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

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<td>(a)</td>
<td>angle between the (x)-axis and (x)-axis.</td>
</tr>
<tr>
<td>(b)</td>
<td>angle between the (y)-axis and (y)-axis.</td>
</tr>
<tr>
<td>(c)</td>
<td>angle between the (z)-axis and (z)-axis.</td>
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<tr>
<td>(c_s)</td>
<td>dissolved-solids concentration, in (M/L^3).</td>
</tr>
<tr>
<td>(c_p)</td>
<td>pure-water concentration, in (M/L^3).</td>
</tr>
<tr>
<td>(\bar{c}_p)</td>
<td>vertically averaged pure-water concentration of an aquifer, in (M/L^3).</td>
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<tr>
<td>(\bar{c}_p)</td>
<td>vertically averaged pure-water concentration of a confining layer, in (M/L^3).</td>
</tr>
<tr>
<td>(g)</td>
<td>acceleration of gravity, in (L/T^2).</td>
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<tr>
<td>(h_o)</td>
<td>freshwater hydraulic head, in (L).</td>
</tr>
<tr>
<td>(\bar{h}_o)</td>
<td>vertically averaged freshwater hydraulic head, in (L).</td>
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<tr>
<td>(h^a)</td>
<td>a quasi-hydraulic head, in (L).</td>
</tr>
<tr>
<td>(\bar{h}^a)</td>
<td>vertically averaged quasi-hydraulic head, in (L).</td>
</tr>
<tr>
<td>(h^a_u)</td>
<td>quasi-hydraulic head at top of aquifer, in (L).</td>
</tr>
<tr>
<td>(h^a_L)</td>
<td>quasi-hydraulic head at bottom of aquifer, in (L).</td>
</tr>
<tr>
<td>(\hat{i}, \hat{j}, \hat{k})</td>
<td>unit vector along the (x)-direction, (y)-direction, and (z)-direction.</td>
</tr>
<tr>
<td>(\hat{j})</td>
<td>mass-flux density of pure water, in (M/L^2T).</td>
</tr>
<tr>
<td>(j_\alpha, j_\beta)</td>
<td>mass-flux density of pure water in the (\alpha)-direction, and in the (\beta)-direction.</td>
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\( \mathbf{k} \), \( \mathbf{k} \) 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 hydraulic conductivity for a layer, in \( L/T \).

\( \bar{K}^c \) 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 \( L/T \).

\( \hat{n} \) outward-directed vector normal to top and bottom aquifer surface with magnitude equal to the secant of the angle between \( \hat{n} \) and \( \hat{y} \).

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

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

\( \dot{q} \) specific discharge of ground water, in \( L/T \).

\( S \) ground-water storage coefficient, dimensionless.

\( d\hat{S} \) 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 \( M/L^2T \).
average aquifer elevation, \((z_u + z_L)/2\).

\(z_u\)  aquifer-top elevation, in L.

\(z_L\)  aquifer-bottom elevation, in L.

\(\Delta z\)  confining-layer thickness, in L.

\(dz\)  differential associated with \(z\)-coordinate.

\(\alpha, \beta, \gamma\)  orthogonal curvilinear coordinates of the \(\alpha\beta\gamma\)-system.

\(\hat{\alpha}, \hat{\beta}, \hat{\gamma}\)  unit vectors along the \(\alpha\)-direction, \(\beta\)-direction, and \(\gamma\)-direction; these are the principal directions of the permeability tensor.

\(d\alpha, d\beta, d\gamma\)  differentials associated with the \(\alpha, \beta, \gamma\)-coordinates.

\(\gamma_x, \gamma_y\)  projection of \(\gamma\) on the \(x\) and \(y\) axes.

\(\mu\)  ground-water viscosity, in \(\text{M/LT}\).

\(\bar{\mu}\)  vertically averaged ground-water viscosity, in \(\text{M/LT}\).

\(\rho\)  ground-water density, in \(\text{M/L}^3\).

\(\bar{\rho}\)  vertically averaged ground-water density, in \(\text{M/L}^3\).

\(\rho_o\)  reference density, here taken as the density of pure water at 4° Celsius and 1 atmosphere pressure.

\(\hat{T}\)  hybrid transmissivity tensor with geometric factors, in \(\text{L}^2/\text{T}\).
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 aligned 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:

\[ \rho = c_s + c_p. \]  \hspace{1cm} (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:

\[ \nabla \cdot \vec{j} + Q = 0 \]  \hspace{1cm} (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:

\[ \vec{j} = c_p \vec{q}. \]  \hspace{1cm} (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 αβγ-system, and the nonorthogonal αβz-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:

\[ \int_{V} \nabla \cdot \vec{j} + \int_{V} Q = 0. \]  \hfill (4)

Using the divergence theorem on the first integral results in:

\[ \int_{S} \vec{j} \cdot d\vec{S} + \int_{V} Q = 0. \]  \hfill (5)
Where the integration over $S$ is over the six faces of the infinitesimal volume element:

$$
\int \vec{j} \cdot d\vec{S} = \int \vec{j}_{\text{sides}} \cdot d\vec{S} + \int \vec{j}_{\text{bottom}} \cdot d\vec{S} + \int \vec{j}_{\text{top}} \cdot d\vec{S}.
$$  \hspace{1cm} (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 $\alpha$- and $\beta$-components of the mass-flux density of pure water are introduced.

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

$$
\int \vec{j} \cdot d\vec{S} = \int j_\alpha (\alpha + d\alpha) \cos a \cos b \, d\beta \, dz \\
- \int j_\alpha (\alpha) \cos a \cos b \, d\beta \, dz + \int j_\beta (\beta + d\beta) \cos a \cos b \, d\alpha \, dz \\
- \int j_\beta (\beta) \cos a \cos b \, d\alpha \, dz.
$$  \hspace{1cm} (7)

Specifically, the first two integrals represent net outflow from $dV$ in the $\alpha$-direction. The next two integrals represent net outflow from $dV$ in the $\beta$-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 $j_\alpha$ is only infinitesimally dependent on $\beta$, the first two integrals of equation 7 become:

$$
[\int j_\alpha (\alpha + d\alpha) \cos a \cos b \, dz - \int j_\alpha (\alpha) \cos a \cos b \, dz] \, d\beta.
$$  \hspace{1cm} (8)
Dividing equation 8 by \( \partial \alpha \partial \beta \) and letting \( \partial \alpha \partial \beta \) approach zero results in:

\[
\frac{3}{3a} \int \cos a \cos b \ j_\alpha(z)dz = \frac{3}{3a} (\cos a \cos b \int j_\alpha(z)dz) . \tag{9}
\]

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, \( j_\alpha \) and \( j_\beta \).

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

\[
\int j(z) \cdot d\hat{s} + \int j(z') \cdot d\hat{s'} = \int j' \cdot d\hat{\hat{s}}. \tag{10}
\]

After equation 10 is divided by \( \partial \alpha \partial \beta \) and \( \partial \alpha \partial \beta \) is made to approach zero, the result is:

\[
\int j(z_u) \cdot \hat{n}_u + \int j(z_L) \cdot \hat{n}_L . \tag{11}
\]

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

\[
\hat{n}_u = \nabla (z-z_u), \quad \hat{n}_L = \nabla (z_L-z) . \tag{12}
\]

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

\[
\lim_{\partial \alpha \partial \beta \to 0} \left[ \int \frac{Qdz}{dV} \partial \alpha \partial \beta \cos a \cos b / \partial \alpha \partial \beta \right] = \int \frac{Q \cos a \cos b dz}{dV} . \tag{13}
\]

Combining equations 7, 11, and 13 results in:

\[
0 = \frac{3}{3a} \left( \cos a \cos b \int j_\alpha(z)dz \right) + \frac{3}{3a} \left( \cos a \cos b \int j_\beta(z)dz \right) + \int j(z_u) \cdot \hat{n}_u + \int j(z_L) \cdot \hat{n}_L + \int Qdz . \tag{14}
\]
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):

$$\dot{q} = -\frac{k}{u}(\nabla p - \rho g).$$  \hspace{1cm} (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

$$h^a = \frac{p}{\bar{\rho} g} + z.$$  \hspace{1cm} (16)

Where $\bar{\rho}$ is the vertically averaged ground-water density within the aquifer.

