX ARRAY                                                  A 620
C     ............................. DELX ..............................    A 630
      READ (5,410) FAC,IVAR,IPRN                                          A 640
      IF (IVAR.EQ.1) READ (5,380) (DELX(J),J=1,J0)                        A 650
      DO 130 J=1,J0                                                       A 660
      IF (IVAR.NE.1) GO TO 120                                            A 670
      DELX(J)=DELX(J)*FAC                                                 A 680
      GO TO 130                                                           A 690
  120 DELX(J)=FAC                                                         A 700
  130 CONTINUE                                                            A 710
      IF (IVAR.EQ.1.AND.IPRN.NE.1) WRITE (6,390) (DELX(J),J=1,J0)         A 720
      IF (IVAR.EQ.0) WRITE (6,360) FAC                                    A 730
C     ............................. DELY ..............................    A 740
      READ (5,410) FAC,IVAR,IPRN                                          A 750
      IF (IVAR.EQ.1) READ (5,380) (DELY(I),I=1,I0)                        A 760
      DO 150 I=1,I0                                                       A 770
      IF (IVAR.NE.1) GO TO 140                                            A 780
      DELY(I)=DELY(I)*FAC                                                 A 790
      GO TO 150                                                           A 800
  140 DELY(I)=FAC                                                         A 810
  150 CONTINUE                                                            A 820
      IF (IVAR.EQ.1.AND.IPRN.NE.1) WRITE (6,400) (DELY(I),I=1,I0)         A 830
      IF (IVAR.EQ.0) WRITE (6,370) FAC                                    A 840
      SUMPST=0.0                                                          A 850
      SUMPSA=0.0                                                          A 860
      SUMPSR=0.0                                                          A 870
      SUMPSJ=0.0                                                          A 880
      DO 160 I=1,I0                                                       A 890
      DO 160 J=1,J0                                                       A 900
      PST(I,J)=0.0                                                        A 910
      PSA(I,J)=0.0                                                        A 920
      PSB(I,J)=0.0                                                        A 930
      PSJ(I,J)=0.0                                                        A 940
      ELEV(I,J)=ELEV(I,J)-THCK(I,J)/2.                                    A 950
  160 CONTINUE                                                            A 960
      I0=I0-1                                                             A 970
      J0=J0-1                                                             A 980
      DO 190 I=2,I0                                                       A 990
      DO 190 J=2,J0                                                       A1000
```

Table 2.--*FORTRAN program to calculate pseudosource terms*--Continued

```
      IF (T(I,J).EQ.0) GO TO 170                                          A1010
C *********************************************************************  A1020
C  HARMONIC MEAN OF HYBRID TRANSMISSIVITY INSURES NO-FLOW BOUNDARIES      A1030
C  CORRECTLY IMPLEMENTED EVEN IN VARIABLE DENSITY CASE..                  A1040
C  CALCULATION OF HARMONIC MEAN HYBRID TRANSMISSIVITY DIVIDED BY THE      A1050
C  DISTANCE BETWEEN NODES FOLLOWS....                                     A1060
C *********************************************************************  A1070
      TAP=2.*T(I,J+1)*T(I,J)/(T(I,J+1)*DELX(J)+T(I,J)*DELX(J+1))          A1080
      TAM=2.*T(I,J)*T(I,J-1)/(T(I,J)*DELX(J-1)+T(I,J-1)*DELX(J))          A1090
      TBP=2.*T(I+1,J)*T(I,J)/(T(I+1,J)*DELY(I)+T(I,J)*DELY(I+1))          A1100
      TBM=2.*T(I,J)*T(I-1,J)/(T(I,J)*DELY(I-1)+T(I-1,J)*DELY(I))          A1110
C****CALC OF DELTA RHO'S AS WEIGHTED AVERAGES ************************     A1120
      DRO=DEN(I,J)-1.                                                     A1130
      DAP=DEN(I,J+1)-1.                                                   A1140
      DAM=DEN(I,J-1)-1.                                                   A1150
      DBP=DEN(I+1,J)-1.                                                   A1160
      DBM=DEN(I-1,J)-1.                                                   A1170
      DNAP=(DAP*DELX(J+1)+DRO*DELX(J))/(DELX(J+1)+DELX(J))                A1180
      DNAM=(DAM*DELX(J-1)+DRO*DELX(J))/(DELX(J-1)+DELX(J))                A1190
      DNBP=(DBP*DELY(I+1)+DRO*DELY(I))/(DELY(I+1)+DELY(I))                A1200
      DNBM=(DBM*DELY(I-1)+DRO*DELY(I))/(DELY(I-1)+DELY(I))                A1210
C *******CALC. OF ELEVATION CHANGES************************************   A1220
      DZAP=ELEV(I,J+1)-ELEV(I,J)                                          A1230
      DZAM=-ELEV(I,J-1)+ELEV(I,J)                                         A1240
      DZBP=ELEV(I+1,J)-ELEV(I,J)                                          A1250
      DZBM=-ELEV(I-1,J)+ELEV(I,J)                                         A1260
      DZA=(DZAP+DZAM)/2.                                                  A1270
      DZB=(DZBP+DZBM)/2.                                                  A1280
C ****CALC OF VARIOUS DELTA-ALPHA'S & DELTA-BETA'S*********************   A1290
      DA=SQRT(DELX(J)**2+DZA**2)                                          A1300
      DB=SQRT(DELY(I)**2+DZB**2)                                          A1310
      COSA=DELX(J)/DA                                                     A1320
      COSB=DELY(I)/DB                                                     A1330
C*********************************************************************  A1340
C     THE END OF FACTOR CALC & THE BEGINNING OF THE CALC OF THE ALPHA & B A1350
C     CONTRIBUTIONS TO HORIZONTAL PSEUDOSOURCE TERM.. THE CALC OF THE VER A1360
C     PSEUDOSOURCE TERM FOLLOWS.                                          A1370
C *********************************************************************  A1380
      PSA(I,J)=-(TAP*DNAP*DZAP-TAM*DNAM*DZAM)*DELY(I)                     A1390
      PSB(I,J)=-(TBP*DNBP*DZBP-TBM*DNBM*DZBM)*DELX(J)                     A1400
      PKL=TKL(I,J)*THKL(I,J)                                              A1410
      PKU=TKU(I,J)*THKU(I,J)                                              A1420
      DDENL=((DEN(I,J)+DENL(I,J))/2.-1.)                                  A1430
      DDENU=((DEN(I,J)+DENU(I,J))/2.-1.)                                  A1440
