1989


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Theoretical and numerical models for heat and mass transport and groundwater flow near salt domes

Evans, David Griffin, Ph.D.
The Louisiana State University and Agricultural and Mechanical Col., 1989

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THEORETICAL AND NUMERICAL MODELS FOR
HEAT AND MASS TRANSPORT AND GROUNDWATER FLOW
NEAR SALT DOMES

A Dissertation
Submitted to the Graduate Faculty of
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy
in
The Department of Geology and Geophysics

by
David Griffin Evans
B.A., The University of California, Berkeley, 1981
M.S., The University of Kansas, 1984
December 1989
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This dissertation is dedicated to the memory of
Paul M. Chesebrough
December 30, 1902 - November 30, 1989
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<td>a, b, c, d, e, f</td>
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<td>$r$</td>
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<tr>
<td>$t$</td>
<td>Time [t]</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature [T]</td>
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<tr>
<td>$u$</td>
<td>Generic dependent variable (C, T or $\Psi$)</td>
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<tr>
<td>$v$</td>
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<td>$\nu$</td>
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**Subscripts and Superscripts**

- $i,j$ Indices for finite difference nodes
- $e,w,n,s$ Indices of interfaces relative to node $i,j$
- $*$ Indicates concentration or temperature of fluid source
- $old, new$ Dependent variable values from previous and current iteration

$L$ is length; $M$ is mass; $E$ is energy; $T$ is temperature
ABSTRACT

Groundwater near salt domes is an inherently complex hydrogeologic system because groundwater is subject to large lateral gradients in salinity and temperature. Moreover, groundwater flow is indirectly coupled to salt tectonics because diapirism alters the salinity and thermal conditions as a sedimentary basin evolves. In order to study this complex environment, mathematical and numerical models are developed which explicitly couple heat and dissolved salt transport to groundwater flow, and account for basin subsidence and salt diapirism. The groundwater flow field is described using a mass stream function which does not require the Boussinesq assumption. The numerical model uses a control volume finite difference scheme and resolves nonlinearities iteratively using under-relaxation.

In order to assess the role of thermohaline convection near salt domes, dimensional analysis is used to simplify the transport equations and reduce the number of model parameters to three: the Rayleigh number, the Lewis number, and the buoyancy ratio. The buoyancy ratio is the ratio of salinity to temperature effects on pore water density, and it is the only dimensionless parameter that appears in the groundwater flow equation. The sense of convective circulation near a salt column depends primarily on the value of the buoyancy ratio and the thermal gradient contrast between the salt and overlying sediments. When the thermal gradient contrast is large or the buoyancy ratio is small, convective circulation
drives groundwater up along the salt edge. These conditions arise over a limited range of geologic circumstances.

A more comprehensive numerical model is used to investigate groundwater flow when salt dissolves preferentially at the crest of a salt dome during diapirism. Simulation results indicate that groundwater will flow down along the salt flank except when regional background salinities are high. Downward groundwater flow leads to low surface heat flow above the dome, in contrast to calculations based on heat conduction alone. Simulation results further indicate that groundwater flow is only weakly dependent on the hydrologic boundary conditions because groundwater density gradients are large. In the absence of high regional salinities, upward flow of groundwater near salt domes is probably driven by the release of geopressured fluids.
CHAPTER 1

STATEMENT OF THE PROBLEM AND METHOD OF SOLUTION

One of the fundamental laws of hydrology is the primeval struggle of subterranean waters and fire.
Raymond Thomassy, 1867
(From Geologie Pratique de la Louisiane)

The purpose of this study is to provide a theoretical context for understanding the complex interaction between groundwater flow and heat and mass transport in the vicinity of salt domes. In particular, inferences that groundwater moves vertically upward near the edges of some salt domes have motivated this study. The study is designed to test various hypotheses about the forces that could be responsible for driving these surprising flow patterns.

Salt domes and ambient sediments represent a complex geologic environment in which there is strong interaction between groundwater temperature, salinity, and flow. These interactions serve to make the salt dome environment one of the most complex that hydrogeologists are likely to encounter. The salt structure provides a local barrier to groundwater flow, provides a source of dissolved salt, and perturbs the local thermal environment. Moreover, salt is often mobile at near surface conditions, so the hydrologic history near salt domes is linked to their structural evolution. The complexity of this environment is born out by recent observations [Hanor, 1987; Leger, 1988; Jensenius and Munksgaard, 1989] that indicate the presence of groundwater
circulation in which flow is vertically upward along the flanks of some salt domes.

Groundwater flow near salt domes will impact not only heat and solute transport, but also sub-surface salt dissolution, salt mobility, petroleum migration, sediment diagenesis, and water quality. Despite its importance, however, groundwater flow near salt domes has only recently received much attention [e.g., Leijnse, 1985; Hanor, 1987; Jensenius and Munksgaard, 1989; Hassanizadeh and Leijnse, 1989; Ranganathan, 1988].

Groundwater near salt domes is inherently unstable because the presence of the salt column produces radial fluid density gradients that drive groundwater flow. The relative effects of lateral heat and salinity gradients near salt domes determine the sense and vigor of groundwater motion in this environment. The thermal effects of the salt diapir can result from the large thermal conductivity of halite relative to overlying and surrounding sediments, which causes isotherms to be pulled up near the salt. In addition, the presence of the salt column produces radial thermal gradients, the physical consequences of which have not previously been considered with respect to fluid flow. Variations in groundwater density will also be influenced by strong salinity gradients in groundwater that result from dissolution of the salt column itself.

Because groundwater density gradients result from both thermal and solute variations introduced by the salt column,
it is apparent that a comprehensive understanding of transport phenomena in this environment requires consideration of fully coupled equations describing groundwater flow, heat transport, and mass transport. In this dissertation I develop mathematical and numerical models that explicitly couple these effects, and I use the model to test hypotheses about the forces that drive upward groundwater flow near salt domes.

1.1 Groundwater flow near salt domes

The presence of upward groundwater flow near some salt domes has recently been inferred from sediment chemistry, groundwater chemistry, and estimates of in situ groundwater density [Hanor, 1987; Leger, 1988; Jensenius and Munksgaard, 1989]. Geochemical and geophysical evidence indicate that kilometer-scale convective circulation occurs in groundwaters next to some salt domes in southern Louisiana (Figure 1.1) [Hanor, 1987; Hanor and Workman, 1986]. The presence of these convection cells is inferred from the spatial distribution of dissolved fatty acids in groundwaters [Hanor and Workman, 1986] and groundwater density estimates based on salinities, temperatures, and pressures determined from electric logs [Bennett and Hanor, 1987; Hanor, 1987]. In the latter case Hanor [1987] was able to estimate the scale and sense of circulation from density estimates by invoking the Dupuit approximation of negligible vertical flow. This work reveals complex circulation patterns near some domes.
Figure 1.1  (a) General sense of groundwater motion and distribution of volatile fatty acids on the west flank of Iberia dome, southern Louisiana. Volatile fatty acids are used here as groundwater tracers [from Hanor and Workman, 1986]. (b) Salinity distribution and inferred flow direction near Welsh Salt Dome in southern Louisiana [after Bennett and Hanor, 1987]. The general flow direction is inferred from density calculations based on salinity and temperature estimates. The important feature of these flow patterns is the presence of upwelling adjacent to the salt. Such upward flow has also been inferred from geochemical data near salt domes in the North Sea [see Jensenius and Munksgaard, 1989].
Specifically, it appears that the sense of convection near some south Louisiana salt domes drives flow up along the salt flank (Figure 1.1). The upward flow is associated with advective transport of dissolved salt, which is manifested as salinity plumes extending above and laterally away from the top of some salt diapirs. The work of Hanor is corroborated to some degree by more recent studies (Figure 1.2) [Leger, 1988; Jensenius and Munksgaard, 1989], but observations and analysis such as those mentioned above are all too rare, and it is unclear whether the observations of Hanor [1987] represent typical or anomalous flow patterns near salt domes. Details of the flow patterns may be controlled by sand-shale distribution and the presence of local faults that commonly flank salt diapirs and serve as groundwater conduits [see Bennett and Hanor, 1987]. The mechanisms that drive convective circulation near these structures, however, remain unknown, although several possible mechanisms have been suggested. Upward groundwater flow near salt domes is a particularly surprising phenomena because of the expectation that groundwater near the dome will be salt-laden and dense, and therefore sink along the salt flank. Indeed, the mechanism that drives flow up along the salt is problematic because it must overcome the downward buoyancy forces produced by the salinity gradient. A variety of mechanisms may be responsible for driving groundwater circulation near salt domes. Several of these mechanisms are discussed below, and include expulsion of geopressured waters, preferential
Figure 1.2 Salinity contours and isotherms near Black Bayou dome in south Louisiana. Arrows indicate inferred direction of groundwater flow [after Leger, 1988].
dissolution near the top of domes, viscous drag from meteoric waters, and thermal effects related to the high thermal conductivity of salt. Each of these mechanisms is likely to be operative to varying degrees near different diapirs.

Upward flow of geopressured water along faults that penetrate the top of overpressured sediments may cause forced convection along the salt flank. Vertical discharge of geopressured waters has been inferred along growth faults in the Gulf of Mexico [Bodner and Sharp, 1988], as well as near salt domes in the North Sea [Jensenius and Munksgaard, 1988]. This mechanism was suggested by Bennett and Hanor [1987] based on observations at Welsh dome in southern Louisiana where mapped faults extend vertically from a localized salinity high at the dome crest to near the top of the geopressure zone. Recent numerical simulations of this type of forced convection remain inconclusive [Ranganathan, 1988], and point to many problems with modeling the release of geopressured water. Further calculations of forced convection are warranted but are not included in this study because of the need to consider simpler models first, and because there is presently a very poor understanding of the transport properties of faults.

Herbert et al. [1988] demonstrated that overturn of groundwater above a salt column can result from viscous drag induced by the flow of shallow meteoric water. This, however, is an inadequate explanation for observations near some domes [e.g., Bennett and Hanor, 1987] where the sense of
inferred circulation is inconsistent with the direction of regional groundwater discharge.

Salt tectonics may play an indirect but important role driving upward flow, particularly when coupled with preferential dissolution of salt at the dome crest. Preferential dissolution at the salt dome crest probably occurs at many salt domes in the Gulf of Mexico because the flanks of many domes are protected by shale sheaths [Atwood and Forman, 1959], and because salt dissolution is most active where the dome is subjected to the flow of meteoric groundwater [Bodenlos, 1970]. The presence of thick masses of cap rock is direct evidence of the importance of salt dissolution at the top of salt domes [Kyle and Price, 1986]. To test this idea it is necessary to use a model that accounts for the salt diapirism and basin subsidence.

Finally, thermally driven convection may provide a simple and plausible mechanism for driving upward groundwater flow near salt domes, provided the thermal effects are not overwhelmed by the salinity effects. Thermohaline convection also provides the simplest model that could be used to explain this phenomena because with any model it is necessary to couple the temperature, salinity, and groundwater flow fields explicitly. If this coupling alone explains the observations, then more complicated models are unnecessary. It is imperative, then, to know the conditions under which thermohaline convection is an important driving mechanism.
Consequently, this is the first model that I present in detail.

1.2 The Role of Numerical Models

As with many hydrogeologic problems there is a paucity of observational data presently available on groundwater flow near salt domes. Most of the information about groundwater flow near salt domes is inferred from groundwater chemistry or from salinity, temperature, and pressure estimates based on well logs [Hanor, 1987]. Inferences about paleohydrology are even more problematic and are generally made from diagenetic studies [e.g., Land, 1984; Jensenius and Munksgaard, 1988]. This being the case, theoretical calculations provide essential and otherwise unobtainable information about physical processes operative in the salt dome-groundwater system. Numerical simulations allow us to test given flow hypotheses as well as to suggest new models that can be tested with independent geochemical or geophysical data, i.e. numerical simulations can indicate what we should be looking for. Moreover numerical calculations provide one of the only means of unravelling and understanding the fundamental physical processes of very complex hydrogeologic systems. The application of numerical models to the study of hydrogeologic models has significant advantages as well as disadvantages. On the one hand we are solving mathematical equations that are known to be excellent predictors of heat and mass transport phenomena (viz. Darcy's
(these include Fick's law, Fourier's law, and Fick's law, and have been studied and tested for well over a century. Accurate solutions to these equations provide an excellent description of the processes of interest. On the other hand, these equations themselves require knowledge about physical parameters (such as permeability, thermal conductivity, and diffusivity) that vary greatly within a given geologic setting, and are often difficult to estimate accurately even when the geology is well known. Consequently there is a direct trade off that needs to be considered in numerically modeling hydrogeologic processes, especially when the modeling is for phenomenological purposes. That tradeoff is between the complexity that is incorporated into the model, and the ease with which the model results can be generalized. This tradeoff is represented schematically in Figure 1.3. When a model is quite simple, then analytical solutions are often available; results from such models are often very useful in trying to understand the basic physics of a particular problem because the model parameters are related in some explicit functional form. Examples of these simple models include linear stability analysis and boundary layer analysis, and are represented by the upper left corner of Figure 1.3. On the other hand we can construct very detailed numerical models that incorporate, for example, heterogeneous and anisotropic medium properties (such models would fall in the lower right corner of Figure 1.3). While such models could accurately predict the transport properties in a
Figure 1.3 A schematic diagram illustrating the tradeoff between the details that are incorporated into a model, and the ease with which model results are generalized. Analytical models would fall into the upper left corner, while detailed numerical models would fall into the lower right corner.
particular circumstances, they provide little insight to the general physical processes at work, and can not be used to make inferences about other hydrogeologic settings. A goal of the work presented herein is to develop mathematical and numerical models which strike a balance between these two extremes, that is to construct models and conduct numerical simulations that are simple enough to provide insight into the important physical processes at work, while being detailed enough to accurately represent the hydrogeology near salt domes.

1.3 Organization of this Dissertation

The following two chapters provide geologic and mathematical background material, respectively, for studying the hydrogeology of the salt dome environment. Chapter 2 is largely a review of geologic material relevant to studying the salt dome environment in the Gulf of Mexico. This includes a discussion of the role of salt in the geologic history of the Gulf as well as a discussion of salt tectonics and properties of rock salt. In Chapter 3 I derive the transport equations in considerable detail, starting with well accepted constitutive laws. In this derivation I introduce the mass stream function, which describes variable density groundwater flow in two dimensions. The mass stream function has several advantages over equations previously used to describe variable density flow, making it especially useful in modeling flow near salt domes.
Having established the general mathematical model for coupled flow near salt domes I provide, in Chapter 4, the details of the numerical representation of the mathematical model. The numerical model presented in Chapter 4 uses a volume-control finite difference technique to discretize the governing equations. Special consideration is given to discretization in cylindrical polar coordinates, and to resolving the nonlinearities inherent in the mathematical model.

The idea that thermohaline convection is responsible for driving upward flow near salt domes is investigated in Chapter 5. In this chapter I simplify the general mathematical model by using dimensional analysis. Dimensional analysis minimizes the number of parameters in the model, thereby providing insight into what conditions are especially important in controlling groundwater flow near salt domes. With dimensional analysis and numerical solutions to dimensionless equations, I am able to investigate the conditions that favor thermally driven upward flow near salt columns. These conditions are considered further in Chapter 6, in which I use simple analytical and numerical calculations to infer the geologic circumstances in which the conditions posited in Chapter 5 are likely to occur.

In Chapter 7 I use a more complicated numerical model to test the hypothesis that the salt dissolution at the top of domes, when combined with salt diapirism, can lead to
salinity conditions that favor upward groundwater flow. This model incorporates time-dependent solute transport, basin subsidence, and salt diapirism. While the results of numerical simulations presented in Chapter 7 indicate that diapirism will not generally produce conditions that lead to upward flow, they reveal several interesting properties of coupled flow near a dome undergoing active diapirism.

In Chapter 8 I summarize the results drawn from simulations in this dissertation. In addition Chapter 8 contains a brief discussion of the role that geopressure may play in controlling groundwater flow near salt domes.
CHAPTER 2

GEOLOGIC BACKGROUND

When diving into the mysteries of the creation of that part of the south-western world which was once comprehended in the limits of Louisiana, will not the geologist himself pause, absorbed in astonishment at the number of centuries which must have been necessary to form the delta of Mississippi? When he discovers successive strata of forests lying many fathoms deep on the top of each other; when he witnesses the exhumation of the fossil bones of mammoths, elephants, or huge animals of the antediluvian race; when he reads the hieroglyphic records of Nature's wonderful doings, left by herself on the very tablets of this country, will he not clasp his hands in ecstasy, and exclaim, "Oh! the dryness of my study has fled; there is poetry in the very foundation of this extraordinary land?"

Charles Gayarre', 1903
(From History of Louisiana)

In the bulk of this study I examine the forces that drive groundwater flow near salt structures, and how these driving mechanisms serve to influence heat and mass transport. This being the case, it is useful to consider idealized geometries and geologic conditions; only rarely will reference be made to specific salt structures. By stripping off the complexities of specific settings we can better assess the general mechanisms that are operative in controlling groundwater flow, and evaluate their importance. Armed with knowledge of which details will be especially important to model accurately, it will then be possible to introduce details of specific locales in future studies.

As with any scientific model, we want our numerical and mathematical transport models to explain a wide variety of
observations (e.g., flow phenomena at most salt domes) while retaining elements of simplicity and precision. In numerically modeling geologic phenomena, however, we are often forced to choose between precise results for specific settings, and simple models for idealized settings. In light of the objectives of this study and the present state of understanding of transport processes near salt domes it is prudent to emphasize simplicity.

Nonetheless, the inferences made from numerical studies are valuable only to the extent that we know what their geologic implications are. That is, we must be able to reconcile the idealized calculations with observations in natural (non-ideal) settings. Moreover, we must be able to see how the general conclusions of such a study would be influenced by the complexities of natural settings. Finally, simplifications and idealizations are only useful in as much as we know what they are idealizations of. For these reasons, the present chapter is devoted to discussing the tectonic and geologic development of salt dome environments in the Gulf of Mexico basin, as well as some properties of salt rock, and the evolution of salt dome structures.

2.1 Salt in the Gulf of Mexico Basin

The Gulf of Mexico Basin is one of the most important petroleum producing basins in the world. In this context, salt is one of the most important sedimentary rocks within the basin. Because of its economic importance, the Gulf of
Mexico has been studied extensively using a variety of geological and geophysical tools. It is somewhat surprising then, that many of the most basic questions about the geologic history of the Gulf of Mexico remain open or have been resolved only within the last few years. In particular, issues of the plate tectonic reconstructions, timing and nature of salt deposition, nature and source of some volcanics, the extent (or existence) of oceanic crust, and the cause of some basement highs remain some of the problems that are still under debate [cf., Pilger, 1981; Nunn et al., 1984; Buffler and Sawyer, 1985; Pindell, 1985; Byerly, 1989].

The presence of salt in the basin contributes to the confusion over the early history of the Gulf of Mexico. Determining the timing of the opening of the Gulf is confounded by the fact that salt is often the basal sedimentary layer. It is nearly impossible to date salt deposits directly; seismic interpretation of the deep basin is made difficult because the salt can introduce high acoustic impedance contrasts that make it difficult to penetrate with seismic energy; and the movement of salt introduces structural and stratigraphic complexities to the overlying sediments.

The geographic distribution of salt within the Gulf of Mexico Basin is generally divided into seven salt provinces [Figure 2.1; Antoine et al., 1974; Murray, 1961]. In the northern Gulf Coast three salt basins are entirely on shore and are sometimes referred to as the Interior Salt Basins;
Figure 2.1 A map of the Gulf of Mexico Basin showing the major salt provinces. E TX SB is the East Texas Salt Basin; N LA SB is the North Louisiana Salt Basin; MS SB is the Mississippi Salt Basin; ISTH SB is the Isthmian Salt Basin; and SDP stands for Salt Dome Province (modified from Antoine et al., [1974]).
these are the East Texas Salt Basin, the North Louisiana Salt Basin, and the Mississippi Salt Basin. The Gulf Coast Salt Basin consists of diapirs on and near shore in Louisiana, Texas, and Mississippi. The Offshore Salt Dome Province extends south into the basin to the Sigsbee Escarpment (Figure 2.1). The Campeche and Sigsbee Knolls in Mexico are salt structures to the west and north of the Yucatan peninsula, and the Isthmian Salt Basin is the onshore, southern extension of the Campeche salt.

In the following section I present a cursory overview of the tectonic and geologic development of the Gulf of Mexico in order to provide a general geologic framework for subsequent chapters.

2.1.1 Early History of the Gulf of Mexico Basin: Salt Deposition

The early opening of the Gulf of Mexico remains somewhat ambiguous and speculative, although a consistent model seems to have emerged in recent years [Pilger, 1981; Pindell, 1985; Salvador, 1987]. The reader is referred to these same references, and references contained within them, for a detailed and comprehensive discussion of the tectonic evolution of the Gulf.

The opening of the Gulf of Mexico Basin was initiated by the breakup of western Panagea from the Late Triassic to Early Jurassic. During this time South America began southerly movement away from the present day northern Gulf Coast. Continental crust was attenuated during extension,
creating topographic lows in which considerable thicknesses of non-marine sediments, predominantly red beds, accumulated [Buffler et al. 1980]. The extensional tectonics created grabens and rift basins that subsided during red bed deposition; consequently the red bed sequences are characterized by abrupt lateral changes in thickness. In the subsurface of the United States Gulf Coast, these red beds are known as the Eagle Mills Formation. Red bed deposition slowed but persisted through the Middle Jurassic during which time the bulk of the present-day Gulf of Mexico was emergent.

Continental attenuation continued through Late Middle Jurassic time causing the Gulf of Mexico to subside below sea level. As this occurred the region was periodically flooded with sea water. The source of the sea water (either from the Pacific or the incipient Atlantic) remains a topic of some discussion [e.g., see Schreiber and Hsu, 1980; Pindell, 1985; Salvador, 1987]. The Gulf of Mexico was largely isolated, and periodic flooding with sea water and subsequent evaporation lead to deposition of areally extensive salt beds. Today salt occurs in two separate masses, the Louann and Campeche salts, which were probably once continuous (Figure 2.2a). Deposition of salt matched subsidence rates, leading to very thick beds (locally 3000 to 4000 m) of nearly pure NaCl. During salt deposition, isolated regions on the northern edge of the Gulf of Mexico remain emergent or nearly so. Over these structures salt is
Figure 2.2  a) The paleogeography of the Gulf of Mexico Basin about 160Ma. Salt deposition was areally extensive and continuous across the basin. Isolated regions on the northern coast remained emergent; specifically the Sabine Uplift is apparent.  b) Late Jurassic paleogeography (about 150Ma) of the Gulf region. Sea floor spreading separates the once continuous salt into two components: the Louann and Campeche salts.  c) Early Cretaceous paleogeography of the Gulf of Mexico. By this time the present-day structural framework of the Gulf was established (modified from Pindell [1985]).
thin or absent. Anhydrite underlies the salt or is laterally equivalent to it elsewhere on the basin periphery. In the northern Gulf coast these are named the Warner anhydrite and they unconformably overlie the Eagle Mills red beds.

Bona fide sea floor spreading began in the Early to Middle-Late Jurassic time. This had two important geologic consequences: 1) it separated the Louann and Campeche salt provinces; and 2) it initiated open marine circulation by establishing a connection between the Gulf of Mexico and the Atlantic (Figure 2.2b). At this time salt deposition ceased and the salt was quickly covered with clastic and carbonate sediments.

2.1.2 Geologic Development Subsequent to Salt Deposition

The Louann salt on the northern edge of the Gulf of Mexico Basin is overlain by the Norphlet Formation. The Norphlet is a thin blanket of red-bed sandstones and conglomerates representing fluvial and eolian deposition. The time-span between cessation of salt deposition and the onset of Norphlet deposition was apparently quite short because the Norphlet protected the Louann from removal by dissolution and erosion [Salvador, 1987].

The Norphlet Formation is overlain by areally extensive carbonate units known as the Smackover Formation. The Smackover is usually divided into two units: the Lower Smackover and Upper Smackover. The Lower Smackover generally consists of dark carbonate muds, representing low energy
carbonate deposition. In contrast, the Upper Smackover represents deposition in a high-energy shallow-water environment, most likely on an extensive carbonate ramp. The Upper Smackover consists mainly of oolitic sands and packstones, and is an important reservoir rock for oil and gas in the northern Gulf. Salt movement in the East Texas Salt Basin and the North Louisiana Salt Basin was probably initiated during Smackover deposition [Jackson and Seni, 1983; Lobao and Pilger, 1985]; the thickness of Smackover in these areas was therefore controlled locally by salt tectonics.

At the end of Smackover deposition, sea level dropped or basin subsidence slowed, exposing much of the Smackover to meteoric conditions [Moore, 1983]. The updip sections of the Smackover were then unconformably overlain by the Haynesville Formation. Haynesville deposition occurred during a continual rise in sea level and gradual basin subsidence. In the East Texas Salt Basin, the earliest Haynesville deposits (the Buckner evaporites) are massive anhydrites deposited in a sabkha environment. As relative sea level continued to rise, more carbonate material was deposited, but the top of the Haynesville (Gilmer Shale) consists of deep water shale units. Farther eastward, in the North Louisiana Salt Basin, the Haynesville consists of mainly deep water carbonates [Moore, 1983]. Deep water deposition continued until the latest Jurassic, at which time massive nonmarine red bed sandstones were deposited on the northernmost edge of the
basin. Little is known about deposition in the more basinward sections of the Gulf of Mexico during this time [Salvador, 1987].

The structural and stratigraphic framework of the present-day Gulf of Mexico was essentially established by the end of the Jurassic.

Lower Cretaceous deposition is marked by three major transgressive-regressive events [MacFarlan, 1977]. Each of these events shifted the ancient shoreline as much as 100km. On the northwestern margin of the Gulf of Mexico there are three corresponding cycles of sedimentation. Each cycle is represented by paired deposition of terrigenous clastics and carbonate rocks which were deposited under conditions ranging from shallow subtidal to supratidal. Each cycle is separated from the next with an upper erosional surface. The lowermost cycle is the most widespread and consists of the Hosston and Sligo Formations. The Hosston Formation lies unconformably on paleozoic strata. It is a marginal-marine to marine unit. On the northwestern margin of the basin the Hosston is predominantly sandstone [Loucks, 1977], but in the North Louisiana Salt Basin it consists of shales and interbedded limestones [Herrmann, 1971]. The Sligo Formation is a marine limestone that was deposited on a broad shelf. The upper portion of the Sligo consists of reefs and grainstones [Bebout, 1977].

Similar transgressive-regressive depositional pairs of clastics and carbonates overlie the Sligo but are thinner and
not as areally extensive as the Hosston-Sligo. These units are known by a variety of stratigraphic names, but the Pearsall and Glen Rose Formations are most commonly used [Loucks, 1977].

Deposition of Lower Cretaceous carbonates extended from East Texas to the Florida Peninsula. Clastic input into the Florida platform was less significant than in the more westward regions of the Gulf Coast. The Florida platform was somewhat isolated from the rest of the Gulf by an extensive reef front that extended south from southern Mississippi to the northern coast of Cuba [Antoine et al., 1974].

By the end of the Early Cretaceous a regional uplift across the northern Gulf margin caused most of northern Louisiana, southern Arkansas, and northeastern Texas to become emergent. Many Lower Cretaceous deposits in these regions were subsequently removed by erosion. Contemporaneous with regional upwarping was igneous activity in the northernmost edges of the Gulf Coast, into Arkansas [Byerly, in press]. This uplift event (called the Mid-Cretaceous unconformity) initiated fluvial deposition of coarse clastics and volcanic detritus on the northern Gulf margin. The Woodbine Formation is the most widespread of these coarse clastics units; it is overlain by the Eagleford shales. In Alabama, the Tuscaloosa Formation is thought to be equivalent to the Woodbine and Eagleford [Livesey, personal communication].

Throughout the Cenozoic a prograding clastic wedge was
built out from the Cretaceous carbonate shelf. Deltas moved laterally across the shelf edge [Woodbury et al., 1973]. Delta shifts and subsidence caused local transgressions, but the clastic wedge moved steadily gulfward [Rainwater, 1964; Winker, 1982]. Figure 2.3 [from Winker, 1982] shows the generalized stratigraphy of the prograding wedge.

Timing of salt diapirism within the Gulf Coast Salt Basin of the northern Gulf Coast is poorly constrained due to the thickness of the section and a lack of public domain data. However, it appears that diapirism was initiated with the rapid influx of clastic sediments during the Tertiary [Woodbury et al., 1973]. This is consistent with the model of clastic deposition triggering diapirism in the interior salt basins [Seni and Jackson, 1983; Lobao and Pilger, 1985].

2.2 Evolution of Salt Structures

Understanding and accurately representing the geometry and tectonic history of salt structures, particularly those in the Gulf of Mexico Basin, are of critical importance in assessing coupled heat and mass transport in adjacent sediments. The geometry and physical properties of salt, as well as the timing and rate of salt movement determine model boundary conditions. The stratigraphy and structure of surrounding sediments affects the physical properties (such as porosity, permeability, and tortuosity) of the model medium. And salt movement affects our choice for steady-state or time-dependent models.
Figure 2.3 A stratigraphic column and Cenozoic depositional trends on the shelf margin in the northwest Gulf of Mexico Basin. The prograding wedge of clastic sediments is clearly evident (modified from Winker [1982]).
In the following two sub-sections I review salt mobility and the stages of salt diapirism as a framework for establishing how these factors generally impinge on the proposed models. These sections are applicable to both the Gulf of Mexico and Zechstein basins. Both are salt basins where salt mobility has been well studied because it has greatly impacted hydrocarbon accumulation.

2.2.1 Salt Mobility

Volumetrically salt is a minor sedimentary rock in the Gulf of Mexico and worldwide. Its unique rheologic, chemical and thermal properties, however, make it one of the most important sedimentary rocks. The rheologic properties of salt are unique because it assumes a ductile rheology at moderate temperatures and confining pressures, yet has negligible porosity. (Shales sometimes exhibit ductile behavior at similar temperatures and pressures as a result of high water content.) The ductility of salt is strongly dependent on temperature. Salt becomes plastic at temperatures of 200°C to 300°C in laboratory studies, but Kent [1979] notes evidence of salt mobility at considerably lower ambient temperatures in the Zechstein basin. Such discrepancies occur because salt rheology depends not only on temperature, but also on the amount of interstitial water, strain rate, and confining pressure. These effects remain poorly understood [Jenyon, 1986]. When plastic, salt rock can become mobilized to form salt diapirs, ridges, pillows,
or lenticular bodies. Salt movement greatly impacts the structure of the surrounding sediments, groundwater chemistry, and the thermal environment — all of which directly affect the groundwater flow field.

Most sediments, including sands, shales, and carbonates, compact with burial as a result of porosity loss. Consequently, the bulk density of sediments generally increases with burial depth. In contrast, the density of salt tends to remain nearly invariant with depth owing to its low porosity and high thermal expansivity. Figure 2.4 [from Dickinson, 1953] shows variations in shale density with depth for shale in the Louisiana Gulf Coast. Also shown is the nearly constant density of salt with depth. At a depth of about 1200m (4000 ft) shale density typically exceeds salt density. Thus if a salt bed is overlain by more than about 1200m of shale, a density inversion exists and the system is gravitationally unstable. When this situation occurs and the salt becomes mobilized, salt diapirs can form in accordance with Rayleigh-Taylor stability theory [see Turcotte and Schubert, 1982; Ramberg, 1981]. However, because the overburden has finite strength, gravitational instability alone is generally insufficient to initiate salt movement [Halbouty, 1967; Kent, 1979; Ramberg, 1981; Jenyon, 1986].

Salt movement in response to gravitational instability is generally referred to as halokinesis. The term halotectonics is used to refer to salt movement that arises from lateral differential stress [Trusheim, 1960]. Because a density
Figure 2.4 A plot of density versus depth for south Louisiana shales and salt. Below a depth of about 1200m the salt is less dense than compacted sediments and a gravitationally unstable condition exists (after Dickinson [1953]).
inversion alone is usually insufficient to mobilize salt, halotectonic effects are probably necessary to initiate salt flow. Halokinesis, however, might become dominant once diapirism begins.

It appears, then, that salt diapirism requires some mechanism for applying lateral stress to the salt layers. This is born out in both scaled laboratory experiments [Ramberg, 1981] and field studies [Halbouty, 1967; Kent, 1979]. Kent [1979] noted that salt forming the Hormuz salt plugs in Iran was not mobilized until the Cretaceous, even though gravitationally unstable conditions probably existed since the Cambrian. The halotectonic requirement for salt movement is seen even more clearly for North American salt basins, where there is a seemingly clear and simple correlation between geologically dynamic settings, and salt mobility [Halbouty, 1967; Jenyon, 1986]. Halbouty [1967] noted that many cratonic basins on North America (e.g. Michigan, Williston, Illinois) have abundant salt layers that have remained immobile throughout the histories of the basins. In contrast, salt layers deposited in continental margin settings are almost always mobilized.

In passive margin settings, such as the Gulf of Mexico, differential stress is applied to the salt layers by variations in sediment load [Humphris, 1978]. As a sediment wedge progrades into the basin salt flows from below the thick sediment wedge in the up dip region of the basin. Net salt migration is basinward, where sediment loading is less
Variations in the overburden thickness introduce lateral stresses that initiate salt flow. The mobilized salt develops ridges with adjacent lows that serve as sediment sinks where sediments accumulate to sufficient thicknesses to promote further diapirism by halokinesis. The Humphris [1978] model is shown diagramatically in Figure 2.5 and is supported by seismic surveys [Humphris, 1978; Jenyon, 1986]. This model appears to apply to other passive margin settings as well, including the Zechstein salts [Trusheim, 1960], the East Texas Salt Basin [Seni and Jackson, 1983], and the North Louisiana Salt Basin [Lobao and Pilger, 1985].

2.2.2 Stages of Diapirism

Some lateral stress in apparently required to initiate salt movement. Once initiated, however, both halotectonic and halokinetic effects can drive further salt flow. Occasionally salt diapirs form by forced intrusion through overlying sediments [Bishop, 1978]. More commonly they develop by a downbuilding process [Barton, 1933; Trusheim, 1960; Seni and Jackson, 1983] in which the top of salt remains static relative to the depositional surface, while the surrounding sediments and overburden subside due to continued deposition.

Salt is provided to the growing salt stock as salt structures develop by evacuating salt from the surrounding salt bed (Figure 2.6). Withdrawal of surrounding salt in turn creates concentric sinks that accumulate thick sequences of
Figure 2.5 A schematic representation of the initiation of salt growth on the continental shelf as a result of sediment loading (from Humphris [1978]).
Figure 2.6 A schematic representation of salt diapir growth and variations in surrounding strata; a) pillow stage, b) diapir stage, and c) post-diapir stage (modified from Trusheim [1960]).
sediments the weight of which contributes to further lateral stress differences and upward buoyant forces. In this way the growth of salt diapirs is coeval with development of adjacent stratigraphy.

Following Trusheim [1960] most studies of the evolution of salt diapirs have invoked a three-stage model in which the structure evolves from bedded salt. These stages are: 1) the pillow stage; 2) the diapir stage; and 3) the post-diapir stage (Figure 2.6). Trusheim [1960] originally applied the three-stage model to Zechstein salts in northern Germany, but subsequent studies indicate that three-stage growth is also quite typical in the northern Gulf of Mexico Basin [Seni and Jackson, 1983; Lobao and Pilger, 1985; Alam and Pilger, 1988]. It should be noted that detailed studies of diapir growth in the Gulf of Mexico have been limited to the interior salt basins due to the lack of public domain data in the more basinward sections. There is no reason to believe, however, that salt domes in the Tertiary section of the Gulf of Mexico experienced a structural evolution distinct from those in other passive margin settings.

2.2.3 Pillow Stage

"Salt pillows are ... concordant anticlinal or laccolithic salt structures with any amplitude/wavelength ratio" [Seni and Jackson, 1983]. In most cases development of pillow structures results from uneven sediment loading and variable rates of deposition on bedded salt [Bishop, 1978].
Present day salt pillows are easily identified by their distinct geometry (Figure 2.6a), while for more evolved structures, thinning of sediments over ancient pillow crests is indicative of sedimentation during this stage. Salt in the crest and flanks of the pillow is supplied by salt withdrawal from surrounding bedded salt, and salt withdrawal creates peripheral lows that accumulate thickened sequences of sediment (Figure 2.6a). These are alternatively called primary peripheral sinks, primary rim synclines, or primary peripheral basins. Because salt pillows can be fairly long wavelength structures, it is not uncommon for the axis of the primary peripheral basin to be tens of kilometers from the pillow crest [Seni and Jackson, 1983; Lobao, 1985]. Overlying sediments can thin dramatically (10-100%) from the peripheral basin over the pillow flank and crest, and sediments overlying the crest are often subjected to erosional removal. The eroded sediments are deposited in the rim syncline thereby accentuating the lateral stress imposed on the salt and promoting further salt movement. During pillow formation, overlying strata will be subject to extensional stress commonly leading to radial faults and fractures in sediments over the pillow crest (Figure 2.6a).

In fluvial-dominated environments, salt pillows serve to divert stream transport. Consequently the primary peripheral basins often contain more sand-rich sediments than do the thinned sediments over the dome crest. This is the case in the East Texas Salt Basin where crestal areas typically
contain 10-20% less sand than the primary peripheral basins [Seni and Jackson, 1983]. In shallow marine environments, the dome crests create bathometric highs on which small reefs can develop [Cantrell et al., 1959; Lobao, 1985]. In deeper marine settings, the bathometric highs created by salt pillows can winnow transported material so that the crestal areas are relatively sand-rich.

2.2.4 Diapir stage

During the diapir stage of salt dome evolution, the salt is mobilized into a cylindrical salt stock, and the salt pillow is deflated (Figure 2.6b). Mechanisms responsible for triggering the transition from salt pillow to diapir remain unclear [Jenyon, 1986], but the onset of diapirism is almost always associated with an increase in deposition rate within the peripheral basins, often with complete erosional removal of sediments from the salt crest [Trusheim, 1960; Seni and Jackson, 1983; Lobao and Pilger, 1985].

Salt diapirs are high amplitude, short wavelength structures relative to salt pillows. The synclinal peripheral basins that existed during the pillow stage is greatly modified by pillow deflation during diapirism. Specifically, the thin sediments deposited on the flanks and crest of the pillow collapse during deflation, while the overthickened sediments near the axis of the primary peripheral basin remain relatively unchanged (Figure 2.6c). The strata that occupied the primary peripheral basin thereby undergo a
structural reversal from synclines to anticlines, creating so-called turtle-structure anticlines [Trusheim, 1960; Seni and Jackson, 1983]. These structures can be effective petroleum traps. Strata that covered the crest and upper flanks of the pillow also undergo structural reversal from anticlines to synclines as a result of pillow deflation (Figure 2.6b). During pillow deflation and diapirism radial faults in the overburden will rotate toward the diapir axis; and commonly displacement across the faults will increase (Figure 2.6b).

The sediment sinks which flank salt diapirs are referred to as secondary peripheral sinks, secondary peripheral basins, or secondary rim synclines. These secondary basins contain thick accumulations of sediments that can be several times the thickness of equivalent units several kilometers from the diapir. Sediments are truncated abruptly at the salt, and the sedimentary record is often absent over the diapir crest as a result of erosion.

2.2.5 Post-diapir Stage

Some late-stage movement of salt often occurs subsequent to active diapirism. Salt movement often occurs as lateral flow near the top of the dome, creating salt overhangs (Figure 2.6c). The post-diapir stage represents the final stage of structural development of a salt dome. Most diapirs in the interior salt basins of the Gulf of Mexico (viz. the East Texas Salt Basin and the North Louisiana Salt Basin)
exhibit evidence for some post diapir movement [Seni and Jackson, 1983; Lobao and Pilger, 1985; Alam and Pilger, 1988].

During the post-diapir stage the crest of the salt dome typically remains at or near the sediment surface even though regional subsidence and deposition may continue. The relatively minor salt uplift during post-diapirism is usually associated with subsidence of surrounding sediments to create tertiary peripheral basins (or third-order rim synclines) (Figure 2.6c). Tertiary peripheral basins are often difficult to detect because of the disruptive effects of faulting and interference from effects of nearby salt structures. The lithostratigraphy of tertiary peripheral basins commonly mimics that of primary peripheral basins. Occasionally, growth faults will form in sediments of the tertiary peripheral basins.

2.2.6 Rates of Diapirism

Establishing growth rate of salt diapirs is one of the most difficult challenges in salt tectonics because sediment deposition rates can vary enormously and because a considerable volume of salt can be lost due to dissolution and surface extrusion. Moreover, estimates of growth rates are possible only when diapirism, occurs by downbuilding; it is virtually impossible to determine growth rates in the event of forced intrusion.

Ramberg [1981] estimated diapir growth rates from scaled
laboratory experiments. His results indicate that rates of diapirism on the order of 2000 m/Ma are likely, and he suggests greater rates are possible during some periods of diapirism.

The most detailed field study of diapir growth rates has been done by Seni and Jackson [1983] for the East Texas Salt Basin. Based on sediment deposition rates in the primary peripheral basin, they estimate net growth rates for salt pillows to be 100-130 m/Ma. Net rise rates during the diapir stage are estimated to be between 150 and 230 m/Ma. Similar diapir growth rates (300m/Ma) were estimated by Trusheim [1960] and Sanneman [1968] for salt Zechstein salt structures. Lobao and Pilger [1985] found very different rates for the pillow growth and diapir growth for salt domes in the North Louisiana Salt Basin. They have estimated diapir growth rates to be between 200 and 1000 m/Ma while pillow growth occurred at only about 75 to 100 m/Ma, in contrast to estimates for the East Texas Salt Basin.

Growth rates of salt structures is expected to be highly variable from one structure to the next, and even during the evolution of a single dome. Rates during all stages of evolution will be strongly affected by a variety of processes and constraints. Most important of these will be the degree and timing of faults, sediment deposition rate, the rheology of salt, salt dissolution, and the strength of the overburden. It is very possible that during diapirism, rates on the order of 1km/Ma are common [see Jenyon, 1986].
2.3 Implications for Groundwater Models

Several factors will combine to drive groundwater flow near salt structures. The most apparent of these will be: 1) flow of shallow meteoric groundwater; 2) salt dissolution; 3) thermal effects from highly conductive salt; and 4) influx of geopressured water either up faults, or through the geopressured sediments. All of these phenomena are strongly coupled to one another, and observational data alone are unlikely to reveal which driving mechanisms are operative or dominant. Many geologic processes, such as rate and timing of diapirism, geologic setting, thermal evolution of the basin, and diagenesis, will influence these driving mechanisms.

The structural and stratigraphic complexity within sediments surrounding salt domes will greatly affect the pathways for fluid flow. The presence of faults can serve to channel flow. Moreover the high variability of sand content within the peripheral basins will make the surrounding medium heterogeneous and anisotropic. Groundwater near salt domes will therefore flow through highly tortuous paths which not even the most detailed numerical model can be expected to accurately describe. Indeed, it will nearly always be the case that groundwater transport models are capable of incorporating considerably more detail than the limited observations warrant. By the same token, our current understanding of transport phenomena near salt domes also
does not warrant the use of particularly precise numerical models.

The goal of this study is to use theoretical and numerical models that simulate transport processes near salt structures in order to evaluate the importance and relative affects of the driving forces near salt domes. In so doing I will make some simplifying assumptions about the salt dome environment and its geologic development. I do so recognizing that the salt dome environment is among the most complex chemical, physical, and hydrodynamic modern environments that geologist and geophysicists are likely to encounter. But understanding the forces that drive fluid circulation in these environments is a critical step in determining their geologic, thermal, and chemical evolution.
CHAPTER 3

MATHEMATICAL DEVELOPMENT OF GOVERNING EQUATIONS

We have observed after much experience that if we want to do certain kinds of things with our concepts, our concepts had better be constructed in certain ways.

Percy Williams Bridgman, 1950
(From Reflections of a Physicist)

In this chapter I derive the transport equations that combine to describe the coupled processes of groundwater flow, dissolved salt advection and diffusion, and heat convection and conduction in a saturated porous medium. Although derivations of some of these equations appear elsewhere [e.g., Bear, 1972; Voss, 1984; Herbert et al., 1988], there remains some inconsistency in formulation. Moreover, the three transport fields are rarely developed together in a systematic way. The following presentation is required to set the notation and mathematical starting point for subsequent chapters. In addition, I derive and use equations for groundwater flow in terms of the mass stream function for variable density fluid, and this requires mathematical considerations that have not been presented previously. An attempt is made in this chapter to develop the governing equations in a complete and general form. The development and presentation of equations in subsequent chapters represent various simplifications of the equations derived forthwith. The specific assumptions used in those chapters are discussed in the appropriate places.
3.1 The Conservation and Constitutive Laws

3.1.1 A Stationary Medium

Three conservation equations and three constitutive flow laws are required to develop transport equations in a porous medium: conservation of fluid mass, conservation of solute mass, and conservation of energy; and Darcy's law, Fick's law, and Fourier's law. These equations are all directly coupled through terms involving groundwater velocity, density, and viscosity. The relevant mass and energy conservation equations are rigorously derived from the theory of mixtures [e.g., Green and Naghdi, 1969]. For the purposes of this presentation it suffices to accept them formally as follows.

Conservation of fluid mass is expressed in general as

\[ \frac{\partial (\phi \rho)}{\partial t} + \nabla \cdot (\rho q) = Q_f \]  (3.1)

where \( q \) is the Darcy flux, \( \phi \) is porosity, \( \rho = \rho(C,T,p) \) is pore water density, and \( Q_f \) represents an internal source of porewater. Conservation of solute of concentration \( C \) in groundwater is given by

\[ \frac{\partial (\phi \rho C)}{\partial t} + \nabla \cdot (\phi J_C) = Q_C \]  (3.2)

where \( J_C \) is the total mass flux of solute, \( Q_C \) is a source term describing the amount of solute contributed to (\( Q_C > 0 \)) or removed from (\( Q_C < 0 \)) groundwater, for example, by chemical
reactions. Equations (3.1) and (3.2) state that the net flux, or divergence, of mass into an elemental volume of a porous medium plus net internal production equals the rate of accumulation of mass within that volume.

