

THERMAL BASIN MODELING AND ANALYSIS
USING THE TIME-TEMPERATURE INDEX

An Improved General Basin Model Incorporating
Compaction, Fluid Flow and Heat Flow

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I. Introduction.

Thermal basin modeling has been a widely- used technique for estimating the maturity of sedimentary basins. Many of the existing thermal basin models compute the time-temperature index (TTI) as a numerical estimate of the maturity of the source beds. The majority of these models are very simple and involve the solution of the heat flow equation with varying thermal gradient and thermal conductivity of the sediments (refs. 1 ,2 ,3).

In the following four sections we present the details of a much more general model. This model involves solution of heat flow, compaction and water flow equations and allows the density, thermal conductivity, compressibility, specific heat, and permeability of sediments to vary with temperature and pressure. Different options are also allowed for modeling the flux changes throughout time. Pertinent equations are presented in section II along with a brief description of the model and the algorithm for the simulation. Section III consists of information regarding choice of model and physical parameters, analysis of results for four different basins, and conclusions. The fourth and final section is a complete description of the use of the computer program. Our purpose is to examine the effect of various phenomena and changes in properties on the iso TTI contours and on the TTI of a given sediment point in a geologic formation. The principal phenomena of interest are:

- 1.) sedimentation rate changes.
- 2.) changes in heat flux and/or thermal conductivity (with discussion of effects of heat flux, thermal conductivity, and specific heat changes on thermal gradient)

To illustrate the effects of sedimentation rate changes and changes in the thermal properties, a Gulf Coast model will be presented at various degrees of complexity. Using the information gained from this analysis, a more detailed Salina basin model will then be analyzed. The Salina basin model will be then used to further study the effects of compaction and water flow. Finally, to demonstrate the affects of realistic changes in heat flux (with time), the results of an Ardmore basin model will be presented.

II. Theoretical Background

The differential equations for compaction, water flow, and heat transfer are presented on the following three pages. In table I a brief explanation of the notation is given (ref. 1). These equations are nonlinear and are thus solved iteratively using the finite difference method. The equations are solved at each time step. Nodes are added (deposition) or subtracted (erosion) as needed. The water flow equation is first solved yielding nodal values for the pressure and water velocity. The heat flow equation is then solved yielding the temperature distribution. The compaction equation is then solved yielding grain velocities. After convergence is checked on pressure, temperature and grain velocity and convergence has been reached, the current value of the TTI for each node in each layer is computed. The TTI is given by eq (10).

The algorithm for the implementation of the model is shown in the form of a flow chart in fig 1.

NOTATION

V_D	- Darcy velocity
σ_T	- Total stress
α	- Compressibility of rock matrix
β	- Compressibility of water
n	- Porosity
p	- Fluid pressure
k	- Permeability
μ	- Water viscosity
ρ_w	- Density of water
ρ_r	- Density of rock matrix
g	- Acceleration of gravity
\hat{z}	- Unit vector in z direction
$\frac{dl}{dt}$	- Sedimentation rate
V_s	- Grain velocity
T	- Temperature
K_r	- Thermal Conductivity of rock matrix
K_w	- Thermal Conductivity of water
c_{pr}	- Specific heat capacity of rock matrix
c_{pw}	- Specific heat capacity of water

Table I. Notation for eqs.. (1) - (9) only

WATER FLOW EQUATION

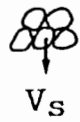
$$(1) \quad \vec{\nabla} \cdot \vec{V}_D = \alpha \frac{d\sigma_T}{dt} - (\alpha + n\beta) \frac{dp}{dt}$$

$$(2) \quad \vec{V}_D = -\frac{k}{\mu} \left[\vec{\nabla} p + \rho_w g \hat{z} \right]$$

$$(3) \quad \frac{d\sigma_T}{dt} = g \left[n \rho_w + (1 - n) \rho_r \right] \frac{dl}{dt}$$

GRAIN VELOCITY OR COMPACTION EQUATION

$$(4) \quad \dot{\bar{V}} \cdot \dot{V}_s = -\alpha \left[\frac{d\sigma_T}{dt} - \frac{dp}{dt} \right]$$



HEAT FLOW EQUATION

$$(5) \quad \vec{\nabla} \cdot [K_{wr} \vec{\nabla} T] - \rho_w c_{pw} \vec{\nabla} \cdot [\vec{V}_w T] = c_{pwr} \rho_{wr} \frac{\partial T}{\partial t}$$

$$(6) \quad \rho_{wr} = n \rho_w + (1-n) \rho_r$$

$$(7) \quad K_{wr} = K_r \left(\frac{K_w}{K_r} \right)^n$$

$$(8) \quad c_{pwr} = (1-n) c_{pr} + n c_{pw}$$

$$(9) \quad \vec{V}_w = V_D / n$$

(10)

$$TTI = \int_{t_o}^t r_B^{2 \left(\frac{T(t) - T_B}{10^\circ C} \right)} dt$$

LOPATIN'S TIME TEMPERATURE INDEX (TTI)

TTI is a measure of the thermal maturity of an oil source rock. It depends on the time the source rock spent at a given temperature. This assumes the maturity reaction rate doubles every $10^\circ C$. T_B is a base temperature and r_B is the reaction rate at that temperature. Lopatin chose $T_B = 105^\circ C$ and $r_B = 1$. t_o is the deposition time of the source rock and t is the time at which the thermal maturity is being calculated.

Waples suggests that oil is generated in an "oil window" between $TTI = 15$ and $TTI = 160$.

COMPUTER PROGRAM FLOW CHART

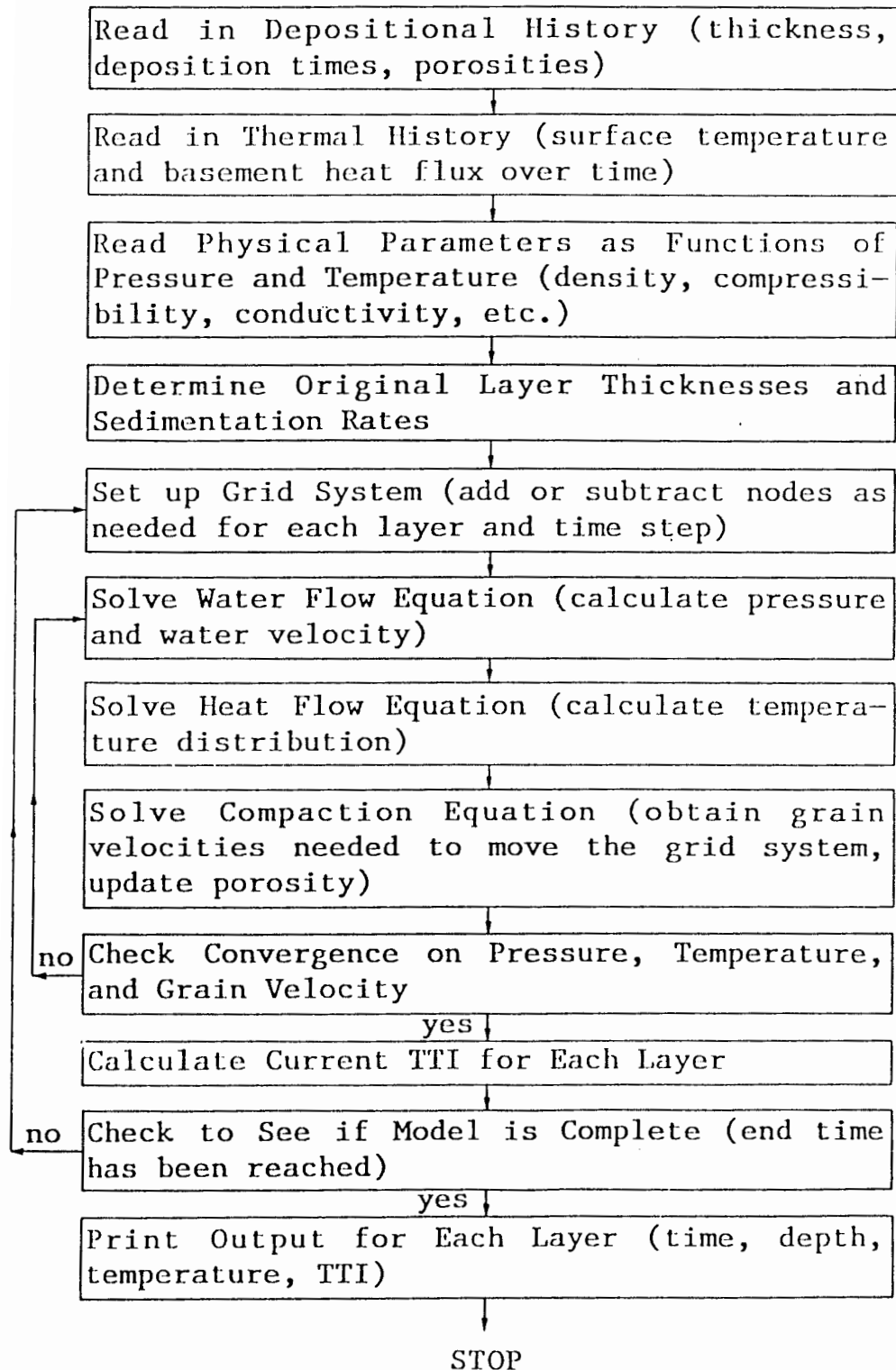


Fig. 1. Algorithm for implementation of model.

III. Application of Model

1) Parameterization

The physical parameters for the rock matrix and water which are allowed to vary with temperature and pressure are listed below along with references to their sources.

PARAMETER	ROCK MATRIX	WATER
thermal conductivity	(4,5,6)	(8)
specific heat	(4,5)	(8)
density	(4,5)	(7)
permeability	(9, 10)	---
compressibility	(9)	(12)

These parameters are included in the model in the form of table whose independent variables are temperature and pressure. The water parameters are obtained by two dimensional linear interpolation between successive table values. Note that the water compressibility may be computed from the water density values (since enough density values were available) by the following relationship:

$$(11) \quad \beta = (\rho_w(p_2) - \rho_w(p_1)) / \rho_w(p_{12}) / (p_2 - p_1)$$

where:

$$\begin{aligned} \beta &= \text{water compressibility} \\ (p_2) &= \text{water density value at } p_2 \\ p_1, p_2 &= \text{different pressure values} \\ p_{12} &= (p_1 + p_2) / 2 \end{aligned}$$

(all at a given temperature T)

Typical initial and final porosities are found in (ref. 13) for shales, (ref. 14) for carbonate rocks and (refs. 10, 11, 13) for sandstone. Initial estimates for initial and final porosities and compressibility functions were made and the model was run repeatedly with new estimates of these parameters until reasonable agreement (within 8%) between final values of the formation thicknesses and porosities and their actual present day values was achieved. Four different methods for the computation of the basement flux were implemented:

1. step changes in the flux with time read from a data file (the flux may be held constant with time if only one flux is input, see section IV)
2. constant flux computed from input geothermal gradient (may input geothermal gradient directly or input depth and bottom hole temperature).
3. flux computed from the isostatic subsidence model of basin formation (ref. 16).
4. 1, 2 or 3 along with a possible magmatic intrusion at the onset of deposition.

Values for the basement heat flux are difficult to find. More commonly they are computed from the average present-day thermal gradient using the relationship below:

$$(12) \quad Q = \bar{k}(T_b - T_0)/L$$

where:

Q = heat flux

\bar{k} = average thermal conductivity

T_b = bottom hole temperature

T_0 = surface temperature

L = bottom hole depth

The average thermal conductivity is computed from the relationship (13):

$$(13) \quad 1/\bar{k} = \left(\sum_i (l_{mid_i} / k_{mid_i}) \right) / L$$

where: $k_{mid_i} = (k(T_{2_i}) - k(T_{1_i})) / 2$

T_{2_i} = temperature at formation bottom
 T_{1_i} = temperature at formation top
 l_{mid_i} = thickness of formation i

Option 2 may be chosen to compute a constant flux from eq 1². Since this equation is an approximation, the model may be rerun with a slightly different flux if the resulting average thermal gradient in the previous run was not satisfactory.

2.) Analysis and Interpretation of Results

A.) Effects of Basin Properties on the TTI of a Sediment Point

Equation (10) may be approximated as a sum:

$$(14) \quad TTI(n,t) = \sum_{m=j+1}^i G(T_{nm}) * \text{delt}t_m$$

where :

$TTI(n,t)$ = is the TTI of a certain sediment point at time t

t = t_i , the current or i th time step since the onset of deposition. Time is descretized in the model

m = the m th point in time

i = the current time point

j = the start time step of deposition of sediment point n

n = a particular sediment point. The sediments in the model are descretized. The first sediment point is deposited at t_0 , the deposition onset. The last one is deposited at the (nodal, see sec. IV) time step before the end time of the last deposition.

