CHAPTER III

THEORITICAL BACKGROUND

3.1 General background

Based on Parsons (1970), earth subsurface can be divided into two zones, the surficial zone and the geothermal zone (Figure 3.1). Within the surficial zone, the temperature is influenced by seasonal warming and cooling of the land surface. Shallow groundwater temperature is ~1 °C to 2 °C higher than the mean annual surface temperature. The amplitude of temperature fluctuations decreases with depth; below ~ 1.5 m, the temperature is not significantly influenced by diurnal fluctuations at the land surface (Silliman and Booth 1993). Temperature profiles in the surficial zone potentially provide information about seasonal recharge / discharge events from precipitation and interchange with surface water.

The geothermal zone is usually below a depth of around 10 m. In the absence of groundwater flow, subsurface temperature in the geothermal zone normally follows the geothermal gradient (Figure 3.1) and usually increases of 1°C per 20 to 40 m of depth. Within the geothermal zone, the temperature profile is not subject to seasonal variations and is expected to be approximately linear except when perturbed by groundwater flow, although changes in thermal conductivity also change curve the thermal profile. Groundwater flow perturbs the geothermal gradient by infiltration of relatively cool water in recharge areas or by upward flow of relatively warm water in discharge areas, causing concave upward profiles in recharge areas and convex upward profiles in discharge areas (Figure 3.1).

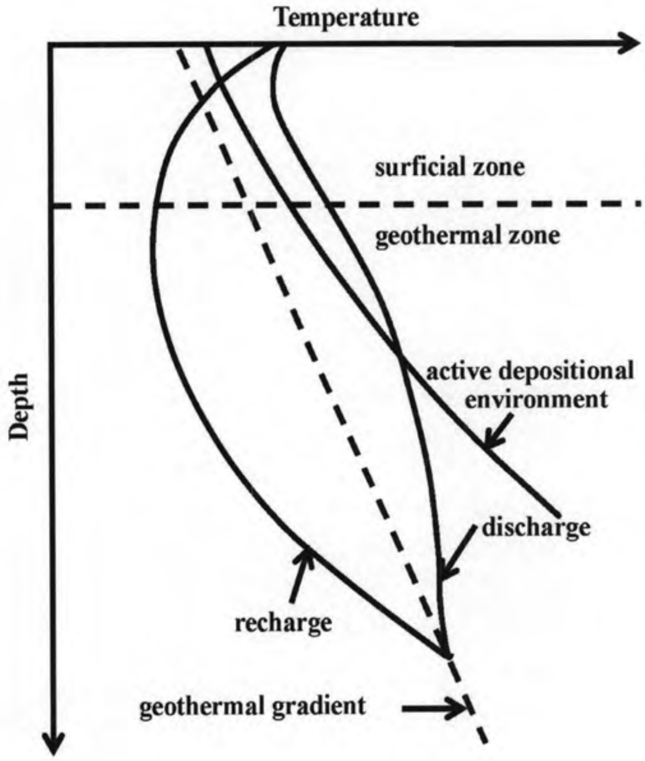

Figure 3.1 Schematic temperature profiles showing deviations of the geothermal gradient caused by surface warming in the surficial zone and convection in the geothermal zone. (modified after Taniguchi 1999a; Domenico and Schwartz 1997)

The profile "recharge" represents downward movement of groundwater that results in concave upward profiles, whereas discharge (upward movement) results in convex upward profiles. The profile "active depositional environment" represents the combined effect of one-dimensional forced convection upward and separation of the boundaries by the accumulation of sediment.

3.2 Heat transport in groundwater flow

Heat can transport from point to point in a porous medium by way of three processes: conduction, convection, and radiation. Conductive transport may be described by a linear law relating the heat flux to the temperature gradient. Convective heat transport is the movement of heat by a moving groundwater. Radiation, better known as thermal electromagnetic radiation, is the radiation emitted through differential temperature of a geologic body. (Domenico and Schwartz, 1997)

In systems where the fluid is moving, there is a convective transport by the fluid motion. When the flow field is caused by external forces, the transport is said to occur by forced convection. Such is the case where groundwater movement takes place in the absence of density gradients such that Darcy's law applies. A second type of transport, called fee convection, occurs when the motion of fluid is due exclusively to density variations caused by temperature gradients. Free convection is probably the dominant type of fluid motion in some hydrothermal systems where the bulk of liquid discharge is in the form of steam or hot water.

A similar phenomenon can occur in mass transport, along fresh water-salt water interfaces in coastal areas where density differences reflect the various salinity differences. For these cases, there are no longer exists a scalar potential so that Darcy's law does not describe the motion. It is emphasized that forced and free convection represent two limiting conditions.