Similarly, heat conservation states that the net flux of heat into an elemental volume plus the net heat production equals the time rate of accumulation of heat within the volume. That is,

\[
\frac{\partial (\rho_m c_m T)}{\partial t} + \nabla \cdot (\phi J_H) = \rho_m Q_H \tag{3.3}
\]

where \( T \) is temperature, \( c \) is the specific heat, \( J_H \) is energy flux, and \( Q_H \) represents an internal heat source. The subscript \( m \) is used to indicate that a certain property applies to the saturated porous medium, for example \( \rho_m \) is the density of the saturated sediments, while \( \rho \) is fluid density. This introduces an important distinction between the heat and mass balance equations which is required because the matrix and fluid are treated as a single phase with respect to heat conservation, but as separate phases with respect to mass conservation. The density of the saturated medium is assumed to be an average of the density of fluid and solid grains:

\[
\rho_m = \phi \rho + (1-\phi) \rho_s \tag{3.4}
\]

The full transport equations combine these conservation laws with the constitutive laws that provide the link between fluid velocity, mass flux, and heat flux, and the intensive,
measurable quantities of pressure, concentration, and temperature. Darcy's law provides a relation between groundwater velocity and pore pressure (or hydraulic head). The generalized form of Darcy's law is

$$\mathbf{q} = \frac{k}{\mu} \cdot (\nabla p - \rho g)$$  \hspace{1cm} (3.5)

where $\mathbf{q}$ is specific discharge (Darcy flux), $\mu$ is the dynamic viscosity of groundwater, $k$ is a tensor describing the intrinsic permeability of the medium, $p$ is pore pressure, and $g$ is the acceleration due to gravity.

Fick's first law provides the needed relation between solute flux and concentration. In a generalized form it is written to include advective as well as diffusive flux of solute:

$$\mathbf{J}_C = \rho v \mathbf{c} - \rho \mathbf{D} \cdot \nabla \mathbf{c}$$  \hspace{1cm} (3.6)

where $\mathbf{v} = \mathbf{q}/\phi$ is the average linear velocity of groundwater through pore spaces, $\mathbf{J}_C$ is total solute flux relative to the solid grains of the sediment, $\mathbf{c}$ is solute concentration in weight percent, and $\mathbf{D}$ is the hydrodynamic dispersion tensor. Each term in equation (3.6) has dimension $[\text{ML}^2\text{t}^{-1}]$. Substituting solute flux in (3.6) into the solute balance equation (3.2), gives

$$\frac{\partial (\rho \phi \mathbf{c})}{\partial t} + \nabla \cdot (\rho \phi \mathbf{v} \mathbf{c} - \rho \phi \mathbf{D} \cdot \nabla \mathbf{c}) = \phi Q_C$$  \hspace{1cm} (3.7)

or, by applying the product rule and separating terms,
But the term in brackets equates to $Q_f$ by equation (3.1), leading to

$$\nabla \cdot (\rho \phi D \cdot \nabla C) - \rho \phi \nabla \cdot \nabla C = \rho \phi \frac{\partial C}{\partial t} + \phi Q_C + C^* Q_f$$  \hspace{1cm} (3.9)$$

where $C^* Q_f$ accounts for the fact that a fluid source may also be a solute source; $C^*$ refers to the solute concentration in the fluid source.

For energy transport Fourier's law relates heat flux to temperature, and is

$$J_H = \rho c_f q T - K \cdot \nabla T$$ \hspace{1cm} (3.10)$$

Here $J_H$ is the total heat flux relative to the solid grains of the medium, and $K$ is the thermal conductivity tensor for the saturated medium. Substituting this into the heat conservation relation given in equation (3.3) gives

$$\frac{\partial (\rho m c_m T)}{\partial t} + \nabla \cdot (\rho c_f q T - K \cdot \nabla T) = \rho m Q_H$$ \hspace{1cm} (3.11)$$

or

$$\frac{\partial (\rho m c_m T)}{\partial t} + \rho q \cdot \nabla (c_f T) + c_f T \nabla \cdot (\rho q) - \nabla \cdot (K \cdot \nabla T) = \rho m Q_H$$ \hspace{1cm} (3.12)$$

But assuming the volumetric heat capacity is an average of that for the fluid and solid grains (i.e. $\rho m c_m = \phi \rho c_f + (1 - \phi) \rho_s c_s$) and that the properties of the solid particles do not
change with time, and by applying fluid mass conservation from equation (3.1), (3.12) reduces to a general second order equation of temperature:

$$\nabla \cdot (K \cdot \nabla T) - \rho q \cdot \nabla (c_f T) = \rho m c_m \frac{\partial T}{\partial t} - T \rho_s c_s \frac{\partial \phi}{\partial t} - \rho_m Q_H + c_f T^* Q_f \quad (3.13)$$

The first term in equation (3.13) describes heat transfer by conduction and the second term describes advective transport of heat by groundwater flow. The first term on the right-hand-side quantifies the accumulation of heat within the saturated medium; the second term represents the loss or gain of heat as the result of changes in porosity; the third term on the right-hand-side represents a heat source in the saturated medium. The last term accounts for the fact that a fluid source can also be a heat source; here $T^*$ is the temperature of the fluid source.

Thus the coupled equations for groundwater flow, solute transport and heat transport in a stationary porous medium are

$$\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho q) = Q_f \quad (3.1)$$

$$q = \frac{k}{\mu} (\nabla p - \rho g) \quad (3.5)$$

$$\nabla \cdot (\rho \phi \mathbf{v} \cdot \nabla c) - \rho \phi \mathbf{v} \cdot \nabla c = \rho \phi \frac{\partial c}{\partial t} + \phi Q_c + C^* Q_f \quad (3.9)$$
\[
\n\n\text{These equations are quite general and describe mass and heat transport relative to the solid grains of the medium. They account for temporal and spatial variations in porosity and permeability, provided the pore space is occluded or enlarged without deforming the medium (e.g., by precipitation or dissolution reactions). They are coupled equations and are written in terms of three unknown variable fields: pressure, concentration, and temperature.}

\text{In addition, the porosity field may also be unknown. If this is the case then an additional condition on porosity is required in order for the problem to be well posed. Because permeability is porosity-dependent, an additional constitutive law specifying this relation would be needed as well.}

\text{3.1.2 A Deforming Medium}

\text{In much of this study I will be interested in evaluating fluid flow, heat and dissolved salt transport during the structural evolution of salt domes. Because most salt domes in the northern Gulf of Mexico evolve through the process of downbuilding (Chapter 2), it is necessary to incorporate basin subsidence directly into the mathematical and numerical models.}

\text{In a moving medium, such as a subsiding sedimentary basin, the mass and energy transported into and out of an elemental}
volume will also depend on the rate of basin subsidence \( V \), and the conservation laws (equations (3.1), (3.2), and (3.3)) must account for this [Cooper, 1966; Bear, 1972; Turcotte and Schubert, 1982]. The appropriate conservation laws, equations (3.1), (3.2), and (3.3), are therefore modified to give conservation of fluid mass,

\[
\nabla \cdot (\rho q^T) = \nabla \cdot (\rho q + \phi V) = -\frac{\partial (\rho \phi)}{\partial t}
\]

(3.14)

conservation of solute mass

\[
\nabla \cdot (\phi J^T_C) = \nabla \cdot (\phi J_C + \phi \rho CV) = -\frac{\partial (\rho \phi C)}{\partial t} \quad (3.15)
\]

and conservation of heat energy

\[
\nabla \cdot (\phi J^T_H) = \nabla \cdot (J_H + \rho m c_m^T V) = -\frac{\partial (\rho m c_m^T)}{\partial t} \quad (3.16)
\]

where the superscript \( T \) indicates flux is measured with respect to fixed spatial coordinates independent of the framework of the porous medium.

In most cases where modeling of groundwater flow is applied to investigate the thermal or chemical evolution of sedimentary basins, it is found that the temporal dependence of temperature and groundwater motion can be neglected, and the steady-state forms of (3.14) and (3.16) are sufficient [e.g., Smith and Chapman, 1983, 1985; Garven and Freeze, 1984; Garven, 1989]. Justification for neglecting the time derivatives in the heat and groundwater equations is
discussed in the references cited, and is discussed further in subsequent chapters of this dissertation. The essence of the argument is that heat and groundwater flow reach steady-state quickly relative to the geologic processes being investigated. In contrast, it is often necessary to explicitly include the temporal variations in solute concentration because dissipation of spatial variations in solute concentration can be relatively inefficient through sediments. Moreover, for the applications in this study it is possible to neglect source terms. The assumptions that serve as the basis for neglecting source terms are: 1) that there is negligible heat production within the sediment column; 2) that there are no solute sources other than those specified through boundary conditions; and 3) that there are no fluid sources within the sediment column (since I will not be considering the presence of geopressed fluids). Except where noted, then, I will use the steady-state form of (3.17) and (3.18) without sources, i.e.

\[ \nabla \cdot (\rho q^T) = \nabla \cdot (\rho q) = 0 \]  
(3.17)

\[ \nabla \cdot (\phi J_c^T) = \nabla \cdot (\phi J_c + \phi v) = - \frac{\partial (\rho \phi c)}{\partial t} \]  
(3.15)

\[ \nabla \cdot (\phi J_H^T) = \nabla \cdot (J_H) = 0 \]  
(3.18)

Equations (3.15), (3.17) and (3.18) can be combined with equations (3.5), (3.6), and (3.10) to describe pressure,
temperature, and dissolved salt concentration in a subsiding sedimentary basin in which steady-state conditions can be assumed for pore fluid flow and heat transport. Numerical experiments presented later indicate that such conditions are applicable to the salt dome environment. Equations (3.6) and (3.10) can be substituted directly into (3.15) and (3.18), as before, to give second order equations for salinity and temperature:

\[
\nabla \cdot [\rho \phi D \nabla C] - \nabla \cdot [\rho \phi (\mathbf{v} + \mathbf{v}) C] = - \frac{\partial (\rho \phi C)}{\partial t} \quad (3.19)
\]

\[
\nabla \cdot [\kappa \nabla T] - \nabla \cdot [\rho c q T] = 0 \quad (3.20)
\]

The groundwater flow equation can be formulated in several ways. Darcy's law (3.5) can be substituted directly into (3.17) to yield an equation in terms of pressure [Voss, 1984]; Darcy's law can be written in terms of equivalent freshwater head, \( h \), by introducing the change of variables \( h = p_0 + \rho - \rho g z \), and then substituted into (3.15), giving a second order equation in terms of \( h \) [Bear, 1972; Graven and Freeze, 1984]. Alternatively, equations (3.15) and (3.5) can be combined through the use of the stream function. For reasons discussed below, the stream function is preferred for the problems considered in this study.
3.2 The Stream Function for Variable Density Fluid

The stream function is a scalar description of the groundwater velocity field such that contours of the stream function represent the paths that fluid packages follow during flow. The difference in the values of the stream function at any two points is a measure of the total flux of fluid across any surface through those points and normal to the plane of view. Use of the stream function as defined in equation (3.21) is of considerable historical and practical importance in hydrogeology. Early solutions to many two-dimensional groundwater flow problems were nearly always achieved through the use of the stream function [e.g. Slichter, 1897]. Even today the stream function provides a useful tool for analytical solutions to many practical groundwater flow problems [see Polubarinova-Kochina, 1962].

The importance of the stream function has stemmed from its application to iso-density flow problems in which hydraulic head is a potential function that completely describes the flow system in which equipotentials are everywhere normal to flow lines. In these circumstances (i.e., for potential flow) the stream function and hydraulic head satisfy the Cauchy-Riemann conditions, thereby lending themselves to solutions using the techniques of complex analysis.

In cases of variable density groundwater, flow is not described by a potential function. However, this does not preclude the use of the stream function as a convenient tool for representing the flow field. Classic papers by Yih
[1961] and de Josselin de Jong [1969] provide notable applications to the flow of inhomogeneous groundwater. In these cases the stream function provides a useful mathematical tool as well as a practical way to visualize flow, and it relates the flow directly to vorticity, which arises from lateral density variations [de Josselin de Jong, 1969].

Nearly all applications of the stream function to groundwater studies have used the stream function as it has been developed historically. In these cases the stream function is related to the velocity field by the well known relations

\[ q_x = -\frac{\partial \psi}{\partial y}, \quad q_y = \frac{\partial \psi}{\partial x} \]  

(e.g., Slichter, 1897; Bear, 1972; and many others). These equations implicitly assume that the fluid continuity equation (equation (3.17)) takes the form

\[ \nabla \cdot \mathbf{q} = 0 \]  

at steady-state. Equation (3.22) represents the condition of volume conservation, as opposed to mass conservation given by (3.17). The omission of the density term in the continuity equation is commonly known as the Boussinesq approximation and is applicable to many groundwater flow problems in which density is only weakly dependent on temperature and solute concentration. The more general form of the continuity
equation is given in (3.17) and should be used in groundwater problems for which significant density gradients can arise, such as near salt domes. Recently it has been the practice to use the more general continuity equation for coupled groundwater-heat transport problems solved on a regional scale [e.g., Smith and Chapman, 1983, 1985; Garven and Freeze, 1984; Garven, 1989].

Although the use of the stream function has several advantages in solving coupled flow problems, it has not been adapted prior to this study for the more general continuity condition. Such a formulation is presented in this section. The aim is to combine the continuity equation and Darcy's law (equations (3.15) and (3.5), respectively) to arrive at a single second-order differential equation that describes groundwater flow.

3.2.1 Cartesian Coordinates

The stream function is defined as being everywhere tangent to the direction of specific discharge [Bear, 1972; de Josselin de Jong, 1969]. That is,

\[ \mathbf{q} \times d\mathbf{r} = 0 \]  

(3.23)

where \( d\mathbf{r} \) is an element of an arc along the stream function.

For two-dimensional flow in Cartesian coordinates, this leads to

\[ \frac{dx}{q_x} = \frac{dy}{q_y} \]  

(3.24)
or,

\[ q_y dx - q_x dy = 0 \]  \hspace{1cm} (3.25)

This equation can be made into an exact differential by multiplying through by density, which becomes an integrating factor:

\[ \rho q_y dx - \rho q_x dy = 0 \]  \hspace{1cm} (3.26)

which is exact because

\[ \frac{\partial (\rho q_y)}{\partial y} = -\frac{\partial (\rho q_x)}{\partial x} \]  \hspace{1cm} (3.27)

by the continuity equation (3.17). Equation (3.26) is solved by writing

\[ \rho q_y dx - \rho q_x dy = d\Psi \]  \hspace{1cm} (3.28)

which has the immediate solution

\[ q_x = \frac{1}{\rho} \frac{\partial \Psi}{\partial y} ; \hspace{0.5cm} q_y = \frac{1}{\rho} \frac{\partial \Psi}{\partial x} \]  \hspace{1cm} (3.29)

in contrast to (3.21). Henceforth references to the stream function, \( \Psi \), are intended to indicate the stream function developed in equation (3.29), which I will also call the mass stream function.

From equations (3.26) through (3.29) it is established that by writing specific discharge, \( q \), in terms of the mass-stream function the continuity equation is satisfied without invoking the Boussinesq assumption. Next I will rewrite
Darcy's law (3.5) to take advantage of this fact, and thereby derive a flow equation in terms of $\Psi$.

Writing the gradients in Darcy's law in two-dimensional Cartesian coordinates gives

$$\rho q_x = -\frac{k_{xx}}{v} \frac{\partial p}{\partial x} = \frac{\partial \Psi}{\partial y}$$  \hspace{2cm} (3.30)

$$\rho q_y = -\frac{k_{yy}}{v} \left[ \frac{\partial p}{\partial y} + \rho g \right] = \frac{\partial \Psi}{\partial x}$$  \hspace{2cm} (3.31)

where $v=\mu/\rho$ represents the kinematic viscosity of groundwater. Isolating the pressure terms and differentiating both sides of (3.30) with respect to $y$ and both sides of (3.31) with respect to $x$ gives

$$\frac{\partial^2 p}{\partial x \partial y} = \frac{\partial}{\partial y} \left[ \frac{v}{k_{xx}} \frac{\partial \Psi}{\partial y} \right]$$  \hspace{2cm} (3.32)

$$\frac{\partial^2 p}{\partial x \partial y} = \frac{\partial}{\partial y} \left[ \frac{v}{k_{yy}} \frac{\partial \Psi}{\partial x} \right] + \frac{\partial p}{\partial x}$$  \hspace{2cm} (3.33)

Subtracting (3.33) from (3.32) gives a second order equation in terms of $\Psi$:

$$\frac{\partial}{\partial x} \left( \frac{v}{k_{yy}} \frac{\partial \Psi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{v}{k_{xx}} \frac{\partial \Psi}{\partial y} \right) = -\frac{\partial p}{\partial x}$$  \hspace{2cm} (3.34)

which will be solved to determine the groundwater flow field for variable density fluid. Once a solution in terms of $\Psi$ is achieved, the components of the specific discharge vector at any point are calculated from (3.29).
3.2.2 Cylindrical Polar Coordinates

In two dimensional cylindrical polar coordinates \((r, \theta, y)\) with no variation in the azimuthal coordinate \(\theta\), the stream function takes a slightly different form and is usually called the Stokes stream function [Bear, 1972]. A second integrating factor of \((1/r)\) is introduced in order to make the continuity equation exact in this coordinate system. That is,

\[
\rho q_r = -\frac{1}{r} \frac{\partial \psi}{\partial y} \quad \rho q_y = \frac{1}{r} \frac{\partial \psi}{\partial r}
\]  

(3.35)

Equations analogous to (3.30) and (3.31) are

\[
\rho q_r = -\frac{k_{rr}}{v} \frac{\partial \rho}{\partial r} = -\frac{1}{r} \frac{\partial \psi}{\partial y}
\]  

(3.36)

\[
\rho q_y = -\frac{k_{yy}}{v} \left[ \frac{\partial \rho}{\partial y} + \rho g \right] = \frac{1}{r} \frac{\partial \psi}{\partial r}
\]  

(3.37)

leading to the flow equation

\[
\frac{\partial}{\partial r} \left( \frac{v}{k_{yy} r} \frac{\partial \psi}{\partial r} \right) + \frac{\partial}{\partial y} \left( \frac{v}{k_{rr} y} \frac{\partial \psi}{\partial y} \right) = -g \frac{\partial \rho}{\partial r}
\]  

(3.38)

3.2.3 Advantages of the Stream Function Formulation

It is now appropriate to mention some of the benefits of using the mass-stream function formulation to calculate the flow field.

(1) A contour of \(\psi\) represents the path along which a package of fluid flows. Consequently the stream function
representation provides an unambiguous picture of the flow field that can be difficult to interpret from discrete velocity arrows. Fluid velocities are proportional to the contour spacing, so the relative magnitude of fluid velocities can also be inferred from a plot of the stream function.

(2) Any solution of the flow field in terms of $\Psi$ guarantees conservation of fluid mass. Numerically, this is perhaps the best reason for using the present formulation. This means that even if the calculated flow field is wrong, or more likely, has not reached numerical convergence, it does conserve mass. This is an especially important consideration for models that couple solute or heat transport to the flow field because the iterative nature of solution techniques presumes that intermediate solutions of the flow field will be incorrect. An assurance of mass conservation makes it likely that intermediate solutions will be physically reasonable and thus promotes convergence. If the calculated flow field fails to conserve mass, errors are easily compounded, leading to divergence.

Surprisingly some commonly-used models do not guarantee mass conservation. In fluid pressure or equivalent fresh water head formulations of the flow equation, great care must be taken in the numerical solutions. Most second-order (central difference) discretization of the pressure or head equations implicitly lead to numerical continuity at alternating nodes, not adjacent ones. This leads to wavy
pressure contours in space. Needless to say, such pressure fields play havoc on calculations of the flow velocities.

(3) Boundary conditions for the stream function are often trivial to specify. In fact, for cases of free convection, boundary conditions vanish.

(4) Velocities are easy to calculate from the stream function (equations (3.29) and (3.35)) and, more importantly, remain consistent from node to node. Velocity calculations are typically very difficult and inaccurate with density-dependent flow even when the pressure or head has been accurately calculated [Yeh, 1981; Voss, 1984]. This problem is eliminated with the stream function formulation.

(5) Solutions of the flow field in terms of the stream function tend to converge more rapidly and be more stable numerically than similar calculations for pressure or head. This is because the total variation in values of \( \Psi \) is small relative to variations in pressure, which can easily range over several orders of magnitude in a single simulation.

3.3 Discussion and Summary

The hydrodynamic complexities of groundwater near salt domes was mentioned in the preceding chapters and is reflected in the mathematical formulation of the transport equations. The groundwater flow equation is directly coupled to the heat and salt transport equations through the Darcy velocity which determines the advective components of heat and salt transport. By the same token the heat and salt
transport equations feedback into the flow equation because they directly affect groundwater density and viscosity. Viscosity variations will alter the hydraulic conductivity and therefore the magnitude of the Darcy velocity. Density effects will be particularly important since density variations produce driving forces or vorticity [de Josselin de Jong, 1969]. A discussion on the actual way that density and viscosity vary with temperature and salinity (and pressure) is postponed until the next chapter.

Density variations in groundwater near salt domes can be quite large owing to the presence of large salinity and temperature gradients. There has been some discussion recently in the literature about the applicability of Darcy's law and Fick's law to problems of brine transport, particularly near salt domes [Hassanizadeh, 1986; Hassanizadeh and Leijnse, 1988]. In as much as these equations were derived originally from experiments with fresh water and dilute solutions, respectively, Hassanizadeh [1988] challenges their use in solutions approaching NaCl saturation and he derives modified constitutive laws for such circumstances [Hassanizadeh, 1986]. There is however, not yet any experimental or field evidence to indicate that the more complex formulation is warranted. Moreover, the more general formulation [Hassanizadeh, 1986] introduces additional physical constants describing medium and fluid properties. Because first-order properties such as permeability and porosity are poorly constrained for most
groundwater models, incorporating additional second-order terms seems imprudent at this time.

Similarly the development presented above neglects temperature-salinity cross diffusion terms. It is well known experimentally that solute flux is weakly dependent on the temperature gradient, as is heat flux on the salinity gradient. Such effects are known as Soret diffusion and Dufour diffusion, respectively. To incorporate these effects into the present model, additive terms of the form $A_S \nabla T$ and $A_D \nabla C$ would need to be included in equations (3.6) and (3.10), respectively [Domenico, 1977]. $A_S$ and $A_D$ are called the Soret and Dufour constants, and little experimental data are presently available for their values [see Lerman, 1979]; in groundwater problems, however, the Soret and Dufour terms are typically two or three orders of magnitude smaller than the terms presented in (3.6) and (3.10) [Domenico, 1977], and their omission is well justified.

In developing the heat and salt transport equations above I assumed no particular coordinate system, but left the equations in general form by using the gradient operator ($\nabla$). In contrast both Cartesian and cylindrical coordinates were considered in developing the stream function because the use of the stream function (as presented) assumes two-dimensional flow. By way of summary, I will rewrite the transport equations below to show the components of the divergence operation in both Cartesian and cylindrical coordinates. The
Transport equations as they appear below are used in subsequent chapters.

In a stationary medium, when heat and groundwater flow are well approximated by steady-state conditions, and when salinity is time-dependent, equations (3.11) (with $V=0$), (3.12) and (3.34) yield the following transport equations.

In two-dimensional Cartesian coordinates groundwater flow is described by

$$\frac{\partial}{\partial x}(v \frac{\partial \psi}{\partial x}) + \frac{\partial}{\partial y}(v \frac{\partial \psi}{\partial y}) = -g \frac{\partial \rho}{\partial x} \tag{3.34}$$

heat transport by

$$\frac{\partial}{\partial x}(k_{yy} \frac{\partial^2 T}{\partial x^2}) + \frac{\partial}{\partial y}(k_{xx} \frac{\partial^2 T}{\partial y^2}) - \frac{\partial}{\partial x}(\rho c q_x T) - \frac{\partial}{\partial y}(\rho c q_y T) = 0 \tag{3.39}$$

and solute transport by

$$\frac{\partial}{\partial x}(\rho \phi D_{xx} \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y}(\rho \phi D_{yy} \frac{\partial c}{\partial y}) - \frac{\partial}{\partial x}(\rho q_x c) - \frac{\partial}{\partial y}(\rho q_y c) = \frac{\partial (\rho \phi c)}{\partial t} \tag{3.40}$$

In cylindrical polar coordinates analogous equations are:

for groundwater flow

$$\frac{\partial}{\partial r}\left(v \frac{\partial \psi}{\partial r}\right) + \frac{\partial}{\partial \theta}\left(v \frac{\partial \psi}{\partial \theta}\right) = -g \frac{\partial \rho}{\partial r} \tag{3.38}$$

for heat transport

$$\frac{1}{r} \frac{\partial}{\partial r}(r K \frac{\partial T}{\partial r}) + \frac{\partial}{\partial \theta}(K \frac{\partial T}{\partial \theta}) - \frac{1}{r} \frac{\partial}{\partial r}(r \rho c q_r T) - \frac{\partial}{\partial \theta}(\rho c q_y T) = 0 \tag{3.41}$$

and for solute transport
To arrive at these equations the following assumptions and approximations were made: flow is well represented in two-dimensions; groundwater flow and heat transport are well approximated by steady-state conditions; Darcy's law, Fick's law, and Fourier's law are all applicable, and cross-diffusion terms are negligible; thermal conductivity is a scalar; off-diagonal terms in the permeability and hydrodynamic dispersion tensors are negligible; and the medium is non-deforming.

For a subsiding medium in which all other assumptions hold, equations (3.40) and (3.42) have additional advective terms that include the subsidence velocity, \( V \), (equation (3.15)). When subsidence is vertical these equations give, respectively,

\[
\frac{1}{r} \frac{\partial}{\partial r} (r \phi \frac{\partial C}{\partial r}) + \frac{\partial}{\partial y} (\rho \phi \frac{\partial C}{\partial y}) - \frac{1}{r} \frac{\partial}{\partial r} (r \rho q_r C) - \frac{\partial}{\partial y} (\rho q_y C) = \frac{\partial (\rho \phi C)}{\partial t}
\]

(3.42)

\[
\frac{\partial}{\partial x} (\rho \phi \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} (\rho \phi \frac{\partial C}{\partial y}) - \frac{\partial}{\partial x} [(\rho q_x + \rho \phi V) C] = \frac{\partial (\rho \phi C)}{\partial t}
\]

(3.43)

and

\[
\frac{1}{r} \frac{\partial}{\partial r} (r \phi \frac{\partial C}{\partial r}) + \frac{\partial}{\partial y} (\rho \phi \frac{\partial C}{\partial y}) - \frac{1}{r} \frac{\partial}{\partial r} (r \rho q_r C) - \frac{\partial}{\partial y} [(\rho q_y + \rho \phi V) C] = \frac{\partial (\rho \phi C)}{\partial t}
\]

(3.44)
Having now established the appropriate governing equations for coupled heat, solute, and groundwater transport, we are faced with the task of attempting to solve them for initial and boundary conditions that are reasonable representations of the salt dome environment. The governing equations are non-linear because they are strongly coupled by density, and specific discharge; care must be taken in order to achieve numerical solutions to these equations that accurately describe the physics of coupled transport near salt domes.
The governing equations presented in the previous chapter are strongly coupled and nonlinear. Consequently it would be unreasonable to expect analytical solutions to exist except in the simplest cases. Simplified problems for which considerable theoretical work has been done include linear stability analysis [Nield, 1968; Tauton et al., 1972; Knobloch, 1986] and boundary layer analysis [Bejan and Khair, 1985; Yucel, 1989]. Even in these problems some computational work is required in order to evaluate the results accurately. In more general problems, such as those that are geologically meaningful, numerical procedures are required in order to solve the differential equations for a given set of complex boundary and initial conditions.

The goal of any numerical model is to map the continuous differential equations (as well as the boundary and initial conditions) onto discrete points in the region of interest, and then solve algebraic equations for values of those variables at the discrete points. Most commonly this is achieved using either finite difference or finite element techniques. For this dissertation I have discretized the governing equations using a control volume finite difference
method [Patankar, 1980]. The finite difference method is preferred because it is relatively easy to implement; it lends itself to efficient solution techniques and code vectorization; it tends to deal with problems involving strong convection more forgivingly than does the finite element method; it is simple and efficient to switch between Cartesian and cylindrical coordinate systems; and finally, it is more intuitive than the finite element method. For most applications, the finite element method has a "veil of mystery about it" [Patankar, 1980].

In this chapter I present a finite difference discretization that is used to solve the transport equations presented in Chapter 3 for coupled flow near salt domes. In this presentation I have chosen to formulate the discrete equations in cylindrical coordinates (i.e., equations (3.38), (3.41), and (3.44)) because this is the geometry relevant to salt dome simulations. The formulations for Cartesian coordinates is a simplified form of what is presented below, and a summary of the discretization for Cartesian coordinates is presented later in a table. Because the control volume finite difference formulation for radially-symmetric cylindrical polar coordinates does not appear elsewhere in the literature and requires some special considerations, that formulation is presented here.
4.1 Linearization by Under-relaxation

Any finite difference formulation will lead to algebraic equations of the form

\[ Au = f \]  \hspace{1cm} (4.1)

where \( A \) is a sparse banded matrix, \( u = [u_{1,1}, u_{1,2}, \ldots, u_{1,M}, \ldots, u_{N,1}, \ldots, u_{N,M}]^T \) is the solution vector containing values of the transport variables (temperature, salinity, or stream function) at \( N \times M \) discrete points, and \( f \) is a constant vector.

In Chapter 5 I present a method for solving equation (4.1) using multigrid, and in Chapter 7 I use a row-by-row method of simultaneous overrelaxation (SOR).

Because the coupled transport variables (\( T, C, \) and \( \Psi \)) depend on one another, the system of governing equations is nonlinear. In as much as any numerical formulation requires a linear form (viz., equation (4.1)), the numerical formulations must impose some method of resolving nonlinearities. Almost always this requires an iterative procedure, most commonly either Newton's method or under-relaxation. The latter of these is often the more efficient and is simple to implement. Consequently, under-relaxation is implemented in the numerical formulation under consideration.

Unrelaxed iterative schemes are of little value in solving brine transport problems (although they are often adequate for coupled groundwater-temperature problems),
because there is such a strong interaction between the groundwater flow and salinity. For example, if we solve for the salinity field based on groundwater flow from the current iteration (which was in turn based on salinities from the previous iteration), the resulting salinities may have little resemblance to salinities calculated previously. When new values of one dependent variable (say \( C \)) are based entirely on the most recent estimates of another variable (say \( \Psi \)), it may take hundreds or thousands of iterations to converge to the correct solution. The idea behind under-relaxation is to put a limit on the degree to which groundwater flow calculated in a given iteration can change the salinity and temperature values that were calculated previously (and vice versa).

Under-relaxation is implemented simply by employing a weighted average of newly calculated values of a variable and previously calculated values:

\[
\hat{u}_{i,j} = \alpha u_{i,j}^{\text{new}} + (1-\alpha) u_{i,j}^{\text{old}}
\]

where \( \alpha \) is called the relaxation parameter, and the superscripts \( \text{old} \) and \( \text{new} \) indicate values of \( u_{i,j} \) for the previous and current iterations, respectively. In my model \( u_{i,j} \) represents either temperature, salinity, stream function, or groundwater velocity at each node. When \( \alpha=1 \) there is no under-relaxation, and when \( \alpha=0 \) the solution does not progress. Values of \( \alpha \) are best determined by numerical
experiments and experience; in the simulations presented below α ranges between 0.2 and 0.8.

4.2 Discretization of Governing Equations

In cylindrical polar coordinates with no azimuthal variation the equations governing groundwater flow, heat transport, and solute transport are given by (Chapter 3)

$$\frac{\partial}{\partial r}(v k_{yy} \frac{\partial \Psi}{\partial r}) + \frac{\partial}{\partial y}(v k_{rr} \frac{\partial \Psi}{\partial y}) = -\frac{\partial p}{\partial r} \quad (3.38)$$

$$\frac{1}{r} \frac{\partial}{\partial r}(r K \frac{\partial T}{\partial r}) + \frac{\partial}{\partial y}(K \frac{\partial T}{\partial y}) - \frac{1}{r} \frac{\partial}{\partial r}(r \rho c_q T) - \frac{\partial}{\partial y}(\rho c_q T) = 0 \quad (3.41)$$

$$\frac{1}{r} \frac{\partial}{\partial r}(r \rho \phi D \frac{\partial C}{\partial r}) + \frac{\partial}{\partial y}(\rho \phi D \frac{\partial C}{\partial y}) - \frac{1}{r} \frac{\partial}{\partial r}(r \rho c_q C) - \frac{\partial}{\partial y}(\rho c_y + \rho \phi V) C = \frac{\partial (\rho \phi C)}{\partial t} \quad (3.44)$$

For each of the three transport equations a cross section of a cylindrical column \((r, 0, y)\) is divided into discrete regions such that the origin of the discretized region is at the cylinder axis (Figure 4.1). The small regions bounded by dark lines in Figure 4.1 are control volumes; one node point (closed circles) is located in the interior of each control volume. Within each control volume medium properties (e.g., \(\phi, K, K,\) and \(D\)) are assumed to be constant, and transport variables are assumed to vary in a smooth way from node point to node point. Each node point is identified by indices \((i, j)\), and has neighboring nodes \((i-1, j)\) and \((i+1, j)\) in the
Figure 4.1  A schematic representation of finite difference discretization in cylindrical polar coordinates. The two dimensional discretization represents a cross-section through a cylindrical annulus.
radial direction, and \((i,j-1)\) and \((i,j+1)\) in the vertical
direction (Figure 4.2). The control volume (the shaded
region of Figure 4.2) associated with node \((i,j)\) is a
cylindrical sector of an annulus bounded by interfaces
indicated as (following the notation of Patankar, [1980]) \(n\),
\(s\), \(e\), and \(w\), respectively.

The finite difference formulation for (3.38) and (3.44)
will be presented in detail, while the temperature
discretization (for 3.41) will be presented by analogy to
that for (3.44). In all cases the discretization produces
matrix equation (4.1) which takes the form

\[
\begin{align*}
\alpha_{i,j}u_{i+1,j} + b_{i,j}u_{i-1,j} + c_{i,j}u_{i,j+1} + d_{i,j}u_{i,j-1} + e_{i,j}u_{i,j} &= f_{i,j}
\end{align*}
\]  

where \(u_{i,j}\) is solution for temperature \((u_{i,j}=T_{i,j})\), salinity
\((u_{i,j}=C_{i,j})\), or stream function \((u_{i,j}=\Psi_{i,j})\) at node \((i,j)\), and
\(\alpha_{i,j}, b_{i,j}, c_{i,j}, d_{i,j}, \) and \(e_{i,j}\) are constants occurring on
diagonal bands of \(A\). In the next section I briefly discuss
how my model calculates fluid velocity and medium properties
at control volume interfaces, and the subsequent three
sections are devoted to determining the values of the
coefficients in (4.3).

4.2.1 Interface Properties

Medium properties are specified and are considered to be
constant within each control volume. The discretization
equations, however, require that medium properties and

Figure 4.2 A diagram showing the details and notation of volume control finite differencing. The control volume is associated with node $i,j$ and is indicated by the stippled region. Control volume interfaces are indicated by $n$, $s$, $e$, and $w$. Each control volume is a cylindrical sector of an annulus.
groundwater velocities be specified at control volume interfaces in order to determine the mass or energy flux into control volumes. Consequently some interpolation method is needed in order to estimate interface properties. The objective of such interpolation is to represent the fluxes across the interfaces accurately. The interpolation of medium properties that most accurately achieves this objective is to estimate interface properties as a harmonic mean of control volume properties because the harmonic mean mimics the conditions of flux continuity through a composite material [Berg and McGregor, 1966; Patankar, 1980].

Referring to Figure 4.3 in which the interface is at an arbitrary location between two nodes, and letting

\[ f_e = \frac{(\Delta r)_e}{(\Delta r)_e + (\Delta r)_i} \]

be the fractional distance of the interface between nodes, some interface property \( \Gamma_e \) (which might represent thermal or hydraulic conductivity, for example) is given by

\[
\Gamma_e = \left[ \frac{1 - f_e}{\Gamma_{i,j}} + \frac{f_e}{\Gamma_{i+1,j}} \right]^{-1}
\]  

(4.4)

When the interface is midway between two nodes (4.4) gives

\[
\Gamma_e = \frac{2\Gamma_{i,j}\Gamma_{i+1,j}}{\Gamma_{i,j} + \Gamma_{i+1,j}}
\]  

(4.5)

For cases in which the medium remains stationary, my model assumes that interfaces are located midway between node points, and (4.5) is used. For calculations involving a subsiding basin this assumption is not used because basin
Figure 4.3 A illustration of how interface properties are calculated between nodes of different properties. $f$ is the fractional distance between nodes, and $\Gamma$ represents any medium property, such as permeability and thermal conductivity.
subsidence can be specified independent of node spacing. In these cases (4.4) is used to estimate interface properties. For the solute and heat transport equations it is also necessary to consider how to estimate advective flux at the control volume interfaces. Using the stream function formulation this is a simple matter. Once values of the stream function have been calculated at each node (section 4.2.2), groundwater velocities are given by equations (3.29) or (3.35), which are easily discretized with second order accuracy midway between node points. Specifically,

\[
(q_x)_e = -\frac{\rho_e}{r_e(\delta r)_e}(\Psi_{i+1,j} - \Psi_{i,j})
\]

\[
(q_x)_w = -\frac{\rho_w}{r_w(\delta r)_w}(\Psi_{i,j} - \Psi_{i-1,j})
\]

\[
(q_y)_n = -\frac{\rho_n}{r_n(\delta r)_n}(\Psi_{i,j+1} - \Psi_{i,j})
\]

\[
(q_y)_s = -\frac{\rho_s}{r_s(\delta r)_s}(\Psi_{i,j} - \Psi_{i,j-1})
\]

where \(r_e\), for example, is the radial distance to the interface between nodes \((i+1,j)\) and \((i,j)\).

Having established how interface properties are calculated, the governing equations are discretized as presented below.

4.2.2 Stream Function Discretization

Integrating equation (3.38) with respect to \(r\) and \(y\) over control volume \((i,j)\) gives
The first and last pairs of integrals in equation (4.7) are straightforward to evaluate, and the integrals in the second term can be rearranged, leading to

\[
\Delta y \left[ \frac{v}{rk_{yy}} \frac{\partial \psi}{\partial r} \right]_w + \int \frac{1}{r} \int \frac{n}{\partial y} \left( \frac{v}{rk_{xx}} \frac{\partial \psi}{\partial y} \right) dy dr = -g \Delta y [\rho]_w
\]  

(4.8)

Evaluating the remaining integrals gives

\[
\Delta y \left[ \frac{v}{rk_{yy}} \frac{\partial \psi}{\partial r} \right]_e + \int \frac{1}{r} \int \frac{n}{\partial y} \left( \frac{v}{rk_{xx}} \frac{\partial \psi}{\partial y} \right) dy dr = -g \Delta y (\rho_e - \rho_w)
\]  

(4.9)

The occurrence of the natural log terms in (4.9) is unique to the stream function discretization in cylindrical coordinates, and arises because the size of control volumes increase exponentially with distance from the cylinder axis.

Now, assuming that \( \psi \) varies linearly from node to node (so that, for example, \( \frac{\partial \psi}{\partial y} |_n = \frac{\psi_{i+1,j} - \psi_{i,j}}{\delta y_n} \)), and evaluating interface properties as described above then

\[
\frac{\Delta y v_e}{r_e (\delta r_e) k_{yye}} (\psi_{i+1,j} - \psi_{i,j}) - \frac{\Delta y v_w}{r_w (\delta r_w) k_{yyw}} (\psi_{i,j} - \psi_{i-1,j}) + \\
\frac{ln \left( \frac{r_e}{r_w} \right) v_n}{(\delta y_n) k_{rrn}} (\psi_{i,j+1} - \psi_{i,j}) - \frac{ln \left( \frac{r_e}{r_w} \right) v_s}{(\delta y_s) k_{rrs}} (\psi_{i,j} - \psi_{i,j-1})
\]

\[= -g \Delta y (\rho_e - \rho_w)
\]  

(4.10)
Because temperature and salinity are assumed to be constant and known at each node, \( \rho \) and \( V \) at the interfaces are considered to be constants in (4.10). From equations (4.10) and (4.3) it is clear that the finite difference coefficients are

\[
\begin{align*}
a_{i,j} &= \frac{\Delta y V_e}{r_e (\delta r_e) k_{yy_e}} \\
b_{i,j} &= \frac{\Delta y V_w}{r_w (\delta r_w) k_{yy_w}} \\
c_{i,j} &= \frac{\ln(r_e / r_w) v_n}{(\delta y_n) k_{rr_n}} \\
d_{i,j} &= \frac{\ln(r_e / r_w) v_s}{(\delta y_s) k_{rr_s}}
\end{align*}
\]

(4.11)

\[
e_{i,j} = -a_{i,j} - b_{i,j} - c_{i,j} - d_{i,j}
\]

\[
f_{i,j} = -g\Delta y (\rho_e - \rho_w)
\]

Here the terms \( f_{i,j} \) represent forcing terms (or source terms for vorticity) at the \((i,j)\)th node. Coefficients \( a_{i,j} \) through \( f_{i,j} \) can be operated on directly by SOR or multigrid algorithms \( \textit{e.g.}, \text{Westlake, 1975; Press et al., 1985}. \) In Cartesian coordinates the coefficients take a similar form: \( r \) represents the horizontal coordinate; the terms \( a_{i,j} \) and \( b_{i,j} \) are multiplied by \( r_e \) and \( r_w \), respectively, and in the expressions for \( c_{i,j} \) and \( d_{i,j} \) the natural log terms are replaced by \( \Delta r \) (see Table 4.1)
4.2.3 Solute Transport Discretization

The finite difference formulation for the dispersion terms in (3.41) is similar to that presented above. The solute transport problem, however, is inherently more difficult to solve numerically because hydrodynamic dispersion is velocity-dependent, because time derivatives must be included in the discretization, and primarily because the advective transport terms tend to be numerically problematic. Discretization of the advection terms is problematic for several reasons: 1) a second-order (volume-centered) differencing scheme makes the off-diagonal terms of the coefficient matrix $A$ numerically dominant, but diagonal dominance is required in order to achieve matrix inversion by iterative methods; 2) discretization of first derivatives leads to false diffusion, i.e., numerical dispersion; 3) a second-order differencing scheme implicitly requires mass conservation between alternating nodes, which can produce wavy numerical results; and 4) the advection coefficients depend directly on estimates of velocity which are often difficult to achieve accurately.

The last of these problems is remedied in part by the use of the stream function as well as by under-relaxation. A partial remedy for the other problems is to use upstream weighting for the derivatives in the advective terms [Laumbach, 1975; Patankar, 1980; Clauser and Kiesner, 1987]. The upstream differencing scheme exploits the fact that when
convection is strong the salinity field is not likely to be linear between nodes. The salinity calculated at a given node will be strongly affected by the salt content of groundwater upstream, but only weakly affected by salinity values downstream. Numerically this approach is first-order accurate in first derivatives; nonetheless it tends to yield numerical results that are physically more accurate than second-order (volume-centered) differences.