      PS3(I,J)=(PKL*DDENL-PKU*DDENU)*DELX(J)*DELY(I)                      A1450
      PST(I,J)=-PSA(I,J)-PSB(I,J)-PS3(I,J)                                A1460
C*********************************************************************  A1470
C       IN ORDER TO MAKE THE CORRESPONDENCE BETWEEN PSA,PSB,PS3 AND THE W A1480
C       DISCHARGE OR RECHARGE OF THE GROUND WATER FLOW CODE OF OPEN FILE   A1490
C       REPORT 75-438 THREE MINUS SIGNS ARE INTRODUCED IN THE EQUATION AB  A1500
```

Table 2.--*FORTRAN program to calculate pseudosource terms*--Continued

```
C       WITH THESE MINUS SIGNS PST(I,J) CAN BE INTRODUCED DIRECTLY AS INP  A1510
C       GROUP IV DATA SET 1 OF REPORT 75-438.  PST<0 CORRESPONDS TO A      A1520
C       DISCHARGING WELL, AND PST>0 CORRESPONDS TO A RECHARGING WELL.      A1530
C*************************************************************************A1540
  170 CONTINUE                                                             A1550
      IF (T(I,J).NE.0) GO TO 180                                           A1560
      PST(I,J)=0.0                                                         A1570
      PSA(I,J)=0.0                                                         A1580
      PSB(I,J)=0.0                                                         A1590
      PS3(I,J)=0.0                                                         A1600
  180 CONTINUE                                                             A1610
      IF (ABS(PST(I,J)).LT.0.2.OR.KCHK.EQ.0) GO TO 190                     A1620
      WRITE (6,250)                                                        A1630
      WRITE (6,280) I,J,DZA,DZB,COSA,COSB,TAP,TAM,TBP,TBM,DNAP,DNAM,DNBP   A1640
     1,DNBM                                                                A1650
      WRITE (6,260)                                                        A1660
      WRITE (6,270) DA,DB                                                  A1670
      WRITE (6,290) PSA(I,J),PSB(I,J),PS3(I,J)                             A1680
      SUMPSA=SUMPSA+PSA(I,J)                                               A1690
      SUMPSB=SUMPSB+PSB(I,J)                                               A1700
      SUMPS3=SUMPS3+PS3(I,J)                                               A1710
  190 CONTINUE                                                             A1720
      SUMPST=SUMPSA+SUMPSB+SUMPS3                                          A1730
      WRITE (6,300)                                                        A1740
      DO 200 I=2,I0                                                        A1750
  200 WRITE (6,350) (PST(I,J),J=2,J0)                                      A1760
      WRITE (6,310)                                                        A1770
      DO 210 I=2,I0                                                        A1780
  210 WRITE (6,350) (PS3(I,J),J=2,J0)                                      A1790
C***** PUNCH OUT RECHARGE DATA FOR SELECTED NODES                         A1800
      DO 220 I=2,I0                                                        A1810
      DO 220 J=2,J0                                                        A1820
      IF (ABS(PST(I,J)).LT.0.2) GO TO 220                                  A1830
      WRITE (6,320) KK,I,J,PST(I,J),PSA(I,J),PSB(I,J),PS3(I,J)             A1840
      WRITE (8,320) KK,I,J,PST(I,J),PSA(I,J),PSB(I,J),PS3(I,J)             A1850
  220 CONTINUE                                                             A1860
      WRITE (6,330) SUMPSA,SUMPSB,SUMPS3,SUMPST                            A1870
      WRITE (6,340)                                                        A1880
      I0=I0+1                                                              A1890
      J0=J0+1                                                              A1900
      STOP                                                                 A1910
C                                                                          A1920
  230 FORMAT (I10)                                                         A1930
  240 FORMAT (3I10)                                                        A1940
  250 FORMAT (T2,'     I  J  DZA      DZB          COSA',',       COSB     T  A1950
     1AP         TAM         TBP',',        TBM          DNAP       DNAM    A1960
     2DNBP         DNBM')                                                  A1970
  260 FORMAT (1H ,7X,'DA',8X,'DB')                                         A1980
  270 FORMAT (1H ,7X,2G10.4)                                               A1990
  280 FORMAT (T5,2I3,11G11.4,/)                                            A2000
```

Table 2.--*FORTRAN program to calculate pseudosource terms*--Continued

```
290 FORMAT (10X,'PSA = ',G10.4,7X,'PSB = ',G10.4,7X,'PSJ = ',G10.4,//)  A2010
300 FORMAT ('1',T50,'PSEUDOSOURCE TOTAL CONTRIBUTION',//)               A2020
310 FORMAT ('1',T50,'PS VERTICAL CONTRIBUTION',//)                      A2030
320 FORMAT (3I10,F10.2,3G10.4)                                         A2040
330 FORMAT (T10,//,50X,'SUM OF P.S. TERMS',/,49X,'******************',/  A2050
   1/,10X,'TOTAL PSA =',F10.4,10X,'TOTAL PSB =',F10.4,10X,'TOTAL PSJ =  A2060
   2',F10.4,10X,'TOTAL PS  =',F15.4,//)                                A2070
340 FORMAT (T10,'NORMAL END OF PROCESSING PROGRAM JD83',/,T10,'PROGRAM  A2080
   1MED BY DOUG LOW  --RASA PROJECTS DENVER',/,T10,'PROGRAM VERSION NU  A2090
   2MBER 6SJ7')                                                        A2100
350 FORMAT (T2,8(G10.4,2X),/,T2,8(G10.4,2X),/,T2,8(G10.4,2X),/,T2,8(G1  A2110
   10.4,2X))                                                           A2120
360 FORMAT ('0',72X,'DELX =',G15.7)                                    A2130
370 FORMAT ('0',72X,'DELY =',G15.7)                                    A2140
380 FORMAT (8G10.0)                                                    A2150
390 FORMAT (1H1,46X,40HGRID SPACING IN PROTOTYPE IN X DIRECTION/47X,40  A2160
   1('-')//('0',12F10.0))                                              A2170
400 FORMAT (1H-,46X,40HGRID SPACING IN PROTOTYPE IN Y DIRECTION/47X,40  A2180
   1('-')//('0',12F10.0))                                              A2190
410 FORMAT (F10.0,2I10,3F10.0,2I10)                                    A2200
    END                                                                A2210-
```

Table 2.--*FORTRAN program to calculate pseudo-source terms*--Continued

```
                                        **********
C     **********                                                        B  10
      SUBROUTINE ARRAY(A,INFT,IOFT,IN,IRN,TF)                           B  20