With these definitions, it follows that:

$$\nabla h^a = \nabla p/\bar{\rho} g + k + \nabla \left(\frac{1}{\rho}\right).$$  \hspace{1cm} (17)

and that

$$\dot{q} = -\frac{k}{\mu} \bar{\rho} g \left(\nabla h^a + \left(\frac{\rho - \bar{\rho}}{\rho}\right) k + \frac{p}{\rho} \nabla \left(\frac{1}{\rho}\right)\right).$$ \hspace{1cm} (18)

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

$$\int j_a dz = -\int c_p \bar{\rho} g/\mu \left(\dot{q} \cdot \left\{\nabla h^a + \frac{\rho - \bar{\rho}}{\rho} k - \frac{p}{\rho} \nabla \left(\frac{1}{\rho}\right)\right\}\right) dz.$$ \hspace{1cm} (19)

The factor $\frac{\rho k}{\rho g/\mu}$ 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:
\[ \int f \, dz = -Cp^2/\bar{\mu} \cdot \hat{a} \cdot \hat{k} \cdot \int \left( \nabla h^a + \frac{\rho}{\bar{\rho}} \frac{\hat{a}}{k} - \frac{p}{g} \frac{1}{\bar{\rho}} \right) \, dz \quad \text{(20)} \]

The last integral of equation 20 can be done immediately:

\[ - \int \frac{p}{g} \nabla \left( \frac{1}{\bar{\rho}} \right) \, dz = - \frac{1}{g} \int \nabla \left( \frac{1}{\bar{\rho}} \right) \, dz = - \frac{p}{g} (z_u - z_L) \frac{1}{\bar{\rho}} \quad \text{(21)} \]

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

\[
\begin{align*}
\int_{z_L}^{z_u} \nabla h^a \, dz &= \nabla \int_{z_L}^{z_u} h^a \, dz - h^a \nabla(z_u - z) + h^a \nabla(z_L - z) \\
&= \nabla \left\{ (z_u - z_L)h^a \right\} - h^a \nabla(z_u - z) + h^a \nabla(z_L - z) \\
&= (z_u - z_L)\nabla h^a + h^a \nabla(z_u - z) - h^a \nabla(z_u - z) + h^a \nabla(z_L - z) \\
&= (z_u - z_L)\nabla h^a + h^a \nabla(z_u - z) - h^a \nabla(z_u - z) + h^a \nabla(z_L - z) \quad \text{(22)}
\end{align*}
\]

Inserting the definitions of \( \hat{n}_u \) and \( \hat{n}_L \) provided in equation 12, and multiplying by \( \hat{a} \cdot \hat{k} \), equation 22 becomes:

\[
\hat{a} \cdot \hat{k} \int_{z_L}^{z_u} \nabla h^a \, dz = (z_u - z_L) \hat{a} \cdot \hat{k} \cdot \nabla h^a - (h^a - h^a_L) \hat{a} \cdot \hat{k} \cdot \hat{n}_L
\]

\[ -(h^a - h^a_u) \hat{a} \cdot \hat{k} \cdot \hat{n}_u \quad \text{(23)} \]

If \( \hat{n}_u \) and \( \hat{n}_L \) are parallel to the \( \gamma \)-axis or have no component along the \( \alpha \)-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 \( \hat{n}_u \) and \( \hat{n}_L \) are parallel to the \( \gamma \)-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 \((h^a_u - h^a)\) and \((h^a_l - h^a)\) 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:

$$
\int j_0 dz \sim -c_p \rho g/ \mu (z_u - z_L) \hat{a} \cdot k \cdot \left( \nabla h^a - \frac{\rho}{\rho_o} \nabla \frac{1}{\rho} \right) .
$$

(24)

Defining the vertically averaged hydraulic head as:

$$
\bar{h}_o = \rho/\rho_o g + z
$$

(25)

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

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

(26)

Combining equations 14, 24, and 26:

$$
\frac{\partial}{\partial \alpha} \left( \frac{1}{c_p} \hat{a} \cdot \hat{t} \cdot \nabla \bar{h}_o \right) + \frac{\partial}{\partial \beta} \left( \frac{1}{c_p} \hat{\beta} \cdot \hat{t} \cdot \nabla \bar{h}_o \right) = \hat{j}(z_u) \cdot \hat{n}_u + \hat{j}(z_L) \cdot \hat{n}_L + \hat{w}

- \frac{\partial}{\partial \alpha} \left( \frac{1}{c_p} \Delta \rho \hat{a} \cdot \hat{t} \cdot \nabla z \right) - \frac{\partial}{\partial \beta} \left( \frac{1}{c_p} \Delta \rho \hat{\beta} \cdot \hat{t} \cdot \nabla z \right)
$$

(27)

where

$$
\Delta \rho = \rho - \rho_o ,
$$

and

$$
\hat{t} = \cos a \cos b \rho_o g (z_u - z_L)/ \mu .
$$

If the approximation leading to equation 24 had been developed with hydraulic head instead of quasi-hydraulic head, then $\hat{t}$ would contain $\rho$ instead of $\rho_o$.

Note that $\nabla \bar{h}_o$ and $\nabla z$ are in the horizontal.
Here,

\[ \hat{t} \] 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

\[ j(z) \cdot \hat{n} \] 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 \( \alpha \) and \( \beta \) are expressed in terms of \( x \), \( y \), and \( z \). Then the restriction that the angles between the \( \alpha \)- and \( x \)-axes and the \( \beta \)- 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 ($\bar{\rho}^c$) is driving an average pure-water concentration ($\bar{c}^p$) 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:

$$\mathbf{j}(z_L) \cdot \hat{n}_L + \mathbf{j}(z_u) \cdot \hat{n}_u = \rho \left( \frac{\partial \rho}{\partial z} + \Delta \bar{\rho}^c / \rho_o \right) - \rho \left( \frac{\partial \rho}{\partial z} + \Delta \bar{\rho}^c / \rho_o \right) \right] \ . \ (28)$$

Here,

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

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

$$K_{YY}^c = \frac{c^p g}{\mu}$$

where

$\overline{k}_{YY}^c$ is the $YY$-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:

\[
\frac{\partial}{\partial x} \left( T_{\alpha\alpha} \frac{3\overline{h}_o}{3x} \right) + \frac{\partial}{\partial y} \left( T_{\beta\beta} \frac{3\overline{h}_o}{3y} \right) = \kappa_{YY} \frac{3\overline{h}_o}{3z} L - \kappa_{YY} \frac{3\overline{h}_o}{3z} u + \frac{W}{\rho_o} \\
- \frac{\partial}{\partial \alpha} \left( T_{\alpha\alpha} \frac{\Delta \rho}{\rho_o} \frac{3z}{3\alpha} \right) - \frac{\partial}{\partial \beta} \left( T_{\beta\beta} \frac{\Delta \rho}{\rho_o} \frac{3z}{3\beta} \right) \\
+ \left( \kappa_{YY} \frac{\Delta \rho}{\rho_o} \right)_L - \left( \kappa_{YY} \frac{\Delta \rho}{\rho_o} \right)_u .
\]  

(29)

Here

\[ T_{\alpha\alpha} \text{ and } T_{\beta\beta} \text{ are the components of a hybrid transmissivity tensor} \]

\[ \text{corresponding to the } \alpha\text{- and } \beta\text{-directions. For example,} \]

\[ T_{\alpha\alpha} = \overline{k}_{\alpha\alpha} \overline{c}_p g (z_u - z_L) / \overline{u} . \]

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:

\[
\frac{c}{\rho} \frac{\partial h}{\partial t} \% 2\cdot S \frac{\partial h}{\partial t}
\]

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:

\[
q = -k \frac{\rho g}{\mu} (\nabla h_o + \Delta \rho/\rho_o k) . \tag{30}
\]

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 aligned with the horizontal and vertical, the orthogonal xyz-system; another is aligned

*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 $\alpha\beta\gamma$-system; and the third is the nonorthogonal $\alpha\beta z$-system (fig. 3).

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

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

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

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

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

where $a$ is positive when $\alpha$ lies above the $xy$-plane, and $b$ is positive when $\beta$ lies above the $xy$-plane. Then:

$$\hat{a} \times \hat{b} = \hat{\gamma}, \text{ and} \quad (M3)$$

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

Similarly:

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

$$\gamma_y = (\hat{a} \times \hat{b})_y = -\sin b = \frac{\partial \gamma}{\partial y}. \quad (M6)$$
Equation M4 is used in the discussion below and follows from equations M1, M2, and M3. Here $\hat{a}$ is the unit vector along the $\alpha$-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:

$$\hat{a} \cdot d\vec{S} = d\hat{\delta} \delta \gamma = \frac{3}{3}(\beta, \gamma) d\hat{\delta} \delta z = \frac{3}{3} \frac{\gamma}{\delta} d\hat{\delta} \delta z = \cos \alpha \cos \beta d\hat{\delta} \delta z.$$  \hspace{1cm} (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 $\alpha$- and $\beta$-components of the mass-flux densities of pure water at the aquifer confining-layer interfaces are approximately equal to or smaller than the $\gamma$-components.
4. The principal directions of the confining layer are the same as those of the aquifer.