$\text{delt}t_m$ = $t_m - t_{m-1}$, the time step size

T_{nm} = temperature at sediment point n at the m th point in time

$G(T_{nm}) = \frac{((T - T_r)/10)}{2}$

$T = \frac{(T_{nm} + T_{nm-1})}{2}$

$T_r = 105 \text{ degrees Celsius}$

For simplicity the sediment point subscript n will be dropped with the understanding that the TTI is computed for a given sediment point which belongs to a certain formation which was deposited starting at time t_j .

The focus of this analysis will be how a set of physical properties of sedimentary basins affects the TTI and thus the relative maturity of sediments in the basin.

These properties may be roughly divided into two groups:

I.) Those which directly affect the depth history of the sediments:

- 1) sedimentation rate
- 2) compressibility

II.) Those which directly affect the thermal history of sediments.

- 1) thermal conductivity
- 2) basement heat flux
- 3) specific heat
- 4) density
- 5) porosity

One must make this division with a bit of caution since there are interrelationships between many of these properties (for instance, compressibility and sedimentation rate affect the depth and thus the temperature of a sediment point. Thermal conductivity, specific heat, and density are temperature dependent. One may note that the properties of the second group have a more direct effect on the average thermal gradient and those of the first group have a direct effect on how rapidly the column forms (how rapidly the temperature changes due to a change in depth.)

In the analysis, when the effects of one property on the time-temperature index were under investigation, the remaining properties (except where indicated) were held fixed.

We are interested in investigating the effects of these properties on two relationships:

- 1) the TTI of a single sediment point vs. time
- 2) the TTI of the entire column as a function of depth and time.

The first relationship will be presented as a two-dimensional curve. It gives a direct analysis of what affects the maturity of a single sediment point throughout time. Rising slopes of this curve indicate an increase in the rate of maturity.

The second relationship is three-dimensional and is therefore depicted as a set of iso-TTI contours on a depth vs. time plot of selected formation barrier sediment points vs. time. In this case we are not necessarily interested in the maturity of a single sediment point as a function of time. We are more interested in the maturity of sediment points at certain depths as a function of time. From this information an "oil window" (refs. 1, 2 and 3) can be determined. Rising slopes of iso-TTI contours may indicate factors favoring maturity or factors causing more mature sediments to be less deep.

a. Sedimentation rate

Case 1: hiatus

It is clear from eqs (4) that if the sedimentation rate is zero (and all other properties remain constant) the depth of a sediment point and thus its temperature remain very nearly constant.

Thus in a period of hiatus when none of the aforementioned properties change, the TTI is very nearly a linear function of time. The slope of this (nearly) linear increase is determined by the G factor. The deeper the sediment point the larger is G and thus the steeper is the slope.

For a period of hiatus the TTI is given by the approximate linear relationship:

$$(15) \quad TTI(t) = TTI_j + G(t-t_j)$$

where:

t = time since onset of deposition

G = temperature dependent factor of TTI
at start of hiatus

t_j = start time of period of hiatus

TTI_j = TTI at the start time of the period
of hiatus

Case 2. Deposition:

During a period of deposition the grains move downward with time and thus the temperature of a sediment point rises (as it lowers in depth with time). The temperature- dependent factor $G(T_i)$ thus increases with each time step.

From eq. (14) it is clear that G increases exponentially with temperature (see definitions following this equation). Since the time step is constant during this period the TTI increase during a period of deposition is a sum of exponentially increasing terms.

If deposition is very rapid each term in the TTI sum at a new time step will be much larger than the sum of the previous terms. In this limiting case the TTI at each value of time is approximately equal to the most recent term:

$$(16) \quad TTI \quad \overset{\sim}{=} \quad G(T)\delta t$$

Where δt is the same throughout a geologic event and is therefore not subscripted.

Since temperature increases with time (at a somewhat less than linear rate due to compaction) one expects a similarly exponential shape of the TTI vs. time curve during a rapid deposition.

From what was previously discussed concerning hiatus and from the above discussion one expects the TTI increase for a period of deposition to be exponential with time. The rate of this exponential increase should depend on the sedimentation rate. For very slow sedimentation rates it should approximate a linear increase. For very large sedimentation rates the TTI should be given approximately by that of the temperature- dependent reaction rate factor G times δt . If one assumes a very small δt and approximates the depth vs. time relationship of a sediment point as linear (for simplicity) an approximate analytical relationship for TTI can easily be derived:

let g = thermal gradient (fixed)
 s = sedimentation rate (fixed for now)
 T_j = temperature of sediment point
at start of period of deposition
 T_r = reference temperature (105 deg. C)
 t_j = start time of this period of deposition if
sediment point was present at this time,
start time of deposition of this particular
sediment point if it was deposited during
this period of deposition.
 TTI_j = TTI at start of period of deposition (zero if
sediment point was deposited during this
period).

If we allow all δt_m to approach zero in eq. (14) we have:

$$(17) \quad TTI(T(t), t) = \int_{t_j}^t G(T(t)) dt + TTI_j$$

Notice that the temperature of a sediment point is (in general) a function of time (thermal parameters held fixed) since temperature is a function of depth and depth is a function of time. If we assume (for simplicity, not accuracy) little or no compaction then the relationship between temperature of a sediment point and time is a linear one (during a period of constant sedimentation rate with all thermal parameters remaining constant):

$$(18) \quad T(t) = \frac{dT(t)}{dt} * (t - t_j) + T_j$$

We have from the chain rule:

$$(19) \quad \frac{dT(t)}{dt} = \frac{(dT(t))}{(dL)} * \frac{(d(L))}{(dt)}$$

where:

L = depth of sediment point

$\frac{dT(t)}{dL} = g$ = thermal gradient

$\frac{dL}{dt} = s$ = sedimentation rate = s

Using the above approximate relationship in eq. (17) yields:

$$(20) \quad TTI(T(t), t) = (2((T_j - T_r - g s t_j)/10)) * 2^{\frac{g s t}{10}} + TTI_j$$

t_j

$$(21) \quad TTI(t) = A(2^{ct} - 2^{ct_j}) + C$$

where:

$$A = \{10/(gs \ln(2))\} * \{2^{**}((T_j - T_r - g s t_j)/10)\}$$

$$c = gs/10$$

$$C = TTI_j$$

$$2^{ct_j} = \text{constant}$$

It is clear from eq. (21) that one can expect an exponentially increasing TTI as time increases and that the rate of this exponential increase increases with increasing thermal gradient and sedimentation rate. It must be emphasized that eq. (21) gives only a rough estimate of the actual TTI since compaction effects will cause the depth vs time relationship to be nonlinear and the thermal gradient to vary smoothly with time (see later sections) even if basement flux and sediment type are held fixed.

In Figs. 2 and 3 we present the simple case in which sediment of a single type is deposited at a fixed rate. All thermal properties for this single formation were held fixed (specific heat for the sediment and water was set to zero to eliminate changes in the thermal gradient due to absorption of heat by the water and rocks. (Thermal conductivity was held fixed at the value for the rock matrix but compaction was allowed.)).

Fig. 2 shows the TTI of the bottom sediment point as a function of time. Since the sedimentation rate for this example was rather rapid (108 M/M.Y.) the present day TTI for the bottom was rather large (over 30000). The functional dependence is clearly exponential and (in this case) very rapidly increasing.

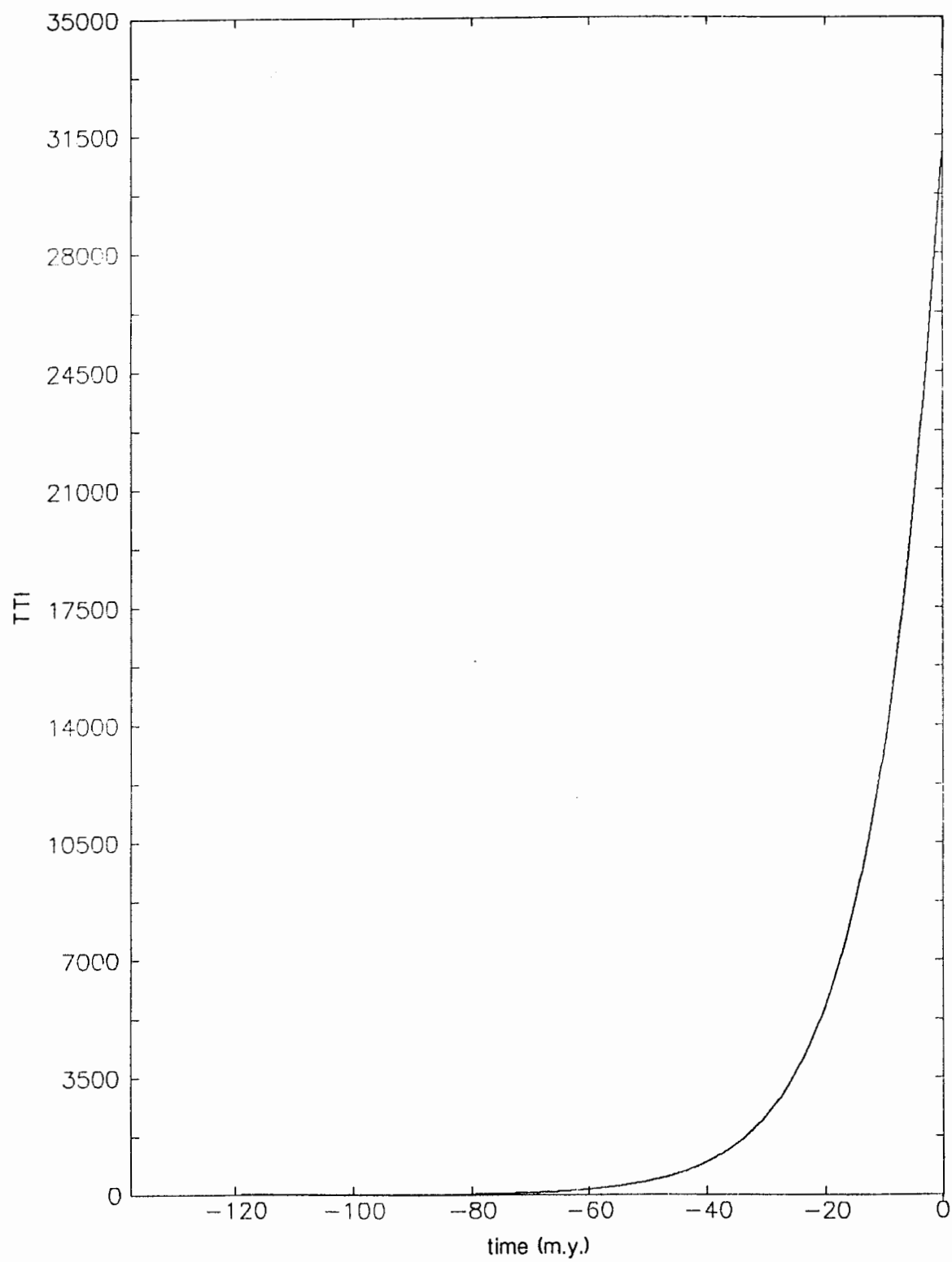


Fig. 2. TTI vs. time for bottom sediment point, single sedimentation rate.