C     **********                                                        B  30
      INTEGER BLK                                                       B  40
      DIMENSION A(21,26), INFT(2,2), IN(6), TF(3), DUM(3), DUM2(4), IOFT B  50
     1(9,4)                                                             B  60
      COMMON /MISC/ I0,J0,K0                                            B  70
      DATA BLK/' '/                                                     B  80
      K=1                                                               B  90
      READ (5,120) FAC,IVAR,IPRN,TF,IRECS,IRECD                         B 100
      IC=4*IRECS+2*IVAR+IPRN+1                                          B 110
      GO TO (10,10,30,30,60,60), IC                                     B 120
   10 DO 20 I=1,I0                                                      B 130
      DO 20 J=1,J0                                                      B 140
   20 A(I,J)=FAC                                                        B 150
      WRITE (6,100) IN,FAC,K                                            B 160
      GO TO 80                                                          B 170
   30 IF (IC.EQ.3) WRITE (6,110) IN,K                                   B 180
      DO 50 I=1,I0                                                      B 190
      READ (5,INFT) (A(I,J),J=1,J0)                                     B 200
      DO 40 J=1,J0                                                      B 210
   40 A(I,J)=A(I,J)*FAC                                                 B 220
   50 IF (IC.EQ.3) WRITE (6,IOFT) I,(A(I,J),J=1,J0)                     B 230
      GO TO 80                                                          B 240
   60 CONTINUE                                                          B 250
      IF (IC.EQ.6) GO TO 80                                             B 260
      WRITE (6,110) IN,K                                                B 270
      DO 70 I=1,I0                                                      B 280
   70 WRITE (6,IOFT) I,(A(I,J),J=1,J0)                                  B 290
   80 CONTINUE                                                          B 300
      IRN=IRN+1                                                         B 310
      DO 90 I=1,6                                                       B 320
   90 IN(I)=BLK                                                         B 330
      RETURN                                                            B 340
C                                                                       B 350
C     ---FORMATS---                                                     B 360
C                                                                       B 370
C                                                                       B 380
C                                                                       B 390
  100 FORMAT (1H0,52X,6A4,' =',G15.7,' FOR LAYER',I3)                   B 400
  110 FORMAT (1H1,45X,6A4,' MATRIX, LAYER',I3/46X,41('-'))              B 410
  120 FORMAT (F10.0,2I10,3F10.0,2I10)                                   B 420
      END                                                               B 430-
```

COMPUTER CODE TO CALCULATE GROUND-WATER DENSITY AND PURE-WATER CONCENTRATION

To calculate pseudosource strengths, it is necessary to know ground-water density throughout the modelled area. Usually, direct determinations of ground-water density are unavailable to model studies. However, it is standard practice to measure dissolved solids in ground water. Combining dissolved-solids data with temperature data and hydraulic-head and elevation measurements, it is possible to obtain a good estimate of ground-water density for brines. The assumption made in the following development is that the density of ground water is the same as the density of a sodium chloride water solution of the same molality, temperature, and pressure. There is some indication in the literature that this is a good approximation, if both solutions are of the same ionic strength (Collins, 1975).

Once this assumption is made, then steam tables for sodium chloride solutions (Potter and Brown, 1977) can be used to calculate ground-water densities. A determination of the molality is necessary to enter the table. Molality of a solution is equal to the number of moles of solute per 1,000 grams of solvent. The formula used to calculate molality is:

$$m = \frac{DS}{MW\ (\rho' - DS/1{,}000)} \qquad (32)$$

where

m is the approximate molality of ground water;

DS is the grams of dissolved solids per liter of ground water at laboratory conditions (20° Celsius and 1 atmosphere);

MW is the gram molecular weight of sodium chloride, 58.4428 grams per mole; and

ρ' is the density of ground water at 20° Celsius and 1 atmosphere, in grams per cubic centimeter.

In the program that follows, the initial density of ground water is assumed to be 1, and a molality is calculated using equation 32. The calculated molality then is substituted into equation 1 of Potter and Brown (1977) to calculate the density at 20° Celsius and 1 atmosphere. This density then is substituted back into equation 32, and a new molality is calculated. The iteration is continued until the last molality calculated is within 0.002 percent of the penultimate molality. When this condition is satisfied, the last molality, field values of pressure (in bars) and temperature (in degrees Celsius) are used to enter the steam tables for sodium chloride solutions to determine a field density (ρ).

This density then is used in equation 33 to calculate the pure-water concentration of ground water as follows:

$$c_p = \rho \left(1 - \frac{1}{\left(1 + \frac{1{,}000}{m \times MW} \right)} \right). \qquad (33)$$

The program is described further in the following flow chart (fig. 6).

Two lacunae inherent in the tables are filled by the density algorithm. First, the lack of data between zero and 0.5 molality is filled by an interpolation. The tables list zero molal densities for only atmospheric pressure. These were used in the interpolation. Second, there are no data for molalities greater than 6.0. To calculate densities for these molalities, an extrapolation is made using a formula that has only been fitted to data at and below 6.0 molality. The interpolation below 0.5 molality might be improved by using table 15 in Potter and Brown (1977), and the fact that a 1 weight percent sodium chloride solution is a 0.1711 molal solution.

The program was run on the U.S. Geological Survey's Amdahl 470 V/7 computer in Reston, Virginia, with an IBM System 360/370, FORTRAN IV, H-extended compiler. Typical central-processing unit time is 2 seconds.