In the case of the former, buoyancy forces are assumed to be negligible. For the latter, fluid motion must be described entirely in terms of buoyancy. When buoyancy forces dominate, the velocity field and the energy field (temperature) are interdependent, and the equations must be solved iteratively. The simplest system to demonstrate forced and free convections, shown in Figure 3.2, is a hypothetical model for flow in hydrothermal areas.

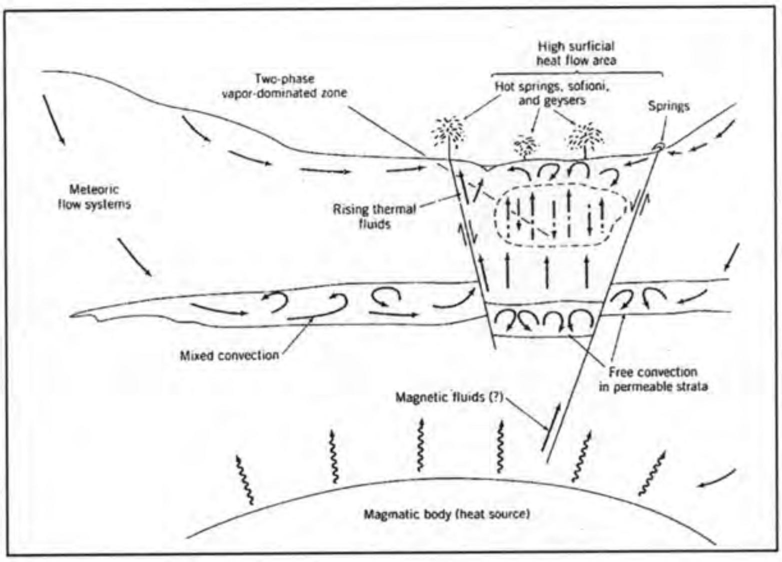

Figure 3.2 Forced, free, and mixed convection in a hydrothermal system (after Sharp and Kyle, 1988)

3.3 Heat transport in active depositional environments

The transient velocity field is responsible for the convective transport of heat. Examining this process from the perspective of the energy transport equations provides some information on the historical pressure - temperature history of a region. Although it is not possible to reconstruct all the factors contributing to the reconstraction of the historical pressure–temperature of basins, mathematical modeling can be used to gain insights of certain processes and for establishing some limiting or threshold conditions. (Domenico and Schwartz, 1997)

In modeling, the conductive gradient is normally depicted as originating due to a heat flux across the lower boundary of an accumulating sedimentary pile (Figure 3.3). Most studies to date have assumed the condition of forced convection although some free convection cannot be ruled out. In addition, it is frequently assumed that the surface temperature remains constant during continual deposition of the sediment. Frequently, a moving coordinates system is used to study this problem. The results of such studies demonstrate that with uniform erosion it will constantly decrease. These facts are shown in Figure 3.4 by profiles 1 and 2 when the distance axis represents the depth from the sediment-water interface to impermeable basement rock.

Profiles 1 and 2 would also be expected from steady one-dimensional flow upward and downward, respectively, where the sedimentary layer remains of uniform thickness (Bredehoeft and Papadopulos, 1965). Profile 3 represents the combined effect of one-dimensional forced convection upward and the separation of the boundaries by the accumulation of sediment. In this case, a zero or near zero velocity at the growing sediment-water interface perturbs profile 1 into the reverse "S" pressure-depth profile 4.

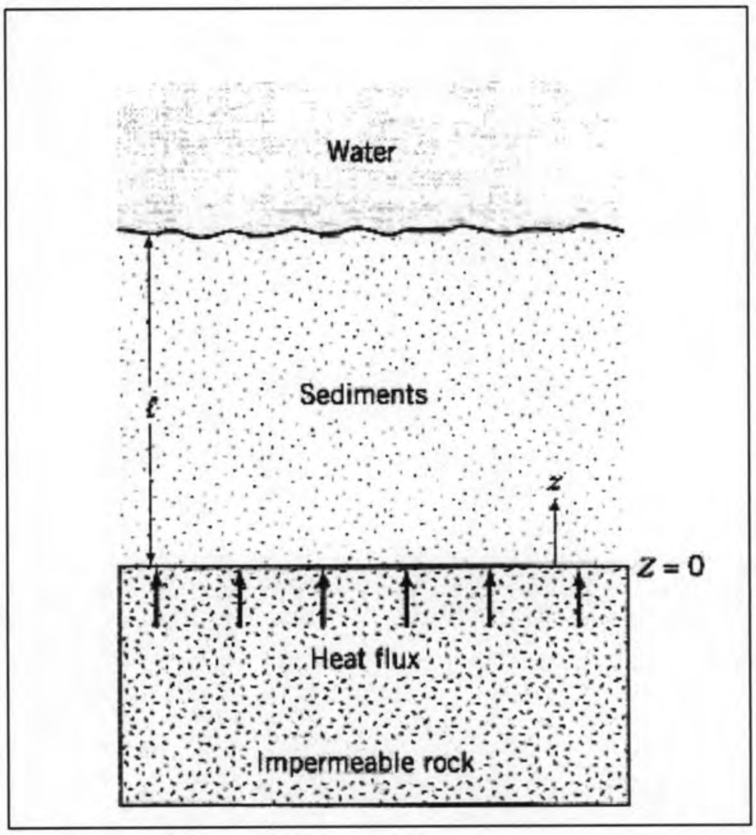

Figure 3.3 Schematic diagram of accumulating sediment with heat flux across the lower boundary. (after Domenico and Schwartz, 1997)