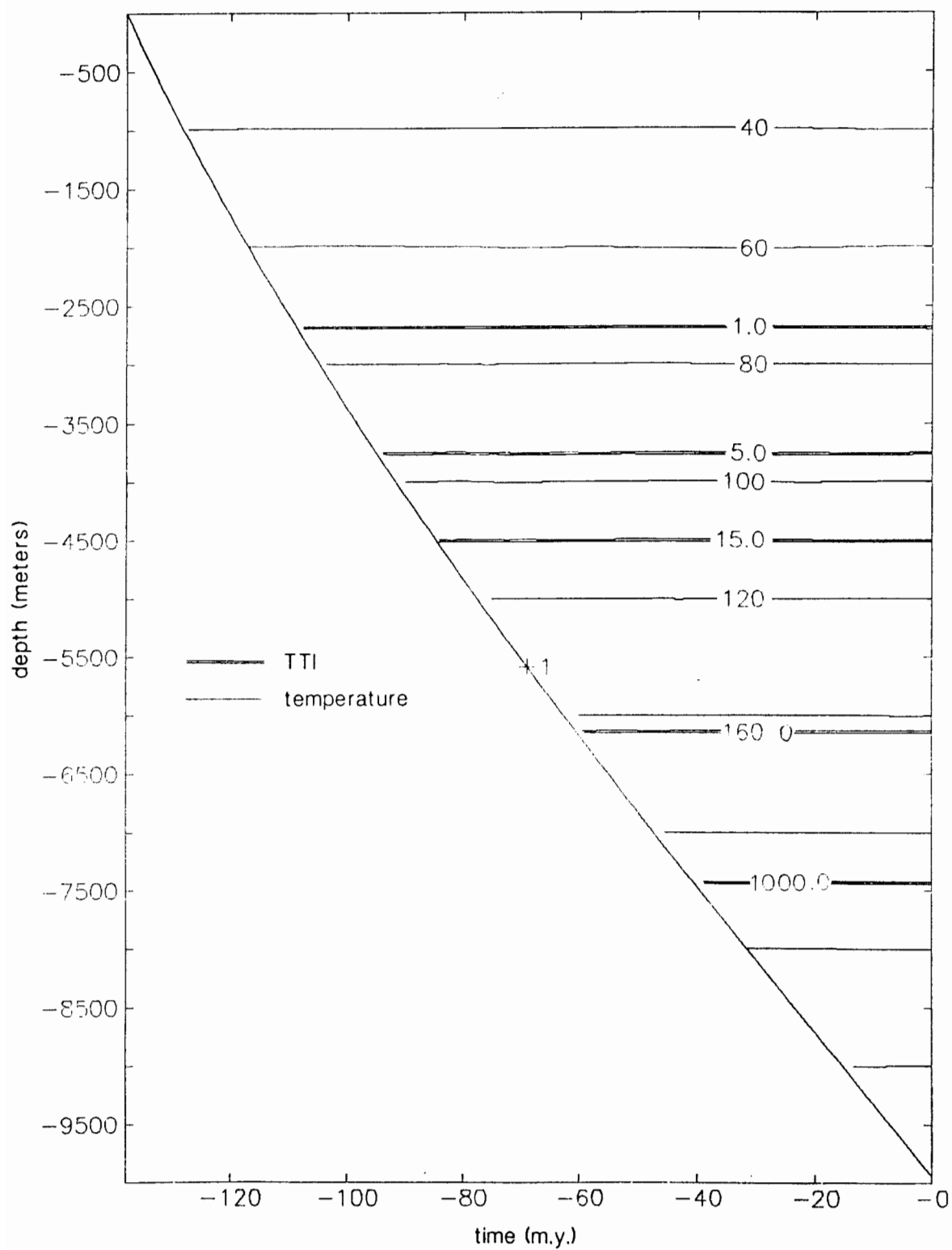


Fig. 3. Depth of basin bottom vs. time, temperature and TTI contours for single sedimentation rate.

Fig. 3 shows the depth versus time plot of the formation bottom upon which is superimposed the TTI (heavy line) and temperature (non-heavy line) contours. The thermal gradient is, of course, constant since all thermal parameters were held fixed. The shape of the TTI contours is worthy of some comment. As one moves across the graph at a fixed depth, since the sedimentation rate is fixed, all sediments took the same amount of time to reach that depth. Thus the age of a sediment point remains constant. Since the thermal gradient is fixed, the temperature at a given depth is also constant throughout time. Since both age and temperature of a sediment point remain constant at constant depth throughout time, from eq. (14) the TTI is constant at constant depth throughout time for this simple case of fixed sedimentation rate and fixed thermal parameters.

Changes in sedimentation rate:

We now consider the case in which formations are deposited at different sedimentation rates (all thermal parameters held fixed). To simplify the discussion, we will consider the deposition of two formations -- each deposited at a different sedimentation rates. We are interested in sediment points which were deposited during or before the first period of deposition under consideration (period j). eq. (21) applies to those sediment points deposited during period k. The results can be generalized for any number of deposition events with different sedimentation rates. From eq. (14) the TTI sum may be rewritten as follows:

$$(22) \quad TTI(T,t) = \sum_{m=j+1}^i G_j(T_m) \Delta t_j + TTI_j \quad \text{if } t_j < t \leq t_k$$

where:

i = current time-step

$T = (T_m + T_{m-1}) / 2$

t_k = start time of second deposition

$$TTI(T, t) = \sum_{m=j+1}^k G_j(T_m) \text{delt}_j + \sum_{m=k+1}^i G_k(T_m) \text{delt}_k + TTI_j \text{ if } t > t_k$$

where: $k + 1$ = first time-step of second deposition

k = time-step at the end of first deposition
(time step after which the second deposition starts)

Where there are, in general, a maximum of N different summations if there are N different sedimentation rates. The appearance of eq. (22) suggests that the shape of the TTI vs. time curve would be a generally exponential relationship whose rate of increase depends on the current sedimentation rate. If we once again allow all delt 's to approach zero and assume a linear depth vs. time relationship, the approximate analytical relationship suggests the same:

$$(23) \quad TTI(T, t) = A_j (2^{gs_j t} - 2^{gs_j t_j}) + C \quad \text{if } t_j < t \leq t_k$$

$$= A_j (2^{gs_j t_k} - 2^{gs_j t_j}) + A_k (2^{gs_k t} - 2^{gs_k t_k}) + C$$

if $t \geq t_k$

where:

s_j = sedimentation rate of first deposition
 s_k = sedimentation rate of second deposition

t_j = start time for first period of
deposition or start time of deposition
of sediment point

 A_j = $\{10/(g s_j \ln(2))\} * \{2^{((T_j - T_r - g s_j t_j)/10)}\}$
 A_k = $\{10/(g s_k \ln(2))\} * \{2^{((T_k - T_r - g s_k t_k)/10)}\}$
 C = TTI_j = start TTI for sediment point

 g = thermal gradient

This analytical relationship also suggests a dependence of rate of exponential increase on the thermal gradient. As will be demonstrated in the next section, The rate of exponential increase of TTI is very sensitive to thermal gradient.

Figure 4 shows the TTI vs. time curve for the bottom sediment points of the first two of a total of three formations of a Gulf Coast (1) model in which all thermal parameters were held fixed. The first formation was deposited at a sedimentation rate of 46 M./M.Y.. The second was deposited at a sedimentation rate of 180 M./M.Y.. The shapes of the curves for the two formation bottom points are similar to what is suggested by the approximate analytical relationship (23). Comparison of the two curves indicates that while the TTI for the second formation bottom point increases exponentially with time with a very rapid rate of increase (large sedimentation rate), The TTI for the first formation bottom point exhibits a slower exponential increase with time before 59 M.Y.B.P ($t_k = 79$ M. Y.) but this rate increases to that of the second formation bottom point after t_k . All of these observations are consistent with the general shape suggested by eq. (23) and suggest that during a period of deposition, if all thermal parameters are held fixed, the TTI of any point in the sedimentary column increases exponentially at a relative rate determined by the relative sedimentation rate.

Changes in sedimentation rate will, of course, affect the shape of the iso-TTI contours also. Figure 5 shows the depth of the bottom point of the bottom formation vs time upon which is superimposed TTI and temperature contours for the model of figure 4 (Note that there is an additional deposition episode in the model (start time 1 m. y . b. p.) which is absent from figure 4). As mentioned previously, if sedimentation rate never changes (all thermal parameters remaining constant), sediment points at the same depth have the same age and temperature and thus the same TTI. If the sedimentation rate suddenly increases, however, the sediments at a given depth reached that depth at a shorter time. Thus if one advances along the graph an amount of time Δt while remaining at fixed depth, the sediments get newer and the iso-TTI contour must descend. As the iso-TTI contour descends the temperature factor rises so that the drop is less than that expected from a mere increase in the grain velocity. If no other changes in sedimentation rate are experienced in the time period in which the contour descends, the sediment points at the same depth will once again have the same age and temperature as soon as sediments in the formation that is currently being deposited are reached. Similarly a sudden drop in the sedimentation rate should cause the TTI contour to rise until sediments deposited at the new (current) sedimentation rate are reached. If, however, numerous changes in the sedimentation rate are experienced as we advance in time at constant depth long before we reach the sediment currently being deposited, the situation is a bit different. An increase in sedimentation rate decreases the **slope** of the TTI contour but does not necessarily cause it to descend. A sudden decrease in the sedimentation rate increases the slope of the TTI contour but does not necessarily cause it to ascend. (See fig. 21 later). It must be strongly emphasized that a

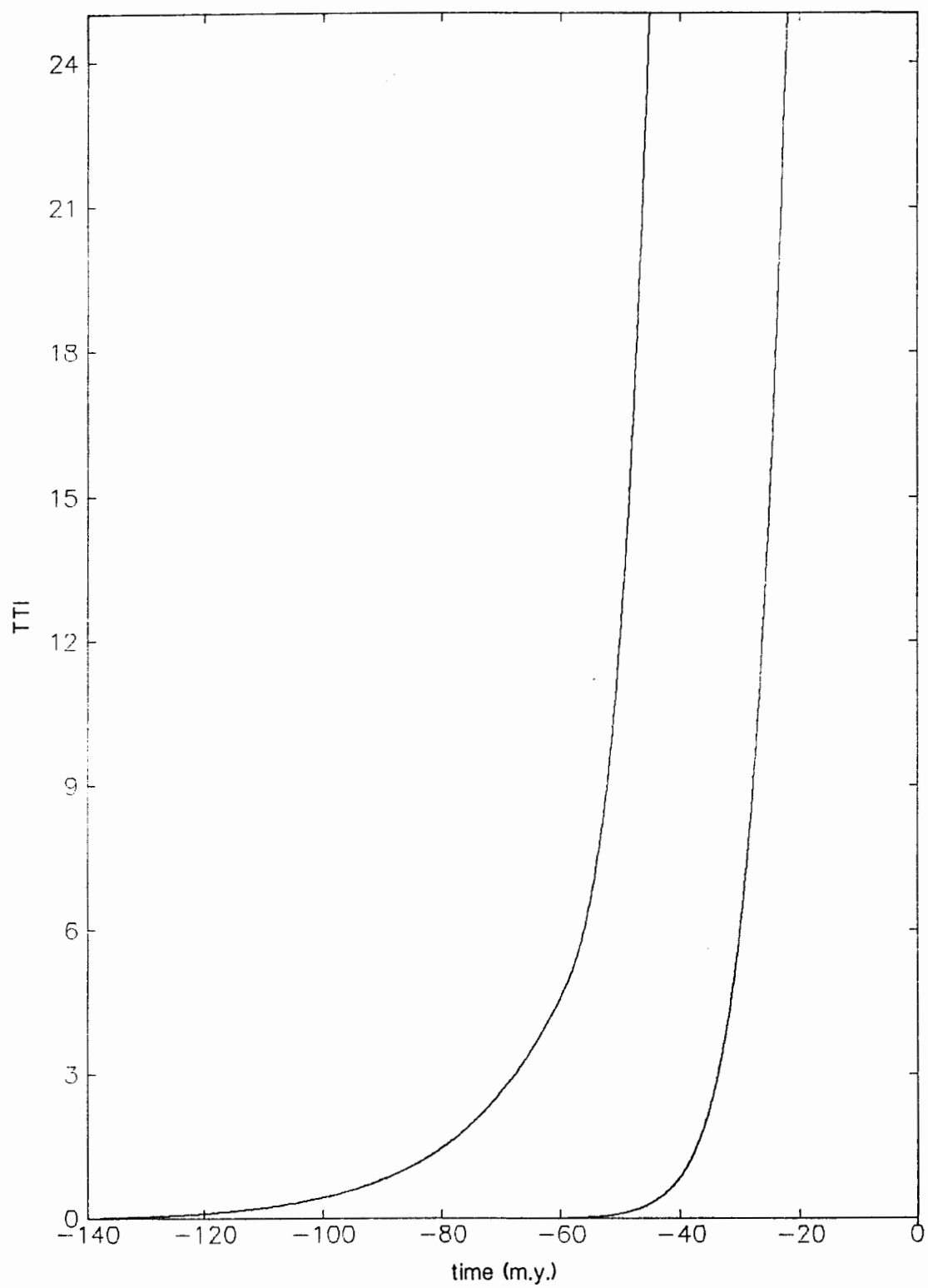


Fig. 4. TTI vs. time for three sedimentation rates (last formation not shown).