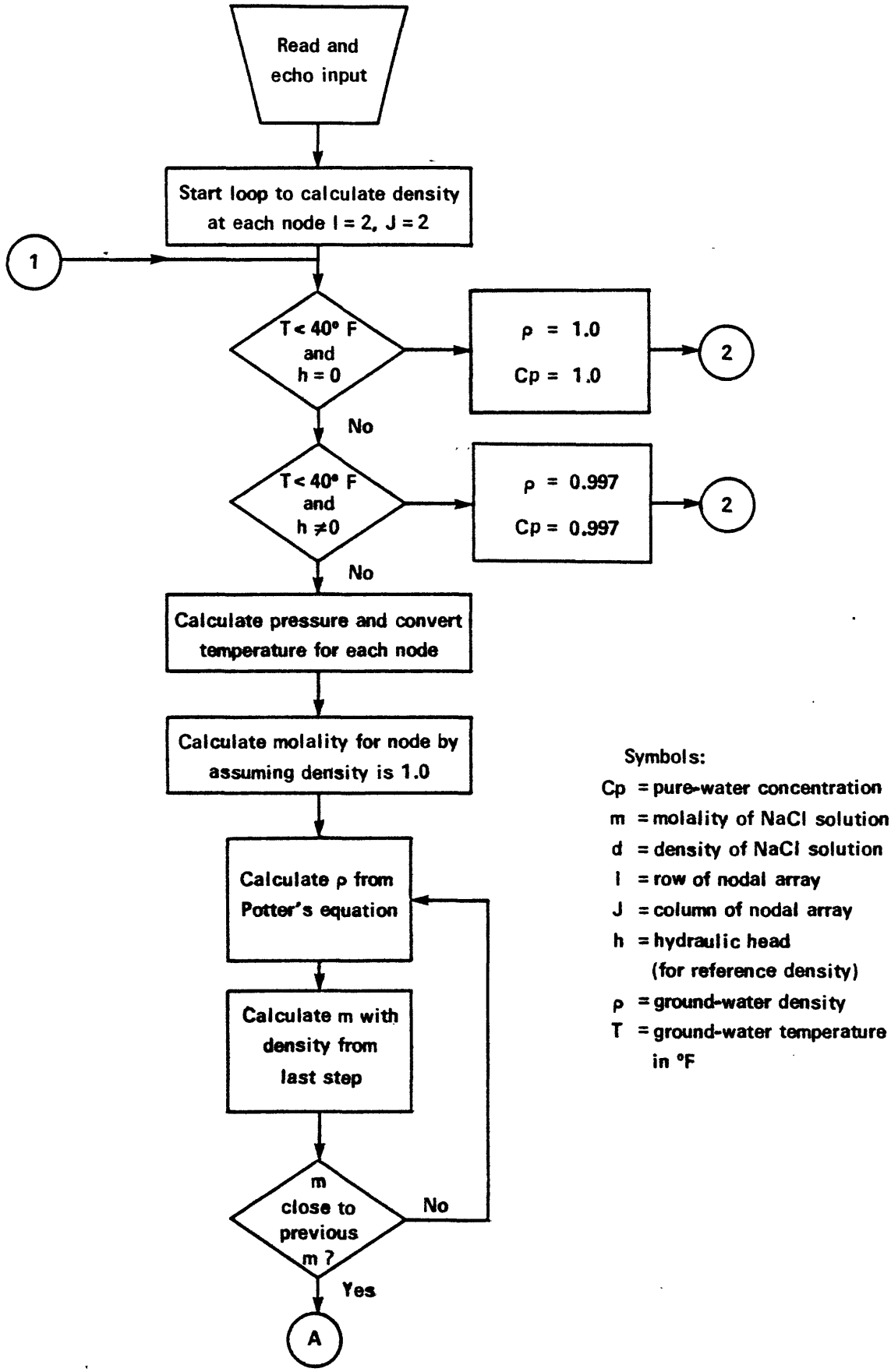

Figure 6.--Flow chart for density calculation program.

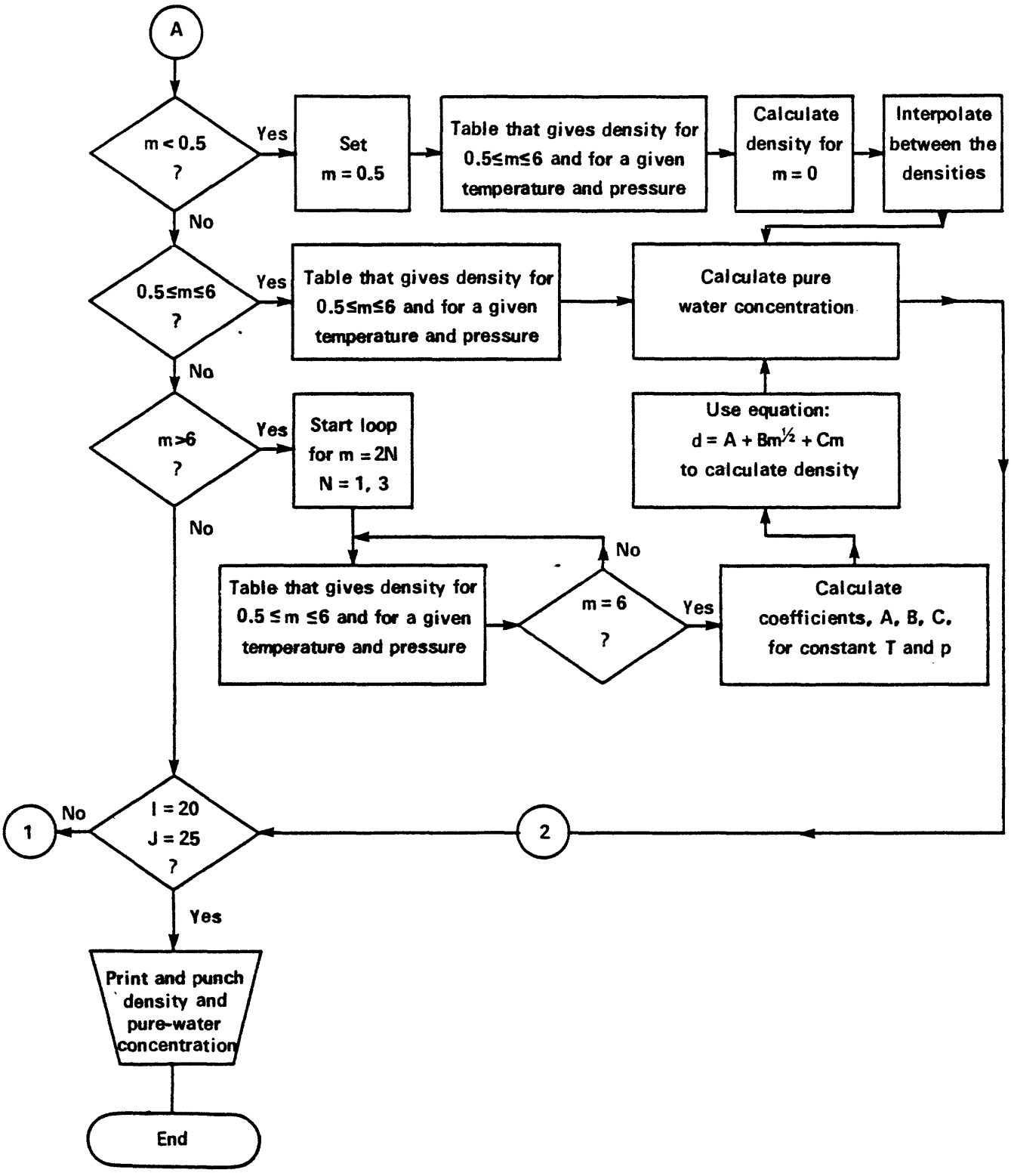

Figure 6.--Flow chart for density calculation program--Continued

Data-Deck Instructions

The following lists the data required for this program and their corresponding formats. Definitions of some density and concentration program variables are given in table 3; density and concentration FORTRAN program is given in table 4. The way to enter data is similar to the way data enters the pseudosource program:

CARD	COLUMN	FORMAT	VARIABLE	DEFINITION
1	1-80	20A4	TITLE	Title of density calculation.