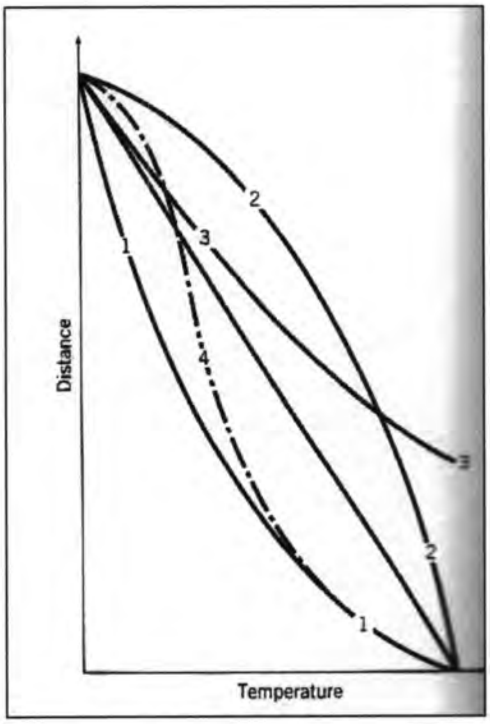

Figure 3.4 Temperature patterns with moving boundaries and convection (after Domenico and Schwartz, 1997)

3.4 Vertical groundwater velocities

The three ideal cases are shown in Figure 3.5, where a one–dimensional velocity field is imposed on a one-dimensional purely conductive thermal field. In Figure 3.5a and 3.5b, the direction of groundwater movement is taken as normal to the conductive isotherms. The hydraulic gradient and the conductive temperature gradient are collinear in the vertical direction so that the streamlines of fluid flow are normal to the isotherms of heat conduction. For these cases, a convection flux is established that will produce the greatest alteration of the conductive temperature distribution. In Figure 3.5a, the resultant temperature gradient will increase with depth, whereas in Figure 3.5b, it will decrease with depth. In addition, the heat flow at the surface will be greater for Figure 3.5b. In Figure 3.5c, the hydraulic gradient and the temperature gradient are normal so that the streamlines of fluid flow are collinear with the isotherms of heat conduction. Here convective transport is eliminated as there is no heat transport along an isotherm.

Geophysicists have long recognized that moving groundwater can affect the flux of heat within the Earth. Van (1934) indicated that the transfer of heat by migrating water could cause variations of temperature gradients within the Earth. He discussed these variations at some length, using illustrative data from the Wall Creek Sands of Salt Creek Oil Field, Wyoming. Because the natural heat–flux density from the Earth is usually small, the upward thermal gradient within the Earth may be affected by groundwater movement. Stallman (1960) presented the basic equations for the simultaneous transfer of heat and water within the Earth and suggested that temperature measurements might provide a means of measuring rates of groundwater movement. The solution to Stallman's general equation for the case of steady-state vertical flow of both groundwater and heat is presented. This solution is of interest to groundwater hydrologists, because it may provide a means for calculating vertical rates of groundwater movement and in some instances, where head relationships are known, vertical permabilities.

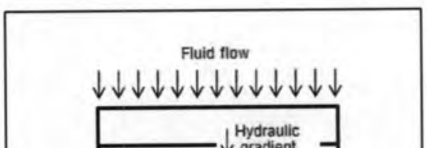

Figure 3.5 Three ideal cases where a field is imposed on a conductive thermal gradient (after Domenico and Schwartz, 1997)

3.5 Groundwater temperature measurement

The identification and quantification mechanisms for replenishing aquifers are important for effective water resource management. Aquifers are replenished by local precipitation along with as interbasin flow, induced stream infiltration, and interaquifer leakage. Generally, some precipitation will percolate through the unsaturated zone to the potentiometric surface of the shallowest aquifer. After the precipation-derived water reaches the saturated zone, its direction and magnitude of flow is governed by the prevailing hydraulic heads and aquifer characteristics.