Multiplying both sides of equation (3.44) by $r$, and integrating with respect to $y$, $r$, and $t$ gives

$$
\int \int \int_{t+\Delta t} \frac{\partial}{\partial t} (r \rho \Phi \frac{\partial C}{\partial r}) \, dy \, dr \, dt +
\int \int \int_{t+\Delta t} \frac{\partial}{\partial y} (r \rho \Phi \frac{\partial C}{\partial y}) \, dy \, dr \, dt -
\int \int \int_{t+\Delta t} \frac{\partial}{\partial r} (r \rho \Phi \frac{\partial C}{\partial r}) \, dy \, dr \, dt -
\int \int \int_{t+\Delta t} \frac{\partial}{\partial y} [(\rho q + \rho \Phi V) C] \, dy \, dr \, dt
$$

\begin{align*}
&= \int \int \int_{t+\Delta t} \frac{\partial (\rho \Phi C)}{\partial t} \, dy \, dr \, dt \\
&\quad (4.12)
\end{align*}

Evaluating the integrals in (4.12) gives
\[
\Delta t \Delta y \left[ r \rho \phi D_{rr} \frac{\partial c}{\partial r} \right]_w + \Delta t \frac{1}{2} r^2 \left[ \rho \phi D_{yy} \frac{\partial c}{\partial y} \right]_s - \Delta t \Delta y \left[ r \rho q r c \right]_w - \Delta t \frac{1}{2} r^2 \left[ (\rho q_y + \rho \phi v) c \right]_s
\]

\[
= \Delta y \left[ \rho c \right]_t^{t+\Delta t}
\]

(4.13)

Using the fact that \[ \frac{1}{2} r^2 \left[ \right]_w = \frac{1}{2} (r_e^2 - r_w^2) = \Delta r \bar{r} \] where \( \bar{r} = \frac{1}{2} (r_e + r_w) \) is the average radius between interfaces, yields

\[
\frac{r_e \Delta y (\rho \phi D_{rr})_e}{\Delta r_e} (C_{i+1,j} - C_{i,j}) - \frac{r_w \Delta y (\rho \phi D_{rr})_w}{\Delta r_w} (C_{i,j} - C_{i-1,j}) + \frac{\Delta r \bar{r} (\rho \phi D_{yy})_n}{\Delta y_n} (C_{i,j+1} - C_{i,j}) + \frac{\Delta r \bar{r} (\rho \phi D_{yy})_s}{\Delta y_s} (C_{i,j} - C_{i,j-1}) - r_e \Delta y (\rho q_r)_e C_e + r_w \Delta y (\rho q_r)_w C_w - \Delta r \bar{r} (\rho q_y + \rho \phi v)_n C_n + \Delta r \bar{r} (\rho q_y + \rho \phi v)_s C_s = \Delta r \bar{r} \Delta y \frac{1}{2\Delta t} [\rho \phi (C_{i,j}^{\text{new}} - C_{i,j}^{\text{old}})]
\]

(4.14)

where \( C_e, C_w, C_n, \) and \( C_s \) are values of solute concentration at the interfaces and are determined by an upstream weighting scheme. For example, in implementing a fully upstream
scheme, the advection terms are calculated by assuming the value of salinity on the upstream side of the control volume edge, so that

\[ C_e = \begin{cases} C_{i,j} & \text{if } (q_r)_e > 0 \\ C_{i+1,j} & \text{if } (q_r)_e < 0 \end{cases} \]

\[ C_w = \begin{cases} C_{i-1,j} & \text{if } (q_r)_w > 0 \\ C_{i,j} & \text{if } (q_r)_w < 0 \end{cases} \]

\[ C_n = \begin{cases} C_{i,j} & \text{if } (q_y)_n > 0 \\ C_{i,j+1} & \text{if } (q_y)_n < 0 \end{cases} \]

\[ C_s = \begin{cases} C_{i,j-1} & \text{if } (q_y)_s > 0 \\ C_{i,j} & \text{if } (q_y)_s < 0 \end{cases} \]

The fully upstream scheme is easy to implement in program code. Unfortunately, it maximizes the numerical dispersion, and in many applications more accurate numerical results are needed. A variety of numerical ploys have been invented in attempts to incorporate the advantages of upstream weighting without introducing excessive false diffusion [Southwell, 1956; Patankar, 1980; Clauser and Kiesner, 1987]. Most of these schemes use three-point volume-centered differences that are exponentially weighted in the upstream direction. Patankar [1980] compares the numerical consequences of several such discretizations and concludes that a power law weighting provides numerical results that most accurately reproduce analytical calculations.
With these discretizations it is helpful to compare the dispersive and advective components of solute flux across control-volume interfaces by introducing the grid Peclet number. Referring to (4.14) we can write the dispersive components at the control volume interfaces as

\[ D_e = \frac{\rho e \Delta y (\rho \phi D_{xx})_e}{\delta r_e} \quad D_w = \frac{\rho w \Delta y (\rho \phi D_{xx})_w}{\delta r_w} \]

\[ (4.16) \]

\[ D_n = \frac{\Delta r \overline{\phi} (\rho \phi D_{yy})_n}{\delta y_n} \quad D_s = \frac{\Delta r \overline{\phi} (\rho \phi D_{yy})_s}{\delta y_s} \]

and the advective components as

\[ F_e = r_e \Delta y (\rho q_x)_e \quad F_w = r_w \Delta y (\rho q_x)_w \]

\[ (4.17) \]

\[ F_n = \Delta r \overline{\phi} (\rho q_y + \rho \phi V)_n \quad F_s = \Delta r \overline{\phi} (\rho q_y + \rho \phi V)_s \]

The grid Peclet numbers are defined as

\[ P_e = \frac{F_e}{D_e} \quad P_w = \frac{F_w}{D_w} \]

\[ (4.18) \]

\[ P_n = \frac{F_n}{D_n} \quad P_s = \frac{F_s}{D_s} \]

With this notation the coefficients in the discretized equation can now be written as
\[
a_{i,j} = D_e F(|P_e|) + \max(-F_e, 0)
\]

\[
b_{i,j} = D_w F(|P_w|) + \max(F_w, 0)
\]

\[
c_{i,j} = D_n F(|P_n|) + \max(-F_n, 0)
\]

\[
d_{i,j} = D_s F(|P_s|) + \max(F_s, 0)
\]

\[
e_{i,j} = a_{i,j} - b_{i,j} - c_{i,j} - d_{i,j} - \frac{\Delta t \Delta y \rho \phi}{2 \Delta t} C_{i,j}^{old}
\]

\[
f_{i,j} = -\frac{\Delta t \Delta y \rho \phi}{2 \Delta t} C_{i,j}^{old}
\]

Here the \(\max()\) represents the maximum value of the terms in parenthesis, and is used as a shorthand notation for equations (4.12); the terms containing \(\Delta t\) are introduced by the discretization of the time derivative, such that \(C_{i,j}^{old}\) is the solute concentration calculated at the previous time step; and \(F[P]\) is an interpolation function that modifies the dispersive component of solute flux according to the magnitude of the Peclet number in order to compensate for numerical dispersion. For example if \(F[P]=1\) the dispersive term is unmodified and full upstream weighting is used. In most of the numerical simulations discussed herein, I use a power law function of the form [Patankar, 1980]

\[
F[P] = \max(0, 1 - 0.1|P|^5)
\]

4.2.4 Heat Transport Discretization

The heat transport equation (3.41) is discretized in a manner exactly analogous to the solute transport equation except that temporal discretization is unnecessary. Thermal Peclet numbers tend to be smaller that those for solute transport because heat conduction is more efficient that solute diffusion through sediments. Because of the analogous form of the heat and solute transport equations it suffices to present only the final form of the finite difference equations (again in cylindrical coordinates). Specifically, the coefficients $a_{i,j}$ through $e_{i,j}$ take exactly the same form as in equations (4.18) and (4.19) except that for heat transport the diffusion (conduction) terms are,

\[
D_e = \frac{r_e \Delta y K_e}{\delta r_e} \quad D_w = \frac{r_w \Delta y K_w}{\delta r_w}
\]

\[
D_n = \frac{\Delta r \bar{r} K_n}{\delta y_n} \quad D_s = \frac{\Delta r \bar{r} K_s}{\delta y_s}
\]

and the convection terms are

\[
F_e = r_e \Delta y (\rho c q_r)_e \quad F_w = r_w \Delta y (\rho c q_r)_w
\]

\[
F_n = \Delta r \bar{r} (\rho c q_y)_n \quad F_s = \Delta r \bar{r} (\rho c q_y)_s
\]
4.2.5 Cartesian Coordinates and Finite Difference Coefficient

Summary

A summary of the finite difference coefficients for the stream function, salinity, and temperature are presented in Tables 4.1, 4.2, and 4.3, respectively. In all three tables the coefficients $a_{i,j}$, $b_{i,j}$, $c_{i,j}$, $d_{i,j}$, $e_{i,j}$, and $f_{i,j}$ represent those in equation (4.3). For heat and solute transport these coefficients depend on some weighting function $F[P]$ of the grid Peclet number, which is given in (4.20). In the absence of basin subsidence the value of $\mathbf{V}$ in Table 4.2 vanishes.

4.3 Equations of State

In the presentation heretofore I have assumed that groundwater density and viscosity are known functions of salinity, temperature, and pressure. Accurate estimates of groundwater density are particularly important in a study such as this because groundwater circulation is driven by lateral density gradients. Moreover, the magnitude of groundwater velocity is inversely related to viscosity since this term appears in the denominator of the hydraulic conductivity.

The density and viscosity of NaCl solutions have been extensively studied for several decades [e.g., Washburn, 1929] and an abundance of experimental results have been compiled [e.g., Newman, 1980]. In most experimental studies the authors attempt to determine a correlation equation that
<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Cylindrical Coordinates</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>ai, j</td>
<td>$\Delta y V_e$</td>
<td>$\Delta y V_e$</td>
</tr>
<tr>
<td></td>
<td>$r_e (\delta r_e) k_{yy_e}$</td>
<td>$(\delta x_e) k_{yy_e}$</td>
</tr>
<tr>
<td>bi, j</td>
<td>$\Delta y V_w$</td>
<td>$\Delta y V_w$</td>
</tr>
<tr>
<td></td>
<td>$r_w (\delta r_w) k_{yy_w}$</td>
<td>$(\delta x_w) k_{yy_w}$</td>
</tr>
<tr>
<td>ci, j</td>
<td>$\ln \frac{r_e}{r_w} V_n$</td>
<td>$\Delta x V_n$</td>
</tr>
<tr>
<td></td>
<td>$(\delta y_n) k_{rrn}$</td>
<td>$(\delta y_n) k_{xxn}$</td>
</tr>
<tr>
<td>di, j</td>
<td>$\ln \frac{r_e}{r_w} V_s$</td>
<td>$\Delta x V_s$</td>
</tr>
<tr>
<td></td>
<td>$(\delta y_s) k_{rrs}$</td>
<td>$(\delta y_s) k_{xxs}$</td>
</tr>
<tr>
<td>ei, j</td>
<td>-$a_i, j - b_i, j - c_i, j - d_i, j$</td>
<td>-$a_i, j - b_i, j - c_i, j - d_i, j$</td>
</tr>
<tr>
<td>fi, j</td>
<td>-$g \Delta y (\rho_e - \rho_w)$</td>
<td>-$g \Delta y (\rho_e - \rho_w)$</td>
</tr>
</tbody>
</table>
Table 4.2 Solute Transport Finite Difference Coefficients

\[ a_{i,j} = D_e F[|F_e|] + \max(-F_e, 0) \]
\[ b_{i,j} = D_w F[|F_w|] + \max(F_w, 0) \]
\[ c_{i,j} = D_n F[|F_n|] + \max(-F_n, 0) \]
\[ d_{i,j} = D_s F[|F_s|] + \max(F_s, 0) \]

\[ e_{i,j} = -a_{i,j} - b_{i,j} - c_{i,j} - d_{i,j} - \frac{\Delta r \Delta y \rho \phi}{2\Delta t} \]
\[ f_{i,j} = -\frac{\Delta r \Delta y \rho \phi}{2\Delta t} c_{i,j} \]

<table>
<thead>
<tr>
<th>Transport Term</th>
<th>Cylindrical Coordinates</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>(D_e)</td>
<td>(r_e \Delta y (\rho \phi D_{rr})_e) / (\delta r_e)</td>
<td>(\Delta y (\rho \phi D_{xx})_e / \delta x_e)</td>
</tr>
<tr>
<td>(D_w)</td>
<td>(r_w \Delta y (\rho \phi D_{rr})_w / \delta r_w)</td>
<td>(\Delta y (\rho \phi D_{xx})_w / \delta x_w)</td>
</tr>
<tr>
<td>(D_n)</td>
<td>(\Delta r \bar{r} (\rho \phi D_{yy})_n / \delta y_n)</td>
<td>(\Delta x (\rho \phi D_{yy})_n / \delta y_n)</td>
</tr>
<tr>
<td>(D_s)</td>
<td>(\Delta r \bar{r} (\rho \phi D_{yy})_s / \delta y_s)</td>
<td>(\Delta x (\rho \phi D_{yy})_s / \delta y_s)</td>
</tr>
<tr>
<td>(F_e)</td>
<td>(r_e \Delta y (pq r)_e)</td>
<td>(\Delta y (pq x)_e)</td>
</tr>
<tr>
<td>(F_w)</td>
<td>(r_w \Delta y (pq r)_w)</td>
<td>(\Delta y (pq x)_w)</td>
</tr>
<tr>
<td>(F_n)</td>
<td>(\Delta r \bar{r} (pq_y + \rho \phi V)_n)</td>
<td>(\Delta x (pq_y + \rho \phi V)_n)</td>
</tr>
<tr>
<td>(F_s)</td>
<td>(\Delta r \bar{r} (pq_y + \rho \phi V)_s)</td>
<td>(\Delta x (pq_y + \rho \phi V)_s)</td>
</tr>
</tbody>
</table>
Table 4.3 Heat Transport Finite Difference Coefficients

\[ a_{i,j} = D_e F[|P_e|] + \max(-F_e, 0) \]
\[ b_{i,j} = D_w F[|P_w|] + \max(F_w, 0) \]
\[ c_{i,j} = D_n F[|P_n|] + \max(-F_n, 0) \]
\[ d_{i,j} = D_s F[|P_s|] + \max(F_s, 0) \]
\[ e_{i,j} = -a_{i,j} - b_{i,j} - c_{i,j} - d_{i,j} \]
\[ f_{i,j} = 0 \]

<table>
<thead>
<tr>
<th>Transport Term</th>
<th>Cylindrical Coordinates</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_e )</td>
<td>( r \Delta y K_e )</td>
<td>( \Delta y K_e )</td>
</tr>
<tr>
<td></td>
<td>( \delta r_e )</td>
<td>( \delta x_e )</td>
</tr>
<tr>
<td>( D_w )</td>
<td>( r \Delta y K_w )</td>
<td>( \Delta y K_w )</td>
</tr>
<tr>
<td></td>
<td>( \delta r_w )</td>
<td>( \delta x_w )</td>
</tr>
<tr>
<td>( D_n )</td>
<td>( \Delta r \bar{r} K_n )</td>
<td>( \Delta x K_n )</td>
</tr>
<tr>
<td></td>
<td>( \delta y_n )</td>
<td>( \delta y_n )</td>
</tr>
<tr>
<td>( D_s )</td>
<td>( \Delta r \bar{r} K_s )</td>
<td>( \Delta x K_s )</td>
</tr>
<tr>
<td></td>
<td>( \delta y_s )</td>
<td>( \delta y_s )</td>
</tr>
<tr>
<td>( F_e )</td>
<td>( r \Delta y (\rho c q_r)_e )</td>
<td>( \Delta y (\rho c q_x)_e )</td>
</tr>
<tr>
<td>( F_w )</td>
<td>( r \Delta y (\rho c q_r)_w )</td>
<td>( \Delta y (\rho c q_x)_w )</td>
</tr>
<tr>
<td>( F_n )</td>
<td>( \Delta r \bar{r} (\rho c q_y)_n )</td>
<td>( \Delta x (\rho c q_y)_n )</td>
</tr>
<tr>
<td>( F_s )</td>
<td>( \Delta r \bar{r} (\rho c q_y)_s )</td>
<td>( \Delta x (\rho c q_y)_s )</td>
</tr>
</tbody>
</table>
reproduces the experimental results to about the same accuracy that is inherent in the data. Consequently many correlation equations exist for determining brine fluid properties. In this study I use correlation equations developed by Phillips et al. [1981, 1983] because these authors have attempted to fit hundreds of data values from a compilation of diverse experimental studies, and because their correlations extend to greater temperatures than many other studies.

Both the density and viscosity of NaCl brines increase with salinity but decrease with temperature; both are only weakly dependent on pressure. The density correlation derived by Phillips et al. [1981] is given by

$$\rho(C, T, p) = 1000(A + B\chi + C\chi^2 + D\chi^3)$$  \hspace{1cm} (4.23)

where

$$\chi = c_1 e^{\lambda_1 C_m} + c_2 e^{\lambda_2 T} + c_3 e^{\lambda_3 p}$$  \hspace{1cm} (4.24)

Here $C_m$ is NaCl concentration in molality, $T$ is in °C, and $p$ is in bars. The constants in equations (4.23) and (4.24) are given in Table (4.4). Densities calculated from (4.23) and (4.24) are contoured as a function of temperature and salinity in Figure 4.4.

Phillips et al. [1981] also present a correlation for dynamic viscosity of high salinity solutions. In their equation, viscosity as a function of temperature and pressure is corrected for the effects of NaCl concentration. Their
Table 4.4 Coefficients for Density Correlation
Equations (4.23) and (4.24)

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3.033405</td>
<td>10.128163</td>
<td>-8.750567</td>
<td>2.663107</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>c1</th>
<th>c2</th>
<th>c3</th>
</tr>
</thead>
<tbody>
<tr>
<td>-9.9559</td>
<td>7.0845</td>
<td>3.9093</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>λ1</th>
<th>λ2</th>
<th>λ3</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.539x10^{-3}</td>
<td>-1.638x10^{-4}</td>
<td>-2.551x10^{-5}</td>
</tr>
</tbody>
</table>
Figure 4.4 A contour plot of groundwater density as a function of temperature and dissolved salt concentration at a confining pressure of 200 bars [as calculated from Phillips et al., 1983].
equation therefore requires a priori estimates of viscosity at a given temperature and pressure. In my model I estimate viscosity as a function of temperature and pressure using a correlation presented by Kestin et al. [1981], and operate on those values using the correlation of Phillips et al. [1981]. Following Kestin et al. [1981] viscosity is first calculated as a function of temperature (in °C)

\[
\mu(T) = 1002 \times 10^\tau
\]  

(4.25)

where

\[
\tau = \frac{\sum_{i=1}^{4} \alpha_i (20-T)^i}{96+T}
\]  

(4.26)

This equation is corrected for the effects of pressure by

\[
\mu(T,p) = \mu(T) \times \left(1 + 10^{-6} \beta_w \frac{P}{1000}\right)
\]  

(4.27)

where

\[
\beta_w = \sum_{i=0}^{4} \beta_i T^i
\]  

(4.28)

Finally, viscosity is corrected for salinity by [Phillips et al., 1981]

\[
\mu(C,T,p) = \mu(T,p) \times \left[ \sum_{i=0}^{4} \gamma_i C_m^i + \epsilon T (1 + e^{\sigma C_m}) \right]
\]  

(4.29)

Values of the constants in equations (4.26), (4.28), and (4.29) are given in Table 4.5. In Figure 4.5, viscosity estimates are plotted versus temperature and salinity using a
Table 4.5 Coefficients for Viscosity Correlation

<table>
<thead>
<tr>
<th>$i$</th>
<th>$\alpha$ (eq. 4.26)</th>
<th>$\beta$ (eq. 4.28)</th>
<th>$\gamma$ (eq. 4.29)</th>
<th>$\varepsilon$ (eq. 4.29)</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-1.297</td>
<td>1.0</td>
<td>6.29x10^{-4}</td>
<td>-0.7</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1.237x10^{-3}</td>
<td>5.74x10^{-2}</td>
<td>8.16x10^{-2}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.303x10^{-3}</td>
<td>-6.97x10^{-4}</td>
<td>1.22x10^{-2}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>3.06x10^{-6}</td>
<td>4.47x10^{-6}</td>
<td>1.28x10^{-4}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>2.55x10^{-8}</td>
<td>-1.05x10^{-8}</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 4.5 A contour plot of groundwater viscosity as a function of temperature and dissolved salt concentration at a confining pressure of 200 bars [as calculated from Kestin et al., 1981, and Phillips et al., 1983].
confining pressure of 200 bars. Viscosity plots at other pressures are very similar.

Variations in thermal conductivity and specific heat in groundwater are considered to be negligible, and no attempt is made in my model to account for these variations. Thermal conductivity and specific heat of NaCl solutions vary only a few percent over the salinity, temperature, and pressures of interest, and the groundwater constitutes a small part (proportional to $\phi$) of the bulk thermal properties of saturated sediments.

4.4 Discussion

Any numerical model is necessarily based on a mathematical model that describes the physical processes of interest through governing equations and boundary and initial conditions. The numerical model consists of a theoretical discretization of the governing equations, the actual computer code that implements the discretization, as well as the finite difference mesh used approximate a given physical problem. The model is distinct from numerical simulations, which are simply runs of the numerical model for a given set of boundary and initial conditions. If numerical simulations are thought of as being analogous to laboratory experiments, then the computer program and finite difference mesh are analogous to the experimental apparatus; the discretization of the governing equations is analogous to the experimental
design; and the simulations themselves are analogous to actually conducting the experiment. In both numerical and laboratory experiments care must be taken at all stages in order that the final results can be meaningfully interpreted.

In this chapter I have outlined how the governing equations are discretized so that they can be solved numerically. The strongly coupled nature of the transport variables near salt domes makes this environment particularly difficult to model numerically. Iterative under-relaxation serves to facilitate convergence under these conditions but does not necessarily guarantee it. Even when convergence is achieved efficiently it may take several hours or tens of hours to run a single simulation. Consequently it is essential to develop a numerical formulation that yields physically reasonable results even when node spacing and time steps are large, so that preliminary simulations still reveal physical attributes of the geologic system in question. The numerical formulation presented here implicitly contains several features that facilitate physically reasonable results for most simulations. For example, 1) this formulation will always produce positive values of temperature and salinity provided the boundary conditions are positive; 2) it does an excellent job of conserving energy and mass; 3) transport variables at a given node will always have values that fall between the values at adjacent nodes; and 4) small changes in one transport variable will not produce excessive changes in another.
The actual coding (in FORTRAN) of the discretization described above is presented as program listings that are included as appendices. At this point I will briefly describe these programs and interject a bit about my programming philosophy and how it is reflected in the code. 1) The programs are highly vectorized (even though simulations were not run on a vector processor). Vectorized code serves to provide consistency in the way arrays are manipulated and, most importantly, it anticipates eventual transfer to supercomputers. 2) Input and output processes, including plotting routines, are completely isolated from calculations so that plotting can be performed in post processing or easily removed if code is migrated to another machine. 3) Simulation input and output files have identical formats so that it is easy to restart or continue terminated simulations. 4) The programs are well structured.

The main program used in this study (program CSDDB) solves the coupled transport equations in either cylindrical polar or Cartesian coordinates. The structure of this code is illustrated in the flow chart in Figure 4.6. Because the general structure of simpler programs is similar to that of CSDDB, this is the only program flow charted here. Essentially, each box in Figure 4.6 is implemented as a subprogram (or group of subprograms) within the FORTRAN code. The flow chart shows how the three transport equations are decoupled and under-relaxed; it also illustrates the iterative loop that is executed for each time step.
Figure 4.6 A flow chart illustrating the structure of the computer code that implements the discretization described in this chapter.
Daily observation teaches us that the water of the ocean and of the atmosphere is never at rest, and so it is with that which occupies the interior of the earth's crust; it, like the others, is constantly in motion, and these motions are at once numerous, extended, and very complex, but may be brought together under three categories — (1) gravitational, (2) thermal, and (3) capillary movements.

Franklin H. King, 1897
From USGS Annual Report 19

Thermally driven convection near salt domes may present a simple and common transport mechanism for driving groundwater up the flanks of salt domes, provided the thermal effects are not overwhelmed by salinity effects. It is clear that thermal environment is affected by the presence of the salt dome, and that the temperature field is strongly coupled to the groundwater flow field. For these reasons the idea that thermohaline convection is responsible for creating the surprising flow patterns near salt domes should be the first hypothesis to be tested. If the temperature field itself provides an adequate explanation of the observed phenomena, then additional hypotheses may be unnecessary, in accordance with Ockham's rule. On the other hand, if the thermal effects are insufficient to provide a reasonable driving mechanism, then other driving forces must be invoked.

In this chapter I attempt to evaluate coupled heat and solute transport as a driving mechanism for groundwater convection near salt diapirs. Specifically, I present math-
ematical and numerical models, and the results of calculations designed to test the hypothesis that the combined effects of temperature and salt concentration variations can produce groundwater convection similar to the patterns observed near some salt domes. Because I am interested in the mechanisms that drive groundwater convection, I present a simplified mathematical model using dimensional analysis. This provides a means to evaluate the relative effects of different dimensionless parameters, and their roles in controlling convection.

The result of dimensional analysis is to reduce to three the number of physical parameters that control the coupled flow problem [see Langhaar, 1951]. This is a significant advantage in the present case because the temperature, salt concentration, and flow fields are controlled by three dimensionless parameters, only one of which asserts direct influence on the flow field. Consequently, we are able to investigate the mechanisms that drive groundwater flow without necessitating an unreasonable number of simulations. The trade-off is that I sacrifice generality by assuming a homogeneous medium and by ignoring mechanical mixing. These assumptions will not affect the conclusions about the nature of free convection near salt domes; but they may make the dimensional analysis approach inappropriate for modelling details of groundwater flow in specific geologic settings.

Problems that are similar to the salt dome problem have
been studied in different contexts, and have some historical importance and relevance to the present chapter. For example, Bejan and his colleagues have studied two-dimensional double-diffusive convection between two isothermal and isosaline plates using both boundary layer analysis [Bejan and Khair, 1985] and dimensional analysis [Trevisian and Bejan, 1985] similar to the dimensional analysis presented below. Natural convection in a porous annulus bounded by isothermal cylinders has been recently discussed by Prasad and Kulacki [1983] and represents the geometry used in some of Wooding's [e.g., 1960] pioneering work on convection in porous medium.

5.1 Mathematical Formulation

5.1.1 Governing Equations

The equations governing groundwater flow, heat and mass transport in a porous medium were derived in Chapter 3 from equations for heat and mass conservation and constitutive flow laws -- viz. Darcy's law, Fourier's law of heat transport, and Fick's first law of diffusion with advection. At this point I simplify these equations by assuming steady conditions and a homogeneous medium. These assumptions lead in a straightforward way to the following governing equations.

\[ \nabla \cdot (\rho q) = 0 \quad (3.17) \]
\[ q = \frac{-k}{\mu} (V_P - \rho g) \quad (3.5) \]

\[ \rho c q \nabla T = k \nabla^2 T \quad (5.1) \]

\[ q \nabla C = \phi D' \nabla^2 C \quad (5.2) \]

where \( q \) is the Darcy flux, \( k \) is the intrinsic permeability of the medium; \( \mu \) and \( \rho \) are the dynamic viscosity and density of the groundwater; \( K \) and \( c \) are the effective thermal conductivity and heat capacity of the saturated medium, and \( D' \) is the effective dispersion coefficient for dissolved species through the saturated medium; \( V_P \) is the pressure gradient; \( g \) is the acceleration of gravity; and \( T \) and \( C \) represent temperature and salt concentration of the groundwater.

Equation (5.1) comes directly from (3.13) by assuming that thermal conductivity and heat capacity are constant; similarly (5.2) comes from equation (3.9) assuming that porosity and hydrodynamic dispersion are constant. In both cases time-dependent and source terms are neglected. In nature permeability \( (k) \), hydrodynamic dispersion \( (D') \), and effective thermal conductivity \( (K) \) all depend on the porosity and the tortuous nature of the sediments. In general \( D' \) should also account for mechanical mixing of dissolved solids and would therefore be velocity dependent [see Bear, 1972]. In order to simplify the analysis and to facilitate
interpretation, I herein neglect this dependence. The consequences of this simplification are discussed in section 5.4. I further simplify the formulation by assuming that groundwater viscosity is constant.

For mathematical simplification, I employ a linear equation of state:

$$\rho(C,T) = \rho_0 [1 + \beta_T (T - T_0) + \beta_C (C - C_0)]$$  \hspace{1cm} (5.3)

which is a reasonable approximation to the elaborate density correlation presented in the previous Chapter. Here $\beta_T$ represents the thermal expansivity of water and has a value of about 0.001°C$^{-1}$, $\beta_C$ is a concentration analog to $\beta_T$ (about -0.025 molal$^{-1}$, as determined from the correlation by Phillips et al. [1983]), and $\rho_0$ is the reference density of water at temperature $T_0=20^\circ$C and concentration $C_0=0$ molal.

As a simple approximation to the salt dome environment I model the salt as a cylindrical column that is overlain by saturated sediments; and I assume that flow occurs in a cylindrical annulus of saturated sediment that surrounds the salt column (Figure 5.1). Accordingly, I write the governing equations in two-dimensional cylindrical polar coordinates $(r,0,y)$ and eliminate the pressure term by invoking the mass stream function (Chapter 3). Assuming that $k$ and $V$ are constant, gives equations for groundwater flow,

$$\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial r^2} - \frac{1}{r} \frac{\partial \psi}{\partial r} = - r \frac{gk \rho_0}{\nu} \left( \beta_T \frac{\partial T}{\partial r} + \beta_C \frac{\partial C}{\partial r} \right)$$  \hspace{1cm} (5.4)
Figure 5.1 A schematic diagram indicating the geometry and boundary conditions used in the numerical model. See text for a discussion of boundary conditions.
heat transport,
\[
\frac{\partial \Psi}{\partial r} \frac{\partial T}{\partial y} - \frac{\partial \Psi}{\partial y} \frac{\partial T}{\partial r} = r \frac{K}{c} \left( \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right)
\] (5.5)

and solute transport,
\[
\frac{\partial \Psi}{\partial r} \frac{\partial C}{\partial y} - \frac{\partial \Psi}{\partial y} \frac{\partial C}{\partial r} = r \phi \frac{D}{\partial y^2} \left( \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right)
\] (5.6)

Here I have multiplied the left-hand-side of equation (5.2) by \(\rho\), and the right-hand-side by \(\rho_0\). This is effectively equivalent to assuming constant thermal and mass diffusivities. Equations (5.4) through (5.6) are directly coupled by the transport variables \(T\), \(C\), and \(\Psi\). For interpretive purposes, however, they represent diffusion of momentum, diffusion and advection of heat, and diffusion and advection of salt, respectively. From the right-hand-side of (5.4) it is apparent that the flow field is strongly controlled by radial variations in the temperature and concentration fields which introduce rotations [de Josselin de Jong, 1969].

5.1.2 Boundary Conditions

Referring to Figure 5.1 I model the salt dome as a cylindrical column overlain by sediments, and solve for flow in a rectangular domain that represents a cylindrical annulus around the salt column. No flow, (streamline) boundary
conditions are imposed on the boundary of the rectangular domain. Concentration boundary conditions are chosen such that the part of the boundary that is modeled as salt has uniformly high concentration \( C_1 \); directly above the salt column lateral salt flux is prohibited. Low concentration \( C_0 \) is specified along the top of the model, and this may be taken to represent uniform mixing with meteoric water. Specifically, concentration boundary conditions are

\[
C = C_1 \quad \text{at} \quad r = \frac{\Delta r}{2},
\]

\[
C = C_0 \quad \text{at} \quad y = H, \quad \text{and}
\]

\[
\frac{\partial C}{\partial n} = 0 \quad \text{elsewhere on the boundary}.
\]

Temperatures are prescribed along the boundaries to reflect the high thermal conductivity of salt (Figure 5.1).

\[
T = T_0 \quad \text{at} \quad y = H,
\]

\[
T = T_1 \quad \text{at} \quad y = 0,
\]

\[
T = a_1(H-y) + T_0 \quad y < y_h \quad \text{at} \quad r = \Delta r/2,
\]

\[
T = a_2(H-y) + b_2 \quad y \geq y_h
\]

and

\[
T = a_0(H-y) + T_0 \quad \text{at} \quad r = 3\Delta r/2
\]

With these boundary conditions the relatively high thermal conductivity of salt is modeled by prescribing a
piecewise linear temperature distribution along the model boundary $r = \Delta R/2$ (Figure 5.1). The relative slopes of the temperature curve along this boundary are chosen such that temperature and heat flux are continuous across the salt-sediment interface $(y_h)$. That is,

$$K_{\text{salt}} \frac{\partial T}{\partial y} \bigg|_{y_h^+} = K_m \frac{\partial T}{\partial y} \bigg|_{y_h^-}$$

and

$$T(y_h^+) = T(y_h^-)$$

at $r = \Delta R/2$. Temperatures at $r = 3\Delta R/2$ vary linearly, so that, at a distance $\Delta R$ from the salt column a constant thermal gradient is maintained.

These somewhat complicated boundary conditions are appropriate because they represent a reasonable approximation of the thermal effects of salt domes and because they facilitate the investigation of the importance of vertically varying thermal gradients in controlling groundwater flow in this environment. The contrast between thermal gradient in salt and overlying sediments can vary widely and will depend on contrasts in thermal conductivity and timing and rate of diapirism. The thermal conductivity contrasts themselves can be quite variable: porosity will largely control the thermal properties of the sediments, while salt conductivity is strongly dependent on temperature and salt purity [NBS monograph 167, 1981]. Both sediment porosity and temperature
of salt will depend on the depth to the top of salt.

5.1.3 Dimensional Analysis

I transform equations (5.4), (5.5), and (5.6) to dimensionless form by introducing the following change of variables:

\[ r_\ast = r/H \]

\[ y_\ast = y/H \]

\[ \psi_\ast = \frac{\psi}{\left(\frac{gk\rho_0 \Delta T \beta_1 H^2}{v}\right)} \]

\[ T_\ast = \frac{T}{(T_1-T_0)} \]

and

\[ C_\ast = \frac{C}{(C_1-C_0)} \]

which yield the dimensionless transport equations

\[ \frac{\partial^2 \psi_\ast}{\partial y_\ast^2} + \frac{\partial^2 \psi_\ast}{\partial r_\ast^2} - \frac{1}{r_\ast} \frac{\partial \psi_\ast}{\partial r_\ast} = r_\ast \left( \frac{\partial T_\ast}{\partial r_\ast} + N \frac{\partial C_\ast}{\partial r_\ast} \right) \quad (5.7) \]

\[ \text{Ra} \left( \frac{\partial \psi_\ast}{\partial r_\ast} \frac{\partial T_\ast}{\partial y_\ast} - \frac{\partial \psi_\ast}{\partial y_\ast} \frac{\partial T_\ast}{\partial r_\ast} \right) = r_\ast \left( \frac{\partial^2 T_\ast}{\partial y_\ast^2} + \frac{\partial^2 T_\ast}{\partial r_\ast^2} + \frac{1}{r_\ast} \frac{\partial T_\ast}{\partial r_\ast} \right) \quad (5.8) \]

\[ \frac{\text{LeRa}}{\phi} \left( \frac{\partial \psi_\ast}{\partial r_\ast} \frac{\partial C_\ast}{\partial y_\ast} - \frac{\partial \psi_\ast}{\partial y_\ast} \frac{\partial C_\ast}{\partial r_\ast} \right) = r_\ast \left( \frac{\partial^2 C_\ast}{\partial y_\ast^2} + \frac{\partial^2 C_\ast}{\partial r_\ast^2} + \frac{1}{r_\ast} \frac{\partial C_\ast}{\partial r_\ast} \right) \quad (5.9) \]
where \( Ra = g \rho_0 c_k \beta_r \Delta T / (KV) \) is the Rayleigh number (i.e. the thermal Rayleigh number); \( Le = K / (\rho_0 c D') \) is the Lewis number, and represents the ratio of thermal to mass diffusivity in the sediments; and \( N = (\beta_c \Delta C) / (\beta_r \Delta T) \) is the buoyancy ratio, which represents the relative effects of concentration and temperature on controlling groundwater density. Because \( \beta_c \) and \( \beta_r \) are assumed to be constant, the buoyancy ratio can also be thought of as a measure of the overall variation in salt concentration versus the overall variation in temperature at steady state. Consequently, the buoyancy ratio will depend on the regional groundwater salinity and ambient temperature.

The solute Rayleigh number, \( S \), is a concentration analog to the thermal Rayleigh number [Nield, 1968], and in the present notation is given by \( S = LeRaN \).

The dimensionless transport equations (5.7), (5.8), and (5.9) reveal several interesting aspects of the coupled flow problem. Equation (5.7) indicates that the flow field will be strongly influenced by the buoyancy ratio because it is the only dimensionless parameter appearing in the diffusion of momentum. The temperature and concentration fields are only indirectly affected by the value of \( N \) through advective modification of isotherms and isopleths. The Rayleigh number serves to weight the importance of advective heat transport (i.e. it multiplies the advective part of equation (5.8)), while the product of the Lewis and Rayleigh numbers weights advective salt transport. For example the greater the Lewis
number, the greater the tendency for isopleths to be dragged parallel to the streamlines. The Lewis and Rayleigh numbers only indirectly influence the flow field by affecting the right-hand-side of equation (5.7). These heuristic comments about the role of $N$, $Ra$, and $Le$ in influencing the transport fields are supported by numerical simulations and sensitivity analysis.

The change of variables chosen here are similar to the convention used by Trevisian and Bejan [1985]. It may seem more natural, however, to have written the transport equations in terms of Prandlt ($Pr$) and Schmidt ($Sh$) numbers by making the change of variables $\Psi* = \Psi/V$. In this case the Prandlt and Schmidt numbers directly modify the amount of advective heat and salt transport. This formulation, however, makes numerical solutions problematic because of the large values that $Pr$ and $Sh$ typically take in porous media. Therefore it is desirable to use the formulation in equations (5.7), (5.8), and (5.9) even though the buoyancy ratio and Lewis number may be less familiar parameters.

The boundary conditions transform in a straightforward way. Specifically, for salt concentration:

$$C_* = 1 \quad \text{at} \quad r_* = 1/2,$$

$$C_* = 0 \quad \text{at} \quad y_* = H/\Delta R,$$

$$\partial C_*/\partial n = 0 \quad \text{elsewhere on the boundary};$$
for temperature,

\[ T^* = 0 \quad \text{at} \quad y^* = 0, \]

\[ T^* = 1 \quad \text{at} \quad y^* = H/\Delta R, \]

\[ T^* = a_0 (H/\Delta T) (1-y^*) \quad \text{at} \quad r^* = 3/2, \]

and

\[ T^* = a_1 (H/\Delta T) (1-y^*) \quad y^*_h < y^* \quad \text{at} \quad r^* = 1/2, \]

\[ T^* = a_2 (H/\Delta T) (1-y^*) + b_2 \quad y^*_h \geq y^* \]

where \( y^*_h \) is the proportion of the vertical scale penetrated by salt. Streamline boundary conditions apply to \( \Psi^* \).

For given boundary conditions and dimensionless parameters, equations (5.7), (5.8), and (5.9) are solved numerically. Copious numerical simulations are required in order to evaluate the specific influences that variations in boundary conditions and dimensionless parameters have on controlling groundwater flow. Nonetheless from the form of the dimensionless equations I am now able to impose a priori reasons for choosing to vary specific parameters and boundary conditions with the goal of evaluating flow near salt columns.

In the numerical calculations presented below I use values of \( \text{Le}=100, \text{Ra}=50 \), and I vary the buoyancy ratio over the range \( 0 \leq \text{Nu} \leq 1.5 \). For \( \text{Le}=100 \) heat will diffuse 100 times faster that dissolved salt over a given distance. This value
is quite reasonable for diffusion through a porous medium. Moreover, even large departures from the chosen values of Le and Ra do not significantly change the groundwater flow patterns.

5.2 Numerical Implementation

Equations (5.7), (5.8), and (5.9) were discretized using Taylor series formulation finite differences with upstream weighting for the temperature and concentration fields. The finite difference analogs to equations (5.7), (5.8), and (5.9) were decoupled and solved iteratively using under-relaxation (Chapter 4). Iterations were repeated until changes in each of the flow variables $T^*$, $C^*$, and $\Psi^*$, were reduced by less than a specified cutoff value between successive iterations. Convergence was verified for several representative cases by starting the simulations with a variety of initial guesses, and by reducing the cutoff value.

The difference equations take the form of sparse matrix equations [e.g., Patankar, 1980]. The form of these equations in my model lends itself to efficient solution techniques. This is an important consideration because a large number of numerical simulations are required in order to make accurate inferences from the calculations, and because the coupled nature of the equations requires iterative numerical procedures that may take scores of
iterations to converge for complex boundary conditions.

In particular, the present model is ideally suited for solution by a multigrid finite difference solution [Brandt, 1977; Jespersen, 1984]. In the multigrid algorithm the partial differential equations are formulated as difference equations on a dense grid. For my purposes node spacing in the radial coordinate is uniform, as is spacing in the vertical direction. The resulting sparse matrix equations are solved by an iterative method (Gauss-Seidel in my model). The advantage of the multigrid method arises in that only a few iterations (2 or 3) are carried out on the original dense grid. The solution vector after these few iterations has large errors which are subsequently corrected by calculations on progressively coarser grids; the correction terms are then interpolated onto the denser mesh. Thus most of the computation is done on coarse grids, for which the iterative procedure is expedient.

The multigrid method exploits the fact that iterative techniques are very efficient in reducing high frequency components of error [Brandt, 1977], but less effective in reducing the low frequency error components. Consequently with most iterative techniques the major computational expense is in reducing low frequency error. With multigriding, low frequency residuals are transferred to a coarser grid on which they are relatively high frequency.

Multigridning is especially appropriate for coupled flow
problems in which transport near the center of the mesh may be important (e.g. salt plumes, or localized cells) and where dense node spacing is required in order to minimize false diffusion. In these cases grids that are fixed \textit{a priori} may not be suitably dense in the regions of interest, and adaptive grids [Thompson \textit{et al.}, 1985] would require separate adaptation for each of the flow fields. In contrast, the multigridding technique subjects each of the flow fields to coarsening grid corrections for each iteration. In each case convergence is called on the basis of calculations done at the finest grid level. In these computations the finest grid contained 31x31 active nodes, with coarsening grid corrections down to 3x3 active nodes in 3 steps. This technique reduced computational time by more than a factor of 3 from that of a pointwise successive overrelaxation technique.

An extensive review of multigridding algorithms is provided by Jespersen [1984], where the author points out that the number of applications of multigridding techniques is small relative to the preponderance of theoretical literature on the method. In part this discrepancy exists because many applications, while being computationally expensive, are not so large as to warrant the additional overhead and programming difficulties associated with multigridding. This is particularly true for very general numerical models in which heterogeneities and general
geometries make multigridging especially cumbersome. To some extent, the latter problems are avoided through the use of dimensional analysis: I seek solutions to simplified equations on a rectangular domain. Furthermore, the computational overhead and programming difficulties pay off here because the same multigridding algorithm is applied similarly to each of the transport equations, and because the nonlinearities in the governing equations require an iterative solution procedure.

Each of the dimensionless transport fields (i.e. equations (5.7), (5.8), and (5.9)) is represented as a second order differential equation of the form.

\[ a_1 \frac{\partial^2 u}{\partial y^2} + a_2 \frac{\partial^2 u}{\partial r^2} + a_3 \frac{1}{r} \frac{\partial u}{\partial r} + a_4 \frac{\partial u}{\partial y} = a_5 \]

which is discretized using a Taylor series finite difference formulation. This leads to a banded matrix equation

\[ A^{(0)} u = f \] (5.10)

In equation (5.10), each row of the matrix equation takes the form

\[ a_{i,j} u_{i+1,j} + b_{i,j} u_{i-1,j} + c_{i,j} u_{i,j+1} + d_{i,j} u_{i,j-1} + e_{i,j} u_{i,j} = f_{i,j} \] (4.3)

In the standard Gauss-Seidel method, equation (4.3) is
solved iteratively:

\[ u_{i,j} = \left( \frac{1}{e_{i,j}} \right) \left[ f_{i,j} - a_{i,j}u_{i+1,j} + b_{i,j}u_{i-1,j} + c_{i,j}u_{i,j+1} + d_{i,j}u_{i,j-1} \right] \quad (5.11) \]

Similarly for the multigrid method iterations of (5.11) are carried out, but typically for only 2 or 3 iterations (Brandt, 1977). In the parlance of multigridning, these iterations are call relaxation sweeps. After a few relaxation sweeps residuals of the form

\[ \mathbf{r}^{(1)} = \mathbf{f} - \mathbf{A}^{(0)}\mathbf{u} \]

are transferred to a coarser grid containing \((\lfloor (N-1)/2+1 \rfloor) \times \lfloor (N-1)/2+1 \rfloor\) active nodes. I transfer residuals by injection (Jespersen, 1984) — that is, by simply dropping alternate nodes. On the coarser grid I then solve the matrix equation

\[ \mathbf{A}^{(1)}\mathbf{e}^{(1)} = \mathbf{r}^{(1)} \quad (5.12) \]

where \(\mathbf{e}^{(1)}\) represents a coarse grid correction to equation (5.11). Equation (5.12) is in turn solved by making a few relaxation sweeps (Gauss-Seidel iterations) and injecting the residuals onto a yet coarser grid to get correction terms \(\mathbf{e}^{(2)}\); relaxation and injection is continued until correction terms are calculated on a sufficiently coarse grid. The coarse-grid corrections are then imposed on successively finer grid levels through bilinear interpolation, and the whole procedure is repeated until convergence in reached.
The elements of the coefficient matrix in equation (5.10) result from finite difference discretization of transport equation; such a discretization results in a value for the spatial distance between nodes occurring in the denominator of each coefficient. Consequently, each coefficient decreases by some power of 2 with each grid coarsening. It is therefore possible for variations in the coefficient matrix at each grid level to be accommodated entirely through the relaxation sweeps, which is expedient.

In discretizing equations (5.8) and (5.9) I use full upstream weighting for advection terms. The coefficients for the diffusive component (i.e., the right-hand side) is unity; upstream weighting is equivalent to increasing this by an additional value proportional to half the node spacing (or 1/64 in these calculations). I conducted additional simulations using 63x63 active nodes, achieving similar results to those for the coarser grid. From these calculations I concluded that the increased numerical precision did not warrant the increased computational expense of using the dense grid for the bulk of the calculations.

5.3 Results

The interaction of temperature and concentration effects leads to a wide variety of calculated flow patterns near salt domes. This is evidenced by the numerical simulations in which I systematically varied the thermal boundary conditions
and the value of the buoyancy ratio. Boundary conditions were varied by prescribing different thermal gradient contrasts between salt and overlying sediments. In this model clockwise circulation produces flow that is up along the salt, and counterclockwise circulation is down along the salt. Figures 5.2 through 5.4 demonstrate that either clockwise (Figure 5.2a) or counterclockwise (Figures 5.3a and 5.4a) convective circulation is possible near the salt column. In the former case the upturned isotherms are sufficient to cause some decrease in density near the salt; this drives groundwater toward the salt boundary and initiates the circulation such that flow is up along the salt column, as observed in Figure 5.2a. Because of the large value of the Lewis number in sediments (Le=100), advective transport dominates over diffusion, and a salt plume extends away from the top of the salt column as a result of upward flow (Figure 5.2b). Advective heat transport does not significantly modify the isotherms because thermal conduction through the salt is relatively efficient given the low Rayleigh numbers used (Figures 5.2b, 5.3b, and 5.4b).

When the isotherms are pulled up less dramatically (Figure 5.3b), or when the absolute value of the buoyancy ratio is larger (Figure 5.4), the radial temperature variations are insufficient to overcome the increased salt content in groundwater; and as salt diffuses away from the boundary, salt-laden groundwater sinks adjacent to the salt
Figure 5.2 Mass stream lines (a), isotherms and concentration contours (b), for simulations using a buoyancy ratio of $N=-0.5$ and boundary conditions representing a thermal conductivity contrast of 8 between the salt and overlying sediments. The stippled region represents that part of the boundary that is modelled as salt. Note that convective flow is up along the salt edge, and that a salt plume forms near the top of the salt column. A weaker, counter-clockwise cell occurs at depth.
Figure 5.3 Mass stream lines (a), isotherms and concentration contours (b), for simulations using a buoyancy ratio of $N=-0.5$ and boundary conditions representing a thermal conductivity contrast of 4 between the salt and overlying sediments. In this case the isotherms are not elevated as dramatically as in Figure 5.2b, consequently salt-laden water sinks adjacent to the salt dome. Upward flow near the top of the salt is very small.
Figure 5.4 Mass stream lines (a), isotherms and concentration contours (b), for simulations using a buoyancy ratio of $N=-1.0$ and the same boundary conditions as in Figure 5.2. Here dissolved salt asserts stronger influence on water density, and salt-laden water sinks.
column (Figures 5.3a and 5.4a). In these cases there is still some clockwise circulation near the top of the salt, but the size and vigor of the upper convection cell is diminished. There is a continuous variation between the flow patterns presented, and in some circumstances the circulation in the upper clockwise cell and the lower counterclockwise cells may be equivalent. It is important to note that the upper (clockwise) cells tend to be localized and are not strongly influenced by the boundary conditions. The lower (counterclockwise) cell extends to the entire radial width of the model, and therefore return flow results for the no flow boundary condition.