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

$$\hat{f}(z_u) \cdot \hat{n}_u = j_\gamma(z_u) - j_\beta(z_u) \frac{3\gamma u}{3\beta} - j_\alpha(z_u) \frac{3\gamma u}{3\alpha} - j_\gamma(z_u).$$  \hspace{1cm} (M8)
Substituting the head parameterization of Darcy's law from equation 30 into equation M8 and applying assumption 4 above results in:

\[ j_{\gamma} = \rho_0 \gamma \left( \frac{\tau^{c}}{k} \cdot \left( \nabla h_o + \Delta \rho / \rho_o k \right) \right) = \rho_0 K^{c}_{\gamma \gamma} \left( \frac{\partial h_o}{\partial y} + \Delta \rho / \rho_o \cos a \cos b \right) \] (M9)

Here

\[ K^{c}_{\gamma \gamma} \] is the \( \gamma \gamma \)-component of the hybrid hydraulic conductivity (containing the concentration of pure water \( c^{c}_{p} \) of the confining layer), and

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

From equations M4, M5, and M6:

\[ \frac{\partial}{\partial y} = \gamma \cdot \nabla = -\sin a \cos b \frac{\partial}{\partial x} - \sin b \frac{\partial}{\partial y} + \cos a \cos b \frac{\partial}{\partial z} \] (M10)

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

\[ \frac{\partial}{\partial y} \approx \cos a \cos b \frac{\partial}{\partial z} \]. (M11)

Using equation M11 in equation M9 yields:

\[ j_{\gamma} \approx \rho_0 K^{c}_{\gamma \gamma} \cos a \cos b \left( \frac{\partial h_o}{\partial z} + \Delta \rho / \rho_o \right) \approx \rho_0 K^{c}_{\gamma \gamma} \left( \frac{\partial h_o}{\partial z} + \Delta \rho / \rho_o \right) \] (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 \( \alpha \)– and \( \beta \)-axes are oriented along principal axes the \( \tau \)-dyadic is diagonal in the \( \alpha \beta \gamma \)-system; that is:

\[ \tau = \tau_{\alpha \alpha} \hat{\alpha} \hat{\alpha} + \tau_{\beta \beta} \hat{\beta} \hat{\beta} + \tau_{\gamma \gamma} \hat{\gamma} \hat{\gamma} \]. (M14)
Equation M14 establishes the notation for what follows. Consider one component of a mixed dyadic: The subscript $a$ corresponds to the $\alpha\beta\gamma$-system, and the subscript $x$, $y$, or $z$ corresponds to the $xyz$-system. Then:

\[ \hat{\alpha} \cdot \hat{\tau} \cdot \hat{i} = \tau_{ax} = \tau_{aa} (\hat{\alpha} \cdot \hat{i}) = \tau_{aa} \cos a , \quad (M15) \]

\[ \tau_{ay} = 0 , \quad (M16) \]

\[ \tau_{az} = \tau_{aa} \sin a . \quad (M17) \]

Equation M16 follows from the restriction that the $\alpha$-axis lies in the $xz$-plane. The last three equations relate some of the components of a mixed dyadic to the principal component $\tau_{aa}$ 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:

\[
\frac{\partial}{\partial \alpha} \left( \frac{-c_p \hat{\alpha} \cdot \hat{\tau} \cdot \overline{V_h}}{\partial \alpha} \right) = \frac{\partial}{\partial \alpha} \left( \frac{c_p}{\partial \alpha} \left( \tau_{ax} \frac{\partial}{\partial x} + \tau_{az} \frac{\partial}{\partial z} \right) \overline{h_o} \right) = \frac{\partial}{\partial \alpha} \left( \frac{c_p}{\tau_{ax}} \frac{\partial \overline{H_o}}{\partial x} \right) . \quad (M18)
\]

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

\[
\left( \frac{\partial}{\partial \alpha} = \hat{\alpha} \cdot \hat{V} = \cos a \frac{\partial}{\partial x} + \sin a \frac{\partial}{\partial z} \right) \left( \frac{c_p}{\tau_{\alpha\alpha}} \cos a \frac{\partial \overline{H_o}}{\partial x} \right) = \cos a \frac{\partial}{\partial x} \left( \frac{c_p}{\tau_{\alpha\alpha}} \cos a \frac{\partial \overline{H_o}}{\partial x} \right) . \quad (M19)
\]

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

\[
\left( \frac{\partial}{\partial \beta} = \hat{\beta} \cdot \hat{V} = \cos b \frac{\partial}{\partial y} \right) \left( \frac{c_p}{\tau_{\beta\beta}} \cos b \frac{\partial \overline{H_o}}{\partial y} \right) = \cos b \frac{\partial}{\partial y} \left( \frac{c_p}{\tau_{\beta\beta}} \cos b \frac{\partial \overline{H_o}}{\partial y} \right) . \quad (M20)
\]
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:

\[
\left( \frac{\partial}{\partial \alpha} - \frac{\partial h_o}{\partial \alpha} \right) + \frac{\partial}{\partial \beta} \left( \frac{\partial}{\partial \beta} - \frac{\partial h_o}{\partial \beta} \right) \approx \frac{\partial}{\partial x} \left( \rho_o T_{\alpha \alpha} \frac{\partial h_o}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho_o T_{\beta \beta} \frac{\partial h_o}{\partial y} \right) \tag{M21}
\]

for combined results of equations M19 and M20. Here

\[ T_{\alpha \alpha} = \frac{k_{\alpha \alpha}}{c_p g} (z - z_L) / \bar{\mu}, \]

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 \( \alpha \)-term below:
Here \((T_{\alpha\alpha})_{j+\frac{1}{2}}\) is the harmonic mean of the hybrid transmissivity between node \(j\) and \(j+1\); along the \(\alpha\)-direction. The harmonic mean needs to be used for proper calculation at boundaries. The factor \((\bar{\Delta\rho}/\rho_o)_{j+\frac{1}{2}}\) 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 \(\alpha\)-term is combined with a \(\beta\)-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 \(\Delta x\) 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:

<table>
<thead>
<tr>
<th>CARD</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>VARIABLE</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>F10.6</td>
<td>PSLL</td>
<td>Print options of intermediate terms.</td>
</tr>
<tr>
<td>2</td>
<td>1-10</td>
<td>I10</td>
<td>IØ</td>
<td>Number of rows.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>I10</td>
<td>JØ</td>
<td>Number of columns.</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>I10</td>
<td>KK</td>
<td>Layer number.</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>COLUMN</th>
<th>FORMAT</th>
<th>VARIABLE</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>G10.0</td>
<td>FAC</td>
<td>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.</td>
</tr>
<tr>
<td>11-20</td>
<td>G10.0</td>
<td>IVAR</td>
<td>0--If no data cards are to be read in for this layer. 1--If data cards for this layer follow.</td>
</tr>
<tr>
<td>21-30</td>
<td>G10.0</td>
<td>IPRN</td>
<td>0--If data for this layer are to be printed. 1--If data for this layer are not to be printed.</td>
</tr>
</tbody>
</table>
When data sets are included, start each row on a new card as follows:

<table>
<thead>
<tr>
<th>DATA SET</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>VARIABLE</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>DENL</td>
<td>Density array of lower aquifer.</td>
</tr>
<tr>
<td>2</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>DENU</td>
<td>Density array of upper aquifer.</td>
</tr>
<tr>
<td>3</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>THKL</td>
<td>Thickness of lower confining bed.</td>
</tr>
<tr>
<td>4</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>THKU</td>
<td>Thickness of upper confining bed.</td>
</tr>
<tr>
<td>5</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>TKL</td>
<td>Hybrid leakance of lower confining bed.</td>
</tr>
<tr>
<td>6</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>TKU</td>
<td>Hybrid leakance of upper confining bed.</td>
</tr>
<tr>
<td>7</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>T</td>
<td>Hybrid-transmissivity array--Inactive nodes need to have transmissivity set to zero, otherwise pseudosource calculation will be wrong.</td>
</tr>
<tr>
<td>8</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>DEN</td>
<td>Aquifer-density array data.</td>
</tr>
<tr>
<td>9</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>ELEV</td>
<td>Aquifer-elevation array data.</td>
</tr>
<tr>
<td>10</td>
<td>1-80</td>
<td>2OF4.0</td>
<td>THCK</td>
<td>Aquifer-thickness array data.</td>
</tr>
<tr>
<td>11</td>
<td>1-80</td>
<td>8G10.0</td>
<td>DELX(J)</td>
<td>Grid spacing in x-direction.</td>
</tr>
<tr>
<td>12</td>
<td>1-80</td>
<td>8G10.0</td>
<td>DELY(I)</td>
<td>Grid spacing in y-direction.</td>
</tr>
</tbody>
</table>
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.
Figure 4.—Data for a symmetrical basin example
<table>
<thead>
<tr>
<th>Layer</th>
<th>Lower Density Data</th>
<th>Upper Density Data</th>
<th>Lower C.R. Impedance</th>
<th>Upper C.R. Impedance</th>
<th>Lower C.R. Leakable</th>
<th>Upper C.R. Leakable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.000000</td>
<td>1.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>2</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>3</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>4</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>5</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>6</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
<tr>
<td>7</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Figure 5.—Output for symmetrical basin example
### Elevation Data

<table>
<thead>
<tr>
<th>Layer</th>
<th>Elevation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Matrix, Layer 1

<table>
<thead>
<tr>
<th>Layer</th>
<th>Matrix Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>-0.5000E01</td>
</tr>
<tr>
<td>4</td>
<td>-0.5000E01</td>
</tr>
<tr>
<td>5</td>
<td>-0.5000E01</td>
</tr>
<tr>
<td>6</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>0.0</td>
</tr>
</tbody>
</table>