Under certain conditions groundwater can move even further downward to deeper aquifers replenishing them at rates which depend upon the rates of vertical groundwater movement. Although recharge rates can be calculated in several ways from direct hydrologic data, this study is concerned with the feasibility of determining recharge rates from subsurface temperature distributions. In a connected system, the exchange of water between the stream and shallow aquifer plays a key role in influencing temperature not only in streams, but also in their underlying sediments. As a result, analysis of subsurface temperature patterns can provide information about seepage flux. Studies, notably in North America, have used temperature monitoring in the stream and underlying sediments as a screening tool for identifying gaining and losing reaches (Silliman and Booth 1993; Stonestrom and Constanz 2003). Recently, heat as a tracer has been demonstrated to be a robust method for quantifying surface water-groundwater exchanges in a range of environments, from perennial streams in humid regions (Lapham 1989; Silliman and Booth 1993) to ephemeral channels in arid locations (Stonestrom and Constanz 2003). Logging devices that measure temperatures at specific time intervals and store the information in memory can be installed both within the stream and at different depths in the sediments below the stream bed. The sensors most often employed are thermocouples, thermistors, resistance temperature devices and integrated circuit sensors. The characteristics of each type of temperature logging equipment along with the advantages and disadvantages and installation methods are presented in Stonestrom and Constantz (2003).

The hydraulic transport of heat enables its use as a tracer with temperature monitoring especially suited for delineating fine-scale flow paths. The heat tracer method has been used to estimate groundwater velocity and aquifer hydraulic properties, and to identify areas of recharge and discharge (Bouyocous 1915; Suzuki 1960; Lee 1985; Lapham 1989; Silliman and Booth 1993; Conant, 2004). One way of using heat tracing in stream-aquifer studies is to compare the temporal patterns evident in stream and shallow sediment temperature. Stream temperatures have a characteristic diurnal pattern overprinting seasonal trends, being influenced by changes in solar radiation, air and ground temperature, rainfall and stream inflows that include groundwater discharge (Sinokrat and Stefan, 1993). These diurnal variations in temperature in the near-stream environment are often large and rapid, providing a clear thermal signal that is easy to measure. In contrast, the temperature of regional groundwater tends to be relatively constant at the daily scale. The movement of heat between surface water and groundwater systems is both advective (associated with fluid movement) and conductive (through the static solid/liquid phase). Ignoring the effect of insitu sources of thermal energy (such as from biological activity), the temperature pattern in the shallow stream sediment profile can be used to evaluate seepage flux.

Advantages

1. Temperature logging devices are robust, simple, relatively inexpensive and available for various scales of measurement. Once installed, loggers can also provide useful time-series data that can provide information on seasonal changes in seepage flux.

2. The temperature signal arrives naturally and the temperature data are immediately available for inspection and interpretation.

3. Temperature monitoring can be used as a screening tool for identifying gaining and losing stream reaches. Such a screening method can be valuable both as a rapid investigative tool for small studies and as a precursor to more detailed studies such as the design/installation of a groundwater monitoring network.

4. Temperature studies are particularly useful in defining small-scale flow paths, as related to stream banks or sand bars. (Stonestrom and Constanz 2003).

Disadvantages

1. Interpretation of the temperature data can be ambiguous when viewed in isolation. It is recommended that temperature monitoring be used in conjunction with other methods such as mini piezometers, seepage meters or hydrographic analysis when interpreting stream-aquifer connectivity. It can be difficult to separate localised effects (such as those associated with weirs or shallow flow) from the broader seepage domain.

2. Temperature measurement is at a point in space and many measurements may be required to obtain information on spatial variability.

It is suggested that temperature loggers can be readily and cheaply incorporated into existing hydrographic networks to provide a supplementary dataset for understanding stream-aquifer connectivity. This is because the water level data can indicate the potential seepage direction and the temperature data can help estimate the magnitude of the seepage. It is also recommended that the existing temperature logging used to calibrate pressure transducers for monitoring water levels be upgraded to sufficient accuracy for heat transfer studies.

3.6 Thermal stability of water columns

Thermal stability of the water column within the well is another critical point in the application of the main equation used for this research. Groundwater temperature obtained from the wells and used in the solution of equation 1 are valid only if the groundwater temperatures inside of the well represent the temperatures of the fluid-porous medium complex adjacent to the well. This is most likely to occur when groundwater within the well is thermally stable. If heat transfer within the well is accomplished through convection, the resulting temperature fluctuations will provide thermal disturbances large enough to invalidate the groundwater temperatures. Thus, convective transfer of heat in the fluid column must be of negligible magnitude.