The trade-off between the thermal boundary conditions and the buoyancy ratio is represented in Figure 5.5, which is based on 24 separate steady-state simulations. In these simulations I systematically varied the thermal gradient contrast on the edge of the model, and the value of the buoyancy ratio. Variations in these two parameters are represented on the axes of Figure 5.5. The horizontal axis in Figure 5.5 represents changes in boundary conditions, or how sharply isotherms are drawn toward vertical near the salt; and the vertical axis gives values of the buoyancy ratio. In this figure I have contoured the sum of the maximum value of the stream function in the lower counterclockwise cell (for which $\Psi_* > 0$) and the upper clockwise cell (for which $\Psi_* < 0$). This sum is a measure of
Figure 5.5 A contour plot of the sum of the minimum and maximum values of the dimensionless mass stream function. These are the values of $\Psi_*$ at the centers of the upper and lower convection cells in Figures 5.2, 5.3, and 5.4. For positive contour values the lower cell dominates and flow is primarily down along the salt edge. For negative values (the shaded region) the upper cell dominates and flow is mainly up along the salt column.
the relative sizes of the two convection cells. When the sum is positive, the lower cell is larger than the upper cell (i.e., it transports more groundwater per radian), and flow is predominantly down along the salt column. For negative values contoured in Figure 5.5 (the shaded region) the upper cell is dominant, and flow is mostly up along the salt. For values of buoyancy ratio and conductivity contrast that fall along the zero contour, two opposing cells are transporting equivalent volumes of groundwater; the zero contour does not indicate the absence of flow.

The values of thermal conductivity contrast and buoyancy ratio shown in Figure 5.5 indicate some of the conditions in which dominantly clockwise or counterclockwise flow is possible. The conductivity contrasts represent the upper extreme of values expected in nature, although other factors can also influence the contrast in thermal gradient (see Discussion). For example, a value of $K_{salt}/K_{sed}=10$ would indicate a contrast between salt and water, and a value of $K_{salt}/K_{sed}=4$ would apply to salt overlain by sediments with 30% to 40% porosity. Values of the buoyancy ratio expected in nature will probably vary between about 0 and -2, with a value of $N=0$ indicating no variation is groundwater salinity, and a value of $N=-2$ indicating salinity varying from fresh water to salt saturation over a temperature difference of 100°C. Over the same temperature difference, salinities that go from fresh to sea water concentrations would give $N=-0.25$. 
For given thermal conditions the buoyancy ratio will depend primarily on the overall regional variation in salt concentration. For example, when groundwater has high salt concentrations regionally, the solute introduced by the salt column may have little effect on the variations in groundwater density; whereas a salt column introduced into fresh groundwater will greatly affect groundwater density. Studies that consider only thermal convection and neglect solute effects on groundwater flow tacitly assume a buoyancy ratio of $N=0$, and studies that consider only solute effects assume an infinite buoyancy ratio.

It is possible to estimate the magnitude of the Darcy flux, $q$, by multiplying the dimensionless mass flux by 
\[(gk\Delta T\beta_T/\nu)\]. For reference I assume values of $g=9.8\text{m/s}^2$, $k=10^{-14}\text{m}^2$ ($\approx 0.01$ Darcy), $\Delta T=100^\circ\text{C}$, $\beta_T=-0.001$, and $\nu=10^{-6}\text{m}^2/\text{s}$.

These values yield maximum velocities of 1.78 cm/year, 1.27 cm/year, and 2.34 cm/year for Figures 5.2a, 5.3a, and 5.4a, respectively. Velocities will scale roughly in proportion with the permeability.

The results presented indicate that it is possible to get thermally induced upward flow along the flank of a salt column even in the presence of salt dissolution. When this occurs, there is likely to be a large contrast in thermal gradient between the salt and overlying sediments, possibly as a result of high sediment porosity. The contour values and spacing in the shaded region of Figure 5.5 indicate that
upward (clockwise) flow has the potential of being much more vigorous than flow driven by sinking salt water. On the other hand, the geologic conditions for which thermally driven convection near salt domes is possible appear to be quite limited.

5.4 Discussion

The dimensional analysis and calculations presented here demonstrate that large variations in the groundwater flow field will occur as a result of fairly subtle changes in the boundary conditions and the dimensionless buoyancy ratio, that is, the ratio of solute to temperature effects on groundwater density. In some circumstances free convection appears to be an adequate mechanism for driving groundwater up along the flank of the salt column when isotherms become sub-vertical near the salt. In these cases, thermal effects decrease fluid density near the salt and induce upward flow provided the buoyancy ratio is not too large. However, flow that is down along the salt dome appears to be the dominant pattern over a large range of buoyancy ratios and boundary conditions. The sense of convection depends on a complex trade-off between how sharply isotherms are pulled up at the salt edge, and the overall variation in salt concentration.

In specifying boundary conditions is this study, the important thermal factor is the contrast in temperature gradients from the salt to the sediments. For convenience, I
have parameterized this contrast with the ratio of thermal conductivities, but other processes may be even more important in elevating isotherms in the salt. Particularly important may be time since diapirism. The effects on groundwater flow will be to induce upward flow along the salt column, even in the presence of larger salinity contrasts. This also suggests that more detailed, time-dependent analysis is warranted. It is worth noting that all observations of upward flow along the salt column have been made in the Tertiary section of the northern Gulf Coast where diapirism has been fairly recent.

Through dimensional analysis I am able to reduce to three the number of parameters that control the simulations: the Rayleigh number, the Lewis number, and the buoyancy ratio. The last of these most strongly affects the flow field, as evidenced by examining the dimensionless transport equations (5.7), (5.8), and (5.9). By formulating the problem in terms of mass flux I avoid imposing the Boussinesq assumption, which can be inappropriate for solutions with large salt concentration gradients.

Dimensional analysis has the desirable consequence of allowing us to more directly investigate the mechanisms that drive flow; in particular it allows us to predict the nature of boundary conditions that are required for free convection to be responsible for the flow patterns that are interpreted from field data [Hanor, 1987]. In order for dimensional
analysis to provide useful insight, it is necessary to make several assumptions about the nature of the medium and fluid. Specifically, I have assumed that the medium is homogeneous and isotropic, that the fluid is of constant viscosity, and that molecular dispersion is negligible (or it is constant and is incorporated into D'). Relaxing these assumptions might change the details of the calculated flow patterns but will not affect the general conclusions of this study.

The general consequences of these assumptions can be examined qualitatively by returning to equations (5.7), (5.8), and (5.9), and the dimensionless parameters. For example, where groundwater flow velocities are high, increased dispersion would locally decrease the Lewis number, so that advective salt transport is decreased somewhat. This would tend to broaden the salt front. Advective salt transport, however, would still be expected to dominate over diffusive-dispersive transport. Similarly, variations in groundwater viscosity would locally alter the importance of heat and salt transport because viscosity appears in the denominator of the Rayleigh number, which multiplies the advective transport terms. This would have the greatest effect on heat transport since advective salt transport is also affected by the Lewis number. The assumption that density varies linearly with temperature and salinity (i.e. that $\beta_T$ and $\beta_C$ are constant) has relatively little consequence compared to limitations imposed by other assumptions.
The most limiting assumption of this analysis is that of a homogeneous, isotropic medium. This assumption may make the dimensional analysis approach inappropriate for studying details of coupled transport near specific salt domes. Variations in stratigraphy near salt domes can be very complex [Seni and Jackson, 1983], and is often structurally modified by halokinesis. In some cases the vertical permeability will be considerably smaller than the horizontal permeability because of interbedded shales and sands. In other cases the effective vertical permeability may be relatively large because vertical faulting is common near salt domes. There is good evidence of groundwater being channeled up along such faults [Bennett and Hanor, 1987; Land et al., 1988; Jensenius and Munksgaard, 1989]. So, sediments near salt domes will be heterogeneous and anisotropic, but it is difficult to make generalizations about the nature of these variations.

As with other assumptions mentioned, the steady-state conditions were used in order to facilitate our understanding of the physical processes. Nonetheless, calculations presented here may have interesting implications for temporal evolution of groundwater flow near salt domes. For example, present-day groundwater salinities in Tertiary sediments of the Gulf Coast are commonly as high as 100 g/l over a large regional extent [Hanor et al., 1986]. In terms of the present analysis, such large regional salinities would lead
to buoyancy ratios with rather small absolute values, increasing the likelihood that circulation is up along the salt edge. In as much as the regional salinities result from salt dissolution [Hanor et al., 1986; Morton and Land, 1987] present values of the buoyancy ratio may be smaller (in absolute value) than values that existed shortly after diapirism. Consequently, it may well be that thermal effects presently have a greater influence on groundwater flow than at previous times. On the other hand, if isotherms are subvertical because of recent diapirism, then the temperature distribution along the vertical boundaries would change with time due to cooling, making the thermal conditions less important with time. With these scenarios convective groundwater flow may actually reverse with time as individual domes and regional salinities develop.

In spite of the limitations mentioned above, these calculations were able to reproduce many of the features of the salinity, temperature, and flow fields that are observed near some salt diapirs [cf. Hanor, 1987], namely upward flow of groundwater flow along the salt edge and a salinity plume that extends from the top of the salt column (Figure 5.2), although these conditions occur for a limited range of buoyancy ratios and boundary conditions. The presence of a salinity plume results from the high value of the Lewis number in porous media, making the salinity field very sensitive to groundwater flow. This is particularly true
near the top of a salt dome when saline fluid is transported advectively upward into relatively fresh groundwater. The details of the groundwater flow paths through actual sediments are difficult to establish either from numerical calculations or from the work of Hanor [1987]. The general trends, however, are in good agreement.
CHAPTER 6

EFFECTS OF THERMAL CONDUCTIVITY CONTRASTS AND SALT DIAPIRISM

To account for the geological behavior of the earth, it is necessary to postulate not only adequate heat sources, but also a "structure" of some kind. A structureless, formless, isotropic sea of heat is geologically useless.

John Verhoogen, 1980
(From Energetics of the Earth)

In the previous chapter I established the thermal boundary conditions and regional salinity variations that are required in order for free thermal convection to drive groundwater up along the edge of a salt column. Specifically, it was established that isotherms must be subvertical near the salt dome flank, causing lateral heat flow into the sediments and salinity variations must not be too severe. These results lead naturally to questions about how and when such conditions arise in the natural salt dome environment. Appropriate values of the buoyancy ratio are likely to arise naturally in the salt dome setting. For example, values of the buoyancy ratio between 0 and about -0.75 appear to be necessary in order for thermal effects to drive groundwater up the flank of a salt dome. Buoyancy ratios within this range will occur when regional salinity varies over about 80 parts per thousand while temperature varies over about 100°C. Constraints on the thermal boundary conditions may be more difficult to satisfy under natural conditions.
In the present chapter I address questions regarding the likelihood that the necessary thermal boundary conditions (as posited in Chapter 3) will result from thermal conductivity contrasts or salt diapirism. That is, I evaluate when these processes could be responsible for causing isotherms to turn up sharply near the salt-sediment interface. The fact that isotherms do become subvertical near salt domes is not at issue here. Such observations have been made by several workers [e.g., Selig and Wallick, 1966; Jensen, 1983; Leger, 1988].

Any combination of three physical mechanisms may be responsible for elevating isotherms near salt domes (as in Figure 5.2b). These were mentioned earlier and are: 1) thermal conductivity contrasts between salt and sediments; 2) rapid diapirism that causes hot salt to be emplaced within cooler sediments; and 3) convective transport of heat by groundwater flow. Each of these is discussed in turn forthwith. The first two mechanisms are discussed in the remainder of this chapter and are found to be unlikely candidates for the requisite thermal conditions. Convective mechanisms are discussed in Chapter 7. Other possible heat sources which are not considered in this dissertation include enthalpy of salt dissolution, frictional heating of sediments during diapirism, and heat of annealing during salt crystal deformation. Salt dissolution is endothermic at the temperatures and pressures of interest [Chase et al., 1985], and so would tend to cool, rather than heat, the surrounding
environment. Little or no data are available on frictional or viscous heating during salt deformation, but it is doubtful that such effects could be responsible for significant heat accumulation. Selig and Wallick [1983] attempted to incorporate frictional heating in some thermal calculations and determined that only a small thermal anomaly resulted even when 100% of the work done by gravity during diapirism went to frictional heating, clearly an extreme estimate.

6.1 Thermal Conductivity Contrasts Between Salt and Sediments

Contrasts in thermal conductivity of materials determines the position of isotherms under steady-state conditions. Under transient conditions temperatures locally are controlled largely by conductivity, but also depend on density and specific heat. The thermal conductivity of rock salt is strongly temperature dependent, whereas the conductivity of sediment depends mostly on porosity. Therefore for given temperature and porosity ranges, we can estimate the expected conductivity contrast and compare the results with the conductivity contrasts required to drive upward flow at a given buoyancy ratio, as indicated in Figure 5.5.

The most common method of estimating the thermal conductivity of saturated porous material is a weighted
average of solid and fluid conductivity values [Dagan, 1972; Voss, 1984; Garven and Freeze, 1984]:

\[ K_m = K_f \phi + (1-\phi)K_s \]  \hspace{1cm} (6.1)

where \( K_f \) and \( K_s \) represent the conductivity of fluid and solid respectively, \( K_m \) is the conductivity of the saturated porous medium, and \( \phi \) is porosity. However, the physical distribution of pore space will also influence conductivity estimates. With this consideration (6.1) represents a maximum thermal conductivity [cf. Domenico, 1977]. Hashin and Shtrikman [1962] suggest that a lower bound on conductivity is given by

\[ K^{\text{lb}} = K_f + \frac{\phi}{1/(K_f-K_s) + \phi/3K_f} \]  \hspace{1cm} (6.2)

These conductivity bounds are shown graphically in Figure 6.1.

The thermal conductivity of rock salt is highly variable and strongly dependent on temperature. In addition, it is influenced by lattice imperfections, and the abundance and type of impurities [NBS Monograph 167, 1981]. Nonetheless, recommended values of rock salt thermal conductivity have been established as a function of temperature [NBS Monograph 167, 1981], and are given in Table 6.1 and Figure 6.2. For computational purposes it is convenient to establish a functional form of conductivity versus temperature, and the
Table 6.1 Recommended Values for the Thermal Conductivity of Rock Salt
(from NBS Monograph 167 [1981])

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Conductivity (Wm⁻¹°C⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-23</td>
<td>8.24</td>
</tr>
<tr>
<td>20</td>
<td>6.65</td>
</tr>
<tr>
<td>27</td>
<td>6.57</td>
</tr>
<tr>
<td>127</td>
<td>4.80</td>
</tr>
<tr>
<td>227</td>
<td>3.67</td>
</tr>
</tbody>
</table>
Figure 6.1 Thermal conductivity of saturated sediments as a function of porosity based on equations (6.1) and (6.2).
Figure 6.2  Thermal conductivity of salt rock versus temperature. Solid circles indicate recommended values \([NBS Monograph 167, 1981]\) and the curve is based on the least squares fit given in equation (6.3).
data in Table 6.1 are well fit by an exponential curve of the form

\[ K_{\text{salt}}(T) = 7.354 \exp(-0.0031575T) \quad (6.3) \]

correlation coefficient, of 0.989). This curve is also plotted in Figure 6.2 for visual comparison. Equation 6.3 is used in this and subsequent chapters to estimate salt conductivity.

Using equations (6.2) and (6.3), it is now possible to estimate contrasts in thermal conductivity that are likely to occur between salt and surrounding sediments, as well as how conductivity contrasts vary with temperature and sediment porosity. Thermal conductivity contrast is represented by the ratio

\[ \frac{K_{\text{salt}}}{K_m} \]

which is contoured in Figure 6.3 for values of \( \phi \) between 0 and 100% and for temperatures between 0°C and 300°C. From Figure 6.3 it is evident that conductivity contrasts greater than about 6 are possible at high porosity and low temperatures, that is, at very shallow depths. Recall that such high contrasts are necessary for free convection to circulate groundwater up salt dome edges, although this is not a sufficient condition because a buoyancy ratio within a specific range is also required.

Superimposed on the contours in Figure 6.3 are curves representative of porosity variation with temperature for
Figure 6.3 A contour plot of the predicted thermal conductivity contrast between salt and sediments as a function of porosity and temperature. The superimposed curves are representative porosity versus temperature curves for sandstones and shales. Conductivity contrasts in excess of 6 are required for dominantly upward convection with a buoyancy ratio of -0.5.
sandstones and shales. For these curves I have simply used well established porosity-depth curves [e.g., Magara, 1980] and assumed that temperature increases by 25°C with every kilometer of depth. The superposition of these porosity-temperature curves on the conductivity contrast surface indicates the conductivity contrasts that are likely to be encountered in nature, and shows that only under very limited conditions will the conductivity contrast be large enough to elevate isotherms to the point that they can drive groundwater up the edge of a salt dome. Thus while free convection may explain the observed groundwater flow patterns, the observation that isotherms are subvertical near the salt is not justified by thermal conductivity contrasts alone, except in rare natural circumstances when the top of salt is near the earth's surface so that sediment porosities are high, or when geothermal gradients are high.

6.2 Elevated Temperatures Following Salt Diapirism

In this section I present calculations on the time-dependent cooling history of salt and sediments in order to establish the extent to which rapid diapirism is responsible for elevating isotherms in sediments. All calculations in this section are for conductive cooling because it will provide a conservative (i.e., an upper bound) estimate of the time of cooling. Two types of calculations are presented: an analytical scaling solution that determines a characteristic time interval for cooling, and a numerical calculation for a
cooling diapir that is emplaced instantaneously. Both calculations indicate that a salt diapir cools at a rate considerably greater than the rate of diapirism, making it unlikely that rapid diapirism is responsible for the subvertical orientation of isotherms near salt domes.

Cooling of an instantaneously emplaced salt diapir is a heat transfer problem that is exactly analogous to the cooling of an igneous intrusion. The latter problem has been studied extensively with both numerical and analytical techniques [e.g., Turcotte and Schubert, 1982; Harrison and Clarke, 1979]. A characteristic time for cooling, $t_c$, can be estimated from simple algebraic considerations. The characteristic time is an estimate of the time required for a point some distance, $y$, to be heated to its maximum temperature following diapirism. In the present case, the characteristic time will be compared to a typical time required for salt to move by forced intrusion over the same distance, $y$.

Consider an instantaneously emplaced diapir of temperature $T_d$, as indicated schematically in Figure 6.4. Vertical heat flow from such a diapir into the surrounding sediments is given dimensionally by

$$q_h = K_m T_d y$$

and the total heat provided (per area) by such a diapir after a time $t_c$ is
Figure 6.4 A schematic diagram illustrating a salt diapir emplaced instantaneously into colder sediments.
Moreover, the total heat accumulated in the sediments (6.5) (per area) is proportional to the depth of emplacement and $T_d \cdot Q_h = cT_d y$

Equating (6.4) and (6.5) and solving for $t_c$ gives

$$t_c = \frac{y^2 \rho c}{K_m}$$

or

$$t_c = \frac{y^2}{K}$$

where $K$ is the thermal diffusivity of the sediments.

Now choosing $y=1$ km (a convenient and realistic value for depth to salt) and assuming $K = 10^{-6}$ m$^2$/sec gives a characteristic cooling time of

$$t_c = 10^{12} \text{sec} = 31,688 \text{ years}$$

Thus it takes on the order of 30,000 years for heat provided by intruded salt to be conducted 1 km. In contrast, it takes on the order of 1 Ma for salt to be intruded by diapirism (Chapter 2). Apparently, heat is removed by conduction at a rate considerably greater than it is supplied by diapirism, and we would expect no significant buildup of heat. Because forced intrusion provides the greatest perturbation to the temperature field, this calculation probably overestimates
the time of cooling, especially for structures that form by downbuilding.

These scaling arguments are verified with a simple numerical calculation of conductive cooling. The geometry sketched in Figure 6.4 is discretized on a finite difference mesh and the heat conduction equation

\[
\frac{1}{r} \frac{\partial}{\partial r} (r K \frac{\partial T}{\partial r}) + \frac{\partial}{\partial y} (K \frac{\partial T}{\partial y}) = \rho c_m \frac{\partial T}{\partial t}
\]  

(6.6)

is solved numerically with a finite difference code (see appendix). The numerical solution allows me to explicitly incorporate the high thermal conductivity of salt into the calculation and also provides for the finite volume of salt. The initial and boundary conditions for this calculation are indicated in Figure 6.5, and represent a hot body of salt at 125°C cooling within a porous medium that initially contains a linear temperature gradient from 0°C to 125°C.

Results of the numerical calculations are given in two graphical forms: contours of the temperature field after 25 thousand, 50 thousand, and 100 thousand years (Figure 6.6), and as a plot of how close the cooling system is to steady-state conditions over a 100,000 year period (Figure 6.7). In both figures it is apparent that the salt-sediment system reaches thermal equilibrium within a few tens of thousands of years. Again this indicates that salt probably cools off by conduction nearly as fast as it is intruded.
Figure 6.5 A diagram illustrating the boundary conditions and finite difference mesh used in finite difference calculations for diapir cooling.
Figure 6.6  Contours of the temperature field around a cooling diapir (that was initially 125°C) after 10, 20, and 50 thousand years.
Figure 6.7 A cooling curve for an instantaneously emplaced salt diapir. This curve represents how close the simulation results are to steady state conditions as a function of time.
6.3 Discussion and Conclusions

In this chapter I have tried to assess the plausibility of two different physical mechanisms that could be responsible for producing the thermal boundary conditions posited in the previous chapter -- boundary conditions that cause significant lateral heat flow near the salt-sediment interface on a salt dome flank. Under some circumstances the contrast in thermal conductivity between salt and overlying sediments can be large enough to elevate isotherms sufficiently for thermal effects to drive upward convection near the salt flank, provided the buoyancy ratio is small enough. These circumstances, however, will be rare and will only occur when the salt is overlain by very high porosity sediment. By the same token diapirism itself cannot supply heat more rapidly than it is conducted away through the sediments. Consequently it is unlikely that isotherms can be elevated very much due to diapirism, even if diapirism occurs at a rate of several kilometers per million years. It is doubtful that this conclusion could be affected by heat provided by friction during diapirism.

In many circumstances, therefore, it is reasonable to conclude that subvertical isotherms observed near some salt domes results from heat advection due to vertical groundwater flow. This inference appears to be at odds with the conclusions of the previous chapter. In Chapter 5 the subvertical orientation of isotherms was used to drive
vertical groundwater flow; while here it was concluded that vertical flow must be responsible for the position of the isotherms. But the latter conclusion could not have been drawn without the former: the calculations in Chapter 5 addressed the question of what conditions are necessary for thermohaline convection to drive groundwater up the salt column, whereas the present chapter has examined when the needed thermal conditions are likely to exist.
CHAPTER 7

COUPLED FLOW NEAR AN EVOLVING SALT DIAPIR

"Communicating then with the great reservoir of salt-water, and fed through submarine fissures, the volcanic caldron had no need of any fuel to produce great masses of salt."

Raymond Thomassay, 1860, on the origins of Louisiana salt volcanoes and salt springs

From Geologie Pratique de la Louisiane

The simulation results presented heretofore used highly simplified models of the salt dome setting and were employed to provide insight into the physical transport processes near salt domes. A comprehensive numerical model of coupled transport in sediments was presented in Chapter 4 and includes variable medium properties, time-dependent solute transport, and basin subsidence. In this chapter I present numerical simulations that employ this more general model. The objectives of these simulations are: 1) to determine the extent to which salt diapirism is responsible for creating salinity inversions that could lead to upward groundwater flow; 2) to more rigorously evaluate the thermal consequences of groundwater flow near an evolving salt diapir; 3) to assess the general sense and magnitude of groundwater flow near a growing salt diapir; and 4) to establish the fundamental nature of the physics of coupled transport near evolving salt diapirs.

In the northern Gulf Coast many salt domes are flanked by producing oil or gas fields. In many cases hydrocarbon emplacement is apparently the result of vertical fluid
migration [Hanor and Sassen, 1989]. This inference is supported by diagenetic studies that indicate that components of some cements are sourced at depth [Land et al., 1987; Posey and Kyle, 1988; McManus, ms. in prep.]. Clearly the migration of hydrocarbons is closely linked to groundwater flow, and our understanding of groundwater, heat, and dissolved salt transport is thus an important step in understanding the migration and emplacement of hydrocarbons.

This study is the first effort to apply a comprehensive numerical model to the study of groundwater near salt domes. The numerical simulations presented below are designed to incorporate the important physical elements of groundwater flow near salt domes. These include explicitly coupling the temperature, salinity, and flow fields; using a radially symmetric cylindrical geometry; incorporating spatial variations in medium properties; and accounting for active diapirism and basin subsidence. The results of these simulations provide insight into the rates and direction of groundwater flow, the thermal consequences of groundwater flow, and the rates and nature of dissolved salt transport near salt domes.

Specifying initial conditions for groundwater salinity can be problematic when simulating hydrologic conditions over millions of years because solute transport may take place at a rate comparable to the structural evolution of the basin. This is especially true near salt domes because the salt structure itself is the solute source. For example, if
solute transport is modeled using a static salt geometry, then the proper initial conditions must reflect the salinity conditions as they existed when the structure first assumed the specified geometry; but we have no way of knowing a priori what those conditions were. For this reason it is important to model flow near salt domes by using a model that accounts for basin subsidence and salt diapirism as well as time dependent solute transport.

In this analysis my emphasis is on whether salt diapirism is responsible for creating upward groundwater flow near salt domes. In as much as a nearly infinite combination of conditions could be incorporated into geologically reasonable simulations, I have chosen to run simulations under conditions that will tend to maximize the possibility of upward flow, provided they are representative of actual salt domes conditions.

7.1 Conceptual Model

The structural evolution of salt diapirs was discussed in some detail in sections 2.2.2 through 2.2.5, and will be briefly reviewed here for the sake of continuity. In the Gulf of Mexico most salt domes develop structurally by a downbuilding processes [Barton, 1933; Seni and Jackson, 1983] in which the top of the salt column remains stationary while the surrounding sediments subside due to continued deposition. Recall that salt dome evolution can be divided into three stages: the pillow stage, the diapir stage, and
the post-diapir stage. In this study I am mainly interested in evaluating groundwater flow during the diapir stage when salt is mobilized into a cylindrical column. During the diapir stage, salt is provided to the growing salt column by deflating the surrounding salt bed (Figure 1.6). Salt deflation creates peripheral basins that fill with sediments. Salt diapirism can be as rapid as several kilometers per million years but more commonly is on the order of a few hundred meters per million years [Ramberg, 1981; Seni and Jackson, 1983; Lobao and Pilger, 1985].

Vertical variations in salt dome solubility result from variations in the lithology of surrounding sediments [Bennett and Hanor, 1987], from the existence of thin shale sheaths that blanket many salt structures [Atwood and Forman, 1959], and from exposure to fresh meteoric groundwaters [Bodenlos, 1970; Kyle and Price, 1986]. Commonly the top of salt will be the primary location for active salt dissolution.

Posey and Kyle [1988] suggested that the speed with which salinity plumes form near salt domes could be indirectly responsible for the occurrence of upward groundwater flow. Preferential dissolution of salt near the top of some domes could conceivably create salinity plumes near the dome crest, in a stratigraphically high position. If this occurs, it would cause groundwater density to decrease with depth, resulting in unstable conditions and leading to convective overturn. The flow of fresh meteoric groundwater across the top of the dome might enhance salt dissolution and extend the
lateral distribution of such salinity plumes.

Consider the schematic diagram of an evolving salt diapir as shown in Figure 7.1. Throughout its evolution the salt crest is exposed to meteoric groundwater flow, and active salt dissolution continually creates high salinity groundwater in a stratigraphically high position. As groundwater flows over the salt it transports dissolved salt laterally away from the incipient diapir (Figure 7.1a) extending high salinities well away from salt. During the diapir stage the surrounding sedimentary basin subsides and the dissolved salt is transported downward into the deep basin (Figure 7.1b). If most groundwater flow continues to be in the lateral direction, the plume that developed early may remain at shallow depths as the basin subsides. If this is the case, then a salinity inversion can occur which, coupled with increasing temperature with depth, would produce a density inversion and groundwater would be unstable. In addition, groundwater flowing away from the dome will create some viscous drag that could create eddy circulation adjacent to the dome. If these effects are strong enough they may allow vertical groundwater flow to extend to the top of the salt column leading to flow and salinity patterns similar to those inferred by Hanor [1987].

Groundwater flow near salt domes, then, is controlled by a combination of driving forces including thermal gradients, salinity gradients, and hydraulic head gradients, all of which are affected indirectly by salt diapirism and basin
Figure 7.1 Conceptual model of groundwater flow and salinity transport near a growing salt dome. Small arrows indicated the active supply of dissolved salt to groundwater near the crest of the dome, in a stratigraphically high position. Large arrows indicate possible directions of groundwater flow; solid lines indicate hypothetical salinity contours. Throughout its evolution the salt crest is exposed to meteoric groundwater flow, and active salt dissolution occurs. (a) Groundwater flowing over the salt pillow transports dissolved salt laterally creating high salinities well away from salt structure. (b) During the diapir stage the surrounding sedimentary basin subsides and the dissolved salt is continuously supplied to groundwater near the dome crest.
evolution. The relative influence of these driving forces will determine the details of the groundwater flow. Because of the strong interplay between these effects their relative importance is difficult to evaluate without a quantitative model that includes them all.

### 7.2 Mathematical Model

Heat and dissolved salt transport and groundwater flow near an evolving salt diapir are adequately described by steady-state heat and groundwater flow equations and time-dependent solute transport (see Chapters 3 and 6). The time-dependent equation must incorporate the effects of basin subsidence by including sediment subsidence in the advection term. The appropriate governing equations were derived in Chapter 3 and are

\[
\frac{\partial}{\partial r}\left(\frac{v}{k_{yy} r} \frac{\partial \psi}{\partial r}\right) + \frac{\partial}{\partial y}\left(\frac{v}{k_{rr} r} \frac{\partial \psi}{\partial y}\right) = -\frac{\partial p}{\partial r} \tag{3.38}
\]

\[
\frac{1}{r} \frac{\partial}{\partial r}\left(r k_T \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial y}\left(r k_T \frac{\partial T}{\partial y}\right) - \frac{1}{r} \frac{\partial}{\partial r}\left(r \rho c_q r T\right) - \frac{\partial}{\partial y}\left(\rho c_q y T\right) = 0 \tag{3.41}
\]

\[
\frac{1}{r} \frac{\partial}{\partial r}\left(r \rho \phi D_{rr} \frac{\partial C}{\partial r}\right) + \frac{\partial}{\partial y}\left(\rho \phi D_{yy} \frac{\partial C}{\partial y}\right) - \frac{1}{r} \frac{\partial}{\partial r}\left(r \rho q_r C\right) - \frac{\partial}{\partial y}\left[(\rho q_y + \rho \phi V) C\right] = \frac{\partial (\rho \phi C)}{\partial t} \tag{3.44}
\]

In order to achieve a solution to these equations, appropriate boundary conditions must be specified for all three transport fields, transport properties of the saturated
sediments must be specified, and discretized equations must be solved algebraically. The method of discretization was detailed in Chapter 4, and it remains to decide on appropriate boundary conditions and a method of solution.

7.2.1 Boundary Conditions

Boundary conditions for the heat transport equations are straightforward and easy to implement. A constant temperature of 20°C is prescribed along the top boundary, a constant heat flux of 60mW/m³ is prescribed on the lower boundary which is 10 km deep. These are representative values for near surface temperatures and regional background heat flow, respectively. The vertical sides are insulated.

Boundary conditions for the stream function and solute transport equations require more consideration. Conditions for the solute transport equation are designed to simulate constant salinity at the crest of the salt dome. Thus control volumes along the top of the salt dome simulate the region at which active salt dissolution takes place. This requires that constant salinity be specified at some internal nodes, not on the boundary of the finite difference mesh, leading to so called "internal boundary conditions." When solving for time-dependent solute transport at such nodes it is sometimes possible to simply reset the concentration values after each time step. This procedure is inelegant and unsatisfactory when several iterations are required for each time step, or when solving for steady-state conditions. A
more appropriate way of handling internal boundary conditions is also easy to implement and works in all circumstances.

Recall that the finite difference equations reduce to the form

\[ a_{i,j} u_{i+1,j} + b_{i,j} u_{i-1,j} + c_{i,j} u_{i,j+1} + d_{i,j} u_{i,j-1} + e_{i,j} u_i = f_{i,j} \]  

(4.3)

where \( u_{i,j} \) is dissolved salt concentration at node \((i,j)\), and \( f_{i,j} \) is determined by either boundary conditions or solute sources. For internal boundary conditions we cannot simply modify the value of \( f_{i,j} \) because we want to specify values of salinity per se, not values of solute flux. To impose internal boundary conditions at node \((i,j)\) such that we want to maintain the salinity there at a value \( u^*_i,j \), let

\[ e_{i,j} = S_{huge} \]

and

\[ f_{i,j} = S_{huge} u^*_i,j \]

where \( S_{huge} \) is a constant much larger than other coefficients in (4.3) (e.g., \( S_{huge} = 10^{30} \)). Then the solution of (4.3) is

\[ u_{i,j} = \frac{f_{i,j}}{e_{i,j}} \frac{S_{huge} u^*_i,j}{S_{huge}} = u^*_i,j \]  

(7.1)

which is the desired result. This is an extension of source-term linearization discussed by Patankar [1980], and is applicable provided an iterative solution procedure is used.

Other boundary conditions for solute transport include no
salinity at the top of the model, and no flux boundaries at the vertical edges. The former condition represents the presence of either shallow, fresh meteoric water at the water table, or the sediment-surface water interface.

The stream function formulation for groundwater flow allows for very general boundary conditions to be specified, [Polubarinova-Kochina, 1962; Bear, 1972]. Some modification of the boundary conditions for the conventional stream function is required in order to accommodate the mass stream function formulation presented in Chapter 3. Nonetheless several factors make application of hydrologic boundary conditions somewhat problematic in the salt dome environment. Salt domes occur in a wide variety of groundwater environments. In some cases the top of salt is actually sub-aerially exposed and subject to surface erosion. In other cases the top of salt may be below subaqueous sediments or quite deep and not exposed to meteoric waters. Indeed, a single dome may by exposed to different hydrologic regimes during different stages of its structural evolution. Salt dissolution is most active when salt is exposed to relatively fresh water aquifers [Bodenlos, 1970]; but aquifers in the northern Gulf Coast are generally recharged hundreds of kilometers north of south Louisiana salt domes [Williamson, 1986], which is well beyond the region that could be practically incorporated into simulations of flow around a single salt dome.

In the simulations presented below I impose a variety of
hydrologic boundary conditions in order to simulate salt
domes in different hydrologic environments and to test the
effects of different boundary conditions. The boundary
conditions I imposed in the simulations include: 1) constant
water table elevation, which represents sub-aerially exposed
sediments above the salt (there is so little relief in the
water table on the Gulf Coastal Plain, that there is no
noticeable distinction between these conditions and
conditions of specified pressure which would represent a dome
in submarine sediments); 2) constant recharge above the salt
column, with constant pressure imposed away from the salt
column itself, which represents a salt island surrounded by
surface water; and 3) constant groundwater velocity above a
salt ridge, which represents flow through an aquifer that is
recharged outside the model boundaries.

Constant pressure boundary conditions are imposed by
recognizing that \( \frac{\partial p}{\partial r} = 0 \), indicating that

\[
q_r = \frac{\partial \Psi}{\partial y} = 0 \tag{7.2}
\]

Constant head conditions are imposed by assuring that, at the
water table

\[
\frac{\partial \Psi}{\partial n} = r \frac{\partial k}{\mu} \frac{\partial h}{\partial r} \tag{7.3}
\]

where \( n \) is the outward unit vector normal to the water table,
\( \mathbf{r} \) is the unit vector parallel to the water table, and \( h \) is
the hydraulic head at the water table. When regions of the
top boundary are subject to a constant recharge rate of $N$, then

$$N = q_y = \frac{1}{\rho} \frac{\partial \Psi}{\partial r}$$  \hspace{1cm} (7.4)

Solving (7.4) for $\Psi$ by integrating gives the appropriate recharge boundary condition:

$$\Psi = \frac{1}{2} r^2 \rho N$$  \hspace{1cm} (7.5)

And finally, constant flow boundary conditions are derived by integrating $q_r = -\frac{\partial \Psi}{\partial y}$ to get

$$\Psi = q_x y + \text{constant}$$  \hspace{1cm} (7.6)

With boundary conditions applied in these ways, the coupled transport equations are well-posed, and, following the discretization discussed in Chapter 4, they are converted to algebraic equations that are solved as follows.

7.2.3 Solution to Algebraic Equations

The finite difference equations for the simulations presented here were solved using a line successive overrelaxation (LSOR) method [Westlake, 1975; also referred to as row-by-row SOR, or block SOR method]. The LSOR technique combines the iterative procedure for sparse matrices with the efficiency of a direct method for solving tridiagonal systems. The LSOR method can be easily visualized with the help of Figure 7.2. The algorithm solves
Figure 7.2 An illustration showing how Line SOR solution is achieved. A solution is achieved a row at a time by using values at neighboring nodes from a previous iteration.
for values of the transport variables one row at a time by assuming that values of that variable are known (from an initial guess or a previous iteration) at nodes on the rows above and below the row of interest. That is, equation (4.3) is rewritten as

\[
\begin{align*}
\alpha_{i,j} u_{i,j+1} + b_{i,j} u_{i,j-1} + e_{i,j} u_{i,j} &= f_{i,j} - c_{i,j} u_{i,\text{old}}^{\text{old}} - d_{i,j} u_{i,\text{old}}^{\text{old}} \\
&= \text{(7.7)}
\end{align*}
\]

where everything on the right-hand-side of (7.7) is considered to be known from previous iterations. Equation (7.7), then, is in a tridiagonal form which is solved efficiently using forward and back substitution. The LSOR algorithm then solves for the next row in the same way. The speed of convergence is improved considerably with overrelaxation which is applied in the usual way [Westlake, 1975].

The LSOR algorithm is considerably more efficient than point-wise SOR routines because it transfers information from the boundaries a row at a time. The solution method is especially appropriate in the present model because the subsiding basin model obviates the need to solve for salinity or groundwater flow below the salt bed, which itself moves vertically through rows of nodes.

7.3 Simulation Results

In the numerical solution of these equations a finite difference grid is set up that includes sediments, salt, and
a region below salt as illustrated schematically in Figure 7.3, where salt is represented by the shaded region. As the basin subsides the salt bed moves vertically downward through the finite difference nodes (Figure 7.3b, 7.3c) and the salt and sediment interfaces are tracked numerically. The equations for solute and groundwater transport are solved numerically at all nodes above the salt layer, and every node within the sediment pile experiences the sediment moving down through it at a constant subsidence velocity. In keeping with the downbuilding model, nodes within and above the salt column experience no sediment movement. No attempt is made in my model to account for variations in vertical subsidence velocity due to sediment compaction or salt deflation. Unlike the solute and groundwater equations, the heat transport equation is solved over all nodes including those below the salt layer.

A detailed sensitivity analysis, *sensu stricto*, was not performed, but model parameters and boundary conditions were changed systematically in order to evaluate qualitatively their relative influence on the transport fields. In Chapter 1 I discussed the trade-off between model complexity and the ease with which numerical results can be generalized. This trade-off is apparent in the simulation results presented in this chapter. Several simulations were run for models with homogeneous sediment properties. These simulations allow us to interpret and understand some of the basic transport properties operative in this complex geologic environment.
Figure 7.3 A schematic model showing how basin subsidence and diapirism are modeled. Each dot represents a finite difference node. The top of the salt column remains stationary while the surrounding basin subside. The region above the salt is filled in with sediment transported across the upper boundary.
Armed with this background, simulations were conducted with more complex medium properties in order to better assess transport processes in salt dome environments representative of the Gulf Coast.

The finite difference grid used in all of the simulations presented in this chapter is shown in Figure 7.4. The shaded region in Figure 7.4 outlines the region that is modelled as salt. As the simulations progress, the basin subsides at a specified rate, and the salt stock grows as illustrated by Figure 7.3; the subsiding basin is filled in with sediment transported across the top of the mesh, while the bottom of the basin moves through the finite difference nodes. Nodes below the bottom of the salt bed are used in temperature calculations, but not in solute transport of groundwater flow calculations. In presenting simulation results I plot only the region above the salt bed.

7.3.1 General Considerations: A Homogeneous Medium

Table 7.1 lists parameters used for simulations that represent the simplest hydrogeologic model near a salt dome: a homogeneous medium with the water table specified on the top boundary of the model. The water table elevation above the salt dome is four meters above that for the rest of the model, where it is level. This represents water table conditions that mimic the surface topography near a salt dome with positive relief. Throughout the northern Gulf Coast, and especially in Louisiana, there is excellent correlation
Figure 7.4  The finite difference grid used in the simulations presented.
Table 7.1 Model Parameters and Boundary Conditions Used for Simulation in Figures 7.5, 7.6, and 7.7

<table>
<thead>
<tr>
<th>Thermal Boundary Conditions:</th>
<th>Basal Heat Flow = 60mW/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Surface Temperature = 20°C</td>
</tr>
<tr>
<td>Hydraulic Boundary Conditions:</td>
<td>Specified head at water table:</td>
</tr>
<tr>
<td></td>
<td>4m increase in head over salt dome. No flow on bottom and edges.</td>
</tr>
<tr>
<td>Salt Geometry:</td>
<td>Cylindrical Stock</td>
</tr>
<tr>
<td>Subsidence Rate =</td>
<td>200m/Ma</td>
</tr>
<tr>
<td>Permeability (k_r) =</td>
<td>10^{-14}m²</td>
</tr>
<tr>
<td>Porosity (ϕ) =</td>
<td>0.20</td>
</tr>
<tr>
<td>Anisotropy (k_r/k_y) =</td>
<td>2.5</td>
</tr>
<tr>
<td>Longitudinal Dispersivity =</td>
<td>10.0m</td>
</tr>
<tr>
<td>Transverse Dispersivity =</td>
<td>1.0m</td>
</tr>
<tr>
<td>Diffusion Coefficient =</td>
<td>10^{-9}m²/sec</td>
</tr>
<tr>
<td>Thermal Conductivity K_{solid} =</td>
<td>2.5 Wm⁻¹°C⁻¹</td>
</tr>
</tbody>
</table>
between water table and land surface elevation [Williams and Williamson, 1989]. In the simulations presented in this section, the sediment permeability is $10^{-14}$ m$^2$ and porosity is 20% which represent sandstone to silty sandstone sediments. These values are actually somewhat low for many sandstones near salt domes in the northern Gulf Coast [McManus, ms. in prep.]. The resulting values of thermal conductivity in saturated sediments yield conductivity contrasts (with respect to the salt) that are insufficient to drive thermohaline convection in the absence of other driving forces.

Figures 7.5, 7.6, and 7.7 illustrate simulation results for this simple model at different times (2 Ma, 10 Ma, and 14 Ma) during salt dome evolution. The rate of salt diapirism and basin subsidence in these simulations is 200m per Ma. When subsidence is initiated large lateral density gradients are present because the dissolved salt diffuses into fresh groundwater (in the context of Chapter 5 this would correspond to a large buoyancy ratio). The density gradient drives groundwater flow laterally into the basin, which in turn carries dissolved salt and serves to rapidly increase salinity throughout the radial basin. In this way a high salinity plume develops and extends across the basin basement. Throughout the simulation groundwater picks up dissolved salt at the dome crest, and saline waters sink along the salt column. Initial groundwater velocities are fairly small (~0.05m/year, Figure 7.5) but increase with
Figure 7.5  (a) Salinity, (b) temperature, (c) stream function, (d) velocity vectors, and (e) surface heat flow after 2 Ma for a simulation in which water table elevation is specified on the upper model boundary (see Table 7.1 for model parameters)
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 2Ma

1 KM
Figure 7.6 A continuation of the simulation presented in Figure 7.5 to 10 Ma.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 10Ma
Figure 7.7 A continuation of the simulation results presented in Figures 7.5 and 7.6 to 14 Ma.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 14 Ma
diapirism because large downward buoyant forces develop as the basin deepens (Figures 7.6, 7.7). The downward buoyant forces are only slightly countered by the effects of increasing temperature with depth.

As groundwater sinks along the salt column, it causes groundwater to be recharged above the edge of the salt column in order to maintain the specified water table elevation. Although the groundwater head at the water table is 4m higher above the dome than it is off to the sides, this has little effect in determining the location of groundwater recharge because the hydraulic forces caused by the head gradient are dwarfed by the forces caused by density gradients. Consequently there is little difference between the simulations presented here and those for which constant pressure is specified along the top boundary. For this reason results from the latter simulations are not shown.

Downward groundwater flow transports heat downward leading to decreased heat flow above and adjacent to the salt column (Figures 7.5e, 7.6e, 7.7e). This result contrasts sharply with thermal conduction models that indicate that salt domes are regions of high surface heat flow [Selig and Wallick, 1966; Jensen, 1983; O'Brien and Lerche, 1988]. Although groundwater velocities are only a few centimeters per year (Figure 7.5d, 7.6d, and 7.7d), advective transport of heat is sufficient to dominate conduction even in the presence of highly conductive rock salt. This is because downward groundwater flow parallels the temperature gradient
thereby maximizing advective transport. The high thermal conductivity of salt is nonetheless apparent in the position of the isotherms within the salt stock itself. The combination of highly conductive salt and downward groundwater flow create a low temperature trough immediately adjacent to the salt edge (Figures 7.6b, 7.7b).