2	1-10	F10.6	CD1FF	Percentage difference allowed for molality iteration to converge.
	11-20	F10.6	PRINT	Print option of intermediate calculations.
3	1-10	I10	IØ	Number of rows.
	11-20	I10	JØ	Number of columns.
	21-30	I10	KØ	Layer number.

All of the following input data require a parameter card either preceding an array or as the sole input for that array.

Every parameter card	COLUMN	FORMAT	VARIABLE	DEFINITION
	1-10	G10.0	FAC	If IVAR = 0, FAC is the value assigned to every element of the matrix for this layer. If IVAR = 1, FAC is the multiplication factor for the following set of data cards for this layer.
	11-20	G10.0	IVAR	0--If no data cards are to be read in for this layer. 1--If data cards for this layer follow.
	21-30	G10.0	IPRN	0--If data for this layer are to be printed. 1--If data for this layer are not to be printed.

When data sets are included, start each row on a new card as follows:

DATA SET	COLUMN	FORMAT	VARIABLE	DEFINITION
1	1-80	16F5.0	TEMP	Temperature, in degrees Celsius.
2	1-80	20F4.0	TDS	Dissolved solids, in grams per liter.
3	1-80	8F10.4	H	Hydraulic head, in feet above sea level.
4	1-80	20F4.0	ELEV	Aquifer elevation, in feet above sea level.

Table 3.--*Definitions of some density and concentration program variables*

Variables	Definitions
A, B, C	Coefficients in the first four columns of table 29 from Potter and Brown (1977).
CDIFF	A value such that when CDIFF is greater than CRTN, the molality iteration stops.
CRTN	Absolute value of the percentage difference between the last calculated molality and the previous calculated molality.
DO	d_o-coefficients of table 28 from Potter and Brown (1977).
DEN	Final floating-point array into which density is put.
DEN1	Density calculated for pure water at field temperature.
DEN3	Density calculated for a 0.5 molality solution.
DENS	Density calculated from equation 1 of Potter and Brown (1977) and used to iterate to a final molality.
DENP	Pure-water concentration array.
E	An array that contains A_o, B_o, and C_o (for 20° Celsius) of table 28 from Potter and Brown (1977).

Table 3.--*Definitions of some density and concentration program variables*--Continued

Variables	Definitions
ELEV	Elevation array.
H	Pure-water (at 20° Celsius and 1 atmosphere) hydraulic-head array.
IDEN	Fixed-point representation of 1,000 x DEN.
IDENP	Fixed-point representation of 1,000 x DENP.
P	Pressure array.
R	Three-element array containing density for molalities of 2.0, 4.0, and 6.0.
RHO	Temporary storage variable for density from steam tables.
TDS	Dissolved-solids array.
TEMP	Temperature array.
TITLE	Alphanumeric variable that contains the first line of input.
X	Three-element array containing molalities equal to 2.0, 4.0, and 6.0.
XMOL	Final iteration molality.
XMOL1	Intermediate iteration molality.
XMOL3	A molality equal to 0.5.

Table 4.--*Density and concentration FORTRAN program*

```
      INTEGER BLK                                                          A  10
      DIMENSION H(21,26), INFT(2,3), IOFT(9,4), IN(6), DUM(3), TF(3)       A  20
      DIMENSION TEMP(21,26), ELEV(21,26), TDS(21,26), P(21,26)             A  30
      DIMENSION DEN(21,26), DENP(21,26), IDEN(21,26), IDENP(21,26)         A  40
      DIMENSION A(13,4), B(13,4), C(13,4), DO(5), TITLE(20), E(3)          A  50
      DIMENSION X(3), R(3)                                                 A  60
C --- E(I) ARE CONSTANTS IN POTTER'S EQ1 FOR 20 DEGREES CENTIGRADE          A  70
      DATA E/15.782,2.0324,0.0744/                                         A  80
      DATA DO/.999839,.997047,.988038,.974844,.974644/                     A  90
      DATA A/1.0059,1.0312,1.049,1.077,1.099,1.117,1.137,1.155,1.168,1.1   A 100
     184,1.198,1.213,1.213,1.021,1.043,1.063,1.081,1.098,1.116,1.135,1.1   A 110
     250,1.166,1.183,1.194,1.210,1.210,1.026,1.047,1.068,1.085,1.102,1.1   A 120
     319,1.135,1.152,1.168,1.183,1.197,1.212,1.212,1.031,1.051,1.071,1.0   A 130
     488,1.107,1.123,1.138,1.154,1.170,1.185,1.199,1.215,1.215/            A 140
      DATA B/-0.318,0.743,1.028,2.769,3.602,4.136,4.746,5.106,5.084,5.33   A 150
     14,5.292,5.428,5.428,0.239,1.200,1.613,1.994,1.666,2.548,3.439,3.74   A 160
     21,4.103,5.588,4.266,4.642,4.642,0.868,1.399,1.869,1.602,1.939,2.23   A 170
     39,2.608,3.354,3.881,3.967,4.066,4.467,4.467,1.077,1.417,1.878,2.22   A 180
     42,2.631,2.894,2.855,3.161,3.688,3.772,3.870,4.294,4.294/             A 190
      DATA C/3.099,2.661,2.413,1.888,1.601,1.378,1.174,1.033,0.980,0.887   A 200
     1,0.858,0.805,0.805,2.974,2.520,2.314,2.276,2.411,1.955,1.593,1.318   A 210
     2,1.165,0.717,1.028,0.885,0.885,2.592,2.336,2.102,2.368,2.173,1.994   A 220
     3,1.820,1.343,1.137,1.091,1.038,0.892,0.892,2.427,2.213,2.001,1.803   A 230
     4,1.635,1.496,1.464,1.338,1.138,1.090,1.043,0.891,0.891/              A 240
      COMMON /MISC/ I0,J0,K0                                               A 250
      DATA INFT/4H(20F,4H4.0),4H(8F1,4H0.4),4H(16F,4H5.0)/                 A 260
      DATA IOFT/'(1H0',',I2,','2X,2','0F6.','1/(5','X,20','F6.1',',))  ',  A 270
     1'    ',',(1H0',',I5,','14F9',',5/(',6X,1',',4F9,',',5)) ',','    ',' A 280
     2  ',',(1H0',',I5,','10E1','2.5/',',(6X,',',10E1','2.5)',')   ',','   ' A 290
     3,',(1H0',',I5.','10E1','1.3/',',(6X.',',10E1','1.3)',')   ',','   '/ A 300
C********                                                                  A 310
      IRN=1                                                                A 320
C******THE MOLECULAR WEIGHT OF NACL AND CONVERSION FACTOR TO CONVERT       A 330
C      FEET OF WATER TO BARS (PRESSURE).....                               A 340
      WT=58.4428                                                           A 350
      CF=.02987712                                                         A 360
C-------READ IN TITLE                                                     A 370
      READ (5,230) TITLE                                                   A 380
C------READ IN CLOSURE CRITERION FOR MOLALITY ITERATION IN PERCENT         A 390
      READ (5,240) CDIFF,PRINT                                             A 400
      WRITE (6,250) CDIFF,PRINT                                            A 410
C------READ IN MATRIX SIZE AND                                            A 420
C------READ IN LAYER NUMBER STARTING AT BOTTOM WITH ONE                   A 430
      READ (5,260) I0,J0,K0                                                A 440
      WRITE (6,270) I0,J0,K0                                               A 450
C---- READ IN TEMPERATURE ARRAY (IN DEGREES FAHRENHEIT)                   A 460
      CALL ARRAY(TEMP,INFT(1,3),IOFT(1,1),'TEMPERATURE (IN FHRNHT)',IRN,   A 470
     1DUM)                                                                 A 480
C---- READ IN DISSOLVED SOLIDS (IN GRAMS PER LITER)                       A 490
      CALL ARRAY(TDS,INFT(1,1),IOFT(1,1),'DISSOLVED SOLIDS IN G/L',IRN,D   A 500
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