Diment (1967), Gretener (1967), and Sammel (1968) had studied problems encountered in obtaining representative groundwater temperatures from wells. Krige (1939) had developed an expression for the critical gradient G_c of a fluid-filled column:

$$G_c = \frac{ga\theta}{c} + \frac{C\mu\alpha}{gar^4} \quad (1)$$

where

g	= acceleration due to gravity (cm/sec^2);
θ	= absolute temperature (°K);
a	= volume coefficient of thermal expansion (1/°C);
α	= thermal diffusivity (cm^2/sec);
μ	= kinematic viscosity of the fluid (cm^2/sec);
r	= radius of the column (cm);
c	= specific heat of groundwater at constant pressure (ergs/gm °C);
C	= a constant, which is equal to 216 cgs units;
G_c	= critical thermal gradient in groundwater (°K/cm)

Sammel (1968) defined the critical gradient G_c as the rate of temperature change with depth at which convective flow is incipient. A case in which convective flow is incipient. A case in which temperature increases with depth, i.e., positive temperature gradient, is thermally unstable when the actual temperature gradient exceeds the critical gradient. In situations where negative gradient exist, G_c cannot be exceeded and thermal stability is maintained. By using Krige's formula, critical thermal gradients were obtained from all monitoring wells used in this research, and compared to their actual thermal gradients. Each thermal gradient is defined as:

$$GT = \frac{(T_{z2} - T_{z1})}{(Z_2 - Z_1)} \tag{2}$$

where

GT= thermal gradient (°C/m);

T_{z2}= groundwater temperature at depth Z_2, deeper than Z_1 (°C)

T_{z1}= groundwater temperature at depth Z_1 (°C);

Z_2= a certain depth within the geological stratum, deeper than Z_1 (meters);

Z_1= a certain depth within the geological stratum (meters);

If the thermal gradient exceeds the critical gradient, then that means the groundwater temperature inside of the well is not representative of the temperature of the water porous medium system next to the well (Arriaga and Leap, 2006)

3.7 Theory of Heat Transport

The general differential equation for simultaneous 3D non-steady heat and fluid flow through isotropic, homogeneous, and fully saturated porous mediums is (Stallman, 1960):

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} - \frac{c_0 \rho_0}{k}\left[\frac{\partial (v_x T)}{\partial x} + \frac{\partial (v_y T)}{\partial y} + \frac{\partial (v_z T)}{\partial z}\right] = \frac{c\rho}{k}\frac{\partial T}{\partial x} \tag{3}$$

where

T = temperature at any point at time t (°C).

c_0 = specific heat of fluid (cal/g °C).

ρ_0 = density of fluid (g/cm^3).

c = specific heat of solid-fluid complex (cal/g °C).

ρ = density of solid-fluid complex (g/cm^3).

k = thermal conductivity of solid-fluid complex (cal/cm sec °C).

v_x, v_y, v_z = components of fluid velocity in the x, y and z direction (cm/sec).

x, y, z = Cartesian coordinates (cm).

t = time since flow started (sec).

In the problem treated below the flow of heat and fluid is one-dimensional (vertical) and steady. Under these conditions the differential equation reduces to

$$\left(\frac{\partial^2 T}{\partial z^2}\right)-\left(\frac{c_0\rho_0 v_z}{k}\right)\left(\frac{\partial T}{\partial z}\right)=0 \tag{4}$$

Bredehoeft and Papadopulos (1965) derived an analytical solution of (4) with the following boundary conditions:

$$T_z=T_0 \quad z=0 \tag{5}$$

$$T_z=T_L \quad z=L \tag{6}$$

where

T_z= temperature at any depth z (°C);

T_0= temperature at z=0 (uppermost temperature measurement) (°C);

T_L= temperature at z=L (lowermost temperature measurement) (°C);

L= vertical distance over which temperatures are being observed (cm).

v_z = vertical groundwater velocity (cm/sec).

In Figure 3.6 gives the conditions under which the model applies. In this diagram, T_0 is an uppermost temperature measurement at z=0, and T_L is a lower-most temperature measurement at z=L.