In order to increase the effects of groundwater flow directly above the salt column I conducted simulations in which recharge was specified directly above the salt dome (Table 7.2). Recharge boundary conditions generally assume that water table accretion occurs at a rate proportional to the average precipitation rate [Freeze and Cherry, 1979]. Forster and Smith [1988] suggest that recharge boundary conditions are generally more appropriate that specified head conditions when modeling hydrogeologic phenomena. It is doubtful that this is the case is southern Louisiana, however, because there is generally a poor correlation between recharge and precipitation [Williamson, 1986]. Recharge rates of 0.1m/year directly above the salt column were simulated by imposing boundary conditions as described in equation (7.4). Recharge rates of 0.1m/year were estimated by Hanor [ms., 1989] for an isolated region of south Louisiana, and this rate is probably an upper extreme of the recharge rate because of the special engineering features present at the study site [Hanor, ms. 1989]. Imposing recharge rates of 0.1m/year above the salt column makes little difference to the simulation results presented
Table 7.2 Model Parameters and Boundary Conditions Used for Simulation in Figure 7.8

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Thermal Boundary Conditions</strong></td>
<td><strong>Basal Heat Flow = 60mW/m²</strong></td>
</tr>
<tr>
<td><strong>Surface Temperature</strong></td>
<td><strong>20°C</strong></td>
</tr>
<tr>
<td><strong>Hydraulic Boundary Conditions</strong></td>
<td><strong>Recharge = 0.1m/Ma directly above the dome; constant pressure elsewhere on top boundary. No flow on bottom and edges.</strong></td>
</tr>
<tr>
<td>Salt Geometry:</td>
<td>Cylindrical Stock</td>
</tr>
<tr>
<td>Subsidence Rate</td>
<td>200m/Ma</td>
</tr>
<tr>
<td>Permeability (kᵢ)</td>
<td>10⁻¹⁴m²</td>
</tr>
<tr>
<td>Porosity (ϕ)</td>
<td>0.20</td>
</tr>
<tr>
<td>Anisotropy (kᵢ/kᵧ)</td>
<td>2.5</td>
</tr>
<tr>
<td>Longitudinal Dispersivity</td>
<td>10.0m</td>
</tr>
<tr>
<td>Transverse Dispersivity</td>
<td>1.m</td>
</tr>
<tr>
<td>Diffusion Coefficient</td>
<td>10⁻⁹m²/sec</td>
</tr>
<tr>
<td>Thermal Conductivity Ksolid</td>
<td>2.5 Wm⁻¹°C⁻¹</td>
</tr>
</tbody>
</table>
in section 7.3.1 (Figure 7.8). In these simulations total
recharge is dominated by the sinking of groundwater adjacent
to the salt column (Figure 7.8d, 7.8d).

Similar flow patterns develop when there is no
groundwater recharge. In Figure 7.9 the upper model boundary
is a streamline boundary (see Table 7.3). This represents
either a steady phreatic surface without recharge, an
impermeable interface, or a sharp interface between
contrast fluids [Bear, 1972]. After ten million years the
transport fields for these boundary conditions resemble those
in the previous simulations (cf. Figure 7.7) with the
exception that there is greater basin wide circulation, which
is an artifact of the noflow boundaries. Streamline boundary
conditions could not exist throughout salt dome evolution
because such conditions must allow for transport of sediment
across the top boundary of the model while preventing
groundwater flow across it. Such conditions might be
approximated during some of the basin’s history, however, by
the deposition of low permeability shales on top of more
permeable sediments. The consequences of such conditions are
discussed in section 7.3.3.

In addition to the simulations presented, several
simulations were conducted in which I changed the rate of
diapirism, medium permeability, and background salinity
values. Maximum groundwater velocity changed roughly in
proportion to the permeability, and concomitant changes in
advective heat and salt transport occurred as expected.
Figure 7.8 Simulation results after 10 Ma when recharge boundary conditions are applied (Table 7.2). A recharge rate of 0.1 m/year was specified directly above the dome, and constant head was specified elsewhere. The component of horizontal flow above the dome is not sufficient to transport dissolved salt laterally away from the crest; the salt laden groundwater at the dome crest sinks along the salt edge. Transport fields are very similar to those in the previous simulation.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 10Ma
Table 7.3 Model Parameters and Boundary Conditions Used for Simulation in Figure 7.9

<table>
<thead>
<tr>
<th>Thermal Boundary Conditions:</th>
<th>Basal Heat Flow = 60mW/m²</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Surface Temperature = 20°C</td>
</tr>
<tr>
<td>Hydraulic Boundary Conditions:</td>
<td>Stream line boundary on top.</td>
</tr>
<tr>
<td></td>
<td>No flow on bottom and edges.</td>
</tr>
<tr>
<td>Salt Geometry:</td>
<td>Cylindrical Stock</td>
</tr>
<tr>
<td>Subsidence Rate =</td>
<td>200m/Ma</td>
</tr>
<tr>
<td>Permeability (k_r) =</td>
<td>10^{-14}m²</td>
</tr>
<tr>
<td>Porosity (ϕ) =</td>
<td>0.20</td>
</tr>
<tr>
<td>Anisotropy (k_r/k_y) =</td>
<td>2.5</td>
</tr>
<tr>
<td>Longitudinal Dispersivity =</td>
<td>10.0m</td>
</tr>
<tr>
<td>Transverse Dispersivity =</td>
<td>1.0m</td>
</tr>
<tr>
<td>Diffusion Coefficient =</td>
<td>10^{-9}m²/sec</td>
</tr>
<tr>
<td>Thermal Conductivity $K_{solid}$ =</td>
<td>2.5 Wm⁻¹°C⁻¹</td>
</tr>
</tbody>
</table>
Figure 7.9 Simulation results after 10 Ma when streamline boundary conditions are applied (Table 7.3). There is no groundwater recharge, and groundwater circulates tending to homogenize the salinities. Here again the transport fields are similar to those in the previous simulations, although the flow velocities are considerably smaller. The flow pattern is dominated by groundwater flowing vertically down the salt column edge.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 10 Ma
Simulations using large permeability values (e.g., $10^{-12} m^2$) encountered numerical stability problems when the sediments thickness reached about 3 kilometers, and these simulations are not presented. These numerical instabilities result from physical instabilities (Rayleigh instabilities) which arise because the critical Rayleigh number is exceeded, causing buoyancy effects to become dominant. Changing the permeability had no qualitative effect on the sense of groundwater motion, and nature of the other transport fields. Similarly, the rate of diapirism did not effect the general conclusions drawn from simulations presented.

When the salt dome intrudes into sediments containing high salinity groundwater then the thermal effects near the salt dome become relatively more important, as seen in Chapter 5. In several simulations I increased the initial groundwater salinity in order to simulate a decrease the absolute value of the buoyancy ratio. When the background salinity exceeded a value of about 14 weight percent thermal effects became dominant and resulted in upward groundwater flow adjacent to the salt column. The effect of high background salinity is illustrated in Figure 7.10, in which the model parameters are the same as those given in Table 7.1 and a background salinity of 16 weight percent is specified. The thermal effects on groundwater density and flow are apparent, and thermally driven convection causes upward flow along most of the salt edge. The upward flow creates a high salinity plume extending from the top of the salt column to
Figure 7.10 Simulation results after 10 Ma when the salt dome builds into sediments containing groundwater with a high background salinity of 16 weight percent. Other parameters are the same as those given in Table 7.1. Because of the high background salinity, thermal effects are relatively more important than in other simulations, and thermally driven convection causes upward flow along the salt column.
**STREAM FUNCTION**

**SPECIFIC DISCHARGE**

**SURFACE HEAT FLOW (mW/m²)**

ELAPSED TIME = 14Ma
the top boundary of the mesh. The effects of salt
dissolution at the top of the dome creates a small amount of
downward flow adjacent to the salt crest.

7.3.2 Constant Groundwater Flow Above a Salt Ridge

With a two-dimensional model it is impossible to simulate
accurately the effects of fresh groundwater in a regional
aquifer flowing over the crest of a salt dome. The
difficulty arises because the problem is inherently three-
dimensional. Even if a regional aquifer is well described in
two-dimensional Cartesian coordinates, because its geometry
remains fairly uniform along strike, the salt column has a
very limited extent along strike. Consequently, with two-
dimensional coordinates there is no way of reconciling these
contrasting geometries. Nonetheless it will be useful to
simulate in some manner the flow of regional groundwater over
a salt dome because such flow will promote salt dissolution
[Bodenlos, 1970; Kyle and Price, 1986], because horizontal
groundwater flow across the salt may drive circulation due to
viscous drag on the lee side of the dome, and because it may
serve to extend salinity plumes well away from the salt.

For the reasons mentioned above I model the effects of
groundwater over a salt ridge rather than over a salt dome.
The salt ridge is modeled in two-dimensional Cartesian
coordinates that represent a cross section through an
elongate feature that extends well into the plane of the
model (Figure 7.11). This geometry is representative of some
Figure 7.11 Schematic diagram of a salt ridge. Simulations are conducted in two-dimensional Cartesian coordinates that represent a cross section through the ridge.
salt diapirs in southern Louisiana [Stipe, 1960], but more importantly, it will tend to maximize the effects of viscous drag near the salt column. The finite difference mesh is the same as that used in previous simulations (Figure 7.4) with the exception that it now represents two-dimensional Cartesian, rather than cylindrical, coordinates. Medium parameters are also similar to those used in previous simulations and are given in Table 7.4. Boundary conditions specifying horizontal flow of 0.1m/year above the salt dome are imposed as indicated in equation (7.6).

With these simulations, as with the previous ones, the groundwater flow is ultimately controlled by the downward flow of dense saline groundwater off of the dome crest. During the early part of ridge development groundwater throughout the shallow basin is dominated by horizontal flow (Figure 7.12). As the basin grows deeper due to basin subsidence, groundwater flowing across the top of the dome cascades down along the salt edge (Figure 7.13) Any effects of viscous drag on the lee side of the salt ridge are unapparent in any of the simulation results.

7.3.3 A Layered Medium: Gulf Coast - Type Model

In this section I present some final simulations that are designed to model coupled transport near a salt dome during the deposition of a layered medium that grossly approximates the stratigraphy in the northern Gulf Coast. The aim here is to take the simulations one step further than those in
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Boundary Conditions:</td>
<td>Basal Heat Flow = 60 mW/m²</td>
</tr>
<tr>
<td></td>
<td>Surface Temperature = 20°C</td>
</tr>
<tr>
<td>Hydraulic Boundary Conditions:</td>
<td>Constant horizontal velocity above ridge.</td>
</tr>
<tr>
<td></td>
<td>No flow on bottom.</td>
</tr>
<tr>
<td></td>
<td>Hydrostatic conditions at edges.</td>
</tr>
<tr>
<td>Salt Geometry:</td>
<td>Elongated Ridge</td>
</tr>
<tr>
<td>Subsidence Rate</td>
<td>200 m/My</td>
</tr>
<tr>
<td>Permeability ( (k_r) )</td>
<td>( 10^{-14} m^2 )</td>
</tr>
<tr>
<td>Porosity ( (\phi) )</td>
<td>0.20</td>
</tr>
<tr>
<td>Anisotropy ( (k_x/k_y) )</td>
<td>2.5</td>
</tr>
<tr>
<td>Longitudinal Dispersivity</td>
<td>10.0 m</td>
</tr>
<tr>
<td>Transverse Dispersivity</td>
<td>1.0 m</td>
</tr>
<tr>
<td>Diffusion Coefficient</td>
<td>( 10^{-9} m^2/sec )</td>
</tr>
<tr>
<td>Thermal Conductivity ( K_{solid} )</td>
<td>( 2.5 \ \text{W} m^{-1} \text{°C}^{-1} )</td>
</tr>
</tbody>
</table>
Figure 7.12  (a) Salinity, (b) temperature, (c) stream function, (d) velocity vectors, and (e) surface heat flow after 4 Ma when groundwater flows at a constant velocity over a salt ridge (see Table 7.4)
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

Elapsed Time = 4Ma

1 KM
Figure 7.13 A continuation of simulation results presented in Figure 7.12 to 8 Ma.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 8 Ma

1 KM
previous sections by modeling deposition of sediments with variable properties in order to gain some insight into the effects of variable lithology, and to investigate the general transport processes that may have been operative during the development of northern Gulf Coast salt domes.

Tertiary sedimentation in the northern Gulf was dominated by the influx of clastic sediments deposited by prograding delta systems (Figure 2.3). Details of the Tertiary stratigraphy of the northern Gulf Coast are complex. Nonetheless, a simple but representative model for Tertiary stratigraphy in the northern Gulf Coast can be given as follows. Lower and Middle Oligocene deep marine sands and interbedded shales (e.g., Vicksburg and Frio sands) are overlain by marine shales that grade into shallow intershelf sands (Oligocene). These in turn are overlain by massive sands of the fluvial deltaic systems (Miocene and younger). The thicknesses of each of these units varies depending on location, but the general trend of sand-shale-sand is consistent throughout the northern Gulf Coast [see Bebout and Guitierrez, 1983].

Simulation results for groundwater flow near a salt diapir that develops structurally into a sand-shale-sand sequence are presented in Figures 7.14, 7.15, and 7.16. Medium parameters and boundary conditions for these simulations are given in Table 7.5. In this simulation the lower sand reaches a total thickness of 2100 m (6890 ft), the intermediate shale unit reaches a thickness of 900 m (2952
Figure 7.14 Transport fields after 4 Ma of subsidence for a simulation that incorporates a layered medium (see Table 7.5). At this time the entire basin is filled with sandstone that will become the basal sedimentary unit.
Figure 7.15  A continuation of simulation results presented in Figure 7.14 to 8 Ma. At this time shale deposition has begun, inhibiting recharge. Circulation is confined to the basal unit. Velocities decrease after this time as dissolved salt in the lower unit becomes homogenized.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME ≈ 8Ma

1 KM
Figure 7.16 A continuation of simulation results presented in Figures 7.14 and 7.15 to 21 Ma. Salinity in the upper sandstone unit resembles that which existed in the lower unit a few million years after subsidence began. Salinity in the lower unit has become well mixed; density in that unit is controlled by temperature, and free thermal convection occurs.
(c) STREAM FUNCTION

(d) SPECIFIC DISCHARGE

ELAPSED TIME = 21 Ma
(e) SURFACE HEAT FLOW (mW/m²)

ELAPSED TIME = 21 Ma

1 KM
<table>
<thead>
<tr>
<th>Table 7.5 Model Parameters and Boundary Conditions Used for Simulation in Figures 7.14, 7.15, and 7.16 (A Layered Medium)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Thermal Boundary Conditions:</strong></td>
</tr>
<tr>
<td>Basal Heat Flow = (60 \text{mW/m}^2)</td>
</tr>
<tr>
<td>Surface Temperature = (20^\circ\text{C})</td>
</tr>
<tr>
<td><strong>Hydraulic Boundary Conditions:</strong></td>
</tr>
<tr>
<td>Specified head at water table: (4\text{m increase in head over salt dome. Hydrostatic conditions at } r=10\text{km. No flow on bottom at } r=0).</td>
</tr>
<tr>
<td><strong>Salt Geometry:</strong></td>
</tr>
<tr>
<td>Subsidence Rate = (200\text{m/Ma})</td>
</tr>
<tr>
<td>Permeability of Lower Sandstone (k_\tau) = (10^{-14}\text{m}^2)</td>
</tr>
<tr>
<td>Permeability of Shale (k_\tau) = (10^{-16}\text{m}^2)</td>
</tr>
<tr>
<td>Permeability of Upper Sandstone (k_\tau) = (10^{-14}\text{m}^2)</td>
</tr>
<tr>
<td>Porosity ((\phi)) = 0.20</td>
</tr>
<tr>
<td>Anisotropy of Lower Sandstone (k_\tau/k_y) = 2.5</td>
</tr>
<tr>
<td>Anisotropy of Shale (k_\tau/k_y) = 10.0</td>
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<tr>
<td>Anisotropy of Upper Sandstone (k_\tau/k_y) = 2.5</td>
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<tr>
<td>Longitudinal Dispersivity = 10.0m</td>
</tr>
<tr>
<td>Transverse Dispersivity = 1.0</td>
</tr>
<tr>
<td>Diffusion Coefficient in Lower Sandstone = (10^{-9}\text{m}^2/\text{sec})</td>
</tr>
<tr>
<td>Diffusion Coefficient in Shale = (5\times10^{-10}\text{m}^2/\text{sec})</td>
</tr>
<tr>
<td>Diffusion Coefficient in Upper Sandstone = (10^{-9}\text{m}^2/\text{sec})</td>
</tr>
<tr>
<td>Thermal Conductivity (K_{\text{solid}}) = 2.5 (\text{Wm}^{-1}\text{C}^{-1})</td>
</tr>
</tbody>
</table>
ft), and the entire sedimentary pile subsides at a constant rate of 200 m/Ma. Prior to the initiation of subsidence, the lower sand is 875 m (2870 ft) thick and is assumed to have reached steady-state salinity conditions.

In the early stages of diapirism, the simulation results (Figure 7.14) are identical to simulation presented earlier (Figures 7.5, 7.6, and 7.7). After 8 million years of subsidence, however, the shale deposition is established (Figure 7.15) and the flow patterns begin to deviate from previous results. At this time recharge is inhibited by the thin shale, and groundwater circulation is largely restricted to the lower sand unit (Figure 7.15c, 7.15d). Even though recharge is inhibited, downward flow along the salt column dominates the circulation pattern. Darcy velocities remain rather high, at 0.09 m/year initially. However, because circulation is driven by radial density gradients, both the density gradients and flow velocities begin to diminish as the dissolved salt content of the lower unit becomes more and more homogenized. The downward flow causes surface heat flow to be low above the edge of the salt column. This effect also diminishes with time as the circulation gets farther from the earth's surface due to subsidence and as velocities decrease.

After 21 million years the upper sand unit is 2075 m (6800 ft) thick (Figure 7.16) and salinity and flow conditions in the upper sand resemble those that existed in the lowest unit a few million years after subsidence started.
(cf. Figure 7.16 and 7.14). As with earlier times in the simulation, groundwater flowing off the crest of the salt dome reduces surface heat flow at the salt edge. By this time the salinity in the lower sand has nearly homogenized and groundwater density is controlled largely by temperature. Thermal effects are sufficient to drive free convection in this unit (Figure 7.16c, 7.16d). The sense of convection, however, drives flow down along the base of the salt column. The circulation direction is partially inherited from earlier circulation because salinities are slightly higher near the salt column than away from it. In addition, the isotherms near the base of salt tend to be pulled down by conduction, and this will also drive convection in the observed direction.

7.4 Discussion and Conclusions

The simulation results presented in this chapter indicate that the groundwater flow near salt domes is only weakly controlled by the hydrologic boundary conditions. This contrasts with groundwater studies in most other geologic settings where it is found that hydrologic boundary conditions are a major factor in controlling flow [Toth, 1963; Freeze and Witherspoon, 1967; Graven and Freeze, 1984]. The salt dome environment is unique in this way because density gradients are large near the salt dome, and because there is very little topographic relief of the water table on the coastal plain.
All of the simulation results presented in this chapter indicate that groundwater should flow down along the salt edge. No combination of boundary conditions and model parameters were able to change the general sense of groundwater motion. It is unlikely that this result would be altered by introducing additional complexities into the present model. This is an important conclusion because it demonstrates that if upward groundwater flow is common near salt domes it is driven by forces that arise from sources other than those created by thermohaline convection or salt dissolution and diapirism. Release of geopressured waters is the likely driving mechanism [cf. Ranganathan 1988; Bennett and Hanor, 1987].

Cases for which thermohaline convection might be the operative mechanism were delineated earlier and will result when the background, or regional, salinity is uniformly high (giving a small buoyancy ratio) or when the contrast in thermal conductivity between salt and adjacent sediment is large (due to high porosities). The former condition has been confirmed for simulations that are otherwise the same as those presented in this chapter.

Because of the specific objectives of this chapter I have not attempted to explicitly model groundwater flow during the post-diapir stage of salt dome development. It is worth noting, however, that the pattern of downward flow persisted in simulations that were run for up to 20 Ma beyond the results presented. This is true even when active diapirism
ceases. Groundwater flow during the post-diapir stage would be influenced by regional groundwater salinity and it is during this stage, when regional salinities are high, that thermohaline convection is most likely to occur. Moreover, the geometric complexities of salt structures during post diapirism (e.g., Figure 2.6) are likely to further complicate groundwater flow.

Temperatures near salt domes are strongly controlled by groundwater flow. Although the high thermal conductivity of salt is apparent in the thermal calculations, the effect of groundwater flow in this environment is especially important because it tends to parallel the temperature gradient which maximizes the advective component of heat transport. The effect of vertical groundwater flow is evident in the surface heat flow above the salt column. For most of the simulations groundwater flow makes the salt dome a region of low surface heat flow. Only when thick shale sequences are present near the top of the model (Figure 7.15) does the surface heat flow reflect the high conductivity of salt rock. Thus thermal models based on conduction alone are likely to be of little value in evaluating the present thermal conditions or the thermal history near salt domes.

These simulations indicate that groundwater salinity will generally decrease with depth in the salt dome environment even when salt dissolution is restricted to the crest of the dome. Moreover, the effects of salt dissolution manifest themselves in salinities several kilometers away from the
dome within a few million years. In simulations using layered sediments, lower sandstones become largely isolated hydrologically after shale deposition occurs. When this happens, homogenization of salinities in the deep sands is achieved through groundwater circulation and solute dispersion, and once the salinity field is homogenized, thermal convection may drive further circulation.

The most important conclusion of these simulations are essentially a negative result to the hypothesis being tested: that diapirism and preferential salt dissolution can lead to salinity and density inversions that drive upward flow. This apparently does not occur, and we are left with the conclusion that either thermohaline convection or release of geopressured fluids is probably responsible for driving upward groundwater flow near salt domes when it does occur. Because thermohaline convection occurs for a limited range of geologic conditions, flow driven by geopressured fluids is the likely driving mechanism if upward flow is a widespread phenomena.

Not all salt diapirs are flanked by geopressured sediments, however. In northern Louisiana and eastern Texas salt domes occur in basins where geopressured sediments are not present [Wallace et al., 1979]. Field-oriented studies such as those of Bennett and Hanor [1987] would be useful in these regions to determine the absence or presence of upward flow. Near West Hackberry dome in southwestern Louisiana, geopressured sediments are at least 3km below the salt dome
crest, and in this region there is apparently no indication of active upward groundwater flow [McManus, ms. in prep.]. In circumstances such as these the simulations presented may accurately model the hydrogeologic development near salt domes.
CHAPTER 8

CLOSING DISCUSSION

Can a fig tree, my brethren, yield olives, or a grapevine figs? No more can salt water yield fresh.

James III:12

A clear understanding of groundwater flow in the salt dome environment is necessary in order to evaluate accurately geologic processes such as sediment diagenesis, hydrocarbon migration, salt dissolution, and heat flow. Unfortunately the salt dome environment is among the most complex that the hydrogeologist is likely to encounter. Field evidence [e.g., Bennett and Hanor, 1987; Hanor and Workman, 1987; Jensenius and Munksgaard, 1989; McManus, ms. in prep., 1989] attests to this complexity and reinforces the need for a better theoretical understanding of groundwater hydrodynamics near salt domes. We currently have only a limited sampling of hydrogeologic conditions near salt domes, we are not in a position to know whether the observations that indicate upward groundwater flow [e.g., Bennett and Hanor, 1987; Hanor and Workman, 1987; Hanor, 1987] represent typical or anomalous conditions near salt domes. There is a growing body of evidence, however, that corroborate the conclusions of Hanor [e.g., Leger, 1988; Jensenius and Munksgaard, 1989] and indicate that upwellng groundwater is a common phenomenon near salt domes.

A quantitative understanding of groundwater flow near salt domes can be gained through the use of mathematical and
numerical models provided these models couple the transport of heat and dissolved salt to groundwater flow. When time-dependent solute transport is considered, the models must also account for basin subsidence and salt diapirism since the structural development of the salt column affects the temporal development of the salinity field.

In establishing a mathematical and numerical model to study groundwater flow near salt domes I have developed the first comprehensive model for simulating coupled transport in this complex environment. The model explicitly couples nonlinear equations describing the groundwater flow, heat transport, and dissolved salt transport, and accounts for basin subsidence and salt diapirism. In this model I have introduced the mass stream function which describes the groundwater flow field in terms of stream lines, but (unlike the conventional use of the stream function) does not require the Boussinseq assumption. The mass stream function is particularly valuable in the present context because it allows for a more accurate estimate of the advective transport terms than flow equations written in terms of hydraulic head. In order to establish general circulatory consequences of thermohaline convection near salt columns, I have used dimensional analysis to simplify the transport equations and minimize the number of controlling parameters. Dimensional analysis is a valuable tool in trying to understand the complexities of coupled transport, but requires assumptions that are too bold to be applicable to a
given salt dome setting.

The general mathematical and numerical models presented here account for basin subsidence and salt movement during heat and mass transport. This is an important consideration in modeling groundwater flow near salt deposits, even in the absence of active salt diapirism, because the regional groundwater salinity may develop at about the same rate as the basin develops mechanically. When this is the case initial conditions can only be specified with confidence when the simulation is started at the time of salt deposition. Subsequent calculations of salt transport must then accommodate basin subsidence.

By conducting simulations that use these models I have attempted to test two hypotheses that might explain the occurrence of upward groundwater flow. These are (1) that thermal effects are responsible for driving flow through thermohaline convection; and (2) that preferential dissolution of salt at the dome crest, combined with the effects of diapirism and viscous drag, can produce stratigraphically high salinity plumes that create density inversions which lead to upwelling of unstable water from depth.

In some cases thermohaline convection might be the operative mechanism. These circumstances occur when regional groundwater salinities are uniformly high or when there exists a large contrast in the thermal conductivity values between salt and saturated sediments. These circumstances
will arise under a limited range of geologic conditions. Calculations presented in Chapter 7 indicate that more commonly groundwater will tend to flow vertically downward off the crest of the salt dome. If upward groundwater flow is a common processes near salt domes then it is probably driven by forces that arise from sources other than those created by thermohaline convection or salt dissolution at the dome crest.

Based on these results it seems likely that the release of geopressured waters is responsible for driving upward groundwater flow near some salt domes in many cases. I have reached this conclusion by using numerical simulations to eliminate the wide spread occurrence of other reasonable causes. This is important for two reasons: (1) the processes that my models simulated represent the simplest hypotheses about forces that could drive upward flow, and any subsequent models must incorporate the effects presented here; and (2) release of geopressured water is very difficult to model accurately [Ranganathan, 1988]. For example Ranganathan [1988] conducted simulations that included the upward flow of geopressured water, and pointed out that his simulations require excessive volumes of pore water.

Unlike groundwater flow in other geologic settings, flow near salt domes is only weakly dependent on water table elevation and recharge because density gradients are large near the salt dome.

Temperatures near salt domes can be modified considerably
by groundwater flow in spite of the high thermal conductivity of salt. This is because groundwater flow tends to parallel the temperature gradient thereby maximizing the heat that it transports. Thus thermal models based on conduction alone are likely to be of little value in evaluating the present thermal conditions or the thermal history near salt domes.
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APPENDIX A

LISTING OF PROGRAM CSDDB FOR COUPLED GROUNDWATER FLOW, HEAT, AND MASS TRANSPORT NEAR A GROWING SALT DIAPIR.
PROGRAM CSDDB
C-------------------------------------------------------------
C Calculate dissolved salt transport, heat transport, and groundwater
C flow near a growing salt dome in which diapirism results from downdrooping
C (i.e., the top of the diapir remains in the same position relative to the
C geoid while the surrounding basin subsides).
C Data input and input format are specified in comments w/in subroutine
C DATAIN. Output files have identical format to input files and can be
C restarted directly.
C Output can also be plotted using NCAR graphics routines. Plotting
C routines are isolated in the latter half of this code and also exist as
C post-processing routines.
C This version requires 2 input files. 1) the main input program
C indicating medium properties, initial and boundary conditions, and sim-
C ulation control information. And 2) a file indicating the position and
C rate of subsidence. The latter is read in subprogram SRATER.
C (Version 1.2 May 12, 1989 -- DGE)
C Note added 06-Jun-1989
C Current version uses Line SOR solution rather than a pointwise SOR
C method.
C Notes added 02-Aug-1989
C (1) The Line SOR routine calculates salinity and groundwater flow only
C for nodes above the salt.
C (2) The off-diagonal terms of the dispersion tensor are not used in
C the calculations of the concentration field.
C----------------------------------------------------------------------------
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101, / Dimension in X-coordinate
1 JDIM=101) / Dimension in Y-coordinate
LOGICAL PRINT,TEMPLT,CONPLT,VELPLT,PSIPLT,GRPLT,ECHO,
2 CNVRCG,CNVRGT,CNVRGP,NEWTS,DOTEMP,DOFLOW,DOCONC,
3 HFLUXBC,ACCRETN,STEADY_STATE
CHARACTER*4 TITLE1 (20), TITLE2 (20)
CHARACTER*23 DATIM
COMMON /PPARAM/
1 PERM(IDIM,JDIM), / Medium physical parameters
2 POR(IDIM,JDIM), / Permeability
3 DCX(IDIM,JDIM), / Diffusion coefficient is X-dir
4 ANISO(IDIM,JDIM), / Anisotropic ratio for PERM
5 ALFAT(IDIM,JDIM), / Transverse therm. dispersion
6 ALFAL(IDIM,JDIM), / Longitudinal therm. dispersion
9 RKS(IDIM,JDIM) / Thermal conductivity of solid
COMMON /COORDS/
1 X(IDIM,JDIM),Y(IDIM,JDIM), / Physical Coordinates
2 ICOSYS / l=>Cartesian o=>Cylindrical
COMMON /FIELDS/
1 TEMP(IDIM,JDIM), / The transport fields
2 CONC(IDIM,JDIM), / Temperature
3 PSI(IDIM,JDIM), / Concentration (not used)
4 VX(IDIM,JDIM), / Pressure
5 VY(IDIM,JDIM), / Velocity in X
1 OLDT(IDIM,JDIM), / Temp from last iteration
1 OLDC(IDIM,JDIM), / Conc from last iteration
2 OLDPSI(IDIM,JDIM), / Psi from last iteration
3 OLDVX(IDIM,JDIM), / Same here for
4 OLDVY(IDIM,JDIM), / Velocity components
5 CLAST(IDIM,JDIM) / CONC from last TIME STEP
COMMON /BNDRYC/
1 HWT(IDIM), / Boundary conditions
2 Q(IDIM), / Head at watertable
2 heat flux on lower boundary
Ld k > 3  WATERTBL, ! Type of flow b c
4  ACCRETN, ! GW accretion at watertable
5  HFLUXBC ! Type of thermal b c
COMMON /SPROP/ ! Scalar properties of medium
1  RHOS, ! Density of solid particles
2  CS, ! Specific heat of solid grains
3  RKF, ! Thermal conductivity of fluid
4  CF, ! Specific heat of fluid
5  RFZERO, ! Reference density of fluid
6  TZERO ! Reference temp for ZER
COMMON /APROP/ ! properties of medium
1  RKSF (IDIM,JDIM), ! Thermal conductivity of medium
2  RHOF (IDIM,JDIM), ! Density of the fluid
A  OLDRHF (IDIM,JDIM), ! Density from last Time Step
3  VISCO (IDIM,JDIM), ! Viscosity of fluid
4  DSPXX (IDIM,JDIM), ! X component of dispersion
5  DSPYY (IDIM,JDIM), ! Y component of dispersion
6  DSPXY (IDIM,JDIM) ! x,y component of dispersion
COMMON /CLOCK/ ! Keep track of time steps
1  ELTIME, ! Elapsed time
2  DT, ! Time step
3  MMTS, ! Increase DT every MMTS steps
4  TSMULT, ! By this much
5  TSMAX, ! Initial time
6  WDT ! Implicit Weighting (not used)
COMMON /ISIZE/ ! Number of node in X and Y
1  NI,NJ, ! Current time step
2  ITIME, ! Maximum number of time steps
3  ITIME ! Logical flags for I/O
COMMON /LFLAGS/ ! Output this iteration or t.s.
1  PRINT, ! Plot TEMP this iter or t.s.
2  TEMPI, ! Plot CONC this iter or t.s.
3  CONPLT, ! Plot VX,VY this iter or t.s.
4  VELPLT, ! Plot Vx,Vy this iter or t.s.
5  PSIPLT, ! Plot Pressure
6  GRPI, ! Plot initial grid
7  ECHO, ! Echo input data
8  CNVGT, ! CONVERGENCE FLAGS Temp,
9  CNVRG, ! concentration, and
*  CNVRG, ! pressure
1  NEWTS, ! New time step flag
2  DOTEMP, ! Solve for temperature
3  DOFLOW, ! Solve for pressure
4  DOCONC, ! Solve for concentration
5  STEADY_STATE ! T for ss conc calculation
COMMON /IOCTRL/ ! Integer values that say what
1  IPRINT, ! iterations to print,
2  IVPLT, ! plot velocities,
3  IPPI, ! plot pressure,
4  ITPLT, ! plot temp, or
5  ICPLT ! plot concentration,
COMMON /RELAX/ ! Under-relaxation parameters
1  RPT, ! Temperature
2  RPC, ! Concentration
3  RPR, ! Pressure
4  RPVEL, ! Velocity
5  SORTEM, MAXTEMI, ! Relax parameter & iterations
6  SORCON, MAXCON, ! for TEMP, CONC
7  SORSI, MAXPSI, ! and PSI
8  GCUTOFF, TCUTOFF, FCUTOFF ! Convergence criteria
COMMON /SUBSID/ ! Subsidence Information
1  TOTS, ! Total subsidence
2  RSRATE, SRATE (IDIM,JDIM), ! Ref subs rate and at nodes
3  JIFTOP (IDIM, JIFTOP (IDIM), ! Node indices of salt bed
Common block $RJACOB$ is defined in subroutine $XYTRAN$

\begin{verbatim}
CALL DATAIN(TITLE1, TITLE2, DATIM, LUNIN, LUNOUT, VE, MAXITER)
IF (GRPLT) CALL GRDPLT(X, Y, NI, NJ, VE, DATIM, TITLE1, TITLE2)
CALL XYTRAN(X, Y, NI, NJ)

Estimate initial density and stuff
CALL EQSTATE
CALL MEDPROP

DO 100 ITIME = 1, ITTIME

Increase size of time step if necessary
IF (.NOT. STEADY_STATE) THEN
  IF (MOD(ITIME, MTS) .EQ. ZERO) THEN
    DTLAST = DT
    DT = TSMULT*DT
  ENDIF
  IF (DT .GT. TSMAX) DT = TSMAX
  ELTIME = ELTIME + DT

And reset old salinity and density values
CALL EQUATE(CONC, CLAST, NI, NJ)
CALL EQUATE(RHOF, OLDRHOF, NI, NJ)
ENDIF

Set logical I/O flags
CALL FLGSET

Do subsidence calculations
CALL SUBSIDE

Initialize physical parameters like dispersion and density
\end{verbatim}
CALL EQSTATE
CALL MEDPROP

C Solve that sucker for this time step
C
C-|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
C-|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
C

DO ITER = 1, MAXITER

C Solve iteratively for PSI and CONC and TEMP
C
CVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVWW

C Calculate velocities using the present stream function
C Only need velocities if were going to plot them or calculate temperatures
C
IF(VELPLT .OR. DOCONC .OR. DOTEMP) THEN

CALL VELCAL

Under-relax the velocity field
IF(RPV .NE. 1) CALL URELAX(VX, OLDVX, RPVEL, NI, NJ)
IF(RPV .NE. 1) CALL URELAX(VY, OLDVY, RPVEL, NI, NJ)

Update dispersion

CALL MEDPROP

ENDIF

C Solve for salt concentration using present velocities
C
IF(DOCONC) THEN

CALL CONSLV(STEADY_STATE)

Under relax the salinity field
IF(RPC .NE. 1) CALL URELAX(CONC, OLDC, RPC, NI, NJ)

Check for convergence of concentration field
CALL CONCHK(CONC, OLDC, NI, NJ, CCUTOFF, CRESID, CNVRGC)

Update density and viscosity

CALL EQSTATE

ENDIF

C Solve for temperature using present velocities
C
IF(DOTEMP) THEN

CALL TEMSLV
Under relax the temperature field

IF(RPT .NE. 1) CALL URELAX(TEMP,OLDT,RPT,NI,NJ)

Check for convergence of temperature field

CALL CONCHK(TEMP,OLDT,NI,NJ,TCUTOFF,TRESID,CNVRGT)

Update density and viscosity

CALL EQSTATE

ENDIF

Solve for Stream function using density from last CONC

IF(DOFLOW) THEN

CALL PSISLV

Underrelax Stream Function values

IF(RPP .NE. 1) CALL URELAX(PSI,OLDSI,RPP,NI,NJ)

Check convergence of Stream Function

CALL CONCHK(PSI,OLDSI,NI,NJ,PCUTOFF,PRESID,CNVRGP)

Update density

CALL EQSTATE

ENDIF

Stop iterations if convergence is reached

IF(CNVRGC .AND. CNVRGF .AND. CNVRGT) GOTO 900
END DO ! End of iteration loop

ITER = ITER-1 ! Come here after convergence
WRITE(*,1000) ITIME,ELTIME,ITER,CRESID,TRESID,PRESID

Then do I/O stuff if necessary

IF(PSIPLT) CALL TPPLOT(PSI,X,Y,NI,NJ,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,' STREAM FUNCTION ')
IF(VELPLT) CALL VPLOT(X,Y,VX,VI,NI,NJ,VE,ELTIME,DT,DATIM,TITLE1,TITLE2)
IF(CONPLT) CALL TPPLOT(CONC,X,Y,NI,NJ,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,' CONCENTRATION ')
IF(TEMPLT) CALL TPPLOT(TEMP,X,Y,NI,NJ,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,' TEMPERATURE ')
IF(PRINT) THEN
CALL DATOUT(LUNOUT,TITLE1,TITLE2,DATIM,VE,MAXITER)
CALL SRATOUT
ENDIF
C
C And time marches on...
C
100 CONTINUE ! End of Time Step Loop
C
C Now we're done w/ the time steps plot final result
C
IF(ICPLT .GT. 0) THEN
  CALL TPPLOT(CONC,X,Y,NI,NJ,VE,ELTIME,DT,
               DATIM,TITLE1,TITLE2,' CONCENTRATION ')
ENDIF
IF(ITPLT .GT. 0) THEN
  CALL TPPLOT(TEMP,X,Y,NI,NJ,VE,ELTIME,DT,
               DATIM,TITLE1,TITLE2,' TEMPERATURE ')
ENDIF
IF(IPPLT .GT. 0) THEN
  CALL TPPLOT(PHI,X,Y,NI,NJ,VE,ELTIME,DT,
               DATIM,TITLE1,TITLE2,' STREAM FUNCTION ')
ENDIF
IF(IVPLT .GT. 0) THEN
  CALL VPLOT(X,Y,VX,VY,NI,NJ,VE,ELTIME,DT,DATIM,
             TITLE1,TITLE2)
ENDIF
C
C Always print out the final calculation
C
CALL DATOUT(LUNOUT,TITLE1,TITLE2,DATIM,VE,MAXITER)
CALL SRATOUT
C
CALL EXIT
1000 FORMAT(1X,15,E14.5,15,' C:',G12.5,' T:',G12.5,' P:',G12.5)
END
C
------------------------------------------------------------------------
C SUBROUTINE DATAIN(TITLE1, TITLE2, DATIM, LUNIN,LUNOUT,VE,MAXITER)
C------------------------------------------------------------------------
C Input variables (numeric values are read in free format)
C
C Line Variables
C ----- -------
C 1 ECHO (NOECHO) (IA4) Echo flag
C 2 DATIM (IA23) Date and time of simulation
C 3 TITLE1 (I20A4) 1st 80 char job comment
C 4 TITLE2 (I20A4) 2nd 80 char job comment
C 5 CSYSTM (IA4) CARTesian or CYLIndrical
C 6 CONCENTRATION (NOCONCENTRATION) (IA4) Do (or don't) conc simulatn
C 7 TEMPERATURE (NOTEMPERATURE) (IA4) Do (or don't) temp simulatn
C 8 STREAM (NOSTREAM) (IA4) Do (or don't) flow simulatn
C
C Temporal control information
C
C 9 ELTIME, DT, MMTS, TSMULT, TSMAX, WPT
C
C I/O control
ITTIME, MAXITER, IPRINT, ITPLT, ICPLT, IPPLT, IVPLT

Relaxation parameters

RPC, RPT, RPP, RPVEL

SOR relaxation parameters and max # of sor iterations

SORCON, MAXCONI, SORTEM, MAXTEMI, SORPSI, MAXPSII

Convergence Criteria for iterations

CCOFF, TCUTOFF, PCUTOFF

Vertical exaggeration

VE

NI, NJ

Number of nodes in x and y

Node number, locations, initial guesses for field parameters

I, J, X(I,J), Y(I,J), CONC(I,J), TEMP(I,J), PSI(I,J)

Node permeability, porosity, diffusion coeff.,
longitudinal and transverse dispersivity, thermal conductivity

PERM(I,J), POR(I,J), DCX(I,J), ANISO(I,J), ALFAL(I,J), ALFAT(I,J), RKS(I,J)

(for J=1 to NJ; for I=1 to NI)

WATERTABLE (STREAM LINE, or ACCRETION) BOUNDARY (1A4) Type of flow bc

Elevation of hydraulic head at watertable

HWT(I) (for I=1 to NI)

HEAT FLUX (TEMPERATURE) BOUNDARY (1A4) Type of thermal b.c.