     1(M)                                                                A 510
C---- READ IN 'FRESH WATER' HEADS (PURE WATER AT STP) IN FEET             A 520
      CALL ARRAY(H,INFT(1,2),IOFT(1,1),'FRESH WATER HEADS IN FT',IRN,DUM  A 530
     1)                                                                  A 540
C---- READ IN AQUIFER ELEVATION (IN FEET ABOVE MSL)                      A 550
      CALL ARRAY(ELEV,INFT(1,1),IOFT(1,4),'AQUIFER ELEV.(IN FT)',IRN,DUM  A 560
     1)                                                                  A 570
      WRITE (6,280)                                                      A 580
      WRITE (6,290) ((A(I,J),I=1,13),J=1,4)                              A 590
      WRITE (6,290) ((B(I,J),I=1,13),J=1,4)                              A 600
      WRITE (6,290) ((C(I,J),I=1,13),J=1,4)                              A 610
      WRITE (6,300) (DO(I),I=1,5)                                        A 620
      I0M1=I0-1                                                          A 630
      J0M1=J0-1                                                          A 640
      DO 110 J=1,J0                                                      A 650
      DO 110 I=1,I0                                                      A 660
      DEN(I,J)=0.0                                                       A 670
      DENP(I,J)=0.0                                                      A 680
  110 P(I,J)=0.0                                                         A 690
      DO 120 I=1,3                                                       A 700
      X(I)=0.0                                                           A 710
  120 R(I)=0.0                                                           A 720
      DO 210 I=2,I0M1                                                    A 730
      DO 210 J=2,J0M1                                                    A 740
      IF (TEMP(I,J).LT.40.AND.H(I,J).EQ.0.0) GO TO 190                   A 750
      IF (TEMP(I,J).LT.40.AND.H(I,J).NE.0.0) GO TO 200                   A 760
      TEMP(I,J)=(TEMP(I,J)-32)*5/9                                       A 770
      P(I,J)=CF*(H(I,J)-ELEV(I,J))                                       A 780
      XMOL=TDS(I,J)*1000/((1000-TDS(I,J))*WT)                            A 790
      N=0                                                                A 800
  130 CONTINUE                                                           A 810
C --- DEN0 IS DENSITY OF PURE WATER AT 20 DEG.C. AND 1BAR                A 820
      DEN0=0.9976054                                                     A 830
      DNM=1000+(E(1)*XMOL+E(2)*(SQRT(XMOL)**3)+E(3)*(XMOL**2))*DEN0      A 840
      DEN$=(1000*DEN0+WT*XMOL*DEN0)/DNM                                  A 850
      N=N+1                                                              A 860
      XMOL1=TDS(I,J)*1000/((DEN$*1000-TDS(I,J))*WT)                      A 870
      CRTN=ABS((XMOL-XMOL1)*100/XMOL)                                    A 880
      XMOL=XMOL1                                                         A 890
      IF (N.EQ.1.AND.PRINT.EQ.1) WRITE (6,310)                           A 900
      IF (PRINT.EQ.1) WRITE (6,320) I,J,K0,N,XMOL1,DEN$,TDS(I,J),CRTN    A 910
      IF (CRTN.GT.CDIFF.AND.N.LT.10) GO TO 130                           A 920
      IF (N.LE.9) GO TO 140                                              A 930
      WRITE (6,330) I,J,K0,N,DEN$,XMOL1,CRTN                             A 940
  140 CONTINUE                                                           A 950
      IF (XMOL.GE.0.5) GO TO 150                                         A 960
      XMOL3=0.5                                                          A 970
      IF (XMOL.EQ.0) DEN3=0.0                                            A 980
      IF (XMOL.NE.0) CALL TABLES(XMOL3,P,I,J,A,B,C,TEMP,DEN3)            A 990
      CALL BELOW(DO,TEMP,I,J,DEN1)                                      A1000
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
      RHO=((0.5-XMOL)*DEN1+XMOL*DEN3)/0.5                                    A1010
  150 IF (XMOL.LT.0.5.OR.XMOL.GT.6.0) GO TO 160                              A1020
      CALL TABLES(XMOL,P,I,J,A,B,C,TEMP,RHO)                                 A1030
  160 IF (XMOL.LE.6.0) GO TO 180                                             A1040
      DO 170 M=1,3                                                           A1050
      X(M)=FLOAT(2*M)                                                        A1060
      Z=X(M)                                                                 A1070
      CALL TABLES(Z,P,I,J,A,B,C,TEMP,Q)                                      A1080
  170 R(M)=Q                                                                 A1090
      DENOM=.272593                                                          A1100
      ANUM=(12-4*SQRT(6.))*R(1)+(2*SQRT(6.)-6*SQRT(2.))*R(2)+(4*SQRT(2.)     A1110
     1-4)*R(3)                                                               A1120
      BNUM=4*R(2)-2*R(1)-2*R(3)                                              A1130
      CNUM=(2-SQRT(2.))*R(3)+(SQRT(6.)-2)*R(1)+(SQRT(2.)-SQRT(6.))*R(2)      A1140
      A1=ANUM/DENOM                                                          A1150
      B1=BNUM/DENOM                                                          A1160
      C1=CNUM/DENOM                                                          A1170
C THE FOLLOWING FORMULA HAS ONLY BEEN VERIFIED FOR MOLALITIES LE  6.0;       A1180
C HERE IT IS USED TO CALCULATE DENSITIES WITH MOLALITIES GT 6.0...           A1190
      RHO=A1+SQRT(XMOL)*B1+XMOL*C1                                           A1200
  180 CONTINUE                                                               A1210
      DEN(I,J)=RHO                                                           A1220
      DENP(I,J)=DEN(I,J)*(1-XMOL*WT/(XMOL*WT+1000))                          A1230
      GO TO 210                                                              A1240
  190 CONTINUE                                                               A1250
      DEN(I,J)=1.0                                                           A1260
      DENP(I,J)=1.0                                                          A1270
      GO TO 210                                                              A1280
  200 CONTINUE                                                               A1290
      DEN(I,J)=0.997047                                                      A1300
      DENP(I,J)=0.997047                                                     A1310
      WRITE (6,340) I,J,K0                                                   A1320
  210 CONTINUE                                                               A1330
      DO 220 J=1,J0                                                          A1340
      DO 220 I=1,I0                                                          A1350
      IDEN(I,J)=IFIX(DEN(I,J)*1000)                                          A1360