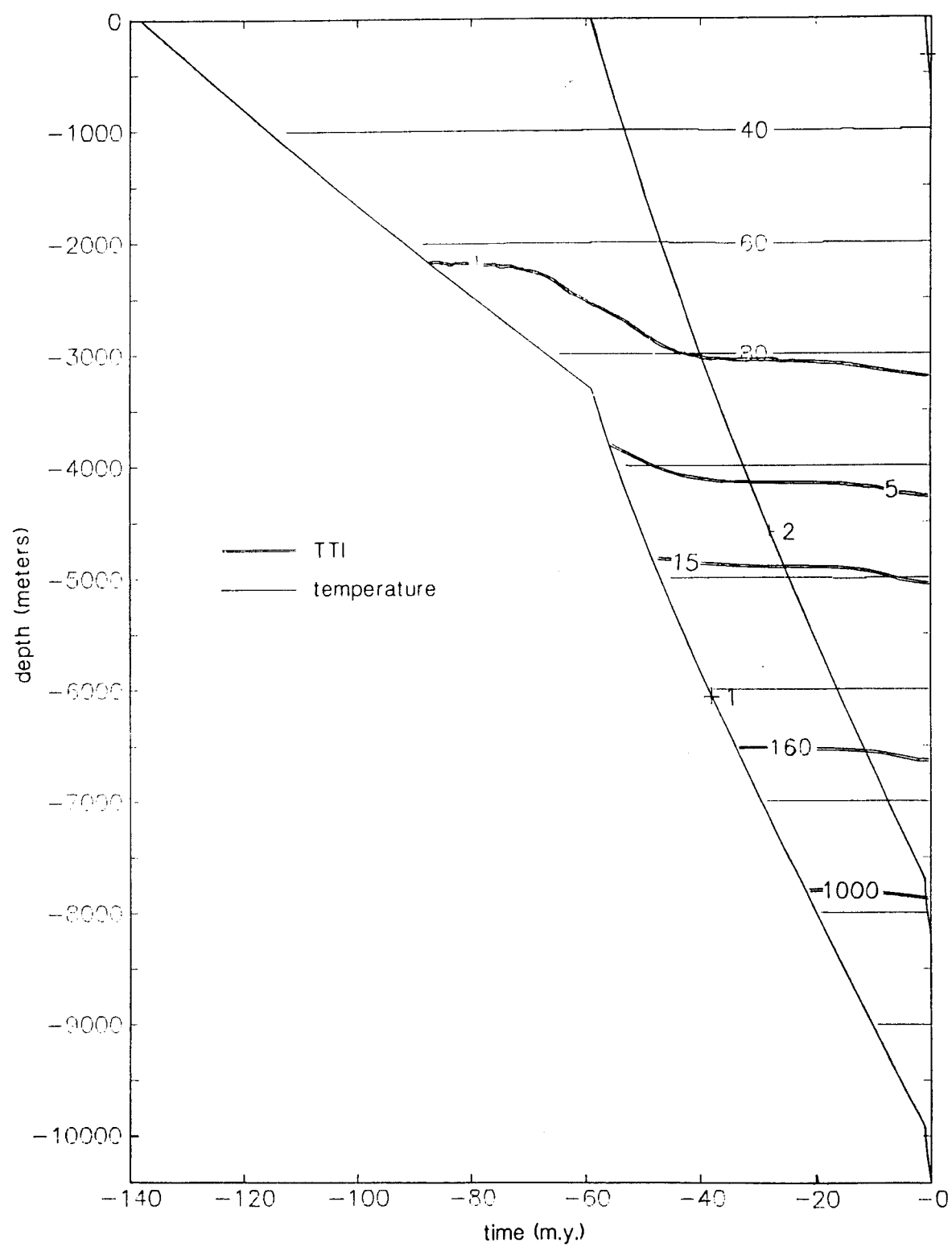


Fig. 5. Depth vs. time, TTI and temperature contours, three sedimentation rates.

sudden descension of a TTI contour never indicates that the TTI of a sediment point is decreasing! The TTI of a particular sediment point never decreases since it is an empirical measure of the extent of an overall reaction that is irreversible. When one traverses the graph of figure 5 at constant depth, one is moving to different (and newer) sediment points which may have newer age (at this new time) and/or lower temperature causing descension of the TTI contour.

Erosion

Since temperature increases with depth and depth decreases with time during a period of erosion, it is clear from eq. (14) and the temperature factor G that smaller and smaller terms are added to the TTI sum during a period of erosion. Thus the functional increase of TTI with time is less than linear with continually decreasing slope. The approximate analytical relationship (21) (with negative sedimentation rates) suggests the same. The function is of the form:

$$TTI(t) = A(2^{-ct_j} - 2^{-ct}) + C, \quad t \geq t_j$$

where $A = - (10/(gs \ln(2)) * (2^{T_j - T_r - gs t_j} / 10))$, a positive, constant factor

$c = -gs/10$ a positive, constant factor

$2^{-ct_j} =$ a constant. (t_j is start time for erosion)

$C =$ TTI, TTI at start time of period of erosion

AT $t = t_j$ the TTI is, of course, equal to the TTI at the start of the period of erosion (C above). As time goes on (during the period of erosion) the rate of increase of eq (24) goes down. If the rate of erosion is large enough, and enough time has passed, TTI may be nearly constant. When the sediment point reaches the surface, its current period of erosion as well as its depth and temperature history have ended. The TTI thus remains constant up to the present.

Fig. 6 shows the TTI vs. time curve for the bottom and middle formations of the Gulf coast model of figs. 4 and 5 during a period of erosion inserted at 30 M. Y. B. P. (ending at 1 M. Y. B. P)

A period of erosion must always cause a rise in the iso-TTI contour. This must be true since during an erosion period sediment points must increase in age as we traverse the Depth-Time Graph at constant depth in the direction of increasing time (see Fig. 7). Older sediment points always have greater TTI than younger ones.

Table 2. summarizes the effect of sedimentation rate on both the shape of the TTI vs time curve for a sediment point and the iso-TTI contours. This summary, of course is an oversimplification, since one must consider the effects of changing the thermal parameters and the compressibility and porosity. These will be discussed in the following sections.

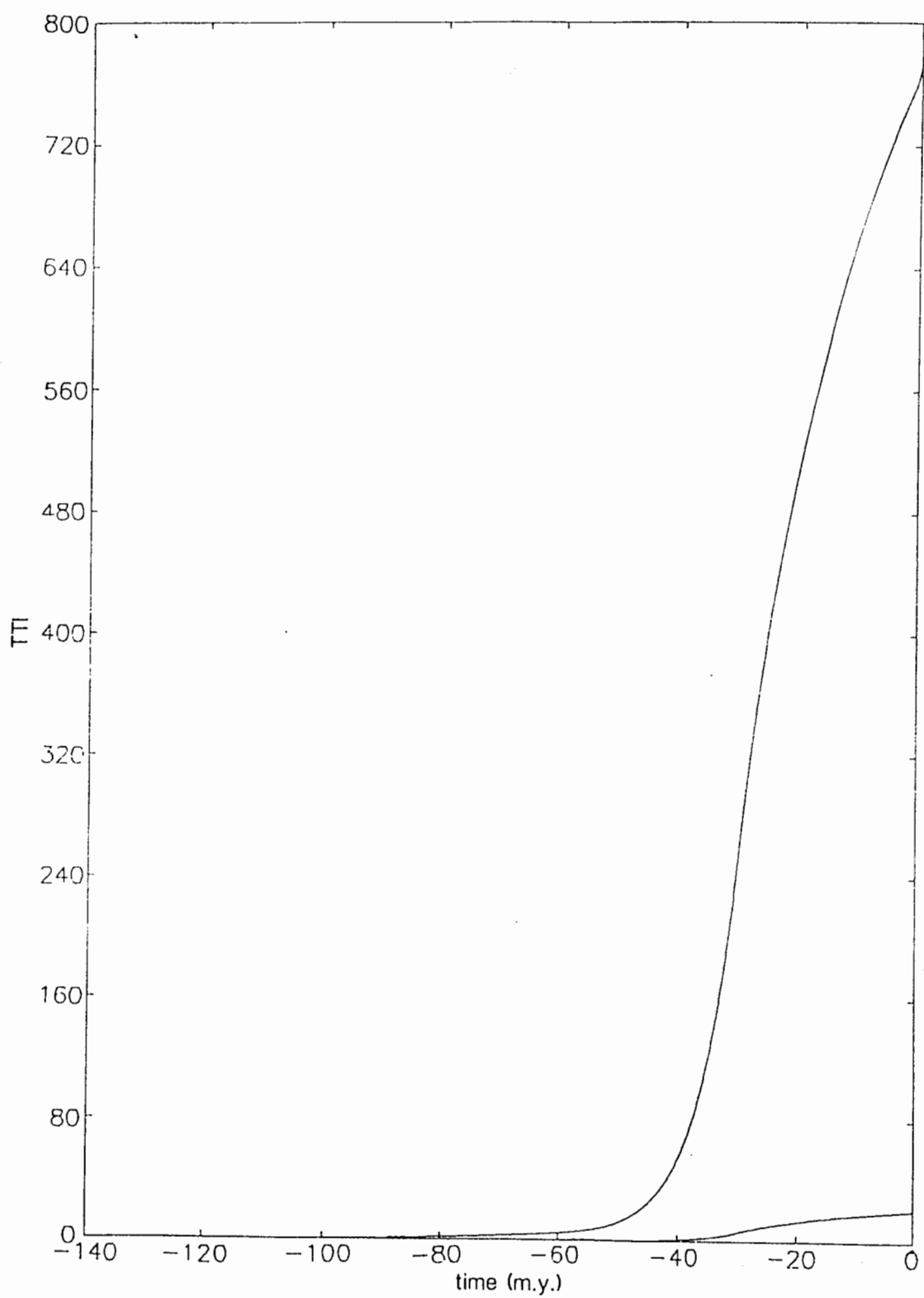


Fig. 6. Similar to Fig. 4 but erosion from 30 to 1 m.y.B.P.

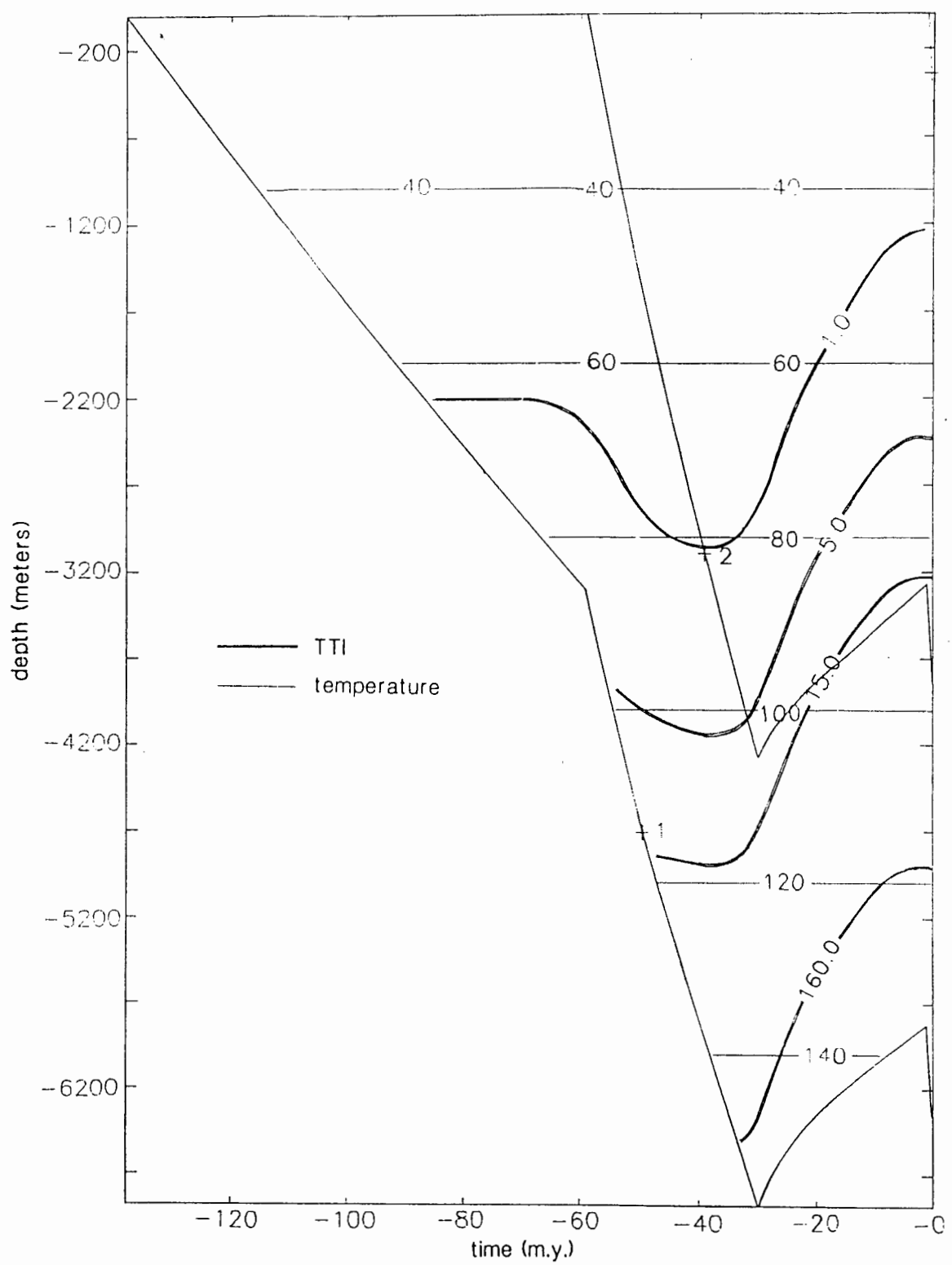


Fig. 7. Same situation as Fig. 5 but erosion at 30 to 1 m.y.B.P.