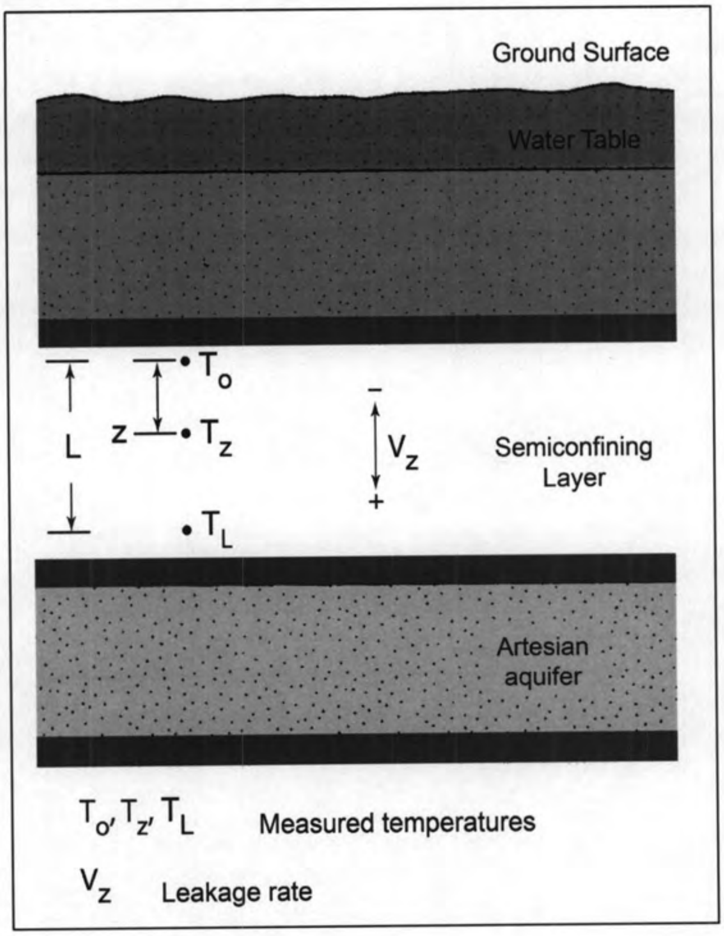

Figure 3.6 Diagrammatic sketch of typical leaky aquifer (modified after Bredehoeft and Papadopulos,1965)

After solving equation (4) and applying boundary conditions (5) and (6), the solution to that differential equation is:

$$\frac{T_z - T_o}{T_L - T_o} = f(\beta, \frac{z}{L}) = \frac{\left(e^{\beta(z/L)} - 1\right)}{(e^{\beta} - 1)} \tag{7}$$

Where

$$\beta = \frac{c_0 \rho_0 v_z L}{k} \tag{8}$$

β is a dimensionless parameter that can be positive or negative depending on whether v_z is downward or upward respectively. Bredehoeft and Papadopulos (1965) provided values of f (β, z/L) for a practical range of parameters and a set of type curves containing arithmetic plots for different values of β.

Ratios $(T_z\text{-}T_o)/\ (T_L\text{-}T_o)$ calculated from measured temperature data are plotted against the depth factor z/L at exactly the same scale as the type curves (Figure 3.7). The values are superimposed on the type curves set keeping the coordinate axes in coincidence. β is obtained from the type curve that best matches the field data curve. β is also related to curvature of a temperature-depth profile at several depths that range from z=0 to z=L. The thickness L is less than or equal to the thickness of the layer through which groundwater is leaking vertically. After obtaining β, it is possible to determine the groundwater velocity, which is calculated from the following relation:

$$v_z = \frac{k\beta}{c_o p_o L} \tag{9}$$

The rest of the parameters in this equation are known and v_z provides the vertical groundwater velocity. It is important to mention that under isotropic and steady-state conditions where groundwater flow does not occur (β=0), the thermal gradient is linear with depth. However, when groundwater movement occurs, the thermal profile curves and the plot of $(e^{\beta\,(z/L)}\text{-}1)/\ (e^{\beta}\text{-}1)$ against z/L is convex upward or downward, depending on the direction of groundwater movement. The thermal profile curvature increases with groundwater velocity because v_z is proportional to β.

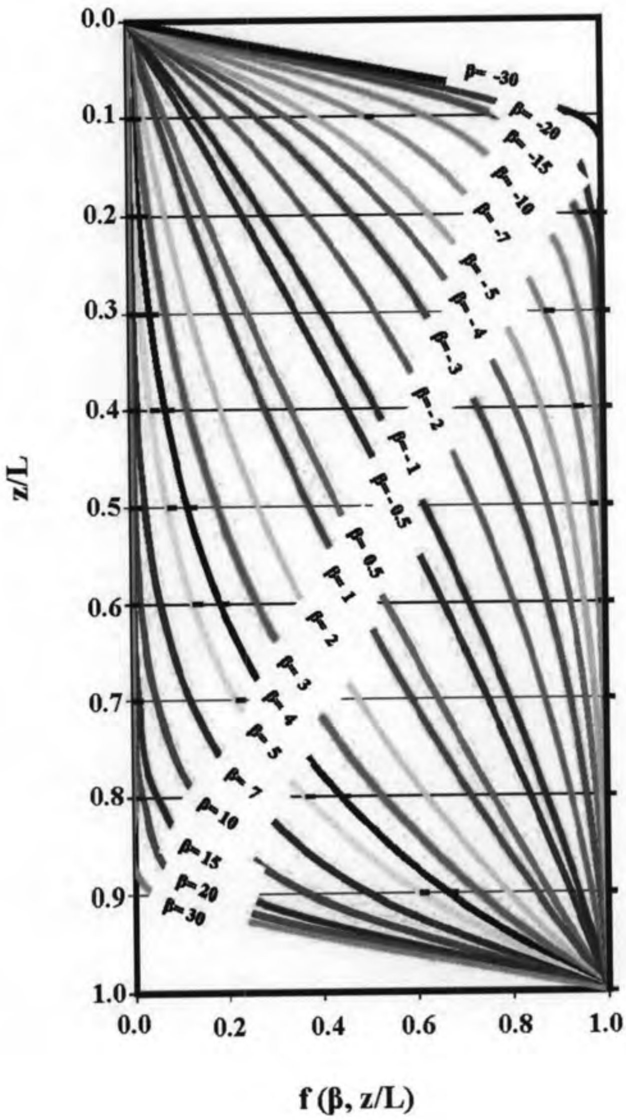

Figure 3.7 Type curves of the function f (β, z/L) (modified after Bredehoeft and Papadopulos, 1965)