Constant heat flux at nodes on lower boundary (where J = 1)
Not needed of temperature boundary condition

Q(I) (for I=1 to NI)

Properties in common block /SPROP / are set w/in this subroutine
but are not read in.
VY(IDIM, JDIM), OLDT(IDIM, JDIM), OLDC(IDIM, JDIM),
OLDSI(IDIM, JDIM), OLDSI, OLDSI, OLDSI, OLDSI, OLDSI,
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READ(LUNIN,100) STRING
IF(STRING .EQ. 'CYLI') THEN
   ICOSYS = 0
   IF(ECHO) WRITE(*,*) 'CYLINDRICAL POLAR COORDINATES'
ELSE IF(STRING .EQ. 'CART') THEN
   ICOSYS = 1
   IF(ECHO) WRITE(*,*) 'CARTESIAN COORDINATES'
ELSE
   STOP 'STOP -- Must specify CYLindrical or CARTesian coordinates'.
ENDIF

Read simulations type (conc, temp, pres, or combination)

READ(LUNIN,100) STRING
IF(STRING .EQ. 'CONC') THEN
   DOCONC = .TRUE.
   CNVRGC = .FALSE.
   IF(ECHO) WRITE(*,*) 'SOLVE FOR CONCENTRATION FIELD'
ELSE IF(STRING .EQ. 'NOCO') THEN
   DOCONC = .FALSE.
   CNVRGC = .TRUE.
   IF(ECHO) WRITE(*,*) 'DO NOT SOLVE FOR CONCENTRATION FIELD'
ELSE
   STOP 'STOP -- Must specify CONCentration or NOConcentration'
ENDIF

READ(LUNIN,100) STRING
IF(STRING .EQ. 'TEMP') THEN
   DOTEMP = .TRUE.
   CNVRGT = .FALSE.
   IF(ECHO) WRITE(*,*) 'SOLVE FOR TEMPERATURE FIELD'
ELSE IF(STRING .EQ. 'NOTE') THEN
   DOTEMP = .FALSE.
   CNVRGT = .TRUE.
   IF(ECHO) WRITE(*,*) 'DO NOT SOLVE FOR TEMPERATURE FIELD'
ELSE
   STOP 'STOP -- Must specify TEMPerature or NOTEmperature'
ENDIF

READ(LUNIN,100) STRING
IF(STRING .EQ. 'STRE') THEN
   DOFLOW = .TRUE.
   CNVRGP = .FALSE.
   IF(ECHO) WRITE(*,*) 'SOLVE FOR STREAM FUNCTION'
ELSE IF(STRING .EQ. 'NOST') THEN
   DOFLOW = .FALSE.
   CNVRGP = .TRUE.
   IF(ECHO) WRITE(*,*) 'DO NOT SOLVE FOR STREAM FUNCTION'
ELSE
   STOP 'STOP -- Must specify STREam function or NOSTream function'
ENDIF

Read temporal control information

READ(LUNIN,* ) ELTIME,DT,MMTS,TSMULT,TSMAX,WPT
IF(DT .LE. ZERO) THEN
   STEADY_STATE = .TRUE.
ELSE
   STEADY_STATE = .FALSE.
ENDIF
IF(ECHO) THEN
   WRITE(*,118) ELTIME,DT,MMTS,TSMULT,TSMAX,WPT
   IF(STEADY_STATE) WRITE(*,*) 'STEADY-STATE SIMULATION'
ENDIF

118  WRITE(118) ELTIME,DT,MMTS,TSMULT,TSMAX,WPT
118 FORMAT(IX,'ELAPSED TIME = ',E14.5/,1X,
1 'TIME STEP = ',E14.5/,1X,
2 'INCREASE DT EVERY ',I5,' TIME STEPS',/1X,
3 'BY A VALUE OF ',E14.5/,1X,
4 'MAXIMUM TIME STEP = ',E14.5/,1X,
5 'WEIGHT IMPLICIT FORM BY ',E14.5)

C Read time steps on wh/ to do I/O

READ(LUNIN,* ) ITTIME,MAXITER,IPRINT,ICPLT,ITPLT,IPPLT,IVPLT
IF(MAXITER .EQ. 0) MAXITER=1
IF(ECHO) WRITE(*,122) ITTIME,MAXITER,IPRINT,ICPLT,ITPLT,
1 IPPLT,IVPLT
122 FORMAT(IX,'MAXIMUM NUMBER OF TIME STEPS = ',I5/,1X,
A 'MAXIMUM ITERATIONS / TIME STEP= ',I5/,1X,
1 'PRINT EVERY ',I5,' TIME STEPS',/1X,
2 'PLOT CONCENTRATION EVERY ',I5,' TIME STEPS',/1X,
3 'PLOT TEMPERATURE EVERY ',I5,' TIME STEPS',/1X,
4 'PLOT STREAM FUNCTION EVERY ',I5,' TIME STEPS',/1X,
5 'PLOT VELOCITY EVERY ',I5,' TIME STEPS')

C Read relaxation parameters

READ(LUNIN,* ) RPC,RPT,RPP,RPVEL
IF(ECHO) THEN
WRITE(*,132) RPC,RPT,RPP,RPVEL
ENDIF
132 FORMAT(IX,'CONCENTRATION RELAXATION = ',E14.5/,1X,
1 'TEMPERATURE RELAXATION = ',E14.5/,1X,
2 'STREAM FUNCTION RELAXATION = ',E14.5/,1X,
3 'VELOCITY RELAXATION = ',E14.5/,1X)
READ(LUNIN,* ) SORCON,MAXCONI,SORTEM,MAXTEMI,SORPSI,MAXPSII
 IF(ECHO) THEN
WRITE(*,134) SORCON,MAXCONI,SORTEM,MAXTEMI,SORPSI,MAXPSII
ENDIF
134 FORMAT(IX, 'SOR RELAXATION FOR CONCENTRATION = ',E14.5,
1 MAXIMUM OF ',15,' ITERATIONS',/1X,
1 'SOR RELAXATION FOR TEMPERATURE = ',E14.5,
1 MAXIMUM OF ',15,' ITERATIONS',/1X,
1 'SOR RELAXATION FOR STREAM FUNCTION = ',E14.5,
1 MAXIMUM OF ',15,' ITERATIONS',/1X)

C Read convergence criteria

READ(LUNIN,* ) CCUTOFF,TCUTOFF,PCUTOFF
IF(ECHO) THEN
WRITE(*,136) CCUTOFF,TCUTOFF,PCUTOFF
ENDIF
136 FORMAT(IX, 'CONVERGENCE CRITERIA',/1X,
1 'CONCENTRATION CUTOFF = ',E14.5/,1X,
1 'TEMPERATURE CUTOFF = ',E14.5/,1X,
1 'STREAM FUNCTION CUTOFF = ',E14.5/,1X)

C Read vertical exaggeration

READ(LUNIN,* ) VE
IF(ECHO) THEN
WRITE(*,140) VE
ENDIF
140 FORMAT(1X, 'VERTICAL EXAGGERATION FOR PLOTTING = ',E14.5/)
IF(ECHO) WRITE(*,142) NI,NJ
142 FORMAT(1X,15,' NODES IN X','16,' NODES IN Y')

Read node numbers, locations and field values for iteration 1

DO 200 IJ=1,NI*NJ
   READ(LUNIN,*) I , J, X(I,J), Y(I,J), CONC(I,J), TEMP(I,J), PSI(I,J),
   PERM(I,J), POR(I,J), DCK(I,J), ANISO(I,J),
   ALFAL(I,J), ALFAT(I,J), RKS(I,J)
1
   OLDTEMP(I,J) = TEMP(I,J)
   OLDCONC(I,J) = CONC(I,J)
   CLAST(I,J) = CONC(I,J)
   OLDPSI (I, J) = PSI(I,J)
200 CONTINUE
   IF(ECHO) THEN
      WRITE(*,152)
   DO 220 J=1,NJ
      DO 210 I=1,NI
         WRITE (*,154) I,J,X(I,J), Y(I,J), CONC(I, J) ,  TEMP ( I, J) ,  PSI ( I , J) ,
         PERM (I, J) ,  POR (I, J), DCK(I,J), ANISO(I,J),
         ALFAL(I,J), ALFAT(I,J), RKS(I,J)
1
      210 CONTINUE
   220 CONTINUE
   ENDIF
152 FORMAT(1X,' NODES, LOCATIONS, FIELD VARIABLES, AND PHYSICAL
1 PARAMETERS')
154 FORMAT(1X,215,5E13,4,/,11X,5E13.4,/,12X,2E13.4)

Read type of thermal boundary condition normal to bottom
READ(LUNIN,100) STRING
IF(STRING .EQ. 'TEMP') THEN
  HFLUXBC = .FALSE.
  IF(ECHO) WRITE(*,*) 'TEMPERATURE SPECIFIED ON BOTTOM BOUNDARY'
  RETURN
ELSE IF(STRING .EQ. 'HEAT') THEN
  HFLUXBC = .TRUE.
  IF(ECHO) WRITE(*,*)
  1  'HEAT FLUX SPECIFIED NORMAL TO BOTTOM BOUNDARY'
ELSE
  STOP 'STOP - Must specify HEAT flux or TEMPerature for bottom bc'
ENDIF
C
C Read in value of heat flux along the lower boundary
C
IF(HFLUXBC) THEN
  READ(LUNIN,*) (Q(I),I=1,NI)
  IF(ECHO) THEN
    WRITE(*,160)
    WRITE(*,162) (I,Q(I), I=1,NI)
  ENDIF
ENDIF
160 FORMAT(IX,'HEAT FLUX AT LOWER BOUNDARY NODES')
162 FORMAT(IX,2(110,E13.4))
C
CLOSE(LUNIN)
RETURN
C There's no place like home
END
C---------------------------------------------------------------------------------
C
SUBROUTINE MEDPROP
C---------------------------------------------------------------------------------

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.00D+00,ONE=1.00D+00,
  1  GRAV=-9.800D+00,THOUS=1.000D+03)
COMMON /COORDS/ X(IDIM,JDIM), Y(IDIM,JDIM), ICOSYS
COMMON /PPARAM/ A
COMMON /FIELDS/ ANISO(IDIM,JDIM), ALFAT(IDIM,JDIM),
  1  ALFAL(IDIM,JDIM), RKS(IDIM,JDIM)
COMMON /FIELDS/ TEMP(IDIM,JDIM), CONC(IDIM,JDIM), PSI(IDIM,JDIM),
  1  VX(IDIM,JDIM),
  1  VY(IDIM,JDIM), OLDT(IDIM,JDIM), OLDC(IDIM,JDIM),
  1  OLDPsi(IDIM,JDIM),
  2  OLdvX(IDIM,JDIM), OLdvY(IDIM,JDIM),
  1  CLAST(IDIM,JDIM)
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /SPROP/ RHOS, CS, RKF, CF, RFZERO, TZERO
COMMON /APROP/ RKSF(IDIM,JDIM), RhoF(IDIM,JDIM),
  1  OLdRhoF(IDIM,JDIM), VISCO(IDIM,JDIM),
  1  DSPXX(IDIM,JDIM), DSPYY(IDIM,JDIM), DSPXY(IDIM,JDIM)
C---------------------------------------------------------------------------------
C
DO 110 J=1,NJ
  DO 100 I=1,NI
    IF(POR(I,J) .LE. ZERO) POR(I,J)=0.02D+00
    IF(DCX(I,J) .LE. ZERO) DCX(I,J)=1.00D-15
Compute composite thermal conductivity

\[ \text{RKS}(I,J) = \text{POR}(I,J) \times \text{RKF} + (\text{ONE} - \text{POR}(I,J)) \times \text{RKS}(I,J) \]

Compute components of hydrodynamic dispersion tensor
(The off-diagonal terms are calculated just to waste CPU time; they are not used in subsequent calculations.)

\[ \text{VMAG} = \sqrt{\text{VX}(I,J)^2 + \text{VY}(I,J)^2} \]

\[ \text{IF} (\text{VMAG} \text{ GT} \text{ ZERO}) \text{ THEN} \]
\[ \text{VX}_2 = \text{VX}(I,J) \times \text{VX}(I,J) \]
\[ \text{VY}_2 = \text{VY}(I,J) \times \text{VY}(I,J) \]
\[ \text{VXY} = \text{VX}(I,J) \times \text{VY}(I,J) \]
\[ \text{DSPXX}(I,J) = \text{DCX}(I,J) + \]
\[ \frac{\text{ALFAL}(I,J) \times \text{VX}_2}{\text{VMAG}} + \]
\[ \frac{\text{ALFAT}(I,J) \times \text{VY}_2}{\text{VMAG}} \]
\[ \text{DSPYY}(I,J) = \frac{\text{DCX}(I,J)}{\text{ANISO}(I,J)} + \]
\[ \frac{\text{ALFAL}(I,J) \times \text{VY}_2}{\text{VMAG}} + \]
\[ \frac{\text{ALFAT}(I,J) \times \text{VX}_2}{\text{VMAG}} \]
\[ \text{DSPXY}(I,J) = (\text{ALFAL}(I,J) - \text{ALFAT}(I,J)) \times \frac{\text{VX}(I,J) \times \text{VY}(I,J)}{\text{VMAG}} \]
\[ \text{DCX}(I,J) \]
\[ \text{DCX}(I,J) / \text{ANISO}(I,J) \]
\[ 1.00 \times 10^{-5} \times \text{DCX}(I,J) \]
\[ \text{ELSE} \]
\[ \text{DSPXX}(I,J) = \text{DCX}(I,J) \]
\[ \text{DSPYY}(I,J) = \text{DCX}(I,J) / \text{ANISO}(I,J) \]
\[ \text{DSPXY}(I,J) = 1.00 \times 10^{-5} \times \text{DCX}(I,J) \]
\[ \text{ENDIF} \]

\[ \text{IF} (\text{DSPXY}(I,J) \text{ EQ} \text{ ZERO}) \text{ DSPXY}(I,J) = 1.00 \times 10^{-5} \times \text{DCX}(I,J) \]
\[ \text{DSPXX}(I,J) = \text{DSPXX}(I,J) \times \text{POR}(I,J) \times \text{RHOF}(I,J) \]
\[ \text{DSPYY}(I,J) = \text{DSPYY}(I,J) \times \text{POR}(I,J) \times \text{RHOF}(I,J) \]
\[ \text{DSPXY}(I,J) = \text{DSPXY}(I,J) \times \text{POR}(I,J) \times \text{RHOF}(I,J) \]

100 CONTINUE
110 CONTINUE

RETURN
END

SUBROUTINE EQSTATE

Computes the density of fluid and viscosity of fluid as a function of Pressure, Salinity, and Temperature

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101, JDIM=101, ZERO=0.00D+00, ONE=1.00D+00,
1 GRAV=9.800D+00, THOUS=1.000D+03, TENTH=0.10D+00)
COMMON /COORDS/ X(IDIM, JDIM), Y(IDIM, JDIM), ICOSYS
COMMON /FIELDS/ TEMP(IDIM, JDIM), CONC(IDIM, JDIM), PSI(IDIM, JDIM),
A VX(IDIM, JDIM),
1 VY(IDIM, JDIM), OLDT(IDIM, JDIM), OLDC(IDIM, JDIM),
B OLDPSI(IDIM, JDIM),
2 OLDVX(IDIM, JDIM), OLVDY(IDIM, JDIM),
C CLAST(IDIM, JDIM)
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /SPROP/ RHOS, CS, RKF, CF, RFZERO, TZERO
COMMON /APROP/ RKSF(IDIM, JDIM), RHOF(IDIM, JDIM),
1 OLDRHOF(IDIM, JDIM), VISCO(IDIM, JDIM),
1 DSPXX(IDIM, JDIM), DSPYY(IDIM, JDIM), DSPXY(IDIM, JDIM)

DO 110 J=1, NJ
DO 100 I=1, NI

Estimate pressure and temperature for equation of state
C
PR = -RFZERO*GRAV*(Y(I,NJ)-Y(I,J))*1.00E-05
C
Convert concentration to molality for equation of state
(Assumes solute is NaCl)
C
CMOLAL = CONC(I,J)*THOUS/(58.00D+00*(ONE-CONC(I,J)))
C
Calculate density of fluid
C
RHOF(I,J) = RHOCALC(TEMP(I,J),CMOLAL,PR)
C
And viscosity
C
VISCO(I,J) = VISCALC(TEMP(I,J),CMOLAL,TENTH*PR)
C
100 CONTINUE
110 CONTINUE
C
. RETURN
END
C------------------------------------------------------------------------
C------------------------------------------------------------------------
SUBROUTINE CONSLV(STEADY_STATE)
C------------------------------------------------------------------------
Solve for CONCentratlon filed for this time step
C------------------------------------------------------------------------
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.00D+00,ONE=1.00D+00)
LOGICAL WATERTBL,HFLUXBC,ACCRETN,STEADY_STATE
COMMON /PPARAM/ PERM(IDIM,JDIM),POR(IDIM,JDIM),DCX(IDIM,JDIM),
A ALFAL(IDIM,JDIM),RKS(IDIM,JDIM)
1 COMMON /COORDS/ X(IDIM,JDIM),Y(IDIM,JDIM),ICOSYS
COMMON /FIELDS/ TEMP(IDIM,JDIM),CONC(IDIM,JDIM),PSI(IDIM,JDIM),
A VX(IDIM,JDIM),
1 Y(IDIM,JDIM),OLDT(IDIM,JDIM),OLDC(IDIM,JDIM),
B OLDPsi(IDIM,JDIM),
2 OLdVX(IDIM,JDIM),OLdVY(IDIM,JDIM),
C CLAST(IDIM,JDIM)
COMMON /CLOCK/ ELTIME,DT,MMTS,TSMULT,TSMAX,WDT
COMMON /BNDRYC/ HWT(IDIM),Q(IDIM),WATERTBL,ACCRETN,HFLUXBC
COMMON /SPROP/ RHOS,CS,RF,CF,RFZERO,TZERO
COMMON /APROP/ RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDRHOF(IDIM,JDIM),VISCOS(IdIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /ISIZE/ NI,NJ,ITIME,ITTIME
 COMMON /RELAX/ RPT,RP,RPP,RPVEL,SORTEM,MAXTEM,SORCON,MAXCONI,
1 SORPSI,MXPSSII,CCUTOFF,TCUTOFF,PCTOFF
COMMON /RJACOB/ X1(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIF(20, IDIM),ZF(20, IDIM),RPERM(20),RPOR(20),
2 RDCX(20),RRKS(20),RANISO(20),NSIF,
2 NONMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces
DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
1 E(IDIM,JDIM),F(IDIM,JDIM)
SAVE ITROLDC,CSIGN,NOMEGA
C------------------------------------------------------------------------
C
Calculate the coefficients of the finite difference
C equation for solute transport
CALL CCOEF(A,B,C,D,E,F,STEADY_STATE)

Modify the coefficients for appropriate boundary conditions

CALL CONCBC(A,B,C,D,E,F,CONC,NI,NJ)

Now solve the sparse matrix equation for CONCetration

CALL SORL(A,B, C, D,E, F,CONC,JIFTOP(NI),NI,NJ,MAXCONI,ITR,SORCON,1
1.0D-08,'CONSLV') ! 1.0D-9*CCUTOFF,)

Update estimate of relaxation factor

IF(ITR .LT. MAXCONI) THEN
NOMEGA = NOMEGA + 1
SORCON = OMEGA_NEW(SORCON,NOMEGA,ITR,ITROLDC,CSIGN)
ENDIF

Adjust concentration of passive nodes

CALL ADJCBC(CONC,NI,NJ)

That's it...

RETURN
END

SUBROUTINE CCOEF(A,B,C,D,E,F,STEADY_STATE)

C--------------------------------------------------------------------------------------------------------------------------------------------------
C
C
C
C Calculate the coefficients of the differential equation that describes solute transport in a porous medium.
C--------------------------------------------------------------------------------------------------------------------------------------------------

IMPLICIT DOUBLE PRECISION(A-H, O-Z)
PARAMETER(IDIM=101, JDIM=101, ZERO=0.0D+00, HALF=0.5D+00, ONE=1.0D+00,
1 TWO=2.0D+00, TENH=0.100D+00, QT=0.25D+00, TEN=1.00D+00)
LOGICAL STEADY_STATE, CYLINDRICAL
COMMON /PPARAM/ PERM(IDIM,JDIM),POR(IDIM,JDIM),DCX(IDIM,JDIM),
A ANISO(IDIM,JDIM),ALFAT(IDIM,JDIM),
1 ALFAL(IDIM,JDIM),RKS(IDIM,JDIM)
COMMON /COORDS/ X (IDIM,JDIM),Y(IDIM,JDIM)
COMMON /FIELDS/ TEMP(IDIM,JDIM),CONC(IDIM,JDIM),PSI(IDIM,JDIM),
1 VX(IDIM,JDIM),
2 OLDPsi(IDIM,JDIM),
3 OLDVX(IDIM,JDIM), OLDVY(IDIM,JDIM),
4 CLAST(IDIM,JDIM)
COMMON /CLOCK / ELTIME, DT, MMTS, TSMULT, TSMAX, WDT
COMMON /ISIZE / NI, NJ, ITIME, ITTIME
COMMON /RJACOB/ X1(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM), Y2(IDIM,JDIM)
COMMON /SPROP / RHOS, CS, RKF, CF, RFZERO, TZERO
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLRHOF(IDIM,JDIM), VISCO(IDIM,JDIM),
2 DSPX(IDIM,JDIM), DSPY(IDIM,JDIM), DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATE, SRATE(IDIM,JDIM), JIFTOP(IDIM),
1 JIP(20, IDIM), ZIP(20, IDIM), RPERM(20), Rпор(20),
2 RDCX(20), RPKS(20), RANISO(20), NSIF,
2 NOMOVE(IDIM), NNM, CTOP, FTOP ! Maximum of 20 interfaces
And the coefficients are...

```
DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
1   E(IDIM,JDIM),F(IDIM,JDIM)
```

```
Define function for upstream weighting

AFUNC(X) = MAX(ZERO, (ONE-TENTH* (MIN(TEN,ABS(X))))**5)
AFUNC(X) = ONE
```

```
First set a couple of logical flags

IF(ICOSYS .EQ. 0 )  THEN
   CYLINDRICAL = .TRUE.
ELSE IF(ICOSYS .EQ. 1 )  THEN
   CYLINDRICAL = .FALSE.
ENDIF
```

```
DO 110 J=2,NJ-1
   DO 100 I=2,NI-1
      Calculate sizes of control volume Interfaces
      DXWEST = X(I,J) - X(I-1,J)
      DXEAST = X(I+1,J) - X(I,J)
      DYSOUTH= Y(I,J) - Y(I,J-1)
      DYNORTH= Y (I , J+l) - Y(I,J)
```

```
Estimate solute diffusion term at Interfaces

DEAST = DCON12(I,J+1,1)*Y2(I,J)/DXEAST
DWEST = DCON12(I-1,J,1)*Y2(I,J)/DXWEST
DNORTH = DCON12(I,J+1,1)*X1(I,J)/DYNORTH
DSOUTH = DCON12(I,J-1,1)*X1(I,J)/DYSOUTH
```

```
REAST = HALF*(RHOF(I,J)+RHOF( 1  + 1 ,  J))
RWEST = HALF*(RHOF(1-1,J)+RHOF(I,J))
RNORTH = HALF*(RHOF(I,J)+RHOF(I, J+l))
RSOUTH = HALF*(RHOF(I,J-l)+RHOF(I, J) )
```

```
FEAST - REAST*VX(I+1,J)*Y2(I,J)
FWEST = RWEST*VX(I,J)*Y2(I,J)
FNORTH= RNORTH*VY(I,J+l)*X1(I,J)
FSOUTH- RSOUTH*VY(I,J)*X1(I, J)
```

```
Modify vertical flux terms to account for subsidence

RPORNO = HALF*(RHOF(I,J+1)*POR(I,J+1)+RHOF(I,J)*POR(I,J))
RPORSO = HALF*(RHOF(I,J)*POR(I,J)+RHOF(I,J-1)*POR(I,J-1))
FNORTH = FNORTH + RPORNO*SRATE(I, J)
FSOUTH = FSOUTH + RPORSO*SRATE(I, J)
```

```
PEAST - FEAST/DEAST
PWEST = FWEST/DWEST
PNORTH = FNORTH/DNORTH
PSOUTH = FSOUTH/DSOUTH
```

```
A(I,J) = DEAST*AFUNC(ABS(PEAST))  + MAX(-FEAST,ZERO)
B(I,J) = DWEST*AFUNC(ABS(PWEST))  + MAX(FWEST,ZERO)
C(I,J) = DNORTH*AFUNC(ABS(PNORTH))  + MAX(-FNORTH,ZERO)
D(I,J) = DSOUTH*AFUNC(ABS(FSOUTH))  + MAX(FSOUTH,ZERO)
```
IF(CYLINDRICAL) THEN
A(I,J) = A(I,J) * HALF*(X(I,J)+X(I+1,J))
B(I,J) = B(I,J) * HALF*(X(I,J)+X(I-1,J))
AVGR = QTR*(X(I+1,J)+TWO*X(I,J)+X(I-1,J)) ! Average radius
C(I,J) = C(I,J) * AVGR
D(I,J) = D(I,J) * AVGR
ENDIF
E(I,J) = - A(I,J) - B(I,J) - C(I,J) - D(I,J) !
F(I,J) = ZERO
100 CONTINUE
110 CONTINUE

For transient solution calculate terms involving time derivatives

IF(.NOT.STEADY_STATE) THEN
DO 160 J=2,NJ-1
DO 150 I=2,NI-1
TIMTRM = X1(I,J)*Y2(I,J)*RHOF(I,J)*POR(I,J)/DT ! Time term
AVGR = QTR*(X(I+1,J)+TWO*X(I,J)+X(I-1,J)) ! Average radius
IF(CYLINDRICAL) TIMTRM » TIMTRM*AVGR
E(I,J) = - A(I,J) - B(I,J) - C(I,J) - D(I,J) - TIMTRM
F(I,J) = F(I,J) - TIMTRM*OLDRHOF(I,J)*CLAST(I,J)/RHOF(I,J)
150 CONTINUE
160 CONTINUE
ENDIF

This Isn't Kansas, Toto
RETURN
END

SUBROUTINE CONCBC(A,B,C,D,E,F,CONC,NX,NY)
C
This adjusts finite difference coefficients for noflow boundary
conditions on sides where Xi is held constant. That is, the normal
derivatives on these boundaries vanish. On input and output A, B, C,
D, E, and F are the coefficients of the finite difference equation in
transformed coordinates; i.e.
C
A(i,j)*CONC(i+1,j) + B(i,j)*CONC(i-1,j) + C(i,j)*CONC(i,j+1) +
D(i,j)*CONC(i,j-1) + E(i,j)*CONC(i,j) = F(i,j)*CONC(i,j)
C
The coordinate transformation is carried out prior to calling CONCBC
and the derivatives of the transformation are passed via common block
RJACOB.
C
See comments in main program segment for general treatment of boundary
conditions.
C
-- Dave Evans Aug. 1988

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.0D0,HALF=0.5D+00,TWO=2.0D+00,
1 HUGE=1.00D+30)
LOGICAL STILL
DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
1 E(IDIM,JDIM),F(IDIM,JDIM),CONC(IDIM,JDIM)
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM)
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDRHOF(IDIM,JDIM), VISCO(IDIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM), DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1
Set NoFlow conditions at the sides of the mesh...

\begin{verbatim}
DO 120 J=2, NY-1
  RJ1 = (X1(2, J) * X2(2, J) + Y1(2, J) * Y2(2, J)) / (X2(2, J) * X2(2, J) + Y2(2, J) * Y2(2, J))
  RJN = (X1(NX-1, J) * X2(NX-1, J) + Y1(NX-1, J) * Y2(NX-1, J)) / (X2(NX-1, J) * X2(NX-1, J) + Y2(NX-1, J) * Y2(NX-1, J))
  A(2, J) = A(2, J) + B(2, J)
  C(2, J) = C(2, J) - RJ1 * B(2, J)
  D(2, J) = D(2, J) + RJ1 * B(2, J)
  B(1, J) = ZERO
  B(2, J) = ZERO
  C(NX-1, J) = C(NX-1, J) + RJN * A(NX-1, J)
  D(NX-1, J) = D(NX-1, J) - RJN * A(NX-1, J)
  B(NX-1, J) = B(NX-1, J) + A(NX-1, J)
  A(NX, J) = ZERO
  A(NX-1, J) = ZERO

120 CONTINUE

And on the edge of the salt column

DO J=JIFBOT(NOMOVE(NNM)), JIFTOP(NOMOVE(NNM))
  DO N=NNM+1, 2, -1
    E(NOMOVE(N), J) = E(NOMOVE(N), J) + B(NOMOVE(N), J)
    B(NOMOVE(N), J) = ZERO
  ENDDO
ENDDO

Modify some interior nodes for specified concentration

DO 130 INM=1, NNM
  E(NOMOVE(INM), JIFTOP(NOMOVE(INM))) = -HUGE
  F(NOMOVE(INM), JIFTOP(NOMOVE(INM))) = -HUGE * CTOP

130 CONTINUE

Modify source terms at top

DO 150 I=1, NX
  F(I, NY-1) = F(I, NY-1) - C(I, NY-1) * CONC(I, NY)
  C(I, NY-1) = ZERO

150 CONTINUE

Set NoFlow at bottom boundary

DO I=1, NX
  STILL=.FALSE.
  DO NI=1, NNM
    IF(I.EQ. NOMOVE(NI)) STILL=.TRUE.
    END DO
  IF(.NOT. STILL) THEN
    E(I, JIFTOP(I)+1) = E(I, JIFTOP(I)+1) + D(I, JIFTOP(I)+1)
    D(I, JIFTOP(I)+1) = ZERO
  ENDIF
END DO

Set constant concentration at the bottom

DO 160 I=1, NX
  F(I, 2) = F(I, 2) - D(I, 2) * CONC(I, 1)
  D(I, 2) = ZERO

1 These lines are for constant concentration along the bottom
SUBROUTINE ADJCBC(U,NX,NY)

ADJust the value of Concentration, U, at passive nodes on Boundaries for which there is no solute flux normal to the boundaries on which xi is 1 or NX.

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.00D+00,HALF=0.5D+00, 
1 TWO=2.00D+00)
LOGICAL STILL
COMMON/RJACOB/XI(IDIM,JDIM),X2(IDIM,JDIM),
Y1(IDIM,JDIM),Y2(IDIM,JDIM),
COMMON/APROP/RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDRHOF(IDIM,JDIM),VISCO(IDIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPY(IDIM,JDIM),DSPXY(IDIM,JDIM),
COMMON/SUBSID/TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIF(20,IDIM),ZIF(20,IDIM),RPERM(20),RPER(20),
2 RDCX(20),RRKS(20),RARISO(20),NSIF,
2 NOMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces
DIMENSION U(IDIM,JDIM)

First to the sides, on which xi is held constant

DO 100 J=1,NY
    ! J=1,NY w/ constant flux bc's
    
    First the right hand side, then the left hand side

    R1 = (X1(2,J)*X2(2,J) + Y1(2,J)*Y2(2,J)) / 
1 (X2(2,J)*X2(2,J) + Y2(2,J)*Y2(2,J))
    RN = (X1(NX-1,J)*X2(NX-1,J) + Y1(NX-1,J)*Y2(NX-1,J)) / 
1 (X2(NX-1,J)*X2(NX-1,J) + Y2(NX-1,J)*Y2(NX-1,J))

    IF (J .EQ. 1) THEN
        U(1,J) = U(3,J) + R1*(U(2,J+1) - U(2,J)) 
        U(NX,J) = U(NX-2,J) + RN*(U(NX-1,J+1) - U(NX-1,J))
    ELSE IF (J .EQ. NY) THEN
        U(1,J) = U(3,J) + R1*(U(2,J) - U(2,J-1))
        U(NX,J) = U(NX-2,J) + RN*(U(NX-1,J) - U(NX-1,J-1))
    ELSE
        U(1,J) = U(3,J) - R1*(U(2,J+1) - U(2,J-1))
        U(NX,J) = U(NX-2,J) + RN*(U(NX-1,J+1) - U(NX-1,J-1))
    ENDIF

100 CONTINUE

Reset concentration at top of salt

DO INM=1,NNM
    U(NOMOVE(INM),JIFTOP(NOMOVE(INM))) = CTOP
END DO

Reset values w/in the salt itself

DO J=JIFBOT(NOMOVE(NNM)),JIFTOP(NOMOVE(NNM))-1
    DO N=NNM,1,-1
        U(NOMOVE(N),J) = U(NOMOVE(N)+1,J)
    ENDDO
END
ENDDO

C Reset passive nodes on basement
C
DO I=1,NX
  STILL=.FALSE.
  DO NI=1,NNM
    IF(I .EQ. NOMOVE(NI)) STILL=.TRUE.
  END DO
  IF(.NOT. STILL) THEN
    U(I,JIFTOP(I)) = U(I,JIFTOP(I)+1)
  ENDIF
END DO

RETURN
END

SUBROUTINE TEMSLV

C Solve for TEMPerature filed for this time step
C
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER( IDIM=101, JDIM=101, ZERO=0.00D+00, ONE=1.00D+00)
LOGICAL WATERTBL,ACCRETN, HFLUXBC
COMMON /PARAM/ PERM(IDIM,JDIM), POR(IDIM,JDIM), DCX(IDIM,JDIM),
  ANISO(IDIM,JDIM), ALPHAT(IDIM,JDIM), ALFAL(IDIM,JDIM), RKS(IDIM,JDIM)
COMMON /COORDS/ X(IDIM,JDIM), Y(IDIM,JDIM), ICOSYS
COMMON /FIELDS/ TEMP(IDIM,JDIM), CONC(IDIM,JDIM), PSI(IDIM,JDIM),
  VX(IDIM,JDIM), VY(IDIM,JDIM), OLDT(IDIM,JDIM), OLDC(IDIM,JDIM),
  OLDSI(IDIM,JDIM), OLDVX(IDIM,JDIM), OLDVY(IDIM,JDIM), CLAST(IDIM,JDIM)
COMMON /CLOCK / ELTIME, DT, MMTS, TSMULT, TSMAX, WDT
COMMON /BNDRYC/ HWT(IDIM), Q(IDIM), WATERTBL, ACCRETN, HFLUXBC
COMMON /SPROP / RHOS, CS, RKSF, CF, RFZERO, TZERO
COMMON /APROP / RKSF(IDIM,JDIM), RHOF(IDIM,JDIM),
  OLDRHOF(IDIM,JDIM), VISCO(IDIM,JDIM), DSPXX(IDIM,JDIM), DSPYY(IDIM,JDIM),
  DSPXY(IDIM,JDIM)
COMMON /ISIZE / NI, NJ, ITIME, ITIME
COMMON /RELAX / RPT, RFC, RPF, RPVEL, SORTEM, SORCON, MAXCONI,
  SORPSI, MAXPSI, CCUTOFF, TCUTOFF, PCUTOFF
COMMON /RJACOB/ XI(IDIM,JDIM), X2(IDIM,JDIM),
  Y1(IDIM,JDIM), Y2(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB, RSRATE, SRATE(IDIM,JDIM), JIFTOP(IDIM),
  JIFBOT(IDIM), ZIP(IDIM,JDIM), ZIPBOT(IDIM), ZIF(IDIM,JDIM), ZIFBOT(IDIM),
  RRKS(20), RRKS(20), RANISO(20), NSIF,
  NOMOVE(IDIM,JDIM), NNM, CTOP, FTOP ! Maximum of 20 interfaces
DIMENSION A(IDIM,JDIM), B(IDIM,JDIM), C(IDIM,JDIM), D(IDIM,JDIM),
  E(IDIM,JDIM), F(IDIM,JDIM)
SAVE ITROLDT, TSIGN, NOMEBA

C Calculate the coefficients of the finite difference
C equation for heat transport
C
CALL TCOEF(A,B,C,D,E,F)

C Modify the coefficients for appropriate boundary conditions
CALL TEMPBC(A,B,C,D,E,F,TEMP,NI,NJ)

Now solve the sparse matrix equation for CONCentration

CALL SORL(A,B,C,D,E,F,TEMP,1,NI,NJ,MAXTEMI,ITR,SORTEM,TCUTOFF, 1  'TEMSLV')

Update estimate of relaxation factor

IF(ITR .LT. MAXTEMI) THEN
  NOMEGA = NOMEGA + 1
  SORTEM = OMEGA_NEW(SORTEM,NOMEGA,ITR,ITROLDT,ITR)
ENDIF

Adjust temperature of passive nodes

CALL ADJTBC(TEMP,NI,NJ)

That's it...

RETURN
END

SUBROUTINE TCOEF(A,B,C,D,E,F)

Calculate the coefficients of the differential equation that describes
heat transport in a porous medium.

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.0D+00,HALF=0.5D+00,ONE=1.0D+00,
  1  TWO=2.0D+00,TENTH=0.100D+00,QUART=0.25D+00,TEN=10.0D+00)
LOGICAL CYLINDRICAL
COMMON /PPARAM/ PERM(IDIM,JDIM),POR(IDIM,JDIM),DCX(IDIM,JDIM),
  1  ANISO(IDIM,JDIM),ALFAT(IDIM,JDIM),ALFAL(IDIM,JDIM),RKS(IDIM,JDIM)
COMMON /COORDS/ X(IDIM,JDIM),Y(IDIM,JDIM),ICOSYS
COMMON /FIELDS/ TEMP(IDIM,JDIM),CONC(IDIM,JDIM),FSI(IDIM,JDIM),
  1  VX(IDIM,JDIM),
  2  VY(IDIM,JDIM),OLDT(IDIM,JDIM),OLDC(IDIM,JDIM),
  3  ODLPSI(IDIM,JDIM),
  4  ODLVX(IDIM,JDIM),OLDVY(IDIM,JDIM),CLAST(IDIM,JDIM)
COMMON /CLOCK / ELTIME, DT, MMTS, TSMULT, TSMAX, WDT
COMMON /ISIZE / NI, NJ, ITIME, ITTIME
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
  1  Y1(IDIM,JDIM),Y2(IDIM,JDIM),
  2  OLDHOF(IDIM,JDIM), VISCO(IDIM,JDIM),
  3  DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSTRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
  1  JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
  2  JIF(20,JDIM),ZIF(20,JDIM),RPERM(20),RPERM(20),
  3  RDCX(20),RRKS(20),RANISO(20),NSIF,
  4  NOMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces
DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
  1  E(IDIM,JDIM),F(IDIM,JDIM)

And the coefficients are...

DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
  1  E(IDIM,JDIM),F(IDIM,JDIM)
DIMENSION FEAST(IDIM,JDIM), PWEST(IDIM,JDIM), PSOUTH(IDIM,JDIM),
          PNORTH(IDIM,JDIM)

Define function for upstream weighting
AFUNC(X) = MAX(ZERO, (ONE-TENTH*(MIN(TEN,ABS(X))))**5)
AFUNC(X) = ONE

First set logical flags for coordinate system
IF(ICSYS .EQ. 0) THEN
  CYLINDRICAL = .TRUE.
ELSE IF(ICSYS .EQ. 1) THEN
  CYLINDRICAL = .FALSE.
ENDIF

DO 110 J=2,NJ-1
  DO 100 I=2,NI-1

Calculate sizes of control volume interfaces
DXWEST = X(I,J) - X(I-1,J)
DXEAST = X(I+1,J) - X(I,J)
DYSOUTH = Y(I,J) - Y(I,J-1)
DYNORTH = Y(I,J+1) - Y(I,J)

Estimate thermal conduction term at interfaces
DEAST = TCON12(I,J-1+1,J)*Y2(I,J)/DXEAST
DWEST = TCON12(I-1+1,J)*Y2(I,J)/DXWEST
DNORTH = TCON12(I,J,J+1)*X1(I,J)/DYNORTH
DSOUTH = TCON12(I,J,J-1)*X1(I,J)/DYSOUTH

Estimate convective term at interfaces
REAST = HALF*(RHOF(I,J)+RHOF(I+1,J))*CF
RWEST = HALF*(RHOF(I,J)+RHOF(I,J-1))*CF
RNORTH = HALF*(RHOF(I,J)+RHOF(I,J+1))*CF
RSOUTH = HALF*(RHOF(I,J-1)+RHOF(I,J))*CF
FEAST = REAST*VX(I+1,J)*Y2(I,J)
FWEST = RWEST*VX(I,J)*Y2(I,J)
FNORTH = RNORTH*VY(I,J+1)*X1(I,J)
FSOUTH = RSOUTH*VY(I,J)*X1(I,J)

Estimate grid Peclet number at interfaces
PEAST(I,J) = FEAST/DEAST
PWEST(I,J) = FWEST/DWEST
PNORTH(I,J) = FNORTH/DYNORTH
PSOUTH(I,J) = FSOUTH/DYSOUTH

A(I,J) = DEAST*AFUNC(ABS(FEAST(I,J))) + MAX(-FEAST,ZERO)
B(I,J) = DWEST*AFUNC(ABS(FWEST(I,J))) + MAX(-FWEST,ZERO)
C(I,J) = DNORTH*AFUNC(ABS(FNORTH(I,J))) + MAX(-FNORTH,ZERO)
D(I,J) = DSOUTH*AFUNC(ABS(FSOUTH(I,J))) + MAX(-FSOUTH,ZERO)

IF(CYLINDRICAL) THEN
  AVGR = QTR*(X(I,J)+X(I+1,J))+TWO*X(I,J)+X(I-1,J)) ! Average radius
  A(I,J) = A(I,J)*HALF*(X(I,J)+X(I+1,J))
  B(I,J) = B(I,J)*HALF*(X(I,J)+X(I-1,J))
  C(I,J) = C(I,J)*AVGR
  D(I,J) = D(I,J)*AVGR
ENDIF

END
This adjusts finite difference coefficients for no flow boundary conditions on sides where \( \xi_1 \) is held constant. That is, the normal derivatives on these boundaries vanish. On input and output \( A, B, C, D, E, \) and \( F \) are the coefficients of the finite difference equation in transformed coordinates; i.e.

\[
\begin{align*}
A(i,j)T(i+1,j) + B(i,j)T(i-1,j) + C(i,j)T(i,j+1) + \\
D(i,j)T(i,j-1) + E(i,j)T(i,j) &= F(i,j)
\end{align*}
\]

The coordinate transformation is carried out prior to calling `TEMPBC` and the derivatives of the transformation are passed via common block `RJACOB`.

See comments in main program segment for general treatment of boundary conditions.

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David Evans Aug. 1988

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IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.0D0,HALF=0.5D+00,TWO=2.0D+00,
1 HUGE=1.0D+09)
LOGICAL HFLUXBC,WATERTBL,ACCRETN
DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
1 E(IDIM,JDIM),F(IDIM,JDIM),T(IDIM,JDIM),
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM),
COMMON /BNDRYC/ HWT(IDIM),Q(IDIM),WATERTBL,ACCRETN,HFLUXBC
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),OLDRHOF(IDIM,JDIM),
1 VISCO(IDIM,JDIM),
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIF(20, IDIM) , ZIF(20, IDIM) , RPERM (20) , RPOR(20),
2 RDCX (20) , RRKS(20) , RANISO (20) , NSIF,
2 NOMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces

Set no flow conditions at the sides of the mesh

DO 120 J=2,NY-1
   RJ1 = (XI(2,J) *X2(2,J) + Y1(2,J) *Y2(2,J) ) / 
1 (X2(2,J) *X2(2,J) + Y2(2,J) *Y2(2,J) )
   RJN = (XI(NX-1,J) *X2(NX-1,J) + Y1(NX-1,J) *Y2(NX-1,J) ) / 
1 (X2(NX-1,J) *X2(NX-1,J) + Y2(NX-1,J) *Y2(NX-1,J) )
   A(2,J) = A(2,J) + B(2,J)
   C(2,J) = C(2,J) - RJ1*B(2,J)
   D(2,J) = D(2,J) + RJ1*B(2,J)
   B(1,J) = ZERO 
   B(2,J) = ZERO 
   C(NX-1,J) = C(NX-1,J) + RJN*A(NX-1,J)
   D(NX-1,J) = D(NX-1,J) - RJN*A(NX-1,J)
   B(NX-1,J) = B(NX-1,J) + A(NX-1,J)
   F(NX-1,J) = F(NX-1,J) - A(NX-1,J) *T(NX,J)
SUBROUTINE ADJTB(C(U,NX,NY))

Adjoint the value of temperature U, at passive nodes on boundaries for which there is no solute flux normal to the boundaries on which xi is 1 or NX.

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.00D+00,HALF=0.5D+00,1 TWO=2.00D+00)
LOGICAL HFLUXBC,WATERTBL,ACCRETN
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM),
COMMON /BNDRCY/ HWT(IDIM),Q(IDIM),WATERTBL,ACCRETN,HFLUXBC
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDHOF(IDIM,JDIM),VISCO(IDIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATES,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIP(20,IDIM),ZIF(20,IDIM),RPERM(20),RPOF(20),
2 RDCX(20),RRKS(20),RANISO(20),NSIF,
2 NOMOVE(IDIM),NM,NCTOP,FTOP ! Maximum of 20 interfaces
DIMENSION U(IDIM,JDIM)

C First to the sides, on which xi is held constant
C
C A(NX,J) = ZERO
A(NX-1,J) = ZERO
120 CONTINUE
C Modify source terms at top
C
DO 150 I=1,NX
F(I,NY-1) = F(I,NY-1) - C(I,NY-1)*T(I,NY)
C(I,NY-1) = ZERO
150 CONTINUE
C
C Set constant temperature or heat flux condition at the bottom
C
IF(.NOT.HFLUXBC) THEN
DO 160 I-1,NX
F(I,2) = F(I,2) - D(I,2)*T(I,1)
D(I,2) = ZERO
160 CONTINUE
ELSE IF(HFLUXBC) THEN
C These lines are for constant heat flux normal to the bottom
DO 220, I=2,NX-1
RI1 = HALF*X2(I,2)/X1(I,2)
GAMMA = -Q(I)*(X1(I,2)*Y2(I,2) - X2(I,2)*Y1(I,2))/
1 (RKSF(I,2)*X1(I,2))
E(I,2) = E(I,2) + D(I,2)
A(I,2) = A(I,2) - RI1*D(I,2)
B(I,2) = B(I,2) + RI1*D(I,2)
F(I,2) = F(I,2) + GAMMA*D(I,2)
D(I,1) = ZERO
D(I,2) = ZERO
220 CONTINUE
ENDIF
C
RETURN
END
C-----------------------------------------------------------------------------------
C SUBROUTINE ADJTB(U,NX,NY)
C Adapt the value of temperature U, at passive nodes on boundaries for which there is no solute flux normal to the boundaries on which xi is 1 or NX.
C
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.00D+00,HALF=0.5D+00,1 TWO=2.00D+00)
LOGICAL HFLUXBC,WATERTBL,ACCRETN
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM),
COMMON /BNDRCY/ HWT(IDIM),Q(IDIM),WATERTBL,ACCRETN,HFLUXBC
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDHOF(IDIM,JDIM),VISCO(IDIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATES,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIP(20,IDIM),ZIF(20,IDIM),RPERM(20),RPOF(20),
2 RDCX(20),RRKS(20),RANISO(20),NSIF,
2 NOMOVE(IDIM),NM,NCTOP,FTOP ! Maximum of 20 interfaces
DIMENSION U(IDIM,JDIM)
C
C First to the sides, on which xi is held constant
C
C A(NX,J) = ZERO
A(NX-1,J) = ZERO
120 CONTINUE
C Modify source terms at top
C
DO 150 I=1,NX
F(I,NY-1) = F(I,NY-1) - C(I,NY-1)*T(I,NY)
C(I,NY-1) = ZERO
150 CONTINUE
C
C Set constant temperature or heat flux condition at the bottom
C
IF(.NOT.HFLUXBC) THEN
DO 160 I=1,NX
F(I,2) = F(I,2) - D(I,2)*T(I,1)
D(I,2) = ZERO
160 CONTINUE
ELSE IF(HFLUXBC) THEN
C These lines are for constant heat flux normal to the bottom
DO 220, I=2,NX-1
RI1 = HALF*X2(I,2)/X1(I,2)
GAMMA = -Q(I)*(X1(I,2)*Y2(I,2) - X2(I,2)*Y1(I,2))/
1 (RKSF(I,2)*X1(I,2))
E(I,2) = E(I,2) + D(I,2)
A(I,2) = A(I,2) - RI1*D(I,2)
B(I,2) = B(I,2) + RI1*D(I,2)
F(I,2) = F(I,2) + GAMMA*D(I,2)
D(I,1) = ZERO
D(I,2) = ZERO
220 CONTINUE
ENDIF
C
RETURN
END
C-----------------------------------------------------------------------------------
C SUBROUTINE ADJTB(U,NX,NY)
C Adapt the value of temperature U, at passive nodes on boundaries for which there is no solute flux normal to the boundaries on which xi is 1 or NX.
C
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.00D+00,HALF=0.5D+00,1 TWO=2.00D+00)
LOGICAL HFLUXBC,WATERTBL,ACCRETN
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM),
COMMON /BNDRCY/ HWT(IDIM),Q(IDIM),WATERTBL,ACCRETN,HFLUXBC
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDHOF(IDIM,JDIM),VISCO(IDIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATES,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIP(20,IDIM),ZIF(20,IDIM),RPERM(20),RPOF(20),
2 RDCX(20),RRKS(20),RANISO(20),NSIF,
2 NOMOVE(IDIM),NM,NCTOP,FTOP ! Maximum of 20 interfaces
DIMENSION U(IDIM,JDIM)
C
C First to the sides, on which xi is held constant
C
C A(NX,J) = ZERO
A(NX-1,J) = ZERO
120 CONTINUE
C Modify source terms at top
C
DO 150 I=1,NX
F(I,NY-1) = F(I,NY-1) - C(I,NY-1)*T(I,NY)
C(I,NY-1) = ZERO
150 CONTINUE
C
C Set constant temperature or heat flux condition at the bottom
C
IF(.NOT.HFLUXBC) THEN
DO 160 I=1,NX
F(I,2) = F(I,2) - D(I,2)*T(I,1)
D(I,2) = ZERO
160 CONTINUE
ELSE IF(HFLUXBC) THEN
C These lines are for constant heat flux normal to the bottom
DO 220, I=2,NX-1
RI1 = HALF*X2(I,2)/X1(I,2)
GAMMA = -Q(I)*(X1(I,2)*Y2(I,2) - X2(I,2)*Y1(I,2))/
1 (RKSF(I,2)*X1(I,2))
E(I,2) = E(I,2) + D(I,2)
A(I,2) = A(I,2) - RI1*D(I,2)
B(I,2) = B(I,2) + RI1*D(I,2)
F(I,2) = F(I,2) + GAMMA*D(I,2)
D(I,1) = ZERO
D(I,2) = ZERO
220 CONTINUE
ENDIF
C
RETURN
END
C-----------------------------------------------------------------------------------

DO 100 J=1,NY / J=1,NY w/ constant flux bc's

First the right hand side, then the left hand side

RL = (X1(2,J)*X2(2,J) + Y1(2,J)*Y2(2,J)) / 
(X2(2,J)*X2(2,J) + Y2(2,J)*Y2(2,J))
RN = (X1(NX-1,J)*X2(NX-1,J) + Y1(NX-1,J)*Y2(NX-1,J)) / 
(X2(NX-1,J)*X2(NX-1,J) + Y2(NX-1,J)*Y2(NX-1,J))

IF (J .EQ. 1) THEN
U(1,J) = U(3,J) + RL*(U(2,J+1) - U(2,J))
U(NX,J) = U(NX-2,J) + RN*(U(NX-1,J+1) - U(NX-1,J))
ELSE IF (J .EQ. NY) THEN
U(1,J) = U(3,J) + RL*(U(2,J) - U(2,J-1))
U(NX,J) = U(NX-2,J) + RN*(U(NX-1,J) - U(NX-1,J-1))
ELSE
U(1,J) = U(3,J) - RL*(U(2,J+1) - U(2,J-1))
U(NX,J) = U(NX-2,J) + RN*(U(NX-1,J+1) - U(NX-1,J-1))
ENDIF

100 CONTINUE

Now do the bottom, on which eta is held constant

IF (HFLUXBC) THEN
DO 200 I=2,NX-1
GAMMA = -Q(I)*X1(I,2)*Y2(I,2) - X2(I,2)*Y1(I,2) / 
(RKSF(I,2)*DSQRT(X1(I,2)*X1(I,2) + Y1(I,2)*Y1(I,2))
RL = (X1(I,2)*X2(I,2) + Y1(I,2)*Y2(I,2)) / 
(X1(I,2)*X1(I,2) + Y1(I,2)*Y1(I,2))
U(1,I) = U(I,3) - TWO*GAMMA - RL*(U(I+1,2) - U(I-1,2))
200 CONTINUE
ENDIF

RETURN
END

SUBROUTINE PSISLV
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ZERO=0.0D+00,HALF=0.5D+00,ONE=1.0D+00,
TWO=2.0D+00,GRAV=-9.80D+00)
LOGICAL STEADY_STATE,HFLUXBC,WATERTBL,ACCRETN
COMMON /PPARAM/ PERM(IDIM,JDIM),POR(IDIM,JDIM),DCX(IDIM,JDIM),
ANISO(IDIM,JDIM),ALFA(IDIM,JDIM),ALFAL(IDIM,JDIM),RKS(IDIM,JDIM)
COMMON /COORDS/ X(IDIM,JDIM),Y(IDIM,JDIM),ICOSYS
COMMON /FIELDS/ TEMP(IDIM,JDIM),CONC(IDIM,JDIM),PSI(IDIM,JDIM),
VX(IDIM,JDIM),VY(IDIM,JDIM),OLDS(1-IDIM,JDIM),OLDC(IDIM,JDIM),
CLAST(IDIM,JDIM)
COMMON /BNDRC/ HMT(IDIM),Q[IDIM],WATERTBL,ACCRETN,HFLUXBC
COMMON /CLOCK/ ELTIME,DT,MT,mT,TSMULT,TSAX,WD
COMMON /ISIZE/ NI,NJ,TIME,ITIME
COMMON /RJACOB/ X1(IDIM,JDIM),X2(IDIM,JDIM),
Y1(IDIM,JDIM),Y2(IDIM,JDIM)
COMMON /RELAX/ RPT,RPC,RPP,REV,SORTED,MAXTEM,SORCON,MAXCONI,
SORPSI,MAXPSII,CCOTOFF,TCOTOFF,PCOTOFF
COMMON /SPROP/ RHOG,CS,RKF,CF,RFZERO,TZERO
COMMON /APROP/ RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
OLDRHOF(IDIM,JDIM),VISCO(IDIM,JDIM)
DIMENSION A(IDIM,JDIM), B(IDIM,JDIM), C(IDIM,JDIM), D(IDIM,JDIM),
E(IDIM,JDIM), F(IDIM,JDIM)

SAVE ITROLDP, PSIGN, NOMEGA

Get coefficients for stream function

CALL PCOEF(A, B, C, D, E, F)

And adjust those babies for the boundary conditions

CALL PSIBC(A, B, C, D, E, F, PSI, NI, NJ)

And solve that sucker

CALL SORL(A, B, C, D, E, F, PSI, JIFTOP(NI), NI, NJ, MAXPSII, ITR, SORPSI,
1 1.D-03*PCUTOFF, 'PSISLV')

Update estimate of relaxation factor

NOMEGA = NOMEGA + 1
SORPSI = OMEGA_NEW(SORPSI, NOMEGA, ITR, ITROLDP, PSIGN)

Reset value of stream function at passive nodes

CALL ADFPBC(PSI, NI, NJ)

RETURN
END

SUBROUTINE PCOEF(A, B, C, D, E, F)

Calculate the finite difference coefficients for the stream function equation

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101, JDIM=101, ZERO=0.0D+00, HALF=0.5D+00, ONE=1.0D+00,
1 TWO=2.0D+00, GRAV=-9.80D+00)
LOGICAL CYLINDRICAL
COMMON /PPARAM/ PERM(IDIM, JDIM), POR(IDIM, JDIM), DCX(IDIM, JDIM),
A ANISO(IDIM, JDIM), ALFAT(IDIM, JDIM),
1 ALFAL(IDIM, JDIM), RKS(IDIM, JDIM)
COMMON /COORDS/ X(IDIM, JDIM), Y(IDIM, JDIM), ICOSYS
COMMON /FIELDS/ TEMP(IDIM, JDIM), CONC(IDIM, JDIM), PSI(IDIM, JDIM),
A VX(IDIM, JDIM),
1 VY(IDIM, JDIM), OLDT(IDIM, JDIM), OLDC(IDIM, JDIM),
B OLDPsi(IDIM, JDIM),
2 OLdVX(IDIM, JDIM), OLdVY(IDIM, JDIM),
C CLAST(IDIM, JDIM)
COMMON /CLOCK/ ELTIME, DT, MMTS, TSMULT, TSMAX, WDT
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /RJACOB/ XI(IDIM, JDIM), X2(IDIM, JDIM),
1 Y1(IDIM, JDIM), Y2(IDIM, JDIM)
COMMON /RELAX/ RPT, RPP, RPVEL, SORTEM, MAXTEMI, SORCON, MAXCONI,
SORPSI, MAXPSII, CCUTOFF, TCUTOFF, PCUTOFF
COMMA /SASPRO / RHO, CS, RK, CF, RFZERO, TZERO
COMMON /APROPS / RKSF (IDIM, JDIM), RHOF (IDIM, JDIM), OLDRHOF (IDIM, JDIM), VISCO (IDIM, JDIM), DSPXX (IDIM, JDIM), DSPYY (IDIM, JDIM), DSPXY (IDIM, JDIM), JIFTOP (IDIM), ZIFTOP (IDIM), JIF (20, IDIM), ZIF (20, IDIM), RPERM (20), RFOR (20), RDCX (20), RRKS (20), RANISO (20), NISIF, NOMOVE (IDIM, JDIM), NN, CTOP, FTOP
DIMENSION A (IDIM, JDIM), B (IDIM, JDIM), C (IDIM, JDIM), D (IDIM, JDIM), E (IDIM, JDIM), F (IDIM, JDIM)

IF (ICOSYS .EQ. 0) THEN
   CYLINDRICAL = .TRUE.
ELSE IF (ICOSYS .EQ. 1) THEN
   CYLINDRICAL = .FALSE.
ELSE
   STOP 'STOP -- in PCOELEM'
ENDIF

DO 110 J = 2, NJ - 1
   DO 100 I = 2, NI - 1

   Estimate hydrologic conductive rho at interfaces
   half-way between nodes.