<u>Change in Sedimentation Rate</u>	<u>effect on TTI</u>	<u>effect on TTI Contours</u>
increase	increases rate of exponential increase with t	decreases slope
decrease	decreases rate of exponential increase with t	increases slope
becomes < 0 (erosion)	increase becomes less than linear. rate of increase decreases with time	causes them to ascend
becomes 0 (hiatus)	increase becomes nearly linear	causes increase or decrease in slope depending on previous sedimentation rate

Table 2. Effects of changes in sedimentation rate on TTI vs t and the TTI contours (on the time-depth graph)

b. Compressibility

From eq. (4) it can be seen that a higher sediment compressibility will result in a greater reduction in the grain velocity of a sediment point with depth, resulting in a shallower depth vs. time dependence. If the compressibility of the sediment is zero everywhere and throughout time, the depth vs. time curve is a linear increase (in depth, not altitude). During the deposition of a highly compressible sediment, the sediment points do not reach as great a depth as in the case of deposition of a sediment with low compressibility. Thus the higher the compressibility, the less pronounced is the rate of exponential increase of TTI during deposition (thermal parameters held fixed). It was desired to include compaction in the models of figures 2 through 7. Thus the compressibility was nonzero and decreased with time for all formations but the empirical functions for all formations were identical. If compressibility were set to zero everywhere and throughout time the TTI vs time curves would be given by eqs. (21) or (23).

As will be shown in a later section, a higher compressibility also will result in a greater reduction in the porosity with time (during deposition) which will cause changes in the thermal parameters of sediments.

In a period of erosion, there will be some decompaction if the compressibility of the most recently deposited sediment was nonzero. The more compressible this sediment is, the more decompaction there will be. But the extent of decompaction during a period of erosion is much less than that of compaction during a period of deposition. Thus the effect on the Temperature vs. time relationship and the TTI vs. time relationship is much less. (See sec. IV for details).

In a period of hiatus, The compressibility has only a small effect on the shape of the TTI vs. time relationship. It is still very nearly a linear increase if all thermal parameters remain fixed.

Thermal Parameters

c. Thermal Conductivity

- 1) Effects of inclusion of water and compaction.

The temperature factor G has an increasing (base 2) exponential dependence on temperature, thus any changes in the temperature of the sediment point cause great changes in the terms of the tti sum (14). Changes in the thermal basin properties will cause changes in the thermal gradient which cause changes in the temperatures along the sedimentary column (temperature profile). Thus the TTIs of sediment points along the column may undergo drastic increases in TTI due to changes in thermal gradient which are caused by changes in the thermal properties.

The thermal gradient at any point in the sedimentary column is related to the basement flux and thermal conductivity by the following relationship:

$$(25) \quad Q = k(z)g(z) = k(z)\left(\frac{\partial T}{\partial L}\right) = -k(z)\left(\frac{\partial T}{\partial z}\right)$$

where:

L = depth below surface

Q = basement flux. This may depend on time but will be held fixed for this section

$k(z)$ = sediment thermal conductivity at altitude z (negative of depth).

$g(z)$ = thermal gradient at altitude z

The sediment thermal conductivity depends on temperature and sediment porosity (and to a very small extent, pressure) which are all functions of altitude (and depth). The sediment thermal conductivity is given by the relationship (26) (a more detailed version of eq. (7)) :

$$(26) \quad k(z) = k_r(z) \{ (k_w(z)) / k_r(z) \} (n(z))$$

From eq. (25) it can be seen that at constant basement flux the thermal gradient is inversely proportional to the thermal conductivity at any point in the sedimentary column. In the previous section, although compaction was allowed, the thermal conductivity was always held fixed at the value of the rock matrix in order to determine the effects of various changes in sedimentation rate on the TTI. Thermal Conductivities for sedimentary rocks typically are in the range 1-5 W/(M DEG C) and may increase or decrease with the temperature depending on the temperature and the rock type. The average (over typical basin temperatures and pressures) thermal conductivity of water is about .63 with a range of .57 -.70 (W/(M DEG. C)). Thus from eq. (26) one can see that neglect of the thermal conductivity of the water which occupies the pore spaces almost always greatly overestimates the thermal conductivity of the sediments. This will cause underestimations of the thermal gradient and the temperature profile. From eqs. (21) and (23) (even though these were derived for a constant thermal gradient g) one might expect that neglect of the thermal conductivity of water would cause disastrous underestimations of the TTI at a sediment point and would predict an oil window that is both too deep and has too late an onset. This is indeed the case.

Figures 8 and 9 are a rerun of the calculation of figures 4 and 5 with the only difference being that in the calculation of figures 4 and 5 the thermal conductivity of the sediments was fixed at a typical value for rocks (2 Watts/(M DEG C)). In the calculation of figures 8 and 9 the thermal conductivity of water was included and the sediment thermal conductivity was allowed to vary according to eq. (26). Comparing figures 4 and 8, one can see that neglecting thermal conductivity of water causes the rate of exponential increases in TTI for the two plotted sediment points to be much too small. The TTI of the bottom sediment point at the present day is calculated to be 21700 if water is neglected. It is calculated to be over 700000 if water is included in the thermal conductivity. Comparison of figures 5 and 9 shows that if water is not included in the calculation of sediment thermal conductivity the onset of oil generation is predicted to be over 20 million years too late. If the thermal conductivity of water is not included, the depth of the top of the oil window at present day is predicted to be over 1500 meters too deep. (For simplicity, in all Gulf Coast type models the thermal conductivity of the rock matrix was not allowed to vary with temperature or pressure).

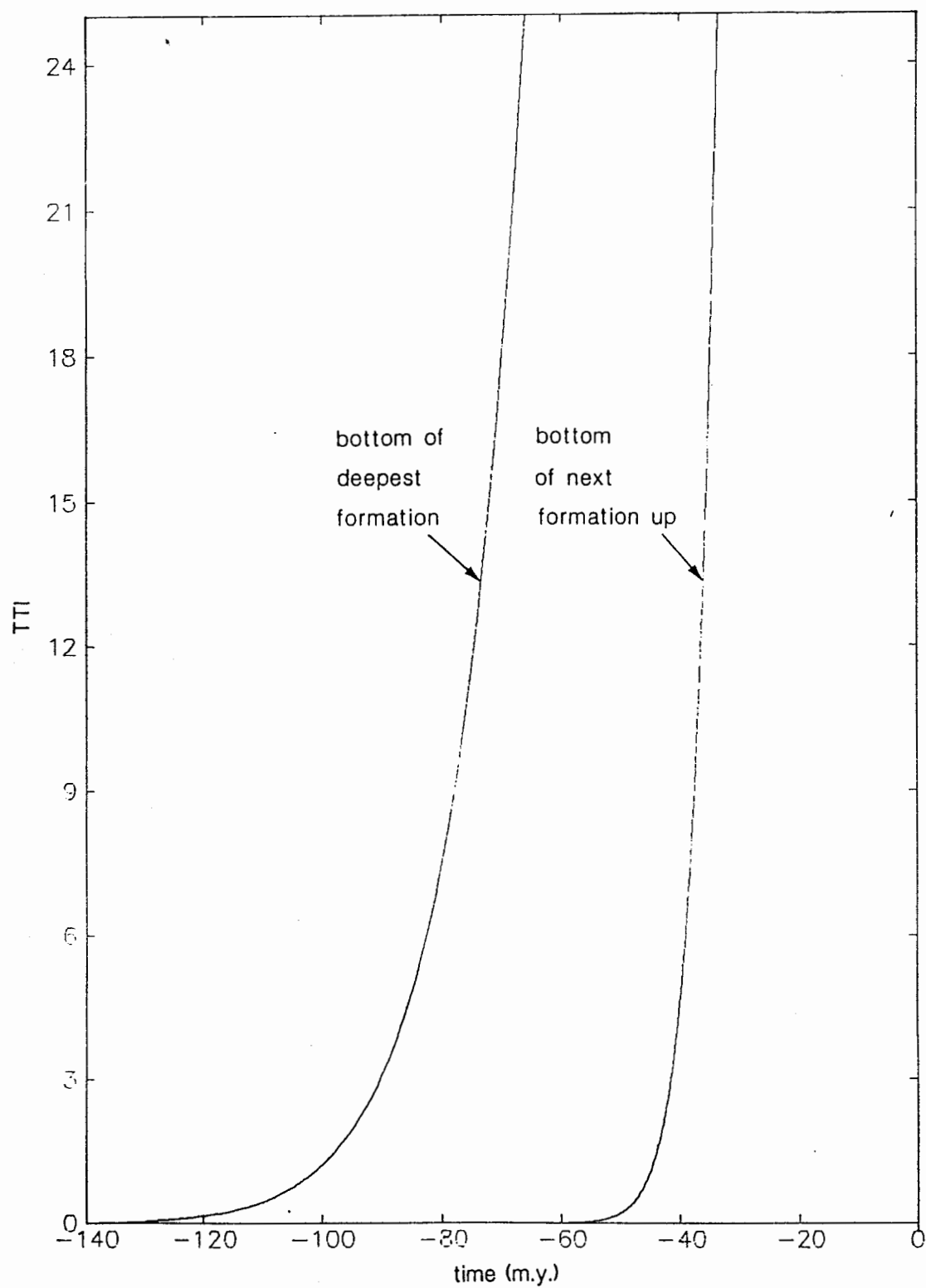


Fig. 8. Similar to Fig. 4 except water-rock thermal conductivity used.

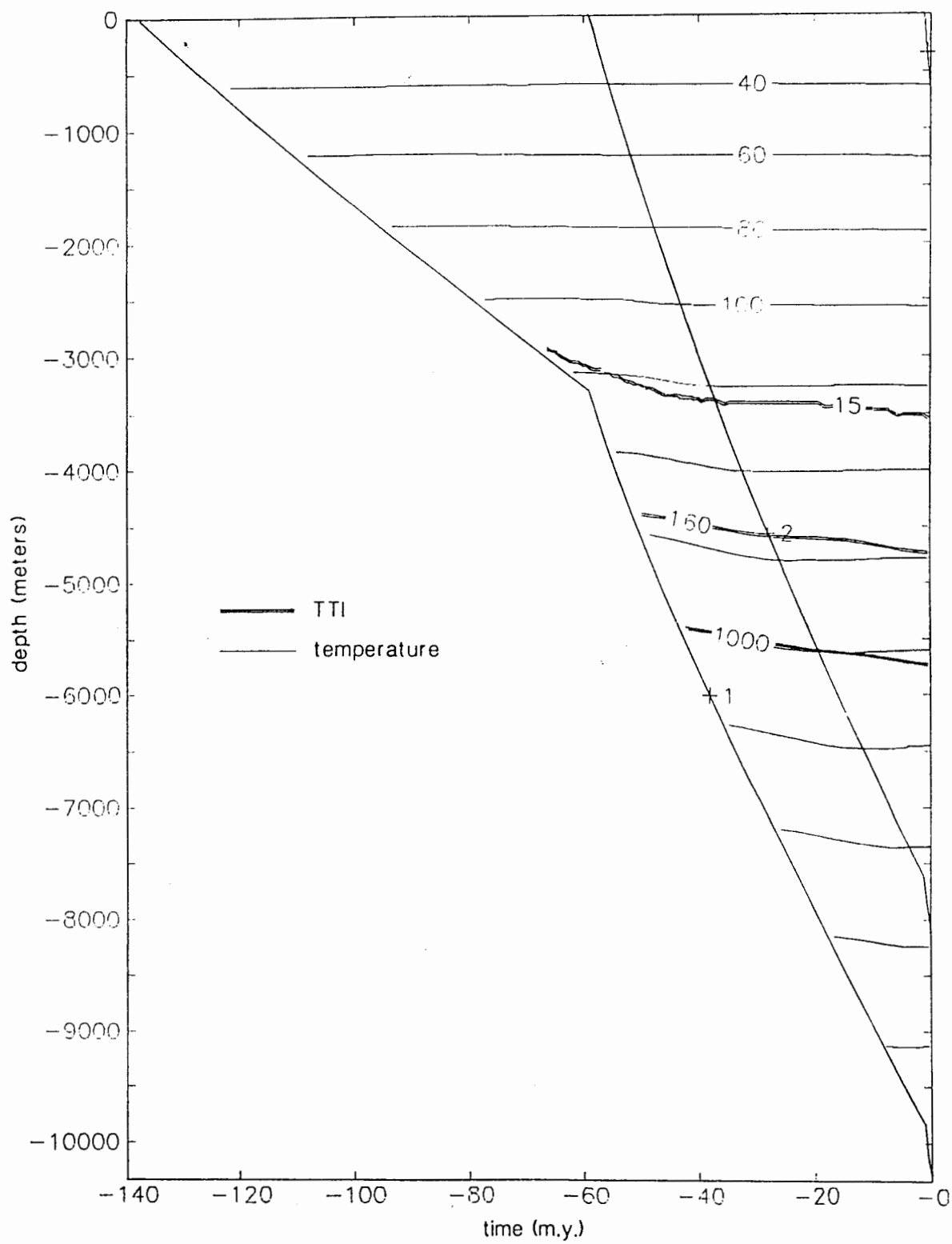


Fig. 9. Similar to Fig. 5 except water-rock thermal conductivity used.