The thermal conductivity of soils is a function of the thermal properties of the solid materials, soil texture, pore size distribution, water content, and the temperature of the medium. The typical value for the thermal conductivity of water-saturated clays is $k= 2\times10^{-3}$ calorie/cm sec °C (Birch et al. 1942). The average value for the thermal conductivity of water-saturated sand and gravel outwash aquifers is $k = 2\times10^{-3}$ calorie /cm sec °C and for water-saturated silts is $k =4\times10^{-3}$ calorie /cm sec °C (Wade 1994).

When water passes from one stratum to another with a different hydraulic conductivity, the direction of the flow path will change (Fetter 1994). Flow lines follow high permeability formations as conduits, and traverse low permeability formations by the shortest route. In aquifer-aquitard systems with permeability contrasts of two orders of magnitude or more, flowlines tend to become almost horizontal in the aquifers and almost vertical in the aquitards (Freeze and Cherry 1979). Boyle and Saleem (1979) presented two different scenarios related to this case. Scenario I represented conditions of positive temperature gradients while scenario II represented conditions of negative temperature gradients (Figure 3.8). The variations in slopes of linear segments in a given profile correspond to changes in the thermal properties associated with various lithologies found in the system. Both scenarios contain three different possibilities for groundwater flow within the aquitard: (a) upward, (b) downward, and (c) no vertical flow. The linear segments (c) with in the aquitard indicate transfer of heat by conduction only (no heat transfer is accomplished by migrating groundwater). On the other hand, the curvilinear segments (a) and (b) indicate vertical transfer of heat by upward and downward flowing groundwater, respectively.

Boyle and Saleem (1979) used a computer procedure to get values of β from the temperature-depth data observed at one–meter spacing over a specified depth interval L. The temperature values were used to compute $(T_z-T_o)/(T_L-T_o)$ as z changes from zero to L. These ratios were compared to the theoretical values of f (β, z/L) computed from the right-hand side of Eq. (7) for $0 \leq z \leq L$ and for specified values of T_o, T_L, L, and β.

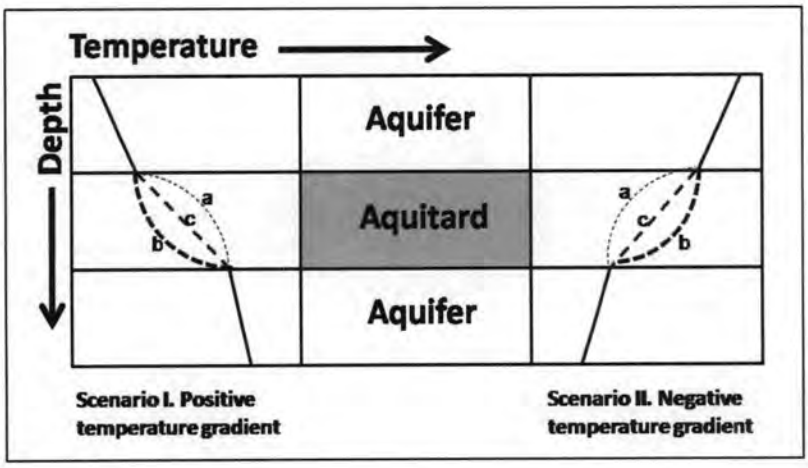

Figure 3.8 Idealized temperature depth profiles that indicate the direction of vertical leakage through an aquitard; upward, downward, and no flow (modified after Boyle and Saleem, 1979)

The program determined the optimum value of β by assigning an initial value to β and then adjusting it until the objective function f (β) was minimized (Saleem 1970),

Where

$$f(\beta) = \sum_{z=0}^{z=L} \left(\frac{T_z - T_o}{T_L - T_o} - \frac{e^{\beta(z/L)} - 1}{e^{\beta} - 1} \right)^2 \qquad (10)$$

The optimum value of β was the one that yielded the minimum value of f (β), for each value of L. It is important to remember that the system resolution is 0.01°C for each temperature difference ratio, the accuracy of the ratios and the resulting value of β is determined by the resolution.