### Thickness Data

- Thickness Data = 1.000000 for Layer 1
- DELX = 1000.000
- DELY = 1000.000

### Pseudosource Total Contribution

<table>
<thead>
<tr>
<th>Layer</th>
<th>Contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-2.885</td>
</tr>
<tr>
<td>2</td>
<td>-5.110</td>
</tr>
<tr>
<td>3</td>
<td>-5.170</td>
</tr>
<tr>
<td>4</td>
<td>-2.885</td>
</tr>
<tr>
<td>5</td>
<td>-5.110</td>
</tr>
<tr>
<td>6</td>
<td>34.67</td>
</tr>
<tr>
<td>7</td>
<td>-5.770</td>
</tr>
<tr>
<td>8</td>
<td>-2.885</td>
</tr>
<tr>
<td>9</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**Figure 5.---Output for symmetrical basin example---Continued**
<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>3</td>
<td>$-2.880.0$</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>4</td>
<td>$-2.880.0$</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>2</td>
<td>$-2.880.0$</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>3</td>
<td>$5.777.885$</td>
<td>$-2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>4</td>
<td>$5.777.885$</td>
<td>$-2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>5</td>
<td>$5.777.885$</td>
<td>$-2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>2</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>3</td>
<td>$5.777.885$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>4</td>
<td>$3.62-17.31$</td>
<td>$-17.31$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>5</td>
<td>$5.777.885$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>6</td>
<td>$2.880.0$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>2</td>
<td>$2.880.0$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>3</td>
<td>$5.777.885$</td>
<td>$-2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>4</td>
<td>$5.777.885$</td>
<td>$-2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>5</td>
<td>$5.777.885$</td>
<td>$-2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>6</td>
<td>$2.880.0$</td>
<td>$0.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>3</td>
<td>$2.880.0$</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>4</td>
<td>$2.880.0$</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>5</td>
<td>$2.880.0$</td>
<td>$2.885.0$</td>
<td>$0.0$</td>
</tr>
</tbody>
</table>

**SUM OF P.S. TERMS**

\[
\begin{align*}
\text{TOTAL PSA} &= 0.0 \\
\text{TOTAL PSB} &= 0.0 \\
\text{TOTAL PS3} &= 0.0 \\
\text{TOTAL PS} &= 0.0
\end{align*}
\]

Normal end of processing program Job 3
Programmed by Doug Low --NASA Projects Denver
Program version number 65J7

Figure 5.--Output for symmetrical basin example--Continued
Table 1.--Definition of some pseudosource program variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>COSA, COSB</td>
<td>Cosines of the angles between the bedding plane and the x- and y-axes.</td>
</tr>
<tr>
<td>DA, DB</td>
<td>Hypotenuse of the right triangle formed by the grid spacing and the bedding plane in the x- and y-directions.</td>
</tr>
<tr>
<td>DAP, DAM</td>
<td>Values of the total differential of alpha in the plus x-direction and minus x-direction from node ((I,J)).</td>
</tr>
<tr>
<td>DELX, DELY</td>
<td>The grid spacing in the x- and y-directions.</td>
</tr>
<tr>
<td>DEN</td>
<td>Average ground-water density for each nodal area.</td>
</tr>
<tr>
<td>DENL, DENU</td>
<td>Average ground-water density for each nodal area in the aquifer below and above the aquifer for which pseudosources are calculated.</td>
</tr>
<tr>
<td>DZA, DZ3</td>
<td>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.</td>
</tr>
<tr>
<td>ELEV</td>
<td>Elevation array for the aquifer for which pseudosources are calculated.</td>
</tr>
<tr>
<td>IO, JO</td>
<td>Number of nodes in the x- and y-directions.</td>
</tr>
<tr>
<td>Variable</td>
<td>Definition</td>
</tr>
<tr>
<td>--------------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>PSA, PSB</td>
<td>The alpha- and beta-terms of the aquifer pseudosource contributions at each node.</td>
</tr>
<tr>
<td>PS3</td>
<td>Confining-layer pseudosource contributions for each node.</td>
</tr>
<tr>
<td>PST</td>
<td>Total pseudosource contribution for each node.</td>
</tr>
<tr>
<td>PSLL</td>
<td>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.</td>
</tr>
<tr>
<td>SUMPST, SUMPSA</td>
<td>PST summed for all nodes, and PSA summed for all nodes.</td>
</tr>
<tr>
<td>T</td>
<td>Hybrid transmissivity.</td>
</tr>
<tr>
<td>TAP, TAM</td>
<td>Harmonic mean of the hybrid transmissivity between nodes (I,J-1) and (I,J), and between the nodes (I,J) and (I,J-1).</td>
</tr>
<tr>
<td>THKL, THKU</td>
<td>Thickness of lower and upper confining layer.</td>
</tr>
<tr>
<td>TKL, TKU</td>
<td>Hybrid leakance of lower and upper confining layer.</td>
</tr>
<tr>
<td>TPSA, TPSB, TPSS</td>
<td>Total aquifer pseudosource contributions, and total confining-layer pseudosource contributions.</td>
</tr>
</tbody>
</table>
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 \( \Delta x \) replacing \( \Delta a \) in equation 31, and with \( (T_{a\alpha})_{j+1} \) calculated as the harmonic mean of \( T_{a\alpha} \) along the \( x \)-direction between nodes \( j \) and \( j+1 \). The aquifer pseudosources from the \( \beta \)-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
C----- FORTRAN PROGRAM TO CALCULATE PSEUOSOURCE TERMS FROM FIELD DATA & M
C----- DATA TESTED ON 16 JUNE 80
C----- IN MAY 1980
C----- INTEGER BLK
C----- DIMENSION T(21,26), DEN(21,26), ELEV(21,26), THCK(21,26), DELX(26)
C----- 1, DELY(21), INFT(2,26), IOFT(2,21), TH(21,26), PS(21,26), PK(21,26)
C----- 2, PS(21,26), WSB(21,26), PSS(21,26), DENL(21,26), THKL(21,26), TMKL(21,26)
C----- 3
C----- COMMON /MISC/ ID, JO, KO
C----- DATA BLK/
C----- DATA ID(20F4.4), 4H4.0, 4H(32X,2HOF6.4,2H4.0)/
C----- DATA IO, JO, K(21H3), 4H(32X,2HOF6.4,2H4.0)/
C----- DATA INFT(I2,4), 4H(32X,2HOF6.4,2H4.0)/
C----- DATA IOFT(I2,4), 4H(32X,2HOF6.4,2H4.0)/
C----- DATA IOFT(I2,4)
C----- DATA INFT(I2,4)
C----- DATA ID(20F4.4), 4H4.0, 4H(32X,2HOF6.4,2H4.0)/
C----- DATA IO, JO, K(21H3), 4H(32X,2HOF6.4,2H4.0)/
C----- DATA INFT(I2,4), 4H(32X,2HOF6.4,2H4.0)/
C----- DATA IOFT(I2,4), 4H(32X,2HOF6.4,2H4.0)/
C----- READ IN PRINT OPTION OF INTERMEDIATE TERMS
C----- READ (5,230) KCHK
C----- READ IN MATRIX SIZE AND
C----- READ IN LOWER DENSITY ARRAY
C----- READ IN UPPER DENSITY ARRAY
C----- READ IN LOWER CONFINING BED THICKNESS ARRAY
C----- READ IN UPPER CONFINING BED THICKNESS ARRAY
C----- READ IN LOWER CONFINING BED LEAKANCE
C----- READ IN UPPER CONFINING BED LEAKANCE
C----- READ IN HYBRID TRANSMISSIVITY ARRAY DATA
C----- INACTIVE NODES MUST HAVE TRANSMISSIVITY SET TO ZERO
C----- OTHERWISE PSEUDOSOURCE CALCULATION WILL BE WRONG
C----- ******************************************
```

36
CALL ARRAY(I,INFT(I,1),IOFT(I,4),TRANSMISSIVITY DATA **,IRN,DH) A 510
THM)
C---- HEAD IN DENSITY ARRAY DATA
CALL ARRAY(I,INFT(I,1),IOFT(I,4),DENSITY DATA **,IRN,DH) A 520
THM)
C---- HEAD IN ELEVATION ARRAY DATA
CALL ARRAY(I,ELEV(I),INFT(I,1),IOFT(I,4),ELEVATION DATA **,IRN,DH) A 530
THM)
C---- HEAD IN THICKNESS ARRAY DATA
CALL ARRAY(I,THC,INFT(I,1),IOFT(I,4),THICKNESS DATA **,IRN,DH) A 540
THM)
C---- HEAD IN DELX ARRAY
C
************** DELX **************
IF (IVAH.EQ.1) READ (5,390) (DELX(J),J=1,JO) A 550
DU 130 J=1,JO A 560
IF (IVAH.NE.1) GO TO 120
DELX(J)=DELX(J)*FAC A 570
GO TO 130
GO TO 120
DELX(J)=FAC A 580
130 CONTINUE
IF (IVAH.EQ.1.AND.IPHN.NE.1) WRITE (6,360) (DELX(J),J=1,JO) A 590
IF (IVAH.EQ.0) WRITE (6,370) FAC A 600
SUMPST=0.0 A 610
SUMPSA=0.0 A 620
SU-1PSB=0.0 A 630
SUMPSJ=0.0 A 640
DU 140 I=1,10 A 650
DO 150 J=1,JO A 660
PST(I,J)=0.0 A 670
SA(I,J)=0.0 A 680
PSB(I,J)=0.0 A 690
PSJ(I,J)=0.0 A 700
ELEV(I,J)=ELEV(I,J)-THC(I,J)/2. A 710
CONTINUE
140 CONTINUE
150 CONTINUE
IF (IVAH.EQ.1.AND.IPHN.NE.1) WRITE (6,400) (PST(I,J),I=1,10,J=1,JO) A 720
IF (IVAH.EQ.0) WRITE (6,400) FAC A 730
SUMPST=0.0 A 740
SUMPSA=0.0 A 750
SU-1PSB=0.0 A 760
SUMPSJ=0.0 A 770
DU 160 I=1,10 A 780
DO 170 J=1,JO A 790
PST(I,J)=0.0 A 800
SA(I,J)=0.0 A 810
PSB(I,J)=0.0 A 820
PSJ(I,J)=0.0 A 830
ELEV(I,J)=ELEV(I,J)-THC(I,J)/2. A 840
CONTINUE
160 CONTINUE
10=10-1 A 850
JO=JO-1 A 860
DU 190 I=2,10 A 870
DU 190 J=2,JO A 880
DO 190 I=2,10 A 890
DO 190 J=2,JO A 900
37
Table 2.—FORTRAN program to calculate pseudosource terms—Continued

IF (I>J, E0=0) GO TO 170

C **************************************************************
C HARMONIC MEAN OF HYBRID TRANSMISSIVITY INSURES NO-FLOW BOUNDARIES
C CORRECTLY IMPLEMENTED EVEN IN VARIABLE DENSITY CASE...
C CALCULATION OF HARMONIC MEAN HYBRID TRANSMISSIVITY DIVIDED BY THE
C DISTANCE BETWEEN NODES FOLLOWS...
C **************************************************************

TBM = T(I,J)*T(I,J)/T(I,J)*DDELX(I)*T(I,J)*DDELX(J)

CALC OF DELTA WH'S AS WEIGHTED AVERAGES ************************

DHO = Denu(J-1)

DAP = FLX(I,J-1) + DRO*DELX(J)

DAM = FLX(J)+DRO*DELX(I)

TAP = (TAP*I)*TAP(I,J)/TAP(I,J)*DDELX(I)*DDELX(J)

TAM = (TAM*I)*TAM(I,J)/TAM(I,J)*DDELX(I)*DDELX(J)

TBM = T(I,J)*T(I,J)*DDELX(I)*DDELX(J)

ONHP = (ONHP*I)*TAP(I,J)/ONHP(I,J)*DDELX(I)*DDELX(J)

ONHM = (ONHM*I)*TAM(I,J)/ONHM(I,J)*DDELX(I)*DDELX(J)

C CALC OF ELEVATION CHANGES *************************************

0£AP = ELEV(I,J)*ELEV(I,J)

OZAM = -ELEV(I-1,J) + ELEV(I,J)

OZAP = ELEV(I,J)*ELEV(I,J)

DDEML = (DDEML(I,J)*DDEML(I,J))/2.

PSA(I,J) = (PSA(I,J)*PSA(I,J))/2.

PSH(I,J) = (PSH(I,J)*PSH(I,J))/2.

PKL(I,J) = (PKL(I,J)*PKL(I,J))/2.

PKU(I,J) = (PKU(I,J)*PKU(I,J))/2.

C THE END OF FACTOR CALC & THE BEGINNING OF THE CALC OF THE ALPHA & B
C CONTRIBUTIONS TO HORIZONTAL PSEUDOSOURCE TERMS, THE CALC OF THE VER
C PSEUDOSOURCE TERM FOLLOWS.
C **************************************************************

PSA(I,J) = (TAP*DAP+DAP+DAP)*TAM(I,J)/ONHP(I,J)*DDELX(I)

PSH(I,J) = (TAP*DAP+DAP+DAP)*TAM(I,J)/ONHM(I,J)*DDELX(J)

PKL(I,J) = (PKL(I,J)*PKL(I,J))/2.

PKU(I,J) = (PKU(I,J)*PKU(I,J))/2.

C IN ORDER TO MAKE THE CORRESPONDENCE BETWEEN PSA+PSH+PSJ AND THE
C DISCHARGE OR RECHARGE OF THE GROUNDWATER FLOW CODE OF OPEN FILE
C REPORT 75-413 THREE MINUS SIGNS WERE INTRODUCED IN THE EQUATION AB

38
Table 2. FORTRAN program to calculate pseudosource terms—Continued