The thermal conductivity at a sediment point almost always increases with depth (we assume for the present time that rock thermal conductivities do not vary with temperature and pressure and the rock type does not change) since the water thermal conductivity is almost always smaller than that of the rock and the porosity at a sediment point generally decreases with increasing depth (see eqs (7) and (26)). Furthermore any increase in the thermal conductivity at a sediment point causes a decrease in the thermal gradient at that sediment point and causes the temperatures in the profile to increase at a slower rate from that point on down to the basin bottom. Since the temperature at a given sediment point is so sensitive to the thermal conductivity at that sediment point and to those of the rock layers above it, and the TTI is so sensitive to variations in the temperature history of the sediment point, the description of the functional dependence of thermal conductivity with depth should be as precise as possible. It is suprising that very often this has not been the case (see refs. 2, 3, and 15).

2). Effects of Differing Rock Type in a Sedimentary Column

Up until now we have been keeping the rock matrix the same in all of our discussions. This is quite adequate if one is only interested in the effects of changing sedimentation rates on the TTI of a sediment point. But in reality the thermal and hydrogeologic properties of different rock types vary over wide ranges. For example, from eqs. (25, 26) it can be seen that sudden deposition of a shale ($k \sim .95 \text{ W/(M DEG C)}$) on top of a sedimentary column consisting entirely of limestone ($k \sim 2.5 \text{ W/(M DEG C)}$) will cause a dramatic lowering of the thermal conductivity near the surface and thus will cause a dramatic raising of the thermal gradient near the surface. Thus the temperatures of all sediment points below the shale will rise suddenly and the terms for this time step in TTI sum will be much larger than those of the last time step. It has also been noted (refs.4,5,6) that the thermal conductivities of some rock types vary quite a bit over typical basin temperature ranges. The variation with pressure is much less and has been ignored in this study. It is very important to use precise thermal conductivities for all rock types at all temperatures since thermal conductivity has such a pronounced effect on the TTI of a sediment point.

Sediments are deposited at and eroded from the top of the basin (i.e., the surface). The addition or removal of sedimentary units of varying lithologies will cause changes in the thermal conductivity near the surface which will affect the temperatures of the sediment points of the entire sedimentary column. Since the precise variation of thermal gradient and thermal conductivity with depth at constant time is not easy to determine, it is both convenient and useful to observe the effect of changes in the average or equivalent vertical thermal conductivity on the average thermal gradient for the entire sedimentary column at time t_i .

The relationship between average thermal conductivity and average thermal gradient is given by eq. (12) of section III.1 where the average thermal gradient is:

$$(27) \quad \bar{g} = (T_b - T_0)/L$$

and the average thermal conductivity for the sedimentary column at time t_i is given by eq. (13). Thus eq. (12) can be rewritten as follows:

$$(28) \quad Q = \bar{k} \bar{g}$$

It can be seen by a slight rearrangement of eq. (28) that as the shale in our example continues to be deposited upon the sandstone, its thickness constitutes a greater and greater percentage of the sedimentary column, thus from eq. (13) it can be seen that the average thermal conductivity will decrease (average thermal gradient will increase) during this period of deposition. The temperatures of all sediment points below the shale will continue to rise and so will the contributions to their TTI sums. Similarly, if the shale is subsequently eroded, the average thermal conductivity will increase, thus the average thermal gradient and the TTI terms will decrease.

In section III.2.A.a we found that the sedimentation rate affected the rate of exponential increase of the TTI of the sediment point with time. The approximate analytical relationships (21) and (23) suggest that it is the product of the thermal gradient and the sedimentation rate that determine the rate of exponential increase. If we use eq (28) to approximate the thermal gradient then eqs. (21) and (23) suggest that the product of the inverse of the average thermal conductivity, the current basement flux and the current sedimentation rate determine (very, very, approximately, of course) rate of exponential increase of the TTI of a sediment point.

If sedimentation rate, basement flux, and, of course, specific heat are held fixed and average thermal conductivity is allowed to decrease (say, by deposition of a shale upon a limestone) one would expect that changes in the shape of the iso-TTI contours would occur throughout the period of deposition. Consider a sediment point at a certain depth below the surface at a time just before the deposition of new material with lower thermal conductivity than that of the current topmost formation. If deposition of the new material begins at the next time step and the new material has a lower thermal conductivity, the thermal gradient at that sediment point and above will increase and the temperature of the sediment point at the same depth at the new time step will have a higher temperature factor G than the previous sediment point at the last time step. Thus the iso-TTI contour slope must increase. As more and more of the new material is deposited, the temperatures of the sediment points at the same depth continue to increase. The amount of increase depends on the thermal gradient. The thermal gradient varies with depth according to eq. (26). As we enter the new material and keep the depth and the sedimentation rate constant and advance in time, the sediment points will again all have the same thermal conductivity (as a function of depth) and the same age. The TTI contours which are high enough to be in the new material will again be horizontal, but since the average thermal conductivity is still decreasing, the temperatures of the sediment points at all depths below the new material are still increasing with time (due to the increase of the percentage of new material in the sedimentary column.) The contours below the new material will thus still have nonzero slope. These contours become horizontal at a time near the point at which they enter the new material.

If the situation is reversed, and a rock material with higher sediment thermal conductivity is deposited atop one of lower thermal conductivity the above discussion still holds but the contours outside the new material will first decrease in slope. The amount of decrease depends on the thermal gradient at that point (a function of depth according to eq. (26)). They will become horizontal when they enter the new material and will remain horizontal until such time when a change in sedimentation rate, thermal conductivity or basement flux occurs.

In fig. 10 the TTI for the bottom sediment point of a model basin in which 3 formations of differing rock thermal conductivities are deposited at the same sedimentation rate is plotted against time.

The first range of thermal conductivities (the variation is due to temperature change) is typical of shales (see ref.4), the second typical of sandstones (ref. 4), the third typical of limestones. At 92 M. Y. B. P. a sudden increase in the rock thermal conductivity caused the rate of TTI increase to go from exponential to less than linear. At 46 M. Y. B. P. a formation of lower rock thermal conductivity is deposited. The average thermal gradient suddenly rises and the rate of TTI increase suddenly increases.

Fig. 11 shows the TTI contours on the depth vs time plot. The slope of all contours suddenly decreases when a formation of higher rock thermal conductivity is deposited. The top contour begins to "level off" as it begins to enter the material being deposited but its slope then increases as a formation of lower thermal conductivity is deposited. It starts to level off again as it approaches the bottom of the topmost formation. The deeper contours also increase in slope but not as much. The thermal gradient at this depth is lower than at shallower depths.

As mentioned previously, it is impossible to make a complete separation of the effects of the parameters in the depth history group from those in the thermal history group. The sedimentation rate affects the rate at which materials are being deposited and thus affects the average thermal conductivity. It also affects the rate of compaction which from eqs. (26)-(28) will affect how rapidly the average sediment thermal conductivity will increase with time due to the greater percentage of low-porosity sediments in the column. Figure 12 demonstrates this. It is a plot of the average thermal gradient vs. time for the Gulf Coast Model of figures 8 and 9. In this figure, the thermal gradient decreases with time because the thermal conductivity is increasing with time due to a greater percentage of rock (and less of water) as time goes on. Notice that the rate of decrease clearly depends on the sedimentation rate.

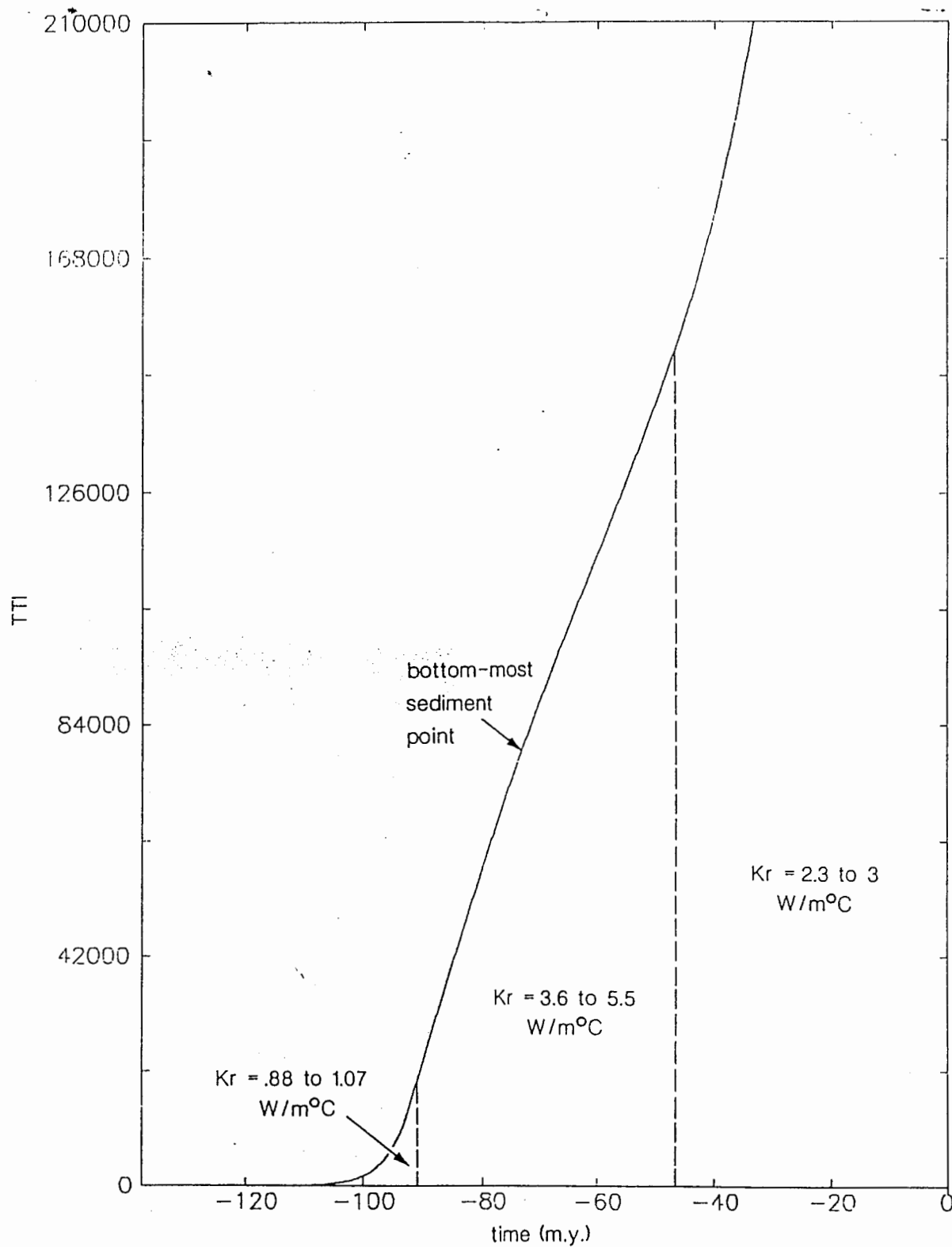


Fig. 10 TTI vs. time (single sedimentation rate, three different ranges of Kr). Rock thermal conductivities (ranges) refer to the material currently being deposited.