  220 IDENP(I,J)=IFIX(DENP(I,J)*1000)                                        A1370
      WRITE (6,350)                                                          A1380
      WRITE (6,390) (TITLE(I),I=1,20)                                        A1390
      WRITE (6,370) ((IDEN(I,J),J=1,26),I=1,21)                              A1400
      WRITE (6,360)                                                          A1410
      WRITE (6,390) (TITLE(I),I=1,20)                                        A1420
      WRITE (6,370) ((IDENP(I,J),J=1,26),I=1,21)                             A1430
      WRITE (7,380) ((IDEN(I,J),J=1,26),I=1,21)                              A1440
      WRITE (7,380) ((IDENP(I,J),J=1,26),I=1,21)                             A1450
      STOP                                                                   A1460
C                                                                            A1470
C                                                                            A1480
  230 FORMAT (20A4)                                                          A1490
  240 FORMAT (2F10.6)                                                        A1500
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
250 FORMAT ('1',T35,'ITERATION CLOSURE CRITERION FOR DENSITY(IN %) =',  A1510
   1F10.6,20X,'PRINT =',F4.1)                                          A1520
260 FORMAT (3I10)                                                      A1530
270 FORMAT (T45,'I0 J0 K0',3I3)                                        A1540
280 FORMAT ('1',T35,'INTERPOLATION COEFFICIENTS A,B,C,&DO',/)          A1550
290 FORMAT (T2,13F8.4)                                                 A1560
300 FORMAT (T2,5F8.6,///)                                              A1570
310 FORMAT (/,T25,'XMOL1',6X,'DEN1',7X,'TDS',7X,'CRTN')                A1580
320 FORMAT (T2,4I5,4F10.5)                                             A1590
330 FORMAT (T2,'GT 10 ITERATIONS',4I5,'DN1=',F10.6,'XMOL=',F10.6,'CRTN A1600
   1=',F8.4)                                                           A1610
340 FORMAT (T2,'HEAD NE 0 BUT TEMP LT 40',3I5)                         A1620
350 FORMAT ('1',T22,'GROUND WATER DENSITY (G/L)',/)                    A1630
360 FORMAT ('1',T22,'PURE WATER CONCENTRATION (G/L)',/)                A1640
370 FORMAT (T12,20I4,/,T12,6I4)                                        A1650
380 FORMAT (20I4,/,6I4)                                                A1660
390 FORMAT (T12,20A4,///)                                              A1670
    END                                                                A1680-
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
      C     ************                                                    A  10
            SUBROUTINE TABLES(XMOL,P,I,J,A,B,C,TEMP,RHO)                    A  20
      C     ************                                                    A  30
            DIMENSION P(21,26), A(13,4), B(13,4), C(13,4), TEMP(21,26)      A  40
      C --- THIS ROUTINE IS NOT GOOD FOR PRESSURES ABOVE 300 BARS OR NACL    A  50
      C     CONCENTRATIONS ABOVE 6.0 MOLALITY OR BELOW 0.5 MOLALITY...      A  60
            IF (P(I,J).GE.100) GO TO 10                                     A  70
            JJ=1                                                            A  80
            P0=1                                                            A  90
         10 CONTINUE                                                        A 100
            IF (P(I,J).LT.100.OR.P(I,J).GE.200) GO TO 20                    B 110
            JJ=2                                                            B 120
            P0=100                                                          B 130
         20 IF (P(I,J).LT.200.OR.P(I,J).GE.300) GO TO 30                    B 140
            JJ=3                                                            B 150
            P0=200                                                          B 160
         30 CONTINUE                                                        B 170
            IF (XMOL.LT.0.5.OR.XMOL.GE.1.0) GO TO 40                        B 180
            II=1                                                            B 190
            XMOL0=0.5                                                       B 200
         40 IF (XMOL.LT.1.0.OR.XMOL.GE.1.5) GO TO 50                        B 210
            II=2                                                            B 220
            XMOL0=1.0                                                       B 230
         50 IF (XMOL.LT.1.5.OR.XMOL.GE.2.0) GO TO 60                        B 240
            II=3                                                            B 250
            XMOL0=1.5                                                       B 260
         60 IF (XMOL.LT.2.0.OR.XMOL.GE.2.5) GO TO 70                        B 270
            II=4                                                            B 280
            XMOL0=2.0                                                       B 290
         70 IF (XMOL.LT.2.5.OR.XMOL.GE.3.0) GO TO 80                        B 300
            II=5                                                            B 310
            XMOL0=2.5                                                       B 320
         80 IF (XMOL.LT.3.0.OR.XMOL.GE.3.5) GO TO 90                        B 330
            II=6                                                            B 340
            XMOL0=3.0                                                       B 350
         90 IF (XMOL.LT.3.5.OR.XMOL.GE.4.0) GO TO 100                       B 360
            II=7                                                            B 370
            XMOL0=3.5                                                       B 380
        100 IF (XMOL.LT.4.0.OR.XMOL.GE.4.5) GO TO 110                       B 390
            II=8                                                            B 400
            XMOL0=4.0                                                       B 410
        110 IF (XMOL.LT.4.5.OR.XMOL.GE.5.0) GO TO 120                       B 420
            II=9                                                            B 430
            XMOL0=4.5                                                       B 440
        120 IF (XMOL.LT.5.0.OR.XMOL.GE.5.5) GO TO 130                       B 450
            II=10                                                           B 460
            XMOL0=5.0                                                       B 470
        130 IF (XMOL.LT.5.5.OR.XMOL.GE.6.0) GO TO 140                       B 480
            II=11                                                           B 490
            XMOL0=5.5                                                       B 500
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
      140 IF (XMOL.NE.6) GO TO 150                                          A 510
          II=12                                                             A 520
          XMOL0=XMOL                                                        A 530