Arriaga (2006) used Microsoft Excel Solver to solve the equation, It is an optimization modeling system that combines the functions of a graphical user interface (GUI), an algebraic modeling language, and optimizers for linear, nonlinear, and integer programs. Each function is integrated into the host spread sheet program. Optimization begins with an ordinary spread sheet model. The spread sheets formula language functions as the algebraic language used to define the model. Through the Solvers GUI, the user specifies an objective and constraints. Solver then analyzes the complete optimization model and produces the matrix form required by the optimizers (Lasdon et al., 1998). Microsoft Excel Solver employs the Generalized Reduced Gradient (GRG2) Algorithm for optimizing non-linear problems and uses the solution values to update the model spread sheet. Solver uses iterative numerical methods that involve plugging in trial values for adjust able cells and observing the results calculated by the constraint cells and the optimum cell. Each trial is called iteration. Because a pure trial and error approach would take such a long time (specially for problems involving many adjustable cells and constraints), Microsoft Excel Solver performs extensive analyses of the observed out puts and their rates of changes as the inputs are varied, to guide these lection of new trial values. In a typical problem, the constraints and the optimum cell are functions of (that is, they depend on) the adjustable cells. The first derivative of a function measures its rate of change as the input is varied. When there are several values entered, the function has several partial derivatives measuring its rate of change with respect to each of the input values; together, the partial derivatives form a vector called the gradient of the function. Derivatives and gradients play a crucial role in iterative methods in Microsoft Excel Solver. They provide clues as to how the adjust able cells should be varied. The main equation used to determine the groundwater velocity is the following:

$$\frac{T_z - T_0}{T_L - T_0} - \frac{e^{\beta(z/L)} - 1}{e^{\beta} - 1} = 0 \qquad (11)$$

In order to use Microsoft Excel Solver, the Solver add in must be downloaded into the system. Typically, this feature is not installed by default when Excel is first set upon the hard disk. To add this facility to the Tools menu, it is necessary to select the menu option Tools Add Ins and then choose the Solver Add-In check box. Add-ins are Excel work sheets that have been saved as Microsoft Excel Add Ins (.xla). Solver provides a less complex method for finding the values needed to obtain the desired results because it has the ability to change the value in multiple cells. Once Solver is used, the Solver Parameters dialog is displayed as shown in Figure 3.9

$$\frac{T_z - T_0}{T_L - T_0} - \frac{e^{\beta(z/L)} - 1}{e^{\beta} - 1} = 0$$

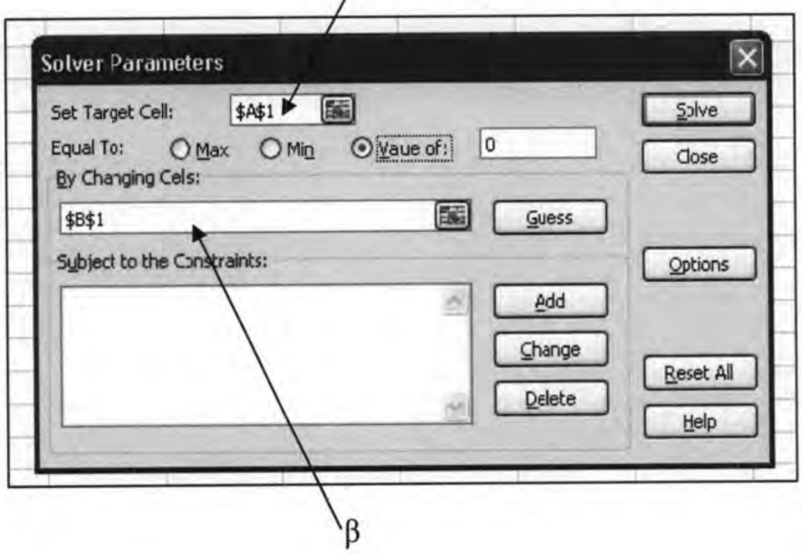

Figure 3.9 The Solver Parameters dialog box

In the Solver Dialog Box, there are several functions: set target cell, by changing cells, subject to constraints, options, and solve. Set target cell specifies the solving target value. This cell must contain a formula and it can be selected by either typing the cell reference in the field or selecting the Collapse Dialog button and clicking on the cell. The target cell used is the left hand side of Equation 11. Once the target cell is specified, the value of the cell is indicated by either setting it to the maximum possible size (Max), minimum size (Min), or a specific value.

According to Equation 10, the target cell is minimized to zero. By changing cells indicates the cells whose values Solver needs to modify in order to obtain the specified results for the target cell. It is possible to specify a maximum of 200 cells. Solver can also automatically select the cells based upon the cells referenced in the target cell formula by selecting the Guess button. The cell that is being constantly modified until the target cell is minimized to zero is the cell that contains the β value. Subject to constraints creates any limitations applied to the changing cells or the target cell. No constraints were specified for any of the cells. Options refine the process by which Solver performs a series of internal calculations to derive values for cells that produce the desired result. Solver attempts to find the results that most closely match the target value and places the results directly in the appropriate cells in the work sheet.