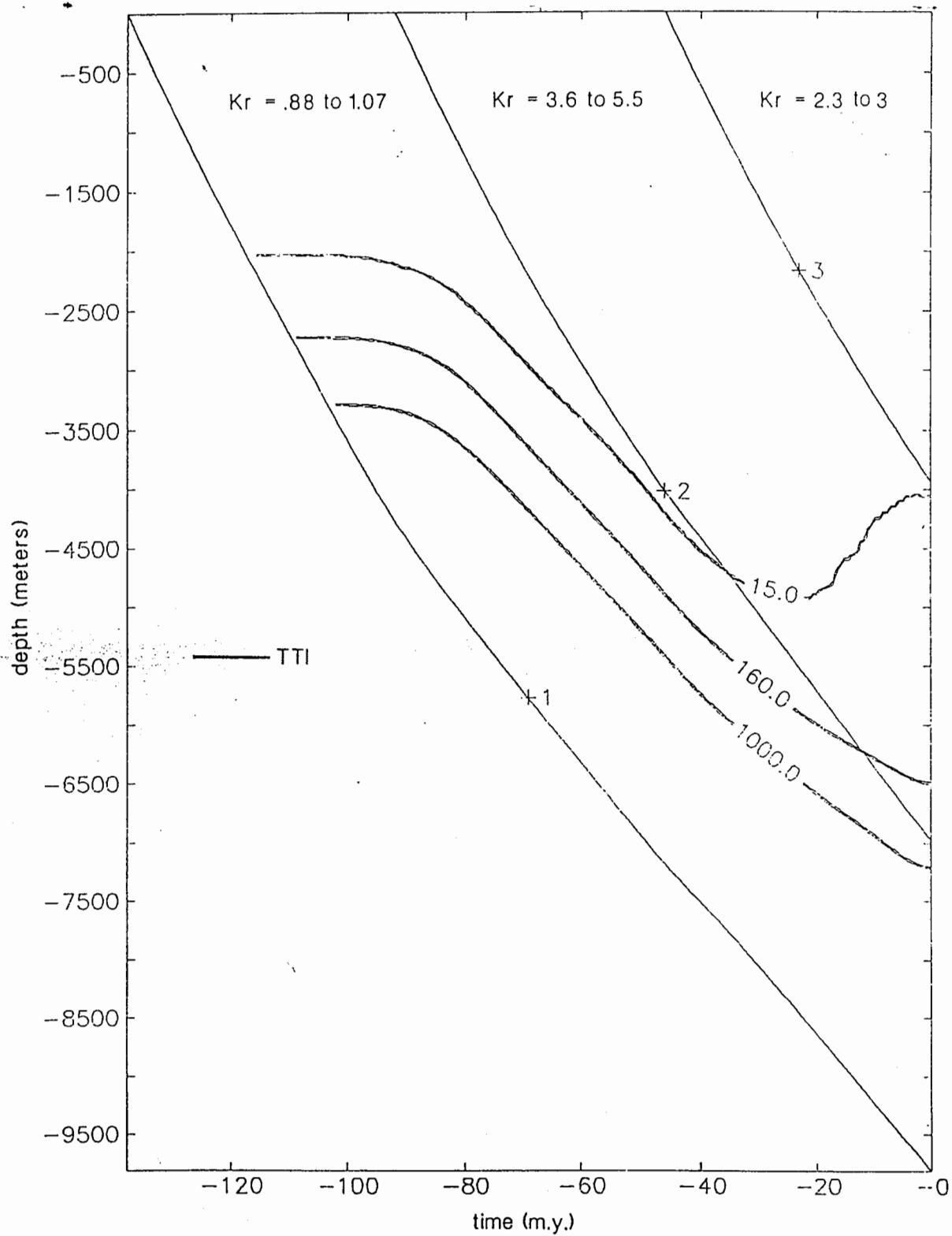


Fig. 11 Burial history with TTI contours (single sedimentation rate, three different Kr ranges). Rock thermal conductivity ranges refer to material currently being deposited.

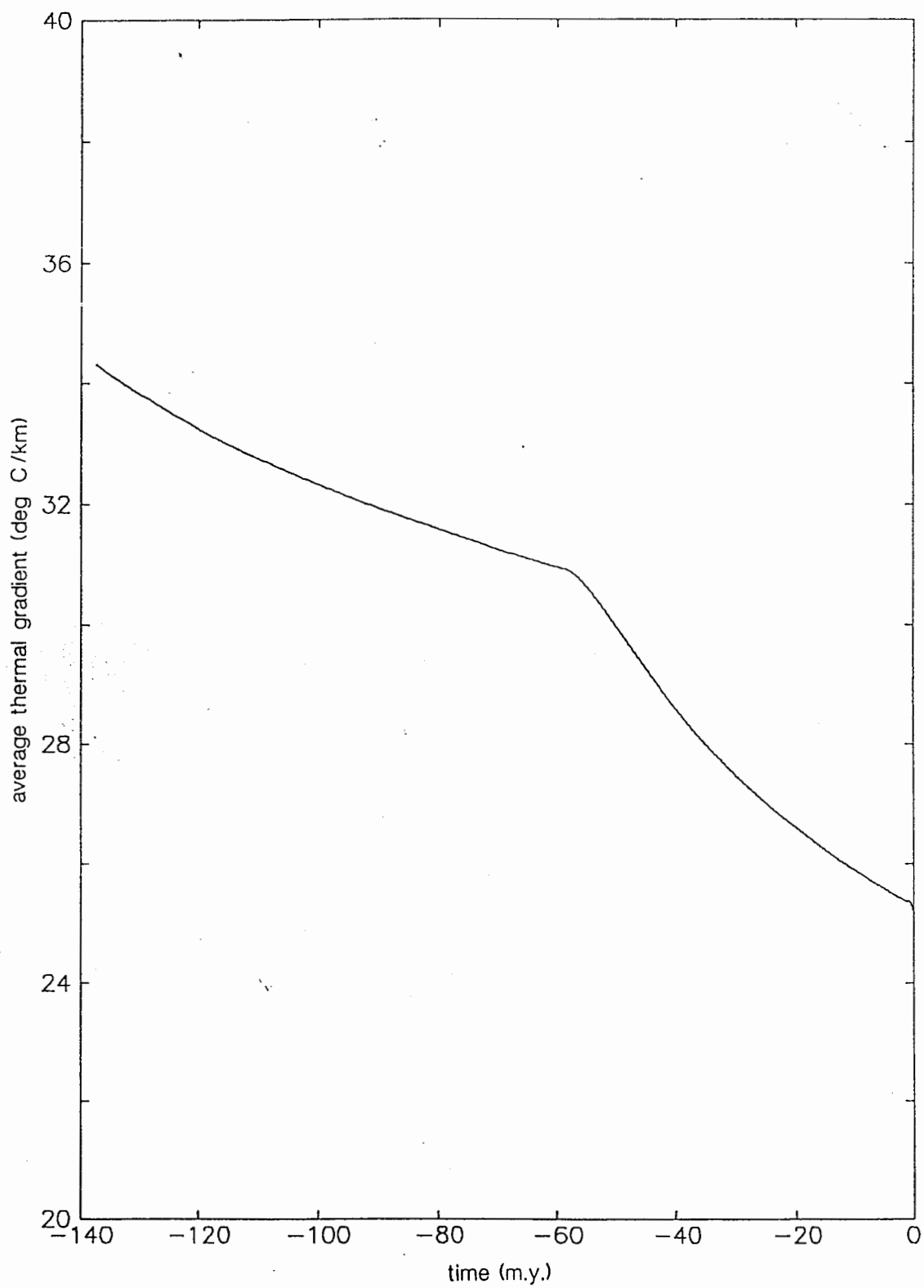


Fig. 12. Average thermal gradient vs. time for Gulf Coast model (specific heats = 0).

The rate of erosion can also affect the average thermal conductivity (and thus the average thermal gradient.) As sediment with a lower thermal conductivity is removed, the average thermal conductivity increases (thermal gradient decreases). How rapidly this occurs depends on the erosion rate. The resulting effect on the TTI sum would be the same as that of depositing a sediment of higher thermal conductivity superimposed upon the affects on the TTI summ due to raising of the sediment point mentioned previously.

The effects of thermal conductivity on the TTI sum of a sediment point and on the shape of an iso-TTI contour are summarized in table 3.

change in thermal conductivity	effect on TTI vs time	effect on shape of TTI contours
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decrease	increases rate of exponential increase	increase in slope
----------	----------------------------------------------	----------------------

increase	decreases rate of exponential increase	decrease in slope
----------	----------------------------------------------	----------------------

Table 3. Effects of thermal conductivity changes on TTI
vs t and the TTI contours

d. Basement Flux

From eqs. (26) and (28) it can be seen that the basement flux affects the thermal gradient in the inverse sense that the thermal conductivity does. If the basement flux increases, so does the average thermal gradient and thus the temperatures at each sediment point. If the flux change is sudden then so are the changes in the temperatures of the sediment points in the sedimentary column. As stated in section III.1 we are interested in four types of flux change:

Constant Flux.

This case has already been considered in the previous subsections of this section.

Step Changes in the Flux

If we now hold the sedimentation rate, thermal conductivity, and specific heat constant and use the same compressibility function throughout, we can model the effects of step changes in the flux on the TTI sum of a sediment point. We will allow the basement flux to remain constant for a certain length of time, then suddenly change at a later time and remain constant at this new value. If we consider only sediment points that were deposited either before or during the first flux period (j), these will experience at least one change in flux. The TTI sum can then be written in the form (22) where in this case the two temperature factor functions G_j and G_k are a result of different values of the basement flux, not different values of the sedimentation rate. The two time periods represented by the two sums are periods of different constant basement flux, not different sedimentation rate. If the flux at the second time period is larger than that of the first, then the rate of increase of the factor G_k with time is greater than that of factor G_j . This suggests that increasing the flux increases the rate of increase of the TTI of a sediment point with time as does increasing the sedimentation rate. If we now let Δt approach zero, approximate the depth vs. time relationship for sediment points as linear, and approximate the thermal gradient during each time step as the average thermal gradient, the result is an approximate analytical relationship similar to that of eq. (23) except that it is the thermal gradient, not the sedimentation rate that is different in the base 2 exponent (and

denominator) of each term. If we substitute eq. (28) for each g in this modified version of eq. (23) we have:

$$(29) \quad TTI(t) = \sum_j A (2^{c_j t} - 2^{c_j t_j}) + C$$

$$t_j < t \leq t_k$$

$$TTI(t) = \sum_j A (2^{c_j t_k} - 2^{c_j t_j}) + \sum_k A (2^{c_k t} - 2^{c_k t_k}) + C$$

$$t > t_k$$

where:

t = current time (from onset of deposition)

t_j = onset time for first flux period under consideration or start time for deposition of a sediment point if it was deposited during the first flux period (j).

t_k = onset time for second flux period under consideration

$$c_j = Q_j s / (10 \bar{k})$$

$$c_k = Q_k s / (10 \bar{k})$$

C = TTI at start of first period (may be zero)

$$A_j = (10 \bar{k} / (Q_j s \ln(2))) * (2^{((T_j - T_r - (Q_j s / \bar{k}) t_j) / 10)})$$

$$A_k = (10 \bar{k} / (Q_k s \ln(2))) * (2^{((T_k - T_r - (Q_k s / \bar{k}) t_k) / 10)})$$

\bar{k} = average thermal conductivity (held constant)

Q_j, Q_k = fluxes at the two time periods under consideration

s = sedimentation rate (held constant)

This approximate result can be generalized to any number of step changes in flux. It suggests also that a flux increase increases the rate of exponential increase of the TTI of a sediment point with time. A flux decrease would decrease this rate. In Figure 13 we present the TTI vs time graph for the same model as shown in figure 2 but this time there are three periods of different (fixed during each period) flux. Notice that initially the rates of exponential increase of figs 2 and 13 are identical, but at 70 M.Y.B.P ($t_k = 68$ M. Y.) the flux increases by a factor of 1.5 and the rate of exponential increase greatly increases. At 55 M.Y.B.P ($t_l = 83$ M. Y.) the flux drops by a factor of 2 and the rate of exponential increase decreases dramatically. The final TTI is just over 14000 compared to nearly 31500 for the constant flux case in fig. 2. A flux drop when the basin is deepest can have an enormous retarding effect on the TTI of a sediment point.

The effect of step changes in flux on the shape of the iso-TTI contours is quite easy to understand. A sudden increase in the flux causes a proportional increase in the average thermal gradient and thus in the magnitude of all temperatures in the sedimentary column at that time step. This causes a sudden jump in the iso - TTI contour regardless of its previous shape. Similarly a sudden drop in the flux causes a sudden drop in the iso-TTI contour. These sudden changes are difficult to graph with contouring methods unless the changes are relatively small.

Sudden Enormous Rise and Rapid Decay of Flux (Magmatic Intrusion).

The magnitude of basement flux due to magmatic intrusion may initially be 25 times as large as that of a typical basement flux, but, according to our results, it decays very rapidly. Fluxes due to magmatic intrusion will be discussed in a later section, when the results for the Ardmore basin are presented.