```fortran
C WITH THESE MINUS SIGNS PST(I,J) CAN BE INTRODUCED DIRECTLY AS INP
C GROUP IV DATA SET 1 OF REPORT 75-43R. PST<0 CORRESPONDS TO A
C DISCHARGING WELL, AND PST>0 CORRESPONDS TO A RECHARGING WELL.
C-----------------------------------------------------------------------------------
170 CONTINUE
   IF (T(I,J),NE.,0) GO TO 180
   PST(I,J)=0.0
   PSH(I,J)=0.0
   PSM(I,J)=0.0
180 CONTINUE
   IF (ABS(PST(I,J)) .LT.0.2 .OR. KCHK.EQ.0) GO TO 190
   WRITE (6,250) I,J,PSH(I,J),PSA(I,J),PSB(I,J),PS3(I,J)
190 CONTINUE
   SUMPS3=SUMPSH*PS3(I,J)
200 WRITE (6,300)
   DO 200 I=2,IO
      WRITE (6,310) (PST(I,J),J=2,JO)
   DO 210 J=2,JO
      IF (ABS(PST(I,J)) .LT.0.2) GO TO 210
      WRITE (6,320) KK,KJ,PST(I,J),PSA(I,J),PSB(I,J),PS3(I,J)
210 CONTINUE
   SUMPS=SUMPSA+SUMPSH+SUMPS3
   SUMPST=SUMPS+SUMPSH+SUMPS3
   WRITE (6,330)
220 CONTINUE
   WRITE (6,330)
   DO 220 J=2,JO
      WRITE (6,330)
230 CONTINUE
   WRITE (6,330)
   STOP
240 FORMAT (11I10)
250 FORMAT (11X,7F7.3)
260 FORMAT (11X,7F7.3)
270 FORMAT (11X,7F7.3)
280 FORMAT (11X,7F7.3)
```

Table 2.—FORTRAN program to calculate pseudosource terms—Continued

```fortran
290 FORMAT (10X,'PSA = ',G10.4,7X,'PSB = ',G10.4,7X,'PS3 = ',G10.4,/
        ,1X,'PS8 = ',G10.4,7X,'PS9 = ',G10.4,7X,'PS10 = ',G10.4,/
        ,1X,'PS11 = ',G10.4,7X,'PS12 = ',G10.4,7X,'PS13 = ',G10.4,/
        ,1X,'PS14 = ',G10.4,7X,'PS15 = ',G10.4,7X,'PS16 = ',G10.4,/
        ,1X,'PS17 = ',G10.4,7X,'PS18 = ',G10.4,7X,'PS19 = ',G10.4,/
        ,1X,'PS20 = ',G10.4,7X,'PS21 = ',G10.4,7X,'PS22 = ',G10.4,/
        ,1X,'PS23 = ',G10.4,7X,'PS24 = ',G10.4,7X,'PS25 = ',G10.4,/
        ,1X,'PS26 = ',G10.4,7X,'PS27 = ',G10.4,7X,'PS28 = ',G10.4,/
        ,1X,'PS29 = ',G10.4,7X,'PS30 = ',G10.4,7X,'PS31 = ',G10.4,/
        ,1X,'PS32 = ',G10.4,7X,'PS33 = ',G10.4,7X,'PS34 = ',G10.4,/
        ,1X,'PS35 = ',G10.4,7X,'PS36 = ',G10.4,7X,'PS37 = ',G10.4,/
        ,1X,'PS38 = ',G10.4,7X,'PS39 = ',G10.4,7X,'PS40 = ',G10.4,/
        ,1X,'PS41 = ',G10.4,7X,'PS42 = ',G10.4,7X,'PS43 = ',G10.4,/
        ,1X,'PS44 = ',G10.4,7X,'PS45 = ',G10.4,7X,'PS46 = ',G10.4,/
        ,1X,'PS47 = ',G10.4,7X,'PS48 = ',G10.4,7X,'PS49 = ',G10.4,/
        ,1X,'PS50 = ',G10.4,7X,'PS51 = ',G10.4,7X,'PS52 = ',G10.4,/
        ,1X,'PS53 = ',G10.4,7X,'PS54 = ',G10.4,7X,'PS55 = ',G10.4,/
        ,1X,'PS56 = ',G10.4,7X,'PS57 = ',G10.4,7X,'PS58 = ',G10.4,/
        ,1X,'PS59 = ',G10.4,7X,'PS60 = ',G10.4,7X,'PS61 = ',G10.4,/
        ,1X,'PS62 = ',G10.4,7X,'PS63 = ',G10.4,7X,'PS64 = ',G10.4,/
        ,1X,'PS65 = ',G10.4,7X,'PS66 = ',G10.4,7X,'PS67 = ',G10.4,/
        ,1X,'PS68 = ',G10.4,7X,'PS69 = ',G10.4,7X,'PS70 = ',G10.4,/
        ,1X,'PS71 = ',G10.4,7X,'PS72 = ',G10.4,7X,'PS73 = ',G10.4,/
        ,1X,'PS74 = ',G10.4,7X,'PS75 = ',G10.4,7X,'PS76 = ',G10.4,/
        ,1X,'PS77 = ',G10.4,7X,'PS78 = ',G10.4,7X,'PS79 = ',G10.4,/
40
Table 2.—FORTRAN program to calculate pseud-source terms—Continued