          PO=P(I,J)                                                         A 540
      150 CONTINUE                                                          A 550
          XXM=(XMOL-XMOL0)/0.5                                              A 560
          XXP=(P(I,J)-PO)/100.                                              A 570
          DAM=(A(II+1,JJ)-A(II,JJ))*XXM                                     A 580
          DAP=(A(II,JJ+1)-A(II,JJ))*XXP                                     A 590
          AA=A(II,JJ)+DAP+DAM                                               A 600
          DBM=(B(II+1,JJ)-B(II,JJ))*XXM                                     A 610
          DBP=(B(II,JJ+1)-B(II,JJ))*XXP                                     A 620
          BB=B(II,JJ)+DBP+DBM                                               A 630
          DCM=(C(II+1,JJ)-C(II,JJ))*XXM                                     A 640
          DCP=(C(II,JJ+1)-C(II,JJ))*XXP                                     A 650
          CC=C(II,JJ)+DCP+DCM                                               A 660
          RHO=AA-(1.E-4)*BB*TEMP(I,J)-(1.E-6)*CC*TEMP(I,J)**2               A 670
          RETURN                                                            A 680
          END                                                               A 690
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
C     ******                                                          C  10
      SUBROUTINE BELOW(DO,TEMP,I,J,DOO)                               C  20
C     ******                                                          C  30
C FOR TEMPERATURES ABOVE 75 DEG.C THIS ROUTINE DOES A LINEAR          C  40
C EXTRAPOLATION FROM POTTER ET AL.   ALSO IT DOES NOT TAKE            C  50
C PRESSURE VARIATION INTO ACCOUNT.                                    C  60
      DIMENSION DO(5), TEMP(21,26)                                    C  70
      IF (TEMP(I,J).GE.25) GO TO 10                                   C  80
      II=1                                                            C  90
      TO=0                                                            C 100
   10 IF (TEMP(I,J).LT.25.OR.TEMP(I,J).GE.50) GO TO 20                C 110
      II=2                                                            C 120
      TO=25                                                           C 130
   20 IF (TEMP(I,J).LT.50.OR.TEMP(I,J).GE.75) GO TO 30                C 140
      II=3                                                            C 150
      TO=50                                                           C 160
   30 IF (TEMP(I,J).LT.75) GO TO 40                                   C 170
      TO=75                                                           C 180
      DOO=(DO(4)-DO(3))/25.                                           C 190
      DOO=(DO(4)+DOO*(TEMP(I,J)-TO))                                  C 200
      GO TO 50                                                        C 210
   40 CONTINUE                                                        C 220
      TXO=(TEMP(I,J)-TO)/25                                           C 230
      DOO=(DO(II+1)-DO(II))*TXO                                       C 240
      DOO=DO(II)+DOO                                                  C 250
   50 CONTINUE                                                        C 260
      RETURN                                                          C 270
      END                                                             C 280-
```

Table 4.--*Density and concentration FORTRAN program*--Continued

```
      C     **********                                                    D  10
            SUBROUTINE ARRAY(A,INFT,IOFT,IN,IRN,TF)                       D  20
      C     **********                                                    D  30
            INTEGER BLK                                                   D  40
            DIMENSION A(21,26), INFT(2,2), IN(6), TF(3), DUM(3), DUM2(4), IOFT  D  50
           1(9,4)                                                         D  60
            COMMON /MISC/ I0,J0,K0                                        D  70
            DATA BLK/' '/                                                 D  80
            READ (5,120) FAC,IVAR,IPRN,TF,IRECS,IRECD                     D  90
            IC=4*IRECS+2*IVAR+IPRN+1                                      D 100
            GO TO (10,10,30,30,60,60), IC                                 D 110
         10 DO 20 I=1,I0                                                  D 120
            DO 20 J=1,J0                                                  D 130
         20 A(I,J)=FAC                                                    D 140
            WRITE (6,100) IN,FAC,K0                                       D 150
            GO TO 80                                                      D 160
         30 IF (IC.EQ.3) WRITE (6,110) IN,K0                              D 170
            DO 50 I=1,I0                                                  D 180
            READ (5,INFT) (A(I,J),J=1,J0)                                 D 190
            DO 40 J=1,J0                                                  D 200
         40 A(I,J)=A(I,J)*FAC                                             D 210
         50 IF (IC.EQ.3) WRITE (6,IOFT) I,(A(I,J),J=1,J0)                 D 220
            GO TO 80                                                      D 230
         60 CONTINUE                                                      D 240
            IF (IC.EQ.6) GO TO 80                                         D 250
            WRITE (6,110) IN,K0                                           D 260
            DO 70 I=1,I0                                                  D 270
         70 WRITE (6,IOFT) I,(A(I,J),J=1,J0)                              D 280
         80 CONTINUE                                                      D 290
            IRN=IRN+1                                                     D 300
            DO 90 I=1,6                                                   D 310
         90 IN(I)=BLK                                                     D 320
            RETURN                                                        D 330
      C                                                                   D 340
      C     ---FORMATS---                                                 D 350
      C                                                                   D 360
      C                                                                   D 370
      C                                                                   D 380
        100 FORMAT (1H0,52X,6A4,' =',G15.7,' FOR LAYER',I3)               D 390
        110 FORMAT (1H1,45X,6A4,' MATRIX, LAYER',I3/46X,41('-'))          D 400
        120 FORMAT (F10.0,2I10,3F10.0,2I10)                               D 410
            END                                                           D 420-
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