   TEAST = ONE / TAU12 (I, J, I + 1, J)
   TEAST = ONE / TAU12 (I - 1, J, I, J)
   TEAST = ONE / TAU12 (I, J, I, J + 1)
   TEAST = ONE / TAU12 (I, J, I - 1, J)
   REAST = TWO * RHOF (I + 1, J) * RHOF (I, J) / (RHOF (I + 1, J) + RHOF (I, J))
   RWEST = TWO * RHOF (I - 1, J) * RHOF (I, J) / (RHOF (I - 1, J) + RHOF (I, J))
   RNORTH = TWO * RHOF (I, J + 1) * RHOF (I, J) / (RHOF (I, J + 1) + RHOF (I, J))
   RSOUTH = TWO * RHOF (I, J - 1) * RHOF (I, J) / (RHOF (I, J - 1) + RHOF (I, J))

   Calculate sizes of control volume interfaces

   DXWEST = X (I, J) - X (I - 1, J)
   DXEAST = X (I + 1, J) - X (I, J)
   DYSOUTH = Y (I, J) - Y (I, J - 1)
   DYNORTH = Y (I, J + 1) - Y (I, J)

   Compute coefficients for stream function

   A (I, J) = TEAST * Y2 (I, J) / DXEAST
   B (I, J) = TWEST * Y2 (I, J) / DXWEST
   C (I, J) = TNORTH * X1 (I, J) / DYNORTH
   D (I, J) = TSOUTH * X1 (I, J) / DYSOUTH

   Modify coefficients for cylindrical coordinates

   IF (CYLINDRICAL) THEN
      ERADIUS = HALF * (X (I, J) + X (I + 1, J))
      WRADIUS = HALF * (X (I, J) + X (I - 1, J))
      A (I, J) = A (I, J) / ERADIUS
      B (I, J) = B (I, J) / WRADIUS
      C (I, J) = C (I, J) * LOG (ERADIUS / WRADIUS) / X1 (I, J)
      D (I, J) = D (I, J) * LOG (ERADIUS / WRADIUS) / X1 (I, J)
   ENDIF

   E (I, J) = - A (I, J) - B (I, J) - C (I, J) - D (I, J)
   F (I, J) = GRAV * Y2 (I, J) * (REAST - RWEST)

100 CONTINUE
SUBROUTINE PSIBC(A,B,C,D,E,F,P,NX,NY)

Modify coefficients for stream function boundary condition such that the stream function is normal to the head gradient on the top boundary.

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM-101,JDIM-101,ZERO=0.0D0,ONE=1.0D+00,
1 HALF=0.5D+00,THO=2.0D+00,GRAV=-9.80D+00)
LOGICAL WATERTBL, HFLUXBC, ACCRETN
COMMON /COORDS/ X(IDIM,JDIM),Y(IDIM,JDIM),ICOSYS
COMMON /BNDRYC/ HWT(IDIM),Q(IDIM),WATERTBL,ACCRETN,HFLUXBC
COMMON /APROP / RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1 OLDRHOF(IDIM,JDIM),VISCO(IDIM,JDIM),
1 DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /PPARAM/ PENH(IDIM,JDIM),POR(IDIM,JDIM),DCX(IDIM,JDIM),
1 ANISO(IDIM,JDIM),ALFAT(IDIM,JDIM),
1 ALFAL(IDIM,JDIM),RKS(IDIM,JDIM)
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1 Y1(IDIM,JDIM),Y2(IDIM,JDIM)
DIMENSION A(IDIM,JDIM),B(IDIM,JDIM),C(IDIM,JDIM),D(IDIM,JDIM),
1 E(IDIM,JDIM),F(IDIM,JDIM),P(IDIM,JDIM)

C..............Set constant Psi at bottom
C
DO I=2,NX-1
F(I,2) = F(I,2) - D(I,2)*P(I,1)
D(I,2) = ZERO
END DO

C..............Either set water table recharge boundary (accretion)
C
IF(ACCRETN) THEN
DO I=2,NX-1
IF(HWT(I) .LT. ZERO) THEN
F(I,NY-1) = F(I,NY-1) - C(I,NY-1)*HWT(I)
ELSE
HP = (HWT(I+1)-HWT(I-1))/(X(I+1,NY)-X(I-1,NY))
A(I,NY-1) = A(I,NY-1) + C(I,NY-1)*HP*Y2(I,NY-1)/XI(I,NY-1)
E(I,NY-1) = E(I,NY-1) + C(I,NY-1)*(ONE+HP*Y2(I,NY-1)/XI(I,NY-1))
ENDIF
C(I,NY-1) = ZERO
END DO ! End of I-loop

C

C..............Set constant Psi on sides
C
DO J=2,NY-1
F(2,J) = F(2,J) - B(2,J)*P(1,J)
B(2,J) = ZERO
F(NX-1,J) = F(NX-1,J) - A(NX-1,J)*P(NX,J)
A(NX-1,J) = ZERO
END DO ! End of J-loop

C

C..............Or set watertable boundary conditions:
C
ELSE IF(WATERTBL) THEN
DO I=2,NX-1

  Set normal derivative of \( \Psi \) = tangential derivative of \( H \)

  \[
  HP = \frac{(HWT(I+1)-HWT(I-1))/(X(I+1,NY)-X(I-1,NY))}{Y(I,NY)-Y(I,NY-1)}
  \]

  \[
  DELTAY = Y(I,NY)-Y(I,NY-1)
  \]

  \[
  ALFA = \frac{ONE}{ANISO(I,NY)*SQRT(ONE/ANISO(I,NY)**2+ONE)}
  \]

  \[
  PROD = DELTAY*HP/ALFA
  \]

  \[
  F(I,NY-1) = F(I,NY-1) + C(I,NY-1)*PROD
  \]

  \[
  E(I,NY-1) = E(I,NY-1) + C(I,NY-1)
  \]

  \( C(I,NY-1) = ZERO \)

END DO

DO J=2,NY-1

  Set no vertical flow on one side, and no flow at \( r=0 \)

  \[
  E(NX-1,J) = E(NX-1,J) + A(NX-1,J)
  \]

  \( A(NX-1,J) = ZERO \)

  \[
  F(2,J) = F(2,J) - B(2,J)*P(1,J)
  \]

  \( B(2,J) = ZERO \)

END DO

ELSE

  ...Or set top boundary = stream line

DO I=2,NX-1

  \[
  F(I,NY-1) = F(I,NY-1) - C(I,NY-1)*P(I,NY)
  \]

  \( C(I,NY-1) = ZERO \)

END DO

DO J=2,NY-1

  Set no vertical flow on sides

  \[
  E(NX-1,J) = E(NX-1,J) + A(NX-1,J)
  \]

  \( A(NX-1,J) = ZERO \)

  \[
  E(2,J) = E(2,J) + B(2,J)
  \]

  \( B(2,J) = ZERO \)

END DO

Set constant \( \Psi \) on sides

DO J=2,NY-1

  \[
  F(2,J) = F(2,J) - B(2,J)*P(1,J)
  \]

  \( B(2,J) = ZERO \)

  \[
  F(NX-1,J) = F(NX-1,J) - A(NX-1,J)*P(NX,J)
  \]

  \( A(NX-1,J) = ZERO \)

END DO

ENDIF

RETURN

END

-----------------------------------------------------------------------

SUBROUTINE ADJPBC(U,NX,NY)

  Adjust the value of the stream function along the top boundary
  to reflect appropriate boundary condition.

IMPLIED DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ONE=1.00D+00)
LOGICAL WATERTBL, ACCRETN, HFLUXBC

-----------------------------------------------------------------------
If stream line boundary condition top needs no adjusting; 
But if water table be need to reset PSI on top boundary

IF (WATERTBL) THEN
  DO I=2,NX-1
    HP = (HWT(I+1)-HWT(I-1))/(X(I+1,NY)-X(I-1,NY))
    DELTAY = Y(I,NY)-Y(I,NY-1)
    PROD = DELTAY*HP*RHOF(I,NY)*PERM(I,NY)/ANISO(I,NY)
    U(I,NY) = U(I,NY-1)+ PROD
  END DO
  DO J=2,NY-1
    U(NX,J) = U(NX-1,J)
    U(1,J) = U(2,J)
  END DO
ELSE IF (ACCRETN) THEN
  DO I=2,NX-1
    IF (HWT(I) .GE. ZERO) THEN
      HP = (HWT(I+1)-HWT(I-1))/(X(I+1,NY)-X(I-1,NY))
      U(I,NY) = U(I,NY-1)+ HP*Y2(I,NY-1)* (U(I+1,NY-1)-U(I,NY-1))/XI(I,NY-1)
    END IF
  END DO
END IF

And on the sides

DO J=2,NY-1
  U(NX,J) = U(NX-1,J)
  U(1,J) = U(2,J)
END DO

RETURN

END

SUBROUTINE VECLCAL

Calculate the Specific Discharge (Darcy Velocity) from the stream function for this iteration or time step.

IMPORTANT NOTE: The velocities are calculated half way between nodes (not at the nodes themselves), such that VX(I,J) represents the x-component of velocity between node (I,J) and node (I-1,J), and VY(I,J) is the y-component between node (I,J) and (I,J-1).

DGE: 08-JUN-1989
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ONE=1.00D+00,HALF=0.5D+00,
1  GRAV=9.8D+00)
LOGICAL CYLINDRICAL
COMMON /PARAM/ PERM(IDIM,JDIM),POR(IDIM,JDIM),DCX(IDIM,JDIM),
A  ANISO(IDIM,JDIM),ALFAT(IDIM,JDIM),
1  ALFAL(IDIM,JDIM),RKS(IDIM,JDIM)
COMMON /COORDS/ X(IDIM,JDIM),Y(IDIM,JDIM),ICOSYS
COMMON /FIELDS/ TEMP(IDIM,JDIM),CONC(IDIM,JDIM),PSI(IDIM,JDIM),
1  VX(IDIM,JDIM),VY(IDIM,JDIM),OLDVX(IDIM,JDIM),OLDVY(IDIM,JDIM),
2  CLAST(IDIM,JDIM)
COMMON /CLOCK/ ELTIME,DT,MTS,TSMULT,TSMAX,WDT
COMMON /ISIZE/ NI,NJ,ITIME,ITTIME
COMMON /RAJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),
1  Y1(IDIM,JDIM),Y2(IDIM,JDIM)
COMMON /RELAX/ RPT,RPC,RPP,RPVEL,SORTEM,MAXTEM,SORCON,MAXCONI,
1  SORPSI,MAXPSII,CCUTOFF,TCUTOFF,PCUTOFF
SROPP/RHOS,CS,RKF,CF,RFZERO,TZERO
COMMON /APROP/ RKSF(IDIM,JDIM),RHOF(IDIM,JDIM),
1  OLDRHOF(IDIM,JDIM),VISC0(IDIM,JDIM),
1  DSPXX(IDIM,JDIM),DSPYY(IDIM,JDIM),DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1  JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
2  JIF(20,IDIM),ZIF(20,IDIM),RPERM(20),RPOR(20),
2  RDCX(20),RRKS(20),RANISO(20),NSIF,
2  NOMOVE(IDIM,NMJ,CTOP,FTOP ! Maximum of 20 interfaces

! Maximum of 20 interfaces
IF(ICOSYS .EQ. 0 ) THEN
CYLINDRICAL = .TRUE.
ELSE
CYLINDRICAL = .FALSE.
ENDIF
!
First save the previous values of velocity
DO J=1,NJ
DO I=1,NI
OLDVX(I,J) = VX(I,J)
OLDVY(I,J) = VY(I,J)
END DO
END DO
!
Calculate X- and Y- components of velocity at interior nodes
!
DO 110 J=2,NJ
DO 100 I=2,NI
VX(I,J) = (PSI(I,J)-PSI(I-1,J))/(Y(I,J)-Y(I-1,J))
VY(I,J) = (PSI(I,J)-PSI(I,J-1))/(X(I,J)-X(I-1,J))
VX(I,J) = VX(I,J)/RHOF(I,J)
VY(I,J) = VY(I,J)/RHOF(I,J)
100  CONTINUE
110 CONTINUE
!
For cylindrical coordinates...
!
IF(CYLINDRICAL) THEN
DO J=2,NJ
DO I=2,NI
RADX = HALF*(X(I,J)+X(I-1,J))
RADY = X(I,J)
VX(I,J) = VX(I,J)/RADX
END DO
END DO

SUBROUTINE SORL(A, B, C, D, E, F, U, JFIRST, NI, NJ, MAXITR, ITR, OMEGA, CUTOFF, SIMTYP)

Line SOR routine that solves the system

\[
a(i, j)u(i, j+1) + b(i, j)u(i-1, j) + c(i, j)u(i, j+1) + d(i, j)u(i-1, j-1) + e(i, j)u(i, j) = f(i, j)
\]

A, B, C, D, E, and F are input as the coefficients of the equation, on a grid of size \( NI \times NJ \), dimensioned with IDIM and JDIM in a parameter statement below. \( U \) is input as the initial guess to the solution, usually zero, and returns with the final value.

The solution begins with row \( JFIRST \) and works up through row \( NJ \). Both rows \( JFIRST \) and \( NJ \) are assumed to contain passive nodes the value of which do not change. \( MAXITR \) is input as the maximum number of sweeps through the mesh, and \( ITR \) is output as the actual number of sweeps made. \( OMEGA \) is input as the relaxation parameter (1<\( OMEGA <2 \)), and \( CUTOFF \) is the convergence criterion such that convergence is called when no node contains a residual value greater than \( CUTOFF \). \( SIMTYP \) is an 8 character string to identify the calling routine; \( SIMTYP \) is echoed when the routine fails to converge.

This routine DOES NOT PIVOTING.

-- Dave Evans 01-JUN-1989

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101, JDIM=101, ONE=1.00D+00, HUGE=1.00D+32, ZERO=0.00D+00)
DIMENSION A(IDIM, JDIM), B(IDIM, JDIM), C(IDIM, JDIM), D(IDIM, JDIM), E(IDIM, JDIM), F(IDIM, JDIM), U(IDIM, JDIM), UU(IDIM)
DIMENSION GAM(IDIM)
CHARACTER*8 SIMTYP

DO ITR = 1, MAXITR
   DO J = JFIRST+1, NJ-1
      BETAV = E(2, J)
      UU(1) = (F(2, J) - D(2, J) * U(2, J-1) - C(2, J) * U(2, J+1)) / BETAV
   END DO
   ! End of I-loop
Back-substitution

DO I=NI-3,1,-1
  UU(I) = UU(I) - GAM(I+1) * UU(I+1)
END DO

Update U w/ over-relaxation

DO I=2,NI-1
  U(I,J) = OMEGA * UU(I-1) + (ONE-OMEGA) * U(I,J)
END DO

Go do next row of nodes

END DO ! End of J-loop

Check convergence

RESMAX = -HUGE
DO J=FIRST+1,NJ-1
  DO I=2,NI-1
    RESMAX = MAX(ABS(RESID), RESMAX)
  END DO ! End of I-loop
END DO ! End of J-loop
IF(ITR.GT.1 .AND. RESMAX.LT.CUTOFF) THEN
  RETURN
ENDIF

If not converged, do another iteration

END DO ! End of ITR-loop

If exceeded max iterations, mention it to user

WRITE(*,100) SIMTYP, RESMAX
PAUSE 'PAUSE in SORL'
RETURN
100 FORMAT(IX,'Conv. failure when called by ',A8,' RESMAX =',G12.5)

END

SUBROUTINE XYTRAN(X,Y,NX,NY)

This subroutine calculates the derivatives of the coordinate transformation from nodes in physical coordinates (X(I,J), Y(I,J), I=1,2,...,NX, J=1,2,...,NY) to curvilinear coordinates (XI,Eta) in which nodes are equally spaced one unit apart, for NX by NY units. The derivatives are stored in a common block RJACOB and are denoted as follows: derivatives w/r/t XI are indicated by 1, and derivatives w/r/t Eta are indicated by 2. So that

\[
\begin{align*}
\frac{dX}{dXI} &= X1, \\
\frac{dY}{dXI} &= Y1, \\
\frac{dX}{dEta} &= X2, \\
\frac{dY}{dEta} &= Y2
\end{align*}
\]

All derivatives are second order correct.

In order to save space the Jacobian is not stored explicitly, but rather
C will must be calculated locally as needed. It is given by

\[
C = \text{Jacobian}(i, j) = X1(i, j)Y2(i, j) - X2(i, j)Y1(i, j)
\]

Dave Evans August 1987 (last update Aug 1989)  

IMPLICIT DOUBLE PRECISION(A-H,O-Z)  
PARAMETER(IDIM=101,JDIM=101)  
PARAMETER(FOURTH=0.25D0,HALF=0.5D0,THREE=0.75D0,ONE=1.0D0,  
TWO=2.0D0,THREE=0.5D0,FOUR=4.0D0,FIVE=5.0D0)  
DIMENSION X(IDIM,JDIM),Y(IDIM,JDIM)  
COMMON /RJACOB/ XI(IDIM,JDIM),X2(IDIM,JDIM),  
Y1(IDIM,JDIM),Y2(IDIM,JDIM)  

Derivatives w/rto XI on the vertical edges

DO 10 J=1,NY
\[
X1(1,J) = \text{HALF}*(X(3,J) + FOUR*X(2,J) - THREE*X(1,J))  
Y1(1,J) = \text{HALF}*(-Y(3,J) + FOUR*Y(2,J) - THREE*Y(1,J))  
X1(NX,J) = \text{HALF}*(X(NX-2,J) - FOUR*X(NX-1,J) + THREE*X(NX,J))  
Y1(NX,J) = \text{HALF}*(-Y(NX-2,J) - FOUR*Y(NX-1,J) + THREE*Y(NX,J))
\]
10 CONTINUE

Derivatives w/rto Eta on the horizontal edges

DO 20 I=1,NX
\[
X2(I,1) = \text{HALF}*(-X(I,3) + FOUR*X(I,2) - THREE*X(I,1))  
Y2(I,1) = \text{HALF}*(-Y(I,3) + FOUR*Y(I,2) - THREE*Y(I,1))  
X2(I,NY) = \text{HALF}*(X(I,NY-2) - FOUR*X(I,NY-1) + THREE*X(I,NY))  
Y2(I,NY) = \text{HALF}*(Y(I,NY-2) - FOUR*Y(I,NY-1) + THREE*Y(I,NY))
\]
20 CONTINUE

The rest of the derivatives along the edges

DO 30 J=2,NY-1
\[
X2(1,J) = \text{HALF}*(X(1,J+1)-X(1,J-1))  
X2(NX,J) = \text{HALF}*(X(NX,J+1)-X(NX,J-1))  
Y2(1,J) = \text{HALF}*(Y(1,J+1)-Y(1,J-1))  
Y2(NX,J) = \text{HALF}*(Y(NX,J+1)-Y(NX,J-1))
\]
30 CONTINUE

DO 40 I=2,NX-1
\[
X1(1,J) = \text{HALF}*(X(I-1,J+1)-X(I-1,J))  
X1(I,NY) = \text{HALF}*(X(I+1,NY)-X(I-1,NY))  
Y1(1,J) = \text{HALF}*(Y(I+1,J+1)-Y(I+1,J))  
Y1(I,NY) = \text{HALF}*(Y(I+1,NY)-Y(I-1,NY))
\]
40 CONTINUE

After all that crap we can finally do the interior points

DO 50 J=2,NY-1
DO 60 I=2,NX-1
\[
X1(I,J) = \text{HALF}*(X(I+1,J)-X(I-1,J))  
X2(I,J) = \text{HALF}*(X(I+1,J+1)-X(I,J-1))  
Y1(I,J) = \text{HALF}*(Y(I+1,J)-Y(I-1,J))  
Y2(I,J) = \text{HALF}*(Y(I,J+1)-Y(I,J-1))
\]
50 CONTINUE
60 CONTINUE

RETURN

END

SUBROUTINE FLGSET
C------------ Set logical I/O flags for this iteration or time step ---------------
C

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IZERO=0)
LOGICAL PRINT,TEMPLT,CONPLT,VELPLT,PSIPLT,GRPLT,ECHO,
2 CNVRGC,CNVRGT,CNVRGP,NEWTS,DOTEMP,DOFLOW,DOCONC,
3 HFLUXBC
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /IOCTRL/ IPRINT, IVPLT, IPPLT, IITPLT, ICPLT
COMMON /LFLAGS/ PRINT,TEMPLT,CONPLT,VELPLT,PSIPLT,GRPLT,ECHO,
1 CNVRGT,CNVRGC,CNVRGP,NEWTS,DOTEMP,DOFLOW,DOCONC,
2 STEADY_STATE

Initialize all flags
PRINT = .FALSE.
TEMPLT = .FALSE.
CONPLT = .FALSE.
VELPLT = .FALSE.
PSIPLT = .FALSE.

Find out if this is an iteration that calls for output

Write output file?
IF(IPRINT .EQ. IZERO) THEN
PRINT = .FALSE.
ELSE IF(MOD(ITIME,IPRINT) .EQ. IZERO) THEN
PRINT = .TRUE.
ENDIF

Plot temperature field?
IF(ITPLT .EQ. IZERO) THEN
TEMPLT = .FALSE.
ELSE IF(MOD(ITIME,ITPLT) .EQ. IZERO) THEN
TEMPLT = .TRUE.
ENDIF

Plot velocity field?
IF(IVPLT .EQ. IZERO) THEN
VELPLT = .FALSE.
ELSE IF(MOD(ITIME,IVPLT) .EQ. IZERO) THEN
VELPLT = .TRUE.
ENDIF

Plot salinity field?
IF(ICPLT .EQ. IZERO) THEN
CONPLT = .FALSE.
ELSE IF(MOD(ITIME,ICPLT) .EQ. IZERO) THEN
CONPLT = .TRUE.
ENDIF
IF(IPPLT .EQ. IZERO) THEN
PSIPLT = .FALSE.
ELSE IF(MOD(ITIME,IPPLT) .EQ. IZERO) THEN
PSIPLT = .TRUE.
ENDIF
RETURN
END

C-----------------------------
SUBROUTINE URELAX(F,FOLD,ALPHA,N,M)

Modify the value of $F(i,j)$ for $i=2,\ldots,N-1$, $j=2,\ldots,N-1$ using underrelaxation.

IMPLICIT DOUBLE PRECISION(A-H,0-Z)

PARAMETER(IDIM=101,JDIM=101,ONE=1.0D+00)

DIMENSION F(IDIM,JDIM),FOLD(IDIM,JDIM)

DO 20 J=1,M
  DO 10 I=1,N
    F(I,J) = ALPHA*F(I,J) + (ONE-ALPHA)*FOLD(I,J)
  10 CONTINUE
  20 CONTINUE

RETURN
END

SUBROUTINE CONCHK(UNEW,UOLD,N,M,RES,RCHECK,CONVRG)

This subroutine checks for iteration convergence using the following algorithm:

\[
\frac{|u_{new}(i,j) - u_{old}(i,j)|}{|u_{new}(i,j)|} < RES \Rightarrow CONVRG = .TRUE.
\]

where $RES$ is a user-specified cutoff value.

Dave Evans Feb 1988

IMPLICIT DOUBLE PRECISION(A-H,0-Z)

PARAMETER(IDIM=101,JDIM=101,ZERO=0.0D+00)

LOGICAL CONVRG

DIMENSION UNEW(IDIM,JDIM), UOLD(IDIM,JDIM)

CONVRG = .FALSE.

SUMDIF = ZERO
SUMNEW = ZERO

DO 20 I=1,N
  DO 10 J=1,M
    SUMDIF = ABS(UNEW(I,J) - UOLD(I,J)) + SUMDIF
    SUMNEW = ABS(UNEW(I,J)) + SUMNEW
    UOLD(I,J) = UNEW(I,J)
  10 CONTINUE
  20 CONTINUE

RCHECK = SUMDIF/SUMNEW

IF(RCHECK .LE. RES) CONVRG = .TRUE.

RETURN

END

SUBROUTINE EQUATE(A,B,N,M)

Equate two 2-dimensional arrays $B=A$, each of which is $N \times M$

IMPLICIT DOUBLE PRECISION(A-H,0-Z)
PARAMETER(IDIM-101, JDIM-101)
DIMENSION A(IDIM, JDIM), B(IDIM, JDIM)
DO J=1,M
DO I=1,N
B(I, J) = A(I, J)
END DO
END DO
RETURN
END

SUBROUTINE DATOUT(LUN, TITLE1, TITLE2, DATIM, VE, MAXITER)

LOGICAL PRINT, TEMPLT, CONPLT, VELPLT, PSIPLT, GRPLT, ECHO,
2 CNVRGC, CNVRGT, CNVRGP, NEWTS, DOTEMP, DOFLOW, DOCONC,
3 HFLUXBC, WATERTBL, ACCRETN, STEADY_STATE
CHARACTER*4 TITLE1(20), TITLE2(20), STRING
CHARACTER*23 DATIM

COMMON /PPARAM/ PERM(IDIM, JDIM), POR(IDIM, JDIM), DCX(IDIM, JDIM),
1 ANISO(IDIM, JDIM), ALFAT(IDIM, JDIM),
COMMON /COORDS/ X(IDIM, JDIM), Y(IDIM, JDIM), ICOSYS
COMMON /FIELDS/ TEMP(IDIM, JDIM), CONC(IDIM, JDIM), PSI(IDIM, JDIM),
1 VX(IDIM, JDIM),
2 VY(IDIM, JDIM), OLDT(IDIM, JDIM), OLDC(IDIM, JDIM),
B OLDPSI(IDIM, JDIM),
2 OLDFX(IDIM, JDIM), OLDFX(IDIM, JDIM),
C CLAST(IDIM, JDIM)
COMMON /BNDRYC/ HWT(IDIM), Q(IDIM), WATERTBL, ACCRETN, HFLUXBC
COMMON /SPROP/ RHOS, CS, CF, RFZERO, ITERO
COMMON /CLOCK/ ELTIME, DT, MMST, TSMULT, TSMAX, WDT
COMMON /ISIZE/ NJ, NJ, ITIME, ITIME
COMMON /LFLAGS/ PRINT, TEMPLT, CONPLT, VELPLT, PSIPLT, GRPLT,
1 ECHO, CNVRGT, CNVRGC, CNVRGP, NEWTS,
2 DOTEMP, DOFLOW, DOCONC, STEADY_STATE
COMMON /IOCTRL/ TPRINT, IPPLT, IPPLT, IPPLT, IPPLT
COMMON /RELAX/ RPT, RPC, RPP, RPVEL, SORTEM, MAXTEMI, SORCON, MAXCONI,
1 SORPSI, MAXPSI, CCUTOFF, TCUTOFF, FCUTOFF

OPEN(UNIT=LUN, CARRIAGECONTROL='LIST', STATUS='NEW')

C.........Write out ECHO flag and iteration number
C
IF(ECHO) THEN
  WRITE(LUN, 110)
ELSE
  WRITE(LUN, 112)
ENDIF
110 FORMAT('ECHO')
112 FORMAT('NOECHO')
C
C.........Get current date and time from the computer and write it
C
ISTAT = LIBSDATE_TIME(DATIM)
WRITE(LUN,114) DATIM
114 FORMAT(1A23)
WRITE title cards

WRITE(LUN,120) (TITLE1(I),I=1,20),(TITLE2(I),I=1,20)
120 FORMAT(20A4,/,20A4)

Specify coordinate system type

IF(ICSYS .EQ. 0 ) WRITE(LUN,130)
IF(ICSYS .EQ. 1 ) WRITE(LUN,132)
130 FORMAT('CYLINDRICAL POLAR COORDINATES')
132 FORMAT('CARTESIAN COORDINATES')

Write out simulation type

IF(DOCONC) THEN
   WRITE(LUN,133)
ELSE
   WRITE(LUN,134)
ENDIF
133 FORMAT('CONCENTRATION SIMULATION')
134 FORMAT('NOCONCENTRATION SIMULATION')

IF(DOTEMP) THEN
   WRITE(LUN,135)
ELSE
   WRITE(LUN,136)
ENDIF
135 FORMAT('TEMPERATURE SIMULATION')
136 FORMAT('NOTEMPERATURE SIMULATION')

IF(DOFLOW) THEN
   WRITE(LUN,137)
ELSE
   WRITE(LUN,138)
ENDIF
137 FORMAT('STREAM FUNCTION SIMULATION')
138 FORMAT('NOSTREAM FUNCTION SIMULATION')

Write out temporal control stuff

WRITE(LUN,139) ELTIME,DT,MTS,TSMULT,TSMAX,WPT
139 FORMAT(1X,2E14.5,I8,3E14.5)

Write out maximum number of iterations and I/O control

WRITE(LUN,140) ITTIME,MAXITER,IPRINT,ICPLT,ITPLT,IPPLT,IVPLT
140 FORMAT(7110)

And the relaxation parameters

WRITE(LUN,150) RPC,RPT,RPP,RPVEL
150 FORMAT(4F15.5)
WRITE(LUN,152) SORCON,MAXCONI,SORTEM,MAXTEMI,SORPSI,MAXPSII
152 FORMAT(3(F11.5,I6))

Write out cutoff values

WRITE(LUN,153) CCUTOFF,TCUTOFF,PCUTOFF
153 FORMAT(3G20.5)

Write out vertical exaggeration for plotting

WRITE(LUN,154) VE
154 FORMAT(1F10.5)

Number of nodes in X and Y

C........................Write title cards
C
WRITE(LUN,120) (TITLE1(I),I=1,20),(TITLE2(I),I=1,20)
120 FORMAT(20A4,/,20A4)
C
C.....................Specify coordinate system type
C
IF(ICSYS .EQ. 0 ) WRITE(LUN,130)
IF(ICSYS .EQ. 1 ) WRITE(LUN,132)
130 FORMAT('CYLINDRICAL POLAR COORDINATES')
132 FORMAT('CARTESIAN COORDINATES')
C
C.....................Write out simulation type
C
IF(DOCONC) THEN
   WRITE(LUN,133)
ELSE
   WRITE(LUN,134)
ENDIF
133 FORMAT('CONCENTRATION SIMULATION')
134 FORMAT('NOCONCENTRATION SIMULATION')

IF(DOTEMP) THEN
   WRITE(LUN,135)
ELSE
   WRITE(LUN,136)
ENDIF
135 FORMAT('TEMPERATURE SIMULATION')
136 FORMAT('NOTEMPERATURE SIMULATION')

IF(DOFLOW) THEN
   WRITE(LUN,137)
ELSE
   WRITE(LUN,138)
ENDIF
137 FORMAT('STREAM FUNCTION SIMULATION')
138 FORMAT('NOSTREAM FUNCTION SIMULATION')
C
C.....................Write out temporal control stuff
C
WRITE(LUN,139) ELTIME,DT,MTS,TSMULT,TSMAX,WPT
139 FORMAT(1X,2E14.5,I8,3E14.5)
C
C.....................Write out maximum number of iterations and I/O control
C
WRITE(LUN,140) ITTIME,MAXITER,IPRINT,ICPLT,ITPLT,IPPLT,IVPLT
140 FORMAT(7110)
C
C.....................And the relaxation parameters
C
WRITE(LUN,150) RPC,RPT,RPP,RPVEL
150 FORMAT(4F15.5)
WRITE(LUN,152) SORCON,MAXCONI,SORTEM,MAXTEMI,SORPSI,MAXPSII
152 FORMAT(3(F11.5,I6))
C
C.....................Write out cutoff values
C
WRITE(LUN,153) CCUTOFF,TCUTOFF,PCUTOFF
153 FORMAT(3G20.5)
C
C.....................Write out vertical exaggeration for plotting
C
WRITE(LUN,154) VE
154 FORMAT(1F10.5)
C
C.....................Number of nodes in X and Y
WRITE(LUN,160) NI,NJ
160 FORMAT(2I5)

WRITE (LUN, 190) I, J, X(I, J), Y(I, J), CONC(I, J), TEMP(I, J), PSI(I, J), PERM(I, J), POR(I, J), DCX(I, J), ANISO(I, J), ALFAL(I, J), ALFAT(I, J), RK(I, J)
170 CONTINUE
180 CONTINUE
190 FORMAT(IX,2I5,5E13.4, / ,11X,5E13.4, / , 11X, 2E13.4)

WRITE(LUN,191)
191 FORMAT('WATER TABLE SPECIFIED ON TOP BOUNDARY')

WRITE(LUN,192) (HWT(I),I=1,NI)
192 FORMAT(6E13.5)

ELSE IF(ACCRETN) THEN
WRITE(LUN,194)
WRITE(LUN,192) (HWT(I),I=1,NI)
194 FORMAT('ACCRETION TO WATER TABLE SPECIFIED ON TOP BOUNDARY')

ENDIF
193 FORMAT('STREAM LINE SPECIFIED ON TOP BOUNDARY')

WRITE(LUN,193)
193 FORMAT(1I13.5)

WRITE(LUN,196)
196 FORMAT('TEMPERATURE BOUNDARY CONDITION ON BOTTOM')

WRITE(LUN,197)
197 FORMAT('HEAT FLUX BOUNDARY CONDITION ON BOTTOM')

WRITE(LUN,198) (Q(I),I=1,NI)
198 FORMAT(6E13.5)

CLOSE(UNIT=LUN)
RETURN

SUBROUTINE SRATOUT
Output subsidence information for current time
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101)
COMMON /CLOCK / ELTIME, DT, MMTS, TSMULT, TSMAX, WDT
COMMON /ISIZE / NI, NJ, ITIME, ITTIME
COMMON /SUBSID/ TOTSUB, RSRATE, SRATE(IDIM, JDIM), JIFBOT(IDIM), JIFTOP(IDIM), RPERM(IDIM), ZIPBOT(IDIM), ZIPFBO(IDIM), RDCX(20), RK(20), RANISO(20), NSIF, NOMOVE(IDIM), NNH, CTOP, FTOP! Maximum of 20 interfaces
LUN=12
OPEN(UNIT=LUN, CARRIAGECONTROL='LIST', STATUS='NEW')
WRITE(LUN,*) RSRATE
WRITE(LUN,*) NSIF
DO I=1, NI
    WRITE(LUN, 120) ZIFBOT(I), ZIFTOP(I), (ZIF(NSL,I), NSL=1, NSIF)
END DO
120 FORMAT(1X, 5G15.5)
DO NSL=1, NSIF+1
    WRITE(LUN,130) RPERM(NSL), RPOR(NSL), RDCX(NSL), RRKS(NSL),
    RANISO(NSL)
END DO
130 FORMAT(5X, 5G15.5)
WRITE(LUN,150) (NOMOVE(I), I=1, NNM)
150 FORMAT(IX, 1017)
WRITE(LUN,*) CTOP, FTOP
WRITE(LUN,*) 'ELAPSED TIME = ', ELTIME
CLOSE(LUN)
RETURN

SUBROUTINE SUBSIDE

Subroutine SUBSIDE reads in the subsidence history curve (rate of subsidence) and tracks two interfaces between media of different properties.

IMPLICIT DOUBLE PRECISION(A-H, O-Z)
PARAMETER(IDIM=101, JDIM=101)
COMMON /COORDS/ X(IDIM, JDIM), Y(IDIM, JDIM), ICOSYS
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /CLOCK/ ELTIME, DT, MMTS, TSMULT, TSMAX, WDT
COMMON /FIELDS/ TEMP(IDIM, JDIM), CONC(IDIM, JDIM), PSI(IDIM, JDIM),
    VX(IDIM, JDIM),
    VY(IDIM, JDIM), OLDT(IDIM, JDIM), OLDC(IDIM, JDIM),
    OLDSPI(IDIM, JDIM),
    OLDVX(IDIM, JDIM), OLDVY(IDIM, JDIM),
    CLAST(IDIM, JDIM),
    CLAP(IDIM, JDIM)
COMMON /SUBSID/ TOTSUB, RSRATE, SRATE(IDIM, JDIM), JIFBOT(IDIM),
    ZIFBOT(IDIM), ZIFTOP(IDIM), JIFTOP(IDIM),
    JIF(20, IDIM), ZIF(20, IDIM), RPERM(20), RPOR(20),
    RDCX(20), RRKS(20), RANISO(20), NSIF,
    NOMOVE(IDIM), NNM, CTOP, FTOP ! Maximum of 20 interfaces
COMMON /PPARAM/ PERM(IDIM, JDIM), POR(IDIM, JDIM), DCX(IDIM, JDIM),
    ANISO(IDIM, JDIM), ALFAT(IDIM, JDIM),
    ALFAL(IDIM, JDIM), RKS(IDIM, JDIM)

On first call, get subsidence rate and interface positions by calling SRATER
IF(ITIME.EQ.1) CALL SRATER
Track the interfaces during subsidence
CALL TRACKR
Assign new values to the medium properties
CALL SETMED
RETURN
SUBROUTINE SRATER

Read in subsidence rate and location of Interfaces

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101)
COMMON /ISIZE/ NI, NJ, ITIME, ITIME
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE,IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIF(20, IDIM),ZIF(20, IDIM),RPERM(20), RPOR(20),
2 RDCX(20), RRKS(20), RANISO(20), NSIF,
2 NOMOVE(IDIM), NNM, CTOP, FTOP ! Maximum of 20 interfaces
SAVE NCALLS
LUN=11

Only execute on first call

NCALLS=NCALLS+1
IF(NCALLS.GT.1)
1 STOP 'STOP -- Second attempt to read subsidence info'

OPEN(LUN,STATUS='OLD',READONLY)

Read subsidence rate (assumed constant)

READ(LUN,* ) RSRATE

Read total number of sediment interfaces

READ(LUN,* ) NSIF

Read interface location for salt-bottom, salt-top, and sediment interfaces

READ(LUN,* ) (ZIFBOT(I),ZIFTOP(I),ZIF(NSL,I),NSL=1,NSIF),I=1,NI)

Read medium properties for sediment layers

READ(LUN,* ) (RPERM(NSL),RPOR(NSL),RDCX(NSL),RRKS(NSL),RANISO(NSL),
1 NSL=1,NSIF+1)

Read total number of nodes that will NOT subside w/rt the top of the model

READ(LUN,* ) NNM

Read node numbers of nodes above which the interface will not subside

READ(LUN,* ) (NOMOVE(I),I=1,NNM)

Finally, read the concentration and salt flux at nodes on the salt crest

READ(LUN,* ) CTOP,FTOP

RETURN
END

C-----------------------------
C-----------------------------
C-----------------------------
C-----------------------------
C-----------------------------
SUBROUTINE TRACER
C
C This subroutine tracks the interfaces during subsidence and stores C the present interface elevations ZIFBOT and ZIFBOT. The node number C of nodes directly below each interface are stored in JIFBOT and JIFTOP, C respectively.
C
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101)
LOGICAL NOTOPMOVE
COMMON /COORDS/ X(IDIM,JDIM), Y(IDIM,JDIM), ICOSYS
COMMON /ISIZE / NI, NJ, ITIME, ITTIME
COMMON /CLOCK / ELTIME, DT, TSMULT, TSMAX, WDT
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM),ZIFBOT(IDIM),ZIFTOP(IDIM),
1 JIF(20, IDIM) ,  ZIF (20, IDIM),  RPERM(20), RFOR(20),
2 RDCX (20) ,RRKS(20),RANISO(20),NSIF,
2 NOMOVE(IDIM),NNM,CTOP,FTOP  !  Maximum of 20 interfaces

First calculate the total subsidence to date

TOTSUB = RSRATE*ELTIME

Now for each column...

DO I=1,NI

Move the bottom interface down...

ZIFBOT(I) = ZIFBOT(I) + RSRATE*DT

Find out if the top Interface for this column moves...

and move that sucker

NOTOPMOVE = .FALSE.

DO INM = 1,NNM

IF(I.EQ.NOMOVE(INM)) NOTOPMOVE = .TRUE.