***************
***************
IN.T.E.R.V.E.H.M.L.K
I(N,6)
C.OM.M.O.N./M.IS.C./I,O,J,K
D.A.T.A.H.L.K/*I/
K=1
K=1
I.C=6*H.E.C.2*I.V.A.R.*P.H.N.*1
G.U.TO.(10,10,30,60,60), I.C
10 UU 20 I=1,10
U 20 J=1,J0
20 A(I,J)=FAC
W.R.T.E.(5*100) I,N+F.A.C.*K
G.U.TO.80
J0 IF (I.C.EQ.3) W.R.I.T.E.(6*110) I,N,K
DO 50 I=1,10
50 IF (I.C.EQ.3) W.R.T.E.(I,N,F.T) I,(A(I,J),J=1,J0)
DO 40 J=1,J0
40 A(I,J)=A(I,J)*FAC
50 IF (I.C.EQ.3) W.R.T.E.(6*110) I,(A(I,J),J=1,J0)
G.U.TO.80
60 C.O.N.T.I.N.U.E.
IF (I.C.EQ.5) G.U.TO.80
W.R.T.E.(6*110) I,N,K
DO 70 I=1,10
70 W.R.T.E.(6*110) I,(A(I,J),J=1,J0)
80 C.O.N.T.I.N.U.E.
I.H.N.=R.N.+1
DO 90 I=1,6
90 I.N.T(I)=H.L.K
W.E.R.T.N.
C.C.C.C
---F.O.R.M.A.T.S---
C.C.C.C
100 F.O.R.M.A.T.(1,H.0.52X,AA4)="+1,15,F.7,1 FOR LAYER+I3"
110 F.O.R.M.A.T.(1,H.0.45X,AA4)="HATW.I.A.LAYER+J3/46X+1(+1)"
120 F.O.R.M.A.T.(F.10.0,2(13,F.10.0,2(10))
E.N.D.

41
To calculate pseudosource strengths, it is necessary to know ground-water density throughout the modeled 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:

\[
m = \frac{DS}{MW \left(\rho' - \frac{DS}{1,000}\right)}
\]

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
- \(\rho'\) 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:

\[ c_p = \rho \left( 1 - \frac{1}{\left( 1 + \frac{1,000}{m \times MW} \right)} \right) \]  \hspace{1cm} (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.
Read and echo input

Start loop to calculate density at each node I = 2, J = 2

T < 40°F and h = 0

No

T < 40°F and h ≠ 0

No

Calculate pressure and convert temperature for each node

Calculate molality for node by assuming density is 1.0

Calculate ρ from Potter's equation

Calculate m with density from last step

m close to previous m?

No

A

Symbols:

- Cp = pure-water concentration
- m = molality of NaCl solution
- d = density of NaCl solution
- I = row of nodal array
- J = column of nodal array
- h = hydraulic head (for reference density)
- ρ = ground-water density
- T = ground-water temperature in °F

Figure 6.—Flow chart for density calculation program.
Set Table that gives density for $0.5 \leq m \leq 6$ and for a given temperature and pressure.

Table that gives density for $0.5 \leq m \leq 6$ and for a given temperature and pressure.

Calculate pure water concentration.

Calculate coefficients, $A$, $B$, $C$, for constant $T$ and $p$.

Use equation: $d = A + Bm + Cm^2$ to calculate density.

Interpolate between the densities.

Print and punch density and pure-water concentration.

End.
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:

<table>
<thead>
<tr>
<th>CARD</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>VARIABLE</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-80</td>
<td>20A4</td>
<td>TITLE</td>
<td>Title of density calculation.</td>
</tr>
<tr>
<td>2</td>
<td>1-10</td>
<td>F10.6</td>
<td>CD1FF</td>
<td>Percentage difference allowed for molality iteration to converge.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>F10.6</td>
<td>PRINT</td>
<td>Print option of intermediate calculations.</td>
</tr>
<tr>
<td>3</td>
<td>1-10</td>
<td>I10</td>
<td>IØ</td>
<td>Number of rows.</td>
</tr>
<tr>
<td></td>
<td>11-20</td>
<td>I10</td>
<td>JØ</td>
<td>Number of columns.</td>
</tr>
<tr>
<td></td>
<td>21-30</td>
<td>I10</td>
<td>KØ</td>
<td>Layer number.</td>
</tr>
</tbody>
</table>
All of the following input data require a parameter card either preceding an array or as the sole input for that array.

<table>
<thead>
<tr>
<th>COLUMN</th>
<th>FORMAT</th>
<th>VARIABLE</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-10</td>
<td>G10.0</td>
<td>FAC</td>
<td>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.</td>
</tr>
<tr>
<td>11-20</td>
<td>G10.0</td>
<td>IVAR</td>
<td>0—If no data cards are to be read in for this layer. 1—If data cards for this layer follow.</td>
</tr>
<tr>
<td>21-30</td>
<td>G10.0</td>
<td>IPRN</td>
<td>0—If data for this layer are to be printed. 1—If data for this layer are not to be printed.</td>
</tr>
</tbody>
</table>
When data sets are included, start each row on a new card as follows:

<table>
<thead>
<tr>
<th>DATA SET</th>
<th>COLUMN</th>
<th>FORMAT</th>
<th>VARIABLE</th>
<th>DEFINITION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1-80</td>
<td>16F5.0</td>
<td>TEMP</td>
<td>Temperature, in degrees Celsius.</td>
</tr>
<tr>
<td>2</td>
<td>1-80</td>
<td>20F4.0</td>
<td>TDS</td>
<td>Dissolved solids, in grams per liter.</td>
</tr>
<tr>
<td>3</td>
<td>1-80</td>
<td>8F10.4</td>
<td>H</td>
<td>Hydraulic head, in feet above sea level.</td>
</tr>
<tr>
<td>4</td>
<td>1-80</td>
<td>20F4.0</td>
<td>ELEV</td>
<td>Aquifer elevation, in feet above sea level.</td>
</tr>
<tr>
<td>Variables</td>
<td>Definitions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>-------------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A, B, C</td>
<td>Coefficients in the first four columns of table 29 from Potter and Brown (1977).</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CDIFF</td>
<td>A value such that when CDIFF is greater than CRTN, the molality iteration stops.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CRTN</td>
<td>Absolute value of the percentage difference between the last calculated molality and the previous calculated molality.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DEN</td>
<td>Final floating-point array into which density is put.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DEN1</td>
<td>Density calculated for pure water at field temperature.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DEN3</td>
<td>Density calculated for a 0.5 molality solution.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DENS</td>
<td>Density calculated from equation 1 of Potter and Brown (1977) and used to iterate to a final molality.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DENP</td>
<td>Pure-water concentration array.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>An array that contains $A_o$, $B_o$, and $C_o$ (for 20° Celsius) of table 28 from Potter and Brown (1977).</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3.--Definitions of some density and concentration program variables--Continued

<table>
<thead>
<tr>
<th>Variables</th>
<th>Definitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>ELEV</td>
<td>Elevation array.</td>
</tr>
<tr>
<td>H</td>
<td>Pure-water (at 20° Celsius and 1 atmosphere) hydraulic-head array.</td>
</tr>
<tr>
<td>IDEN</td>
<td>Fixed-point representation of 1,000 x DEN.</td>
</tr>
<tr>
<td>IDENP</td>
<td>Fixed-point representation of 1,000 x DENP.</td>
</tr>
<tr>
<td>P</td>
<td>Pressure array.</td>
</tr>
<tr>
<td>R</td>
<td>Three-element array containing density for molalities of 2.0, 4.0, and 6.0.</td>
</tr>
<tr>
<td>RHO</td>
<td>Temporary storage variable for density from steam tables.</td>
</tr>
<tr>
<td>TDS</td>
<td>Dissolved-solids array.</td>
</tr>
<tr>
<td>TEMP</td>
<td>Temperature array.</td>
</tr>
<tr>
<td>TITLE</td>
<td>Alphanumeric variable that contains the first line of input.</td>
</tr>
<tr>
<td>X</td>
<td>Three-element array containing molalities equal to 2.0, 4.0, and 6.0.</td>
</tr>
<tr>
<td>XMOL</td>
<td>Final iteration molality.</td>
</tr>
<tr>
<td>XMOL1</td>
<td>Intermediate iteration molality.</td>
</tr>
<tr>
<td>XMOL3</td>
<td>A molality equal to 0.5.</td>
</tr>
</tbody>
</table>
Table 4.--Density and concentration FORTRAN program

INTEGER BLK
DIMENSION H(21,26), INFT(2,3), IOFT(9,4), IV(6), DUM(3), TF(3)
DIMENSION TEMP(21,26), ELEV(21,26), TDS(21,26), P(21,75)
DIMENSION DTM(21,26), DEP(21,26), IOTP(21,26), IP(21,26), IT(21,26)
DIMENSION A(13,4), B(13,4), C(13,4), DUM(5), TITLE(20), E(3)
DIMENSION X(3), 9(3)

C    E(I) ARE CONSTANTS IN POTTER'S Eq.11 FOR 20 DEGREES CENTIGRADE
DATA E/15.782, 2.0324, 0.0744/
DATA DO/. 999839, .997047, .988038, .974044, .974044/

C    THE MOLECULAR WEIGHT OF NaCl AND CONVERSION FACTOR TO CONVERT
C FEET OF WATER TO BARS (PRESSURE)......
*T=s158.4428
*CF=.02987712
C    READ IN TITLE
3EAO (5,230) TITLE
C    READ IN CLOSURE CRITERION FOR MOLALITY ITERATION IN PERCENT
READ(5,240) COIF, PRINT A 410
WRITE(6*250) COIF, PRINT A 420
C    HEAD IN MATRIX SIZE AND
C    READ IN LAYER NUMBER STARTING AT BOTTOM WITH ONE
READ(5,260) IO,JO,KO
WRITE(6*270) IO,JO,KO
C    READ IN TEMPERATURE ARRAY (IN DEGREES FAHRENHEIT)
CALL ARRAY(TEMP,INFT(1,3),IOFT(1,1),TEMPERATURE (IN FHNCMT),IT, DUM)
C    READ IN DISSOLVED SOLIDS (IN GRAMS PER LITER)
CALL ARRAY(TDS,INFT(1,3),IOFT(1,1),DISSOLVED SOLIDS IN G/L, I, DUM)
C    READ IN DISSOLVED SOLIDS (IN GRAMS PER LITER)
Table 4.—Density and concentration FORTRAN program—Continued

<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>104</td>
<td>C----</td>
<td>HEAD IN FRESH WATER HEADS (PURE WATER AT TP) IN FEET</td>
</tr>
<tr>
<td>105</td>
<td>CALL</td>
<td>ARRAY(H,1,FNT(1,2),IOFT(1,1),&quot;FRESH WATER HEADS IN FT&quot; ,I=1,N,J=1,M)</td>
</tr>
<tr>
<td>110</td>
<td>C----</td>
<td>HEAD IN AQUIFER ELEVATION (IN FEET AOVE MSL)</td>
</tr>
<tr>
<td>111</td>
<td>CALL</td>
<td>ARRAY(ELEV,INFT(1,1),IOFT(1,4),&quot;AQUIFER ELEVATION IN FT&quot; ,I=1,N,J=1,M)</td>
</tr>
<tr>
<td>115</td>
<td>WRITE</td>
<td>(6,280)</td>
</tr>
<tr>
<td>116</td>
<td>WRITE</td>
<td>(6,290)</td>
</tr>
<tr>
<td>117</td>
<td>WRITE</td>
<td>(6,300)</td>
</tr>
<tr>
<td>120</td>
<td>DO 110</td>
<td>I=1,10</td>
</tr>
<tr>
<td>121</td>
<td>DO 120</td>
<td>J=1,10</td>
</tr>
<tr>
<td>122</td>
<td>IF</td>
<td>TEMP(I,J) LT 40 AND H(I,J) EQ 0.0 GO TO 190</td>
</tr>
<tr>
<td>123</td>
<td>IF</td>
<td>TEMP(I,J) LT 40 AND H(I,J) NE 0.0 GO TO 200</td>
</tr>
<tr>
<td>124</td>
<td>TEMP</td>
<td>(I,J) = (TEMP(I,J) - 32) * 5/9</td>
</tr>
<tr>
<td>125</td>
<td>P(I,J)</td>
<td>= CF * (H(I,J) - ELEV(I,J))</td>
</tr>
<tr>
<td>126</td>
<td>XMOL</td>
<td>= 1000 * (1000 - TDS(I,J)) / WT</td>
</tr>
<tr>
<td>127</td>
<td>XMOL1</td>
<td>= XMOL</td>
</tr>
<tr>
<td>128</td>
<td>CONTINUE</td>
<td></td>
</tr>
<tr>
<td>130</td>
<td>C ---</td>
<td>DENO IS DENSITY OF PURE WATER AT 20 DEG.C. AND 1DBA</td>
</tr>
<tr>
<td>131</td>
<td>DENO</td>
<td>= 0.9976054</td>
</tr>
<tr>
<td>132</td>
<td>UNM</td>
<td>= 1000 * (E(1) * XMOL * E(2) * (SQRT(XMOL) ** 3) * E(3) * (XMOL ** 2) ** DENO)</td>
</tr>
<tr>
<td>133</td>
<td>DENS</td>
<td>= 1000 * DENO * WT * XMOL * DENO) / UNM</td>
</tr>
<tr>
<td>134</td>
<td>N=1</td>
<td></td>
</tr>
<tr>
<td>135</td>
<td>XMOL</td>
<td>= TDS(I,J) * 1000 / ((DENS * 1000 - TDS(I,J)) * WT)</td>
</tr>
<tr>
<td>136</td>
<td>XMOL1</td>
<td>= XMOL</td>
</tr>
<tr>
<td>137</td>
<td>CRYN</td>
<td>= ABS1(XMOL * XMOL1 * 100 / XMOL)</td>
</tr>
<tr>
<td>138</td>
<td>IF</td>
<td>(N.EQ.1 AND PRINT.EQ.1) WRITE (6,310)</td>
</tr>
<tr>
<td>139</td>
<td>IF</td>
<td>(PRINT.EQ.1) WRITE (6,320) I,J,K0,N,XMOL1,DENS,TDS(I,J),CRYN</td>
</tr>
<tr>
<td>140</td>
<td>CONTINUE</td>
<td></td>
</tr>
<tr>
<td>140</td>
<td>IF</td>
<td>XMOL.GE.0.5 GO TO 150</td>
</tr>
<tr>
<td>141</td>
<td>XMOL3</td>
<td>= 0.5</td>
</tr>
<tr>
<td>142</td>
<td>IF</td>
<td>XMOL.EQ.0.0 DENS=0.0</td>
</tr>
<tr>
<td>143</td>
<td>IF</td>
<td>XMOL.NE.0.0 CALL TABLES(XMOL3,P,I,J,A,B,C,TEMP,DENS)</td>
</tr>
<tr>
<td>144</td>
<td>CALL</td>
<td>RELO(100,TEMP,I,J,DENS)</td>
</tr>
</tbody>
</table>

52
Table 4.—Density and concentration FORTRAN program—Continued

RHO = (0.5 - XMOL) * DEN1 + XMOL * DEN3 / 0.5

150 IF (XMOL LT 0.5 OR XMOL GT 6.0) GO TO 140
     CALL TABLES(XMOL, P, I, J, A, B, C, TEMP, H2O)

160 IF (XMOL LE 6.0) GO TO 180
     DO 170 M = 1, 3
           X(M) = FLOAT(2.0**M)
           Z(M) = A(M)
     CALL TABLES(Z, P, I, J, A, B, C, TEMP, Q)
     R(M) = Q
     OEN = 272593
     ANUM = (12 - 4 * SQRT(6.)) * R(1) + (2 * SQRT(6.)) * R(2) + (4 * SQRT(2.)) * R(3)
     AI = ANUM / DENOM
     BI = ANUM / DENOM
     CI = CNUM / DENOM

C THE FOLLOWING FORMULA HAS ONLY BEEN VERIFIED FOR MOLALITIES LE 6.0;
C HERE IT IS USED TO CALCULATE DENSITIES WITH MOLALITIES GT 6.0...

180 CONTINUE
     DEN1 = RHO
     DEN1(J) = DEN1(J) * (1 - XMOL * WT / (XMOL * WT + 1000))
     GO TO 210

190 CONTINUE
     DEN1(J) = 1.0
     DENP(J) = 1.0
     GO TO 210

200 CONTINUE
     DEN1(J) = 0.997047
     DENP(J) = 0.997047
     WRITE (6, 340) I, J, K0

210 CONTINUE
     DO 220 J = 1, 10
           IDEN1 = IFIX(DEN1(J) * 1000)
           IDENP = IFIX(DENP(J) * 1000)
           WRITE (6, 350)
           WRITE (6, 370) (TITLE(I), I = 1, 20)
           WRITE (6, 370) (IDEN1(J), J = 1, 26, I = 1, 21)
           WRITE (6, 360)
           WRITE (6, 330) (TITLE(I), I = 1, 20)
           WRITE (6, 330) (IDENP(J), J = 1, 26, I = 1, 21)
           WRITE (7, 380) (IDEN1(J), J = 1, 26, I = 1, 21)
           WRITE (7, 380) (IDENP(J), J = 1, 26, I = 1, 21)
     STOP