END DO

IF(.NOT.NOTOPMOVE) THEN

END ZIFTOP(I) = ZIFTOP(I) + RSRATE*DT

ENDIF

DO NSL=1,NSIF

ZIF(NSL,I) = ZIF(NSL,I) + RSRATE*DT

ENDIF

Now find the nodes that bound the Interfaces below

DO J=1,NJ-1

IF(ZIFBOT(I),GE,Y(I,J),AND.ZIFBOT(I).LT.Y(I,J+1)) JIFBOT(I)=J

IF(ZIFTOP(I),GE,Y(I,J),AND.ZIFTOP(I).LT,Y(I,J+1)) JIFTOP(I)=J

DO NSL=1,NSIF

IF(ZIF(NSL,I),GT,Y(I,NJ)) THEN ! Interface is above model top

JIF(NSL,I)=NJ

ELSE IF(ZIF(NSL,I),GE,Y(I,J),AND.ZIF(NSL,I).LT,Y(I,J+1)) THEN

JIF(NSL,I)=J

ENDIF

ENDIF

END DO

END DO

RETURN

END
SUBROUTINE SETMED
C
Set new medium values to nodes due to subsidence
C
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,HALF=0.5D+00,ONE=1.0D+00,TWO=2.0D+00,
1
THOUS=1.0D+03,ZERO=0.000D+00)
LOGICAL NMOVE
COMMON /COORDS/ X(IDIM,JDIM), Y(IDIM,JDIM), ICOSYS
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /FIELDS/ TEMP(IDIM,JDIM), CONC(IDIM,JDIM), PSI(IDIM,JDIM),
1 VX(IDIM,JDIM),
1 VV(IDIM,JDIM), OLDT(IDIM,JDIM), OLDC(IDIM,JDIM),
2 OLDSL(IDIM,JDIM), OLDVY(IDIM,JDIM),
C CLAST(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB, RSRATE, SRATE(IDIM,JDIM), JIFBOT(IDIM),
1 JIFTOP(IDIM), ZIFBOT(IDIM), ZIFTOP(IDIM),
1 JIF(20, IDIM), ZIF(20, IDIM), RPERM(20), RPOR(20),
2 RDXX(20), RRRK(20), RANISO(20), NSIF,
2 NOMOVE(IDIM), NNH, CTOP, FTOP ! Maximum of 20 interfaces
COMMON /PPARAM/ PERM(IDIM,JDIM), POR(IDIM,JDIM), DCX(IDIM,JDIM),
1 ANISO(IDIM,JDIM), ALFA(IDIM,JDIM),
1 ALFALD(IDIM,JDIM), RKS(IDIM,JDIM)
C
Set porosity as a function of depth and permeability
as a function of porosity
C
CPOR(DEPTH) = PHI0*EXP(RCDEPTH*DEPTH)
CPERM(PHI) = PKC1*PHI**5 + PKC0
where
PKC1=9.7655274D-12
PKC0=9.9902000D-18
C
Set constant porosity and permeability
CPOR(DEPTH) = 0.2D+00
CPERM(PHI) = 1.00E-14
DO I=1,NI
DO J=1,NJ
C
IF BELOW the salt...
IF(J.LE.JIFBOT(I)) THEN !---------------------------------!
PERM(I,J) = 1.00D-20
POR(I,J) = 0.020D+00
DCX(I,J) = 1.000D-15
RKS(I,J) = 2.8D+00
ANISO(I,J) = 1.0
SRATE(I,J) = RSRATE
ELSE IF(J.GT.JIFBOT(I) .AND. J.LT.JIFTOP(I)) THEN
PERM(I,J) = 1.00D-20
POR(I,J) = 0.020D+00
DCX(I,J) = 1.000D-15
RKS(I,J) = RRSALT(TEMP(I,J))
ANISO(I,J) = 1.0
C
WITHIN the salt...
C
ELSE IF(J.LE.JIFTOP(I)) THEN
PERM(I,J) = 1.00D-20
POR(I,J) = 0.020D+00
DCX(I,J) = 1.000D-15
RKS(I,J) = RRSALT(TEMP(I,J))
ANISO(I,J) = 1.0
If node is w/in the column itself,
then subsidence rate is zero

NMOVE = .FALSE.
DO INM = 1, NNM
   IF(I .EQ. NOMOVE(INM)) NMOVE = .TRUE.
END DO
IF(NMOVE) THEN
   SRATE(I,J) = ZERO
ELSE
   SRATE(I,J) = RSRATE
ENDIF

ABOVE the salt

ELSE
NMOVE = .FALSE.
DO INM = 1, NNM
   IF(I .EQ. NOMOVE(INM)) NMOVE = .TRUE.
END DO
IF(NMOVE) THEN
   SRATE(I,J) = 0.000D+00
ELSE
   SRATE(I,J) = RSRATE
ENDIF

IF( J .LE. JIF(1,1)) THEN
   PERM(I,J) = RPERM(1)
   POR(I,J) = RPOR(1)
   DCX(I,J) = RDCX(1)
   RKS(I,J) = RRKS(1)
   ANISO(I,J) = RANISO(1)
ELSE
   DO NSL=1, NSIF-1
      IF(J.GT.JIF(NSL,1).AND.J.LE.JIF(NSL+1,1)) THEN
         PERM(I,J) = RPERM(NSL+1)
         POR(I,J) = RPOR(NSL+1)
         DCX(I,J) = RDCX(NSL+1)
         RKS(I,J) = RRKS(NSL+1)
         ANISO(I,J) = RANISO(NSL+1)
      ENDIF
   ENDDO
ENDIF

IF( J > JIF(NSIF,1)) THEN
   PERM(I,J) = RPERM(NSIF+1)
   POR(I,J) = RPOR(NSIF+1)
   DCX(I,J) = RDCX(NSIF+1)
   RKS(I,J) = RRKS(NSIF+1)
   ANISO(I,J) = RANISO(NSIF+1)
ENDIF

ENDIF

The following do-loop resets concentration at top of dome

DO INM = 1, NNM
   POR(NOMOVE(INM), JIFTOP(NOMOVE(INM))) = RPOR(1)
   PERM(NOMOVE(INM), JIFTOP(NOMOVE(INM))) = RPERM(1)
   DCX(NOMOVE(INM), JIFTOP(NOMOVE(INM))) = RDCX(1)
   CONC(NOMOVE(INM), JIFTOP(NOMOVE(INM))) = CTOP
END DO
RETURN
DOUBLE PRECISION FUNCTION RKSALT(T)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(A=7.354D+00,B=-3.1575E-03)
RKSALT = A*EXP(B*T)
RETURN
END

DOUBLE PRECISION FUNCTION DCON12(I1,J1,I2,J2)

Estimate the hydrodynamic dispersion at a point between two nodes
w/ indices (I1,J1) and (I2,J2) by using an harmonic average

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,HALF=0.5D+00,ONE=1.0D+00, TWO=2.0D+00)
COMMON /COORDS/ X(IDIM,JDIM), Y(IDIM,JDIM), ICOSYS
1
COMMON /ISIZE / NI, NJ, ITIME, ITTIME
COMMON /APROP/ RKSF(IDIM,JDIM), RHOF(IDIM,JDIM),
1 OLRHOF(IDIM,JDIM), VISC0(IDIM,JDIM),
1 DSXX(IDIM,JDIM), DSPY(IDIM,JDIM), DSPXY(IDIM,JDIM)
COMMON /SUBSID/ TOTSUB,RRSF,IDIM,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP(IDIM), ZIFBOT(IDIM), ZIFTOP(IDIM),
1 JIF(20, IDIM), ZIF(20, IDIM), RPERM(20), RPOR(20),
2 DDCX(20), RRRS(20), RANISO(20), NSIF,
2 NOMOVE(IDIM),NM,CTOP,FTOP ! Maximum of 20 interfaces
FRACD=HALF
1 ! Node below no interface
D1 = DSPYY(I1,J1)
D2 = DSPYY(I2,J2)
IF(J1.EQ.J2) THEN ! Side-by-side nodes
FRACD = HALF
D1 = DSPXX(I1,J1)
D2 = DSPXX(I2,J2)
ELSE IF(J1.EQ.JIFBOT(I1)) THEN ! Node below bottom salt interface
FRACD=(Y(I2,J2)-ZIFBOT(I1))/(Y(I2,J2)-Y(I1,J1))
D1 = DSPYY(I1,J1)
D2 = DSPYY(I2,J2)
ELSE IF(J1.EQ.JIFTOP(I1)) THEN ! Node below top salt interface
FRACD=(Y(I2,J2)-ZIFTOP(I1))/(Y(I2,J2)-Y(I1,J1))
D1 = DSPYY(I1,J1)
D2 = DSPYY(I2,J2)
ELSE
DO NSL=1,NSIF
IF(J1.EQ.JIF(NSL,I1)) THEN ! Node below interface NSL
FRACD=(Y(I2,J2)-ZIF(NSL,I1))/(Y(I2,J2)-Y(I1,J1))
D1 = DSPYY(I1,J1)
D2 = DSPYY(I2,J2)
END IF
ENDDO
ELSE
DO NSL=1,NSIF
IF(J1.EQ.JIF(NSL,I1)) THEN ! Node below interface NSL
FRACD=(Y(I2,J2)-ZIF(NSL,I1))/(Y(I2,J2)-Y(I1,J1))
D1 = DSPYY(I1,J1)
D2 = DSPYY(I2,J2)
END IF
ENDDO
END IF
END IF
END IF
END IF
END IF
END IF
END IF
ENDDO
C
DCONR=(ONE-FRACD)/D1 + FRACD/D2 ! Reciprical conductivity at interface
DCON12 = ONE/DCONR ! Conductvty at interface
RETURN
END
DOUBLE PRECISION FUNCTION TCON12(I1, J1, I2, J2)
C-----------------------------------------------------------------------------
C     Estimate the thermal conductivity at a point between two nodes
C     w/ indices (I1, J1) and (I2, J2) by using an harmonic average
C-----------------------------------------------------------------------------
IMPLICIT DOUBLE PRECISION (A-H, O-Z)
PARAMETER (IDIM=101, JDIM=101, HALF=0.5D+00, ONE=1.0D+00, TWO=2.0D+00)
COMMON /COORDS/ X(IDIM, JDIM), Y(IDIM, JDIM), ICOSYS
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /APROP/ RKSF(IDIM, JDIM), RHOF(IDIM, JDIM),
1   OLRHOF(IDIM, JDIM), VISCO(IDIM, JDIM),
1   DSRXX(IDIM, JDIM), DSRYY(IDIM, JDIM), DSRXY(IDIM, JDIM)
COMMON /SUBSID/ TOTSUB, RSRATE, SRATE(IDIM, JDIM), JIFBOT(IDIM),
1   JIFTOP(IDIM), ZIFBOT(IDIM), ZIFTOP(IDIM),
2   RDCX(20), RRRS(20), RANISO(20), NSIF,
2   NOMOVE(IDIM), NN, CTOP, FTOP
C-----------------------------------------------------------------------------
FRACD=HALF
D1 = RKSF(I1, J1)
D2 = RKSF(I2, J2)
IF (J1.EQ.J2) THEN
   ! Side-by-side nodes
   FRACD = HALF
ELSE IF (J1.EQ.JIFBOT(I1)) THEN
   ! Node below bottom salt interface
   FRACD = (Y(I2, J2)-ZIFBOT(I1))/(Y(I2, J2)-Y(I1, J1))
ELSE IF (J1.EQ.JIFTOP(I1)) THEN
   ! Node below top salt interface
   FRACD = (Y(I2, J2)-ZIFTOP(I1))/(Y(I2, J2)-Y(I1, J1))
ELSE
   DO NSL=1, NSIF
      IF (J1.EQ.JIF(NSL, I1)) THEN
         ! Node below Interface 1
         FRACD = (Y(I2, J2)-ZIF(NSL, I1))/(Y(I2, J2)-Y(I1, J1))
      ENDIF
   ENDDO
ENDIF
C
TCONR = (ONE-FRACD)/D1 + FRACD/D2
TCON12 = ONE/TCONR
RETURN
C-----------------------------------------------------------------------------
DOUBLE PRECISION FUNCTION TAU12(I1, J1, I2, J2)
C-----------------------------------------------------------------------------
C     Estimate the product (hydraulic conductivity) * (reference density)
C     at a point between two nodes w/ indices (I1, J1) and (I2, J2) by using an
C     harmonic average
C-----------------------------------------------------------------------------
IMPLICIT DOUBLE PRECISION (A-H, O-Z)
PARAMETER (IDIM=101, JDIM=101, HALF=0.5D+00, ONE=1.0D+00, TWO=2.0D+00, GRAV=9.8D+00)
COMMON /COORDS/ X(IDIM, JDIM), Y(IDIM, JDIM), ICOSYS
COMMON /ISIZE/ NI, NJ, ITIME, ITTIME
COMMON /APARAM/ PERM(IDIM, JDIM), POR(IDIM, JDIM), DCX(IDIM, JDIM),
1   A ANISO(IDIM, JDIM), ALFAT(IDIM, JDIM),
1   ALFAD(IDIM, JDIM), RKS(IDIM, JDIM)
COMMON /APROP/ RKSF(IDIM, JDIM), RHOF(IDIM, JDIM),
1   OLRHOF(IDIM, JDIM), VISCO(IDIM, JDIM),
1   DSRXX(IDIM, JDIM), DSRYY(IDIM, JDIM), DSRXY(IDIM, JDIM)
COMMON /APROP/ LHSR, CS, RKF, CP, RPZERO, TZERO
COMMON /SUBSID/ TOTSUB, RSRATE, SRATE(IDIM, JDIM), JIFBOT(IDIM),
1   JIFTOP(IDIM), ZIFBOT(IDIM), ZIFTOP(IDIM),
2   RDCX(20), RRRS(20), RANISO(20), NSIF,
2 NOMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces

Set values of hydraulic conductivity at each node

A1 = PERM(I2,J1)*RHOF(I2,J1)/VISCO(I2,J1)
A2 = PERM(I2,J2)*RHOF(I2,J2)/VISCO(I2,J2)

IF(J1.NE.J2) THEN
A1 = A1/ANISO(I1,J1)
A2 = A2/ANISO(I1,J1)
ENDIF

Now see if nodes are separated by salt-sed interface

FRACD=HALF
! Node below no interface
IF(J1.EQ.J2) THEN
FRACD = HALF
ELSE IF(J1.EQ.J1FBIOT(I1)) THEN
FRACD=(Y(I2,J2)-YFBIOT(I1))/(Y(I2,J2)-Y(I1,J1))
ELSE IF(J1.EQ.J1FITOP(I1)) THEN ! Node below top interface
FRACD=(Y(I2,J2)-YFITOP(I1))/(Y(I2,J2)-Y(I1,J1))
ELSE
DO NSL=1,NSIF
IF(J1.EQ.J1F(NSL,I1)) THEN ! Node below Interface 1
FRACD=(Y(I2,J2)-YF(NSL,I1))/(Y(I2,J2)-Y(I1,J1))
ENDIF
ENDDO
ENDIF

And estimate hydraulic conductivity at interface

TAUR=(ONE-FRACD)/A1 + FRACD/A2
TAU12 = ONE/TAUR
RETURN
END

DOUBLE PRECISION FUNCTION RHOCALC(T,CM,P)
Calculate solution density as a function of Temperature (deg C), NaCl Concentration (molal), and Pressure (bars) for the range

10 < T < 350 deg C
0.25 < C < 5 molal
vapor sat < P < 500 bar

(The value of C1 has been corrected as per Sid Philips, pers. comm.)

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(A=-3.033405, B=10.128163, C=-8.750567, D=2.663107,
1 A1=-0.004539, A2=-0.0001638, A3= 0.00002551,
2 C1=-9.9559, C2= 7.0845, C3= 3.9093)
RHOCALC = 1.000D+03*(A + B*X + C*X**2 + D*X**3)
RETURN
END

DOUBLE PRECISION FUNCTION VISCALC(T,CM,P)
Calculate solution viscosity (in Pa*sec) as a function of Temperature (T in degC), NaCl concentration (CM in molal), and Pressure (P in MPa) for the range:

10 < T < 200 deg C
0 < CM < 5 molal
0.1 < P < 50 MPa

Water viscosity as a function of P and T is calculated from the correlation given by:


Corrections for salinity effects is calculated from the correlation given by:


The limits on T result from the applicability of the Kestin et al. correlation for water. The Phillips et al. correlation for salinity correction can be extended to 350 deg C, but another algorithm would need to be used in this code to calculate ETAW.

--- Dave Evans - 04-Aug-1989 --------------------------------------------------

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(A0=0.024192D+00,BO=571.1716D+00,TO=133.15D+00,
1 PA=0.0816D+00,PB=0.0122D+00,PC=0.00128D+00,
2 PD=0.000629D+00,PK=0.70D+00,ETA20=1002.D+00,
3 T20=20.0D+00,T96=96.0D+00,THOUS=1.0D+03,ZERO=0.00D+00,
4 ONE=1.00D+01, TEN=1.0D+01, RMICRO=1.00D-06)
DIMENSION ALFA(1:4),BETA(1:4)
DATA (ALFA(I),I=1,4) /1.2378D+00, -1.303D-03, 3.06D-06, 2.55D-08/
DATA (BETA(I),I=0,4) /-1.297, 5.74D-02, -6.97D-04, 4.47D-06,
1 -1.05D-08/
SAVE ALFA,BETA

Viscosity as a function of Temperature

SUM1=ZERO
DO I=1,4
SUM1 = SUM1 + ALFA(I)*(T20-T)**I
END DO
EXPON=SUM1/(T96+T)
ETA0T=ETA20*TEN**EXPON

Pressure correction

BETAW=ZERO
DO I=0,4
IF(T.EQ.ZERO .AND. I.EQ.0) THEN
  BETAW = BETAW + ZERO
ELSE
  BETAW = BETAW + BETA(I)*T**I
ENDIF
END DO

Water Viscosity

ETAW = ETA0T*(ONE+BETAW*P/THOUS)*RMICRO

Philips et al. correlation for salinity correction:

ETAR = ONE + PA*CM + PB*CM**2 + PC*CM**3 + PD*T*(ONE-EXP(PK*CM))
DOUBLE PRECISION FUNCTION OMEGA_NEW(OMEGA,TIMSTP,ITR,ITROLD,SSIGN).

Estimate the relaxation factor for SORL based on current and previous value of OMEGA and ITR

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
INTEGER*4 TIMSTP
OMEGA_NEW = OMEGA

Change in Omega will be larger early on...

IF(TIMSTP .LE. 10) THEN
  DOMEGA = 0.02
ELSE
  DOMEGA = 0.01
ENDIF

If first call, just save ITR and return

IF(TIMSTP .EQ. 1) THEN
  ITROLD = ITR
  SSIGN = 1.00D+00
  OMEGA_NEW = OMEGA + DOMEGA
  RETURN
ENDIF

If needed fewer iterations than last time, then keep changing OMEGA in same direction

IF(ITR .LT. ITROLD) THEN
  OMEGA_NEW = OMEGA + SSIGN*DOMEGA
ELSE IF(ITR .GE. ITROLD) THEN
  SSIGN = -SSIGN
  OMEGA_NEW = OMEGA + SSIGN*DOMEGA
ENDIF

If OMEGA_NEW is too high, reduce it
IF(OMEGA_NEW.GE.2.0D+00) OMEGA_NEW = 1.95
IF(OMEGA_NEW.LE.1.0D+00) OMEGA_NEW = 1.05
ITROLD = ITR
RETURN
END
SUBROUTINE TPPLOT(U,X,Y,NX,NY,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,
   SUBTTL)

Contour the field U which is calculated on an NX x NY grid, with node points at locations X(i,j), Y(i,j), i=1,...,NX, j=1,...,NY. The plot uses a vertical exaggeration of VE and is annotated with the iteration number (ITR), two 80 character TITLE cards, and a 16 character SUBTITLE.

Dave Evans 19-Aug-1988

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101, IRES=40)

Plotting variables need to be single precision
REAL*4 SU(IDIM,JDIM),SX(IDIM*JDIM),SY(IDIM*JDIM),SVE,WK,SCRARR
DIMENSION U(IDIM,JDIM),X (IDIM,JDIM),Y (IDIM,JDIM),GU(IDIM,JDIM)

Dimension work arrays for CONRAN
DIMENSION WK(13*IDIM*JDIM),IWK(31*IDIM*JDIM),SCRARR(IRES*IRES)

Arrays for subsidence and stuff
COMMON /SUBSID/ TOTSUB,RSRATE,SRATE(IDIM,JDIM),JIFBOT(IDIM),
1 JIFTOP (IDIM),ZIFBOT (IDIM),ZIFTOP (IDIM),
1 JIF (20, IDIM), ZIF (20, IDIM), RPERM(20), RPOR(20),
2 RDCX(20), RRKS(20), RANISO(20), NSIF,
2 NOMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces

Set up string variables and equivalent for annotations
CHARACTER*4 TITLE1(20),TITLE2(20),SUBTTL(5)
CHARACTER*23 DATIM

Regrid results
NGX=51
NGY=51
CALL BLGRID(X,Y,U,NX,NU,NGX)

Plot border and annotate plot
CALL BDRPLT(X,Y,UX,UY,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,SUBTTL)

Draw the outline of the mesh
CALL OUTLIN(X,Y,UX,UY)

Convert gridded data to single precision
SVE=SGRL(VE)
DO J=1,NGY
DO I=1,NGX
SUBROUTINE VPLOT(X,Y,VX, VY,NX, NY, VE, ELTIME, DT, DATIM, TITLE1, TITLE2)

// Plot velocity vectors w/ vector tail at node point and vector length scaled to velocity magnitude.

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ONE=1.0D+00, HALF=0.5D+00,
1 SPERY=3.15576E+07)

REAL*4 SX(IDIM,JDIM),SY(IDIM,JDIM),SVX(IDIM,JDIM),SVY(IDIM,JDIM),
1 SVE,VMAG,VMAGMX,PROP,SCALE,XTIP,YTIP,XTAIL,YTAIL,XMID,VMID
DIMENSION X(IDIM,JDIM),Y(IDIM,JDIM), VX(IDIM,JDIM),VY(IDIM,JDIM)

// Set up string variables and equivalent for annotations
CHARACTER*4 TITLE1(20),TITLE2(20),SUBTTL<5>
CHARACTER*12 VSTR
CHARACTER*23 DATIM
DATA SUBTTL/' SPE','CIFI','C DI','SCHA', 'RGE '/

// Set X, Y, VX, VY to single precision, and get bounds on X and Y
CALL SPCOPY (X, SX, NX, NY, ONE)
CALL SPCOPY (Y, SY, NX, NY, VE)
CALL SPCOPY (VX, SVX, NX, NY, ONE)
CALL SPCOPY (VY, SVY, NX, NY, ONE)
CALL SPMNX(SX,SY,NX,NY,SPMIN,SPMAX,SPYMIN,SPYMAX)
SVE = SNGL(VE)

// Scale the velocity vectors
K=0
VMAGMX=0.0
DO 50 J=1,NY
   DO 40 I=1,NX
      K=K+1
      VMAG=SQRT(SVX(I,J)**2 + SVY(I,J)**2)
      VMAGMX = MAX(VMAGMX, VMAG)
   40 CONTINUE
50 CONTINUE

// Now try scaling velocity vectors to set scale
If first iteration or zero velocity field, return

IF(VMAGMX.EQ.ZERO) THEN
  TYPE*,'No Non-zero Velocity Vectors -- Velocity Field Not Drawn'
  RETURN
ENDIF

Draw mesh outline and annotate plot

CALL BDRPLT(X,Y,NX,NY,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,SUBTTL)

Draw the outline of the mesh

CALL OUTLIN(X,Y,VE,NX,NY)

Set scaling stuff, PROP is the proportion of grid size

CALL DRAWSALT(X,Y,VE,NX,NY)

PROP=0.1*(SPXMAX-SPXMIN)
SCALE=PROP/VMAGMX

Plot arrows

ISTEP=1
JSTEP=1
WRITE(*,*),'Enter increment for velocity arrows (I and J)'
READ(*,*) ISTEP,JSTEP
DO 210 J=2,NY-1,JSTEP
  DO 200 I=2,NX-1,ISTEP
    VMAG=SQRT(SVX(I,J)**2 + SVY(I,J)**2)
    IF(VMAG.EQ.ZERO) GOTO 200
    XTAIL=SPXMAX-VMAGMX*SCALE
    XTIP=XTAIL+VMAG*SCALE
    XMID=HALF*(XTIP-XTAIL)
    YMID=HALF*(YTIP-YTIP)
    XTAIL=XTAIL-XMID
    YTIP=YTIP-YMID
    CALL ARROW1(XTAIL,YTAIL,XTIP,YTIP,SVE,1.E-15)
  200 CONTINUE
210 CONTINUE

Plot a reference vector in the lower right

YTIP=SPYMIN-0.05*(SPYMAX-SPYMIN)
XTAIL=SPXMAX-VMAGMX*SCALE
XTIP=XTAIL+XTIP/2.
XTIP=XTIP/2.
YTIP=SPYMIN-0.092*(SPYMAX-SPYMIN)
WRITE(VSTR,4) VMAGMX*SPERYR
  4  FORMAT(1X,E11.4)
CALL PWRT(IXTIP,YTIP,AREF(VSTR),12,11,0,0)
CALL PLOT_END
RETURN
END
SUBROUTINE OUTLIN(X, Y, VE, NX, NY)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101, JDIM=101)
DIMENSION X(IDIM, JDIM), Y(IDIM, JDIM)
REAL*4 PX(4*IDIM), PY(4*IDIM), SVE

Store perimeter points in PX, PY arrays

SVE=SNGL(VE)
HALF=0.5
K=1
PX(K)=HALF*(SNGL(X(1,1)) + SNGL(X(2,1)))
PY(K)=HALF*(SVE*SNGL(Y(1,1)) + SVE*SNGL(Y(1,2)))
DO I=2,NX-1 ! Across the Bottom
  K=K+1
  PX(K)=HALF*(SNGL(X(I,1)) + SNGL(X(I,2)))
  PY(K)=HALF*(SVE*SNGL(Y(I,1)) + SVE*SNGL(Y(I,2)))
END DO
K=K+1
PX(K)=HALF*(SNGL(X(NX-1,1)) + SNGL(X(NX,1)))
PY(K)=HALF*(SVE*SNGL(Y(NX,1)) + SVE*SNGL(Y(NX,2)))
DO J=2,NY-1 ! Up the right side
  K=K+1
  PX(K)=HALF*(SNGL(X(NX-1,J)) + SNGL(X(NX,J)))
  PY(K)=HALF*(SVE*SNGL(Y(NX-1,J)) + SVE*SNGL(Y(NX,J)))
END DO
K=K+1
PX(K)=HALF*(SNGL(X(NX-1,NY)) + SNGL(X(NX,NY)))
PY(K)=HALF*(SVE*SNGL(Y(NX-1,NY)) + SVE*SNGL(Y(NX,NY)))
DO I=NX-1,2,-1 ! Across the Top
  K=K+1
  PX(K)=HALF*(SNGL(X(I,NY)) + SNGL(X(I,NY-1)))
  PY(K)=HALF*(SVE*SNGL(Y(I,NY)) + SVE*SNGL(Y(I,NY-1)))
END DO
K=K+1
PX(K)=HALF*(SNGL(X(1,NY)) + SNGL(X(2,NY)))
PY(K)=HALF*(SVE*SNGL(Y(1,NY)) + SVE*SNGL(Y(1,NY)))
DO J=NY-1,2,-1 ! Down the left side
  K=K+1
  PX(K)=HALF*(SNGL(X(1,J)) + SNGL(X(2,J)))
  PY(K)=HALF*(SVE*SNGL(Y(1,J)) + SVE*SNGL(Y(2,J)))
END DO
K=K+1
PX(K)=PX(1)
PY(K)=PY(1)

CALL CURVE(PX, PY, K)

RETURN
END

SUBROUTINE DRAWSALT(X, Y, VE, NX, NY)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101, JDIM=101)
DIMENSION X(IDIM, JDIM), Y(IDIM, JDIM)
INTEGER*2 IDASHPAT
REAL*4 SX1, SX2, SY1, SY2, HALF, SVE
COMMON /SUBSID/ TOTSUB, RSRATE, RSRATE(IDIM, JDIM), JIFBOT(IDIM),
  1 JIFTOP(IDIM), ZIFBOT(IDIM), ZIFTOP(IDIM),
  1 JIF(20, IDIM), ZIF(20, IDIM), RPERM(20), RIOR(20),
  2 RDCX(20), RRKS(20), RANISO(20), NSIF,
NOMOVE(IDIM),NNM,CTOP,FTOP ! Maximum of 20 interfaces

Now plot the position of the salt layer

IDASHPAT = 7070
HALF = 0.5
SVE = SNGL(VE)

Draw the bottom

CALL DASHD(IDASHPAT)
SX1 = HALF*(SNGL(X(1,1)) + SNGL(X(2,1)))
SY1 = SVE*SNGL(ZIFBOT(1))
SX2 = HALF*(SNGL(X(NX-1,1)) + SNGL(X(NX,1))
SY2 = SY1
CALL LINED(SX1,SY1,SX2,SY2)

And the Top of Salt

DO I=2,NX-1
SX1 = HALF*(SNGL(X(I,1)) + SNGL(X(I-1,1)))
SX2 = HALF*(SNGL(X(I,1)) + SNGL(X(I+1,1)))
SY1 = SNGL(ZIFTOP(I))
SY2 = SNGL(ZIFTOP(I+1))
IF (SY1 .EQ. SY2) THEN
CALL LINED(SX1,SY1,SX2,SY2)
ELSE
CALL LINED(SX1,SY1,SX2,SY1)
CALL LINED(SX2,SY1,SX2,SY2)
ENDIF
END DO

RETURN
END

SUBROUTINE BDRPLT(X,Y,NX,NY,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,
1 SUBTTL)

Plot the border of the mesh, and annotate the plotting area.

The plot uses a vertical exaggeration of VE and is annotated w/ the
Iteration number [ITR], two 80 character TITLE cards, and a 16 character
SUBTITLE.

Dave Evans

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ONE=1.00D+00,S_PER_YR=3.15576D+07)

Plotting variables need to be single precision

REAL*4 AR,SVE,SPXMIN,SPXMAX,SPYMIN,SPYMAX,WK,SPX1,SPX2,
1 SPY1,SPY2,SX(IDIM,JDIM),SY(IDIM,JDIM),XI,YI,SDX,
2 SBAR
DIMENSION X(IDIM,JDIM),Y(IDIM,JDIM)

Set up string variables and equivalent for annotations

CHARACTER*2 STBAR(4)
CHARACTER*3 STVE(10),STVE9
CHARACTER*4 TITLE1(20),TITLE2(20),SUBTTL(5),STR1,TSTRIT,STRIT(4)
CHARACTER*5 ST_TIME(7),ST_DTIME(7)
CHARACTER*6 STBR13
CHARACTER*10 ST_ELTIME,ST_DT
CHARACTER*23 DATIM
EQUIVALENCE(ST_ELTIME,ST_TIME(4))
EQUIVALENCE(ST_DT,ST_DTIME(4))
EQUIVALENCE(STVE9,STVE(9))
EQUIVALENCE(STBR13,STBAR(1))
DATA (STVE(I),I=1,10) /'VER','TIC','AL ','EXA','RAT','IoN',','1,'/
DATA (ST_TIME(I),I=1,3) /'ELAPS','ED TI','ME = '/
DATA (ST_DTIME(I),I=1,3) /'TIME ','STEP ','= '/
DATA SPXMIN/1.E+30/, SPXMAX/-1.E+30/, SPYMIN/1.E+30/, SPYMAX/-1.E+30/
DATA STBAR(4) /' M'/

Start by getting date and time
WRITE(ST_ELTIME,2) ELTIME/S_PER_YR
WRITE(ST_DT,2) DT/S_PER_YR
2 FORMAT(E10.4)

Search boundary coordinates for extreme values
SVE = SNGL(VE)
CALL SPCOPY(X,SX,NX,NY,ONE)
CALL SPCOPY(Y,SY,NX,NY,VE)
CALL SPMNMX(SX,SY,NX,NY,SPXMIN,SPXMAX,SPYMIN,SPYMAX)

Set aspect ratio for plotting
AR=(SPYMAX-SPYMIN)/(SPXMAX-SPXMIN)

Write vertical exaggeration to string variable for annotation
WRITE(STVE9,3) NINT(SVE)
3 FORMAT(I3)

Call set w/ appropriate vertical exaggeration
CALL SET(0.05,0.77,0.1,0.1+0.72*AR,
SPXMIN,SPXMAX,SPYMIN,SPYMAX,1)

Write titles and stuff...
CALL GETSET(MXA,MBX,MYA,MYB,SPX1,SPX2,SPY1,SPY2,LTYPE)
CALL PWRITE(512,MYB+160,%REF(TITLED),80,12,0,0)
CALL PWRITE(512,MYB+110,%REF(TITLE2),80,12,0,0)
CALL PWRITE(410,MYB+50,%REF(SUBTTL),20,18,0,0)
CALL PWRITE(960,103,%REF(STVE),30,14,90,-1)
CALL PWRITE(925,103,%REF(ST_DTIME),35,14,90,-1)
CALL PWRITE(890,103,%REF(DATIM),35,14,90,-1)
CALL PWRITE(855,103,%REF(DATIM),17,14,90,-1)

Draw and annotate scale bar in lower left corner
SDX=SPXMAX-SPXMIN
SDY=SPYMAX-SPYMIN
IF(SDX .GE. 0.0 .AND. SDX .LT. 100.) SBAR = 10.
IF(SDX .GE. 100.0 .AND. SDX .LT. 1000.) SBAR = 100.
IF(SDX .GE. 1000.0 .AND. SDX .LT. 10000.) SBAR = 1000.
IF(SDX .GE. 10000.0 .AND. SDX .LT. 100000.) SBAR = 10000.
IF(SDX .GE. 100000.0) SBAR = 100000.
WRITE(STBR13,4) INT(SBAR)
4 FORMAT(I6)
SUBROUTINE ARR0W1(XI,Y1,X2,Y2,VE,SHORT)

FUNCTION: Subroutine ARR0W uses NCAR calls to plot a vector from (XI,Y1) to (X2,Y2), with the tip of arrow head being at (X2,Y2).

INPUT:
X1,Y1,X2,Y2 = The coordinates of the tail and tip of the vector, respectively.
VE = Vertical exaggeration of plot
SHORT = The length of the shortest vector to be plotted

Dave Evans and Steve Jones, May 1986

IMPLICIT REAL*4(A-H,O-Z)

XYL=SQRT((X2-X1)**2+(Y2-Y1)**2)
IF(XYL.LT.SHORT) RETURN ! Skip short vectors
PI=3.141592654 ! Pi
PSI=28. ! Convert to radians
PHI=ATAN(TAN(PHI)/VE)
X1T=X1-X2 ! Translate tip to origin
Y1T=Y1-Y2
THETA=ATAN2(Y1T,X1T) ! Angle of vector
CALL LINE(X1,Y1,X2,Y2) ! Plot the vector stem
D=0.2*XYL ! Length of arrow head
X2T=0.
Y2T=0.
IF(ABS(X1T).LT.1.0E-08) X1T=1.0E-08 ! Don't divide by 0
X=D*COS(THETA+PHI) + X2 ! Plot vector tip
Y=D*SIN(THETA+PHI) + Y2
CALL LINE(X2,Y2,X,Y)
X=D*COS(THETA-PHI) + X2
Y=D*SIN(THETA-PHI) + Y2
CALL LINE(X2,Y2,X,Y)
RETURN
END
Plot location of grid points \( [X(i,j), Y(i,j), \ldots, X_N, Y_j, \ldots, Y_N] \) using a vertical exaggeration of \( \mathcal{V}E \).

Dave Evans 19-Aug-1988

```
C- Plot location of grid points \( [X(i,j), Y(i,j), \ldots, X_N, Y_j, \ldots, Y_N] \)
C using a vertical exaggeration of \( \mathcal{V}E \).
C
Dave Evans 19-Aug-1988

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ONE=1.0D+00)
DIMENSION X(IDIM,JDIM),Y(IDIM,JDIM)
REAL*4 SX(IDIM,JDIM), SY(IDIM,JDIM), SPXMIN, SPXMAX, SPYMIN, SPYMAX,
1 AR,RAR,SVE
CHARACTER*4 TITLE1(20),TITLE2(20),SUBTTL(5)
DATA SUBTITL/1 DI1,'FFER', 'ENCE', 'GRI'/'

CALL SPCOPY(X,SX,NX,NY,ONE)
CALL SPCOPY(Y,SY,NX,NY,VE)
CALL BDRPLT(X,Y,NX,NY,VE,ELTIME,DT,DATIM,TITLE1,TITLE2,SUBTTL)
SVE=SNGL(VE)

Plot each row of nodes

DO 210 J=1,NY
   DO 200 I=1,NX-1
      CALL LINE(SX(I,J),SY(I,J),SX(I+1,J),SY(I+1,J))
   200 CONTINUE
210 CONTINUE

Plot each column of nodes

DO 310 I=1,NX
   DO 300 J=1,NY-1
      CALL LINE(SX(I,J),SY(I,J),SX(I,J+1),SY(I,J+1))
   300 CONTINUE
310 CONTINUE

CALL PLOT_END

RETURN
END
```

SUBROUTINE BLGRID(X,Y,Z,NI,NJ,GZ,NGPX,NGPY)

This subroutine regrids values on an uneven orthogonal grid such
that the gridded values are on evenly spaced grid points. The gridding
is done with BI-LINEAR interpolation. \( X(i,j) \) and \( Y(i,j) \) \((i=1,2,\ldots,NI)\)
\((j=1,2,\ldots,NJ)\) are the coordinates of an arbitrary orthogonal grid with
values of \( Z \) specified at each grid point. These values are regridded
on \( NGPX \) evenly spaced grid points in the \( X \)-direction and \( NGPY \) evenly
spaced points in the \( Y \)-direction, and the regridded values are stored
in \( GZ \).

Dave Evans Last update 31-Jul-1989

```
C- This subroutine regrids values on an uneven orthogonal grid such
C that the gridded values are on evenly spaced grid points. The gridding
C is done with BI-LINEAR interpolation. \( X(i,j) \) and \( Y(i,j) \) \((i=1,2,\ldots,NI)\)
C \((j=1,2,\ldots,NJ)\) are the coordinates of an arbitrary orthogonal grid with
C values of \( Z \) specified at each grid point. These values are regridded
C on \( NGPX \) evenly spaced grid points in the \( X \)-direction and \( NGPY \) evenly
C spaced points in the \( Y \)-direction, and the regridded values are stored
C in \( GZ \).
C
Dave Evans Last update 31-Jul-1989

IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101,ONE=1.00D+00)
DIMENSION X(IDIM,JDIM),Y(IDIM,JDIM),Z(IDIM,JDIM),GZ(IDIM,JDIM)

DX=(X(NI,1)-X(1,1))/FLOAT(NGPX-1) ! X-step size
DY=(Y(1,NJ)-Y(1,1))/FLOAT(NGPY-1) ! Y-step size

Step through \( NGPX \) by \( NGPY \) points and estimate \( Z \)
```
DO IG=1,NGPX
DO JG=1,NGPY
   GX=DX*FLOAT(IG-1)
   GY=DY*FLOAT(JG-1)
   C
   Find the nodes that bound (GX,GY)
   C
   DO I=1,NI-1
      IF(X(I,1).LE.GX .AND. GX.LT.X(I+1,1)) GOTO 100
   END DO
   I=I-1 ! if it falls through, assume pt is on border
100 CONTINUE
   DO J=1,NJ-1
      IF(Y(1,J).LE.GY .AND. GY.LT. Y(I,J+1)) GOTO 200
   END DO
   J=J-1 ! if it falls through, assume pt is on border
200 CONTINUE
   AND now interpolate
   C
   T=(GX-X(I,J))/(X(I+1,J)-X(I,J))
   U=(GY-Y(I,J))/(Y(I,J+1)-Y(I,J))
   GZ(IG,JG)=(ONE-T)*(ONE-U)*Z(I,J)
         +T*(ONE-U)*Z(I+1,J)
         +T*U*Z(I,J+1)
         +(ONE-T)*U*Z(I,J+1)
   END DO
   END DO
   C
   Save the Whales
   RETURN
END

C------------------------------------------------------------------------
C------------------------------------------------------------------------
C SUBROUTINE SPMMNX(X,Y,N,M,XMIN,XMAX,YMIN,YMAX)
C------------------------------------------------------------------------
C SINGLE PRECISION subroutine to get the maximum values from the
C perimeter of two two-dimensional arrays X and Y, each dimension NxM.
C------------------------------------------------------------------------
IMPLICIT REAL*4(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101)
DIMENSION X(IDIM,JDIM),Y(IDIM,JDIM)
YMIN = 1.E+30
XMIN = 1.E+30
YMAX = -YMIN
XMAX = -XMIN
DO 230 I=1,N
   YMIN = MIN(YMIN,Y(I,1))
   YMAX = MAX(YMAX,Y(I,M))
230 CONTINUE
DO 240 J=1,M
   XMIN = MIN(XMIN,X(I,1))
   XMAX = MAX(XMAX,X(N,J))
240 CONTINUE
RETURN
END

C------------------------------------------------------------------------
C------------------------------------------------------------------------
C SUBROUTINE SPCOPY(X,SX,N,M,SCLR)
C------------------------------------------------------------------------
C Multiply two-dimensional array X by the scalar SCLR, and copy the
C product into single precision array SX.
C Both X and SX are two dimensional of size NxM.
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
PARAMETER(IDIM=101,JDIM=101)
DIMENSION X(IDIM,JDIM)
REAL*4 SX(IDIM,JDIM)
SPSCLR=SNGL(SCLR)
DO J=1,M
   DO I=1,N
      SX(I,J) = SPSCLR*SNGL(X(I,J))
   END DO
END DO
RETURN

C     Bob's Your Uncle
END
APPENDIX B

SAMPLE INPUT FILES FOR PROGRAM CSDDB
NOECHO
4-OCT-1989 14:07:45.41
SAMPLE INPUT FILE FOR PROGRAM CSDDB — THIS FILE WAS USED IN SIMULATIONS
GIVEN IN FIGURES 7.5, 7.6, AND 7.7 IN THIS DISSERTATION

Cylindrical Polar Coordinates
Concentration Simulation
Temperature Simulation
Stream Function Simulation

<table>
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<tr>
<th>Cylinder</th>
<th>Radius</th>
<th>Concentration</th>
<th>Temperature</th>
<th>Stream Function</th>
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</thead>
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<td>0.0000E+00</td>
<td>0.0000E+00</td>
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<td>0.1000E-01</td>
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<td>0.0000E+00</td>
<td>0.2392E+03</td>
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<td>0.1000E-14</td>
<td>0.1000E+10</td>
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<tr>
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<td>3</td>
<td>1.0000E+04</td>
<td>0.0000E+00</td>
<td>0.2392E+03</td>
</tr>
<tr>
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<td></td>
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<td>0.1000E-14</td>
<td>0.1000E+10</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>0.1100E+04</td>
<td>0.0000E+00</td>
<td>0.2392E+03</td>
</tr>
<tr>
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<td></td>
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<td>0.1000E-14</td>
<td>0.1000E+10</td>
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<td>0.1000E-14</td>
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<td>0.0000E+00</td>
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Note: The values are in scientific notation.
<p>| 20 | 7 | 0.6000E+04 | 0.3000E+04 | 0.0000E+00 | 0.1741E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 21 | 7 | 0.6500E+04 | 0.3000E+04 | 0.0000E+00 | 0.1741E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 22 | 7 | 0.7000E+04 | 0.3000E+04 | 0.0000E+00 | 0.1741E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 23 | 7 | 0.7500E+04 | 0.3000E+04 | 0.0000E+00 | 0.1741E+03 | 0.0000E+00 |
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| 24 | 7 | 0.8000E+04 | 0.3000E+04 | 0.0000E+00 | 0.1742E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 25 | 7 | 0.8500E+04 | 0.3000E+04 | 0.0000E+00 | 0.1742E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 26 | 7 | 0.9000E+04 | 0.3000E+04 | 0.0000E+00 | 0.1742E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 27 | 7 | 0.9500E+04 | 0.3000E+04 | 0.0000E+00 | 0.1742E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 28 | 7 | 1.0000E+04 | 0.3000E+04 | 0.0000E+00 | 0.1742E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 29 | 8 | 0.5000E+03 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 30 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 31 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 32 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 33 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
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| 34 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
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| 35 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
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| 36 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
|    |   | 0.1000E+19 | 0.2000E+01 | 0.1000E+14 | 0.1000E+01 | 0.1000E+02 |
| 37 | 8 | 0.1000E+04 | 0.3500E+04 | 0.0000E+00 | 0.1628E+03 | 0.0000E+00 |
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**WATER TABLE SPECIFIED ON TOP BOUNDARY**

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**HEAT FLUX BOUNDARY CONDITION ON BOTTOM**

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VITA

David Griffin Evans was born February 6, 1956, in Redwood City California. He is the youngest of three children born to Proctor and Shirley Evans of San Carlos California. He graduated from Carlmont High School in May, 1974. In December, 1981 he received a Bachelor of Arts degree in geophysics from the University of California at Berkeley. He earned a Master of Science degree from the University of Kansas in 1984, and wrote a thesis titled Seismicity of the Sleepy Hollow Oil Field, Red Willow County, Nebraska. While at the University of Kansas he was awarded the Erasmus Haworth Honors Award for outstanding M.S. student in geology, and he passed his Master's degree general exam with honors. After completing his M.S. degree he worked for the Kansas Geological Survey for one year before entering the Ph.D. program at Louisiana State University in August, 1985. For four years at LSU he was an LSU Alumni Federation Fellow, and during the last few months of his studies there he received a research assistantship. Dave was married to Lisa Ann Willey, of Redwood City California, on July 30, 1983. His daughter, Eileen Louise, was born on August 30, 1985, the day after he began his Ph.D. program. His son, Ian Willey, was born on August 26, 1989. After his graduate studies, he joined the faculty at the University of Maine, Orono, as an Assistant Professor of Geological Sciences.
DOCTORAL EXAMINATION AND DISSERTATION REPORT

Candidate: David Griffin Evans

Major Field: Geology

Title of Dissertation:
Theoretical and Numerical Models for Heat and Mass Transport and Groundwater Flow Near Salt Domes

Approved:

[Signatures]

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination:

November 20, 1989