C

230 FORMAT (20A4)
240 FORMAT (2F10.6)
Table 4.—Density and concentration FORTRAN program—Continued

```fortran
250 FORMAT (11, *135, 'ITERATION Closure criterion FOR Density (in %) =', 1F10.6, 'PRINT =*F=*1')
260 FORMAT (310)
270 FORMAT (T45, 'I0 K0 X133)
280 FORMAT (11, *135, 'INTERPOLATION COEFFICIENTS A+B+C+D+O+O+/')
290 FORMAT (T2, 13F4.4)
300 FORMAT (T2, 5F8.6+/)
320 FORMAT (T2, 415, 4F10.5)
330 FORMAT (T2, 'GT 10 ITERATIONS', 415, 'DEN1=*,F10.6, 'XMOL=*,F10.6, 'CRTN=*,F8.4)
340 FORMAT (T2, 'HEAD NE 0 BUT TEMP LT 40', 315)
350 FORMAT (11, *122, 'GROUNDER DENSITY (G/L)'),
360 FORMAT (11, *122, 'PURE WATER CONCENTRATION (G/L)'),
370 FORMAT (T12, *122, 'T12, 314)
380 FORMAT (2014, /, 614)
390 FORMAT (T12, 20A4, /)
END
```

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

```fortran
C ---------
SUBROUTINE TABLES(XMOL,P,I,J,GE,TEMP,RHO)
C ----------
DIMENSION P(21,26), A(13,4), B(13,4), C(13,4), TEMP(21,26)
C THIS ROUTINE IS NOT GOOD FOR PRESSURES ABOVE 300 ARMS OR
CONCENTRATIONS ABOVE 6.0 MOLALITY OR BELOW 0.5 MOLALITY...
IF (P(I,J).GE.100) GO TO 10
J=1
P0=1
10 CONTINUE
IF (P(I,J).LT.100.OR.P(I,J).GE.200) GO TO 20
J=2
P0=100
20 CONTINUE
IF (P(I,J).LT.200.0R.P(I,J).GE.300) GO TO 30
J=3
P0=200
30 CONTINUE
IF (XMOL.LT.0.5.OR.XMOL.GE.1.0) GO TO 40
II=1
XMOL=0.5
40 IF (XMOL.LT.1.0.OR.XMOL.GE.1.5) GO TO 50
II=2
XMOL=1.0
50 IF (XMOL.LT.1.5.OR.XMOL.GE.2.0) GO TO 60
II=3
XMOL=1.5
60 IF (XMOL.LT.2.0.OR.XMOL.GE.2.5) GO TO 70
II=4
XMOL=2.0
70 IF (XMOL.LT.2.5.OR.XMOL.GE.3.0) GO TO 80
II=5
XMOL=2.5
80 IF (XMOL.LT.3.0.OR.XMOL.GE.3.5) GO TO 90
II=6
XMOL=3.0
90 IF (XMOL.LT.3.5.OR.XMOL.GE.4.0) GO TO 100
II=7
XMOL=3.5
100 IF (XMOL.LT.4.0.OR.XMOL.GE.4.5) GO TO 110
II=8
XMOL=4.0
110 IF (XMOL.LT.4.5.OR.XMOL.GE.5.0) GO TO 120
II=9
XMOL=4.5
120 IF (XMOL.LT.5.0.OR.XMOL.GE.5.5) GO TO 130
II=10
XMOL=5.0
130 IF (XMOL.LT.5.5.OR.XMOL.GE.6.0) GO TO 140
II=11
XMOL=5.5
```

Table 4.—Density and concentration FORTRAN program—Continued

```
      51 140 IF (XMQL.NE.6) GO TO 150
      52    I=12
      53    XMOL0=XMOL
      54    PO=P(I,J)
      55 150 CONTINUE
      56      XXM=(XMOL-XMOL0)/0.5
      57      XXP=(P(I,J)-PO)/100.
      58      DAM=(A(I+1,JJ)-A(I+JJ))*XXM
      59      DAP=(A(I+J)+1)-A(I+JJ))*XXP
      60      AA=A(I+JJ)*DAP+DAM
      61      DB=B(I+1,JJ)-B(I+JJ))*XXM
      62      DHP=(B(I+JJ)+1)-B(I+JJ))*XXP
      63      HR=A(I+JJ)*DAP+DAM
      64      DCM=C(I+1,JJ)-C(I+JJ))*XXM
      65      DCP=C(I+JJ)+1)-C(I+JJ))*XXP
      66      CC=C(I+JJ)*DCP+DCM
      67      RHO=AA-(1.E-4)*HH*TE4P(I,J)-(1.E-6)*CC*TEMP(I,J)*2
      68      RETURN
      69      END
```
1 C
2 SUBROUTINE ELO(00, TEMP, I, J, 000)
3 C
4 C FOR TEMPERATURES ABOVE 75 DEG.C THIS ROUTINE DOES A LINEAR
5 C EXTRAPOLATION FROM POTTER ET AL. ALSO IT DOES NOT TAKE
6 C PRESSURE VARIATION INTO ACCOUNT.
7 DIMENSION 00(5), TEMP(21,26)
8 IF (TEMP(I,J).GE.25) GO TO 10
9 II=1
10 TO=0
11 10 IF (TEMP(I,J).LT.25.0 OR TEMP(I,J).GE.50) GO TO 20
12 II=2
13 TO=25
14 20 IF (TEMP(I,J).LT.50.0 OR TEMP(I,J).GE.75) GO TO 30
15 II=3
16 TO=50
17 30 IF (TEMP(I,J).LT.75) GO TO 40
18 TO=75
19 000=(00(I,F)+00(3))/25.
20 000=(00(I,F)*00*(TEMP(I,J)-TO))
21 GO TO 50
22 40 CONTINUE
23 TX0=(TEMP(I,J)-TO)/25
24 000=00(I)+00(I)*TX0
25 000=00(I)+000
26 50 CONTINUE
27 RETURN
28 END
Table 4.--Density and concentration FORTRAN program--Continued

<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>C</td>
</tr>
<tr>
<td>2</td>
<td>SUBROUTINE ARRAY(A,INFT,IOFT,IN,IRN,TF)</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
</tr>
<tr>
<td>4</td>
<td>INTEGER 8I_K</td>
</tr>
<tr>
<td>5</td>
<td>DIMENSION A(21,26), INFT(2,2), IN(6), TF(3), DUM(3), NUM2(4), IOFT</td>
</tr>
<tr>
<td>6</td>
<td>COMMON /MISC/ IO,JO,KO</td>
</tr>
<tr>
<td>7</td>
<td>DATA 8I_K/10,10,10/</td>
</tr>
<tr>
<td>8</td>
<td>READ (5,120) FAC,IVAR,IPRN,TF,IXECS,IRECO</td>
</tr>
<tr>
<td>9</td>
<td>IC=IC+IRECS+2*IVAR+IPRN+1</td>
</tr>
<tr>
<td>10</td>
<td>GO TO (10,10,30,30,60,60) IC</td>
</tr>
<tr>
<td>11</td>
<td>10 DD 20 I=1,IO</td>
</tr>
<tr>
<td>12</td>
<td>DO 20 J=1,JO</td>
</tr>
<tr>
<td>13</td>
<td>20 A(I,J)=FAC</td>
</tr>
<tr>
<td>14</td>
<td>WRITE (6,100) IN,FAC,KO</td>
</tr>
<tr>
<td>15</td>
<td>GO TO 80</td>
</tr>
<tr>
<td>16</td>
<td>30 IF (IC.EQ.3) WRITE (6,110) IN,KO</td>
</tr>
<tr>
<td>17</td>
<td>DO 50 I=1,IO</td>
</tr>
<tr>
<td>18</td>
<td>READ (5,INFT) (A(I,J),J=1,J0)</td>
</tr>
<tr>
<td>19</td>
<td>50 DO J=1,JO</td>
</tr>
<tr>
<td>20</td>
<td>60 CONTINUE</td>
</tr>
<tr>
<td>21</td>
<td>60 IF (IC.EQ.3) GO TO 90</td>
</tr>
<tr>
<td>22</td>
<td>WRITE (6,110) IN,KO</td>
</tr>
<tr>
<td>23</td>
<td>DO 70 I=1,IO</td>
</tr>
<tr>
<td>24</td>
<td>70 WRITE (6,IOFT) I,(A(I,J),J=1,J0)</td>
</tr>
<tr>
<td>25</td>
<td>80 CONTINUE</td>
</tr>
<tr>
<td>26</td>
<td>80 IF (IC.EQ.3) WRITE (6,110) IN,KO</td>
</tr>
<tr>
<td>27</td>
<td>90 IF (IC.EQ.3) WRITE (6,IOFT) I,(A(I,J),J=1,J0)</td>
</tr>
<tr>
<td>28</td>
<td>RETURN</td>
</tr>
<tr>
<td>29</td>
<td>---FORMATS---</td>
</tr>
<tr>
<td>30</td>
<td>100 FORMAT (1H0,52X,AA**1 =I,G15.7,I FOR LAYER*IJ)</td>
</tr>
<tr>
<td>31</td>
<td>110 FORMAT (1H1,45X,AA**1 MATRIX LAYER<em>I3/46X,41(</em>-1))</td>
</tr>
<tr>
<td>32</td>
<td>120 FORMAT (F10.0,2I10,3F10.0,2I10)</td>
</tr>
<tr>
<td>33</td>
<td>END</td>
</tr>
</tbody>
</table>

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REFERENCES