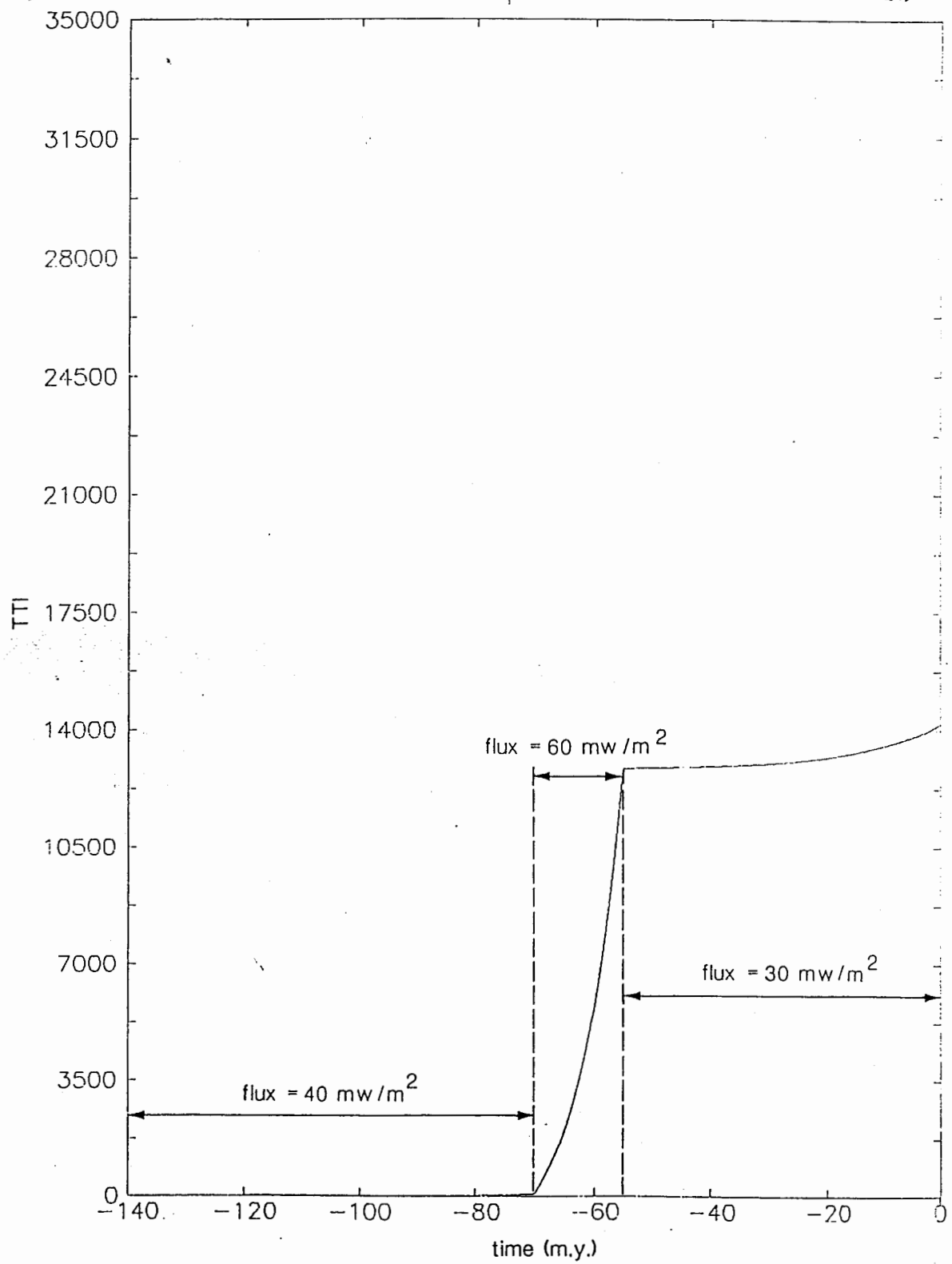


Fig. 13. TTI vs. time for basin bottom; single sedimentation rate with fluxes shown.

Gradual Decrease of Flux Due to Isostatic Subsidence of Basin.

If the flux is allowed to gradually decrease according to the isostatic model of basin subsidence (ref. 16), the average thermal gradient continues to decrease with time. If sedimentation rate is fixed the temperature factors G in the TTI sum (14) may increase with each successive term, but each G factor will be smaller than what it would be if the flux had remained constant at its initial (largest) value. In fact, if the rate of flux decrease from time-step to time-step is large enough (or the sedimentation rate slow enough) that each successive temperature of the sediment point is smaller than the previous one, smaller and smaller terms will be added to the TTI sum. Thus in this case one may expect to observe the same kind of functional dependence (TTI vs. time) as is observed for erosion at constant values for thermal parameters (Fig 6.). At very low sedimentation rate and relatively high flux decrease it is theoretically possible for the TTI to remain nearly constant. At high sedimentation rate and very small flux drop, the increase in TTI for the sediment point would be rapid and exponential, similar to the case of figure 2.

From our discussions of the effects of flux on thermal gradient it is relatively obvious that a gradual decrease in flux would cause a gradual decrease in the slope of the TTI contour (other parameters remaining constant, of course).

In a later section, we will present an Ardmore basin model in which the isostatic subsidence model was used to determine the basement flux.

e. Specific Heat

Up until this point we have assumed that the system is in equilibrium. That is, all of the heat entering the system through the basement leaves the system through the surface. None of it is absorbed by the rock matrix or the water in the pore spaces. All time dependence of the temperatures at each sediment point in the sedimentary column has come from changes in the thermal conductivity or basement flux. This is what is known as steady-state behavior. If we now allow the specific heat to have a nonzero value in eq.(5) we have a non-steady-state or nonequilibrium process and the sediments will absorb some of the heat coming in from the basement. The sediments absorb heat until equilibrium is reached. But when new sediment is continually added, the system never reaches equilibrium. The faster the sedimentation rate, the more new sediment is added to the column per unit time. Thus if we have a sudden increase in sedimentation rate, we suddenly have a lot more new sediment. The more new sediment we have, the further from equilibrium the system is and the faster the rocks and water will absorb heat. Since more sediment is added per unit time, there will be more new sediment at each time step to absorb heat. Since the heat is being absorbed at each time step in the non-steady-state process, we might expect then that the average thermal gradient is generally lower for the non-steady-state process than for the steady-state process throughout time with the greatest difference occurring at the start of the most rapid deposition with the highest density and specific heat (see eq. 5). Figure 14 suggests that the drop in thermal gradient relative to the steady-state process increases with increasing sedimentation rate (compare with fig. 12, which is Traced on fig. 14 with a dotted line).

f. Density

The density affects the thermal gradient in the same way that the specific heat does (see eq. 5). The higher the density is, the more the sediments will absorb heat and lower the thermal gradient. A higher density toward the top of the sedimentary column also increases the stress rate which then increases the grain velocity, thus causing a greater amount of compaction of lower strata per unit time (see eqs. 3 and 4). This will cause all thermal parameters to change at a higher rate. The (sediment) thermal property with the greatest influence seems to be thermal conductivity, which lowers thermal gradient when increased.

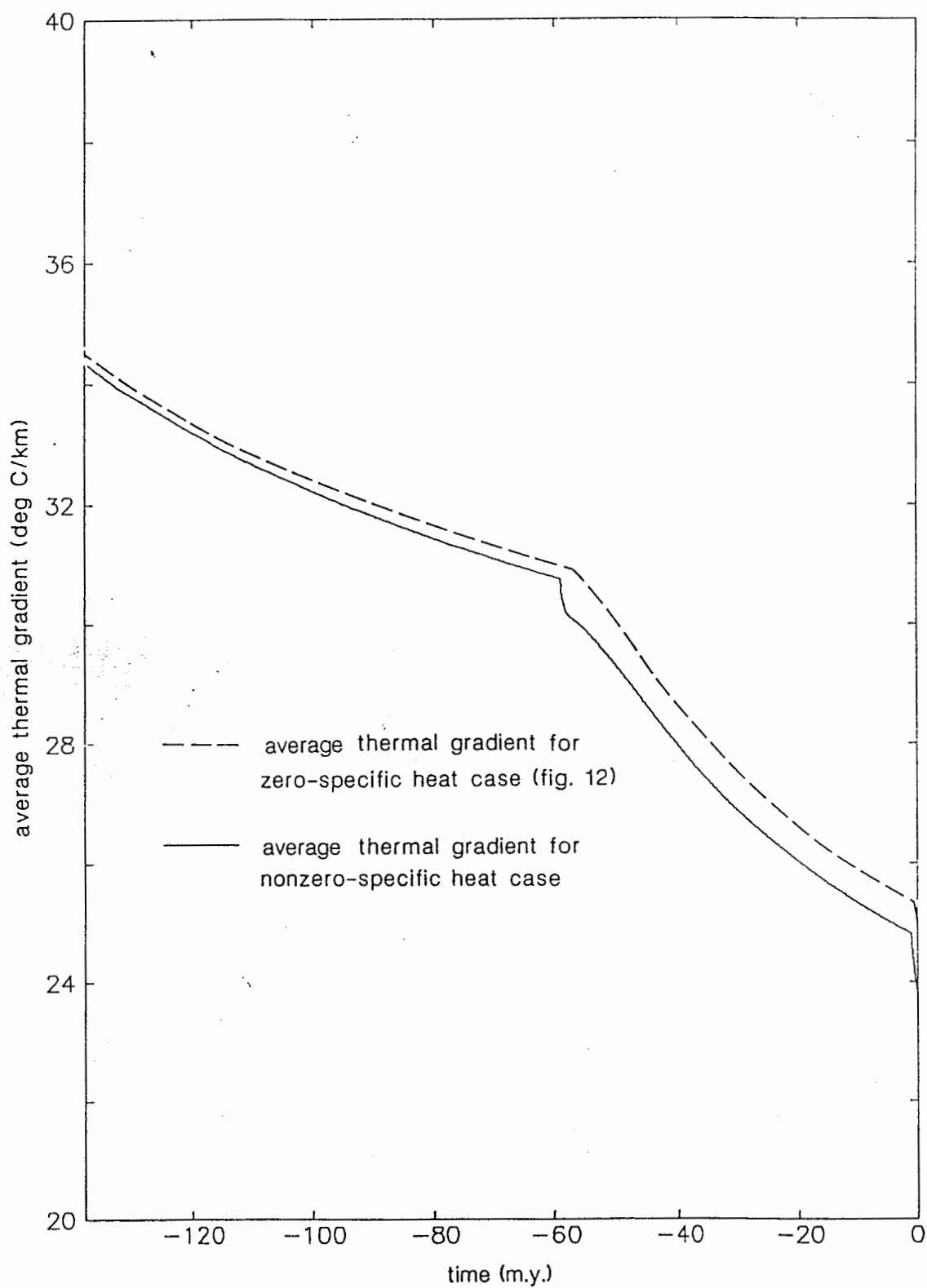


Fig. 14. Average thermal gradient vs. time, nonzero specific heat, Gulf Coast model.

g. Summary

A summary of the net effects of changes in each of the properties on the TTI of a sediment point in a sedimentary column is presented in table 4. If the lithology, burial history, and thermal history of the basin is known, very rough estimates as to the maturity of the basin can be made by superposition of these effects. They may also be used to analyze the resulting TTI's of points in basin formations and the TTI contours of a complicated basin model. This will be of help in determining the correctness of results obtained from a model. But the main goal is a more detailed understanding of what contributes to the maturity of sedimentary basins. These will be done in the following two sections.

Table 5. lists some of the characteristics which might be associated with a mature basin and those which might be associated with an immature one.

In the following two sections we present the results of two rather complex basin models. We will use the relationships developed in the previous sections to analyze the TTI data and to explain the shape of TTI and temperature contours.

change in property	effect on TTI vs t	effect on TTI contours (on time-depth graphs)
increase in sedimentation rate	increases exp. rate of increase	decreases slope
decrease in sedimentation rate	decreases the exp. rate of increase	increases slope
increase in thermal conductivity	decreases exp. rate of increase	decreases slope
decrease in thermal conductivity	increases exp. rate of increase	increases slope
step increases in basement flux	increases exp. rate of increase	causes step increases in contours
step decreases in basement flux	opposite of above	opposite of above
gradual changes in basement flux	opposite of thermal conductivity	opposite of thermal conductivity (see table 3.)
nonzero specific heat	decreases rate of exp increase	decreases slopes

Table 4. Summary of effects of various properties on TTI contours and TTI vs time curves.

Factors contributing to
the maturity of a sedi-
mentary basin.

Factors detracting from
the maturity of a sedi-
mentary basin

rapid sedimentation rates

slow sedimentation rates

low thermal conductivities
(of sediments)

high thermal
conductivities
(of sediments)

low specific heats of sediments

high specific heats
(of sediments)

high basement flux

low basement flux

generally higher porosity
of sediments

generally low
porosities of
sediments

relatively few and/or relatively
slow erosions

relatively many
and/or relatively
rapid erosions

generally low compressibilities
of sediments

generally high
compressibilities
of sediments

Table 5. Characteristics associated with mature and immature
basins.

B.) Salina Basin Model Results

a. Maturity of basin

In Figs 15-17 we present the results of a very realistic Salina Basin Model based on actual well data (lithology, present day thicknesses, average thermal gradient, bottom hole temperature, depth of basin bottom and geologic history. At the location of this well, the basin consists primarily of relatively thin formations which are an alternating sequence of limestone and shale. Sedimentation rates varied widely but there were four major periods of erosion, including one which constituted the final event and lasted from 65 M.Y.B.P to the present. There were a total of 39 formations. These were grouped into the five larger formations (shown in Figure 15) for discussion. Table 6. summarizes the present day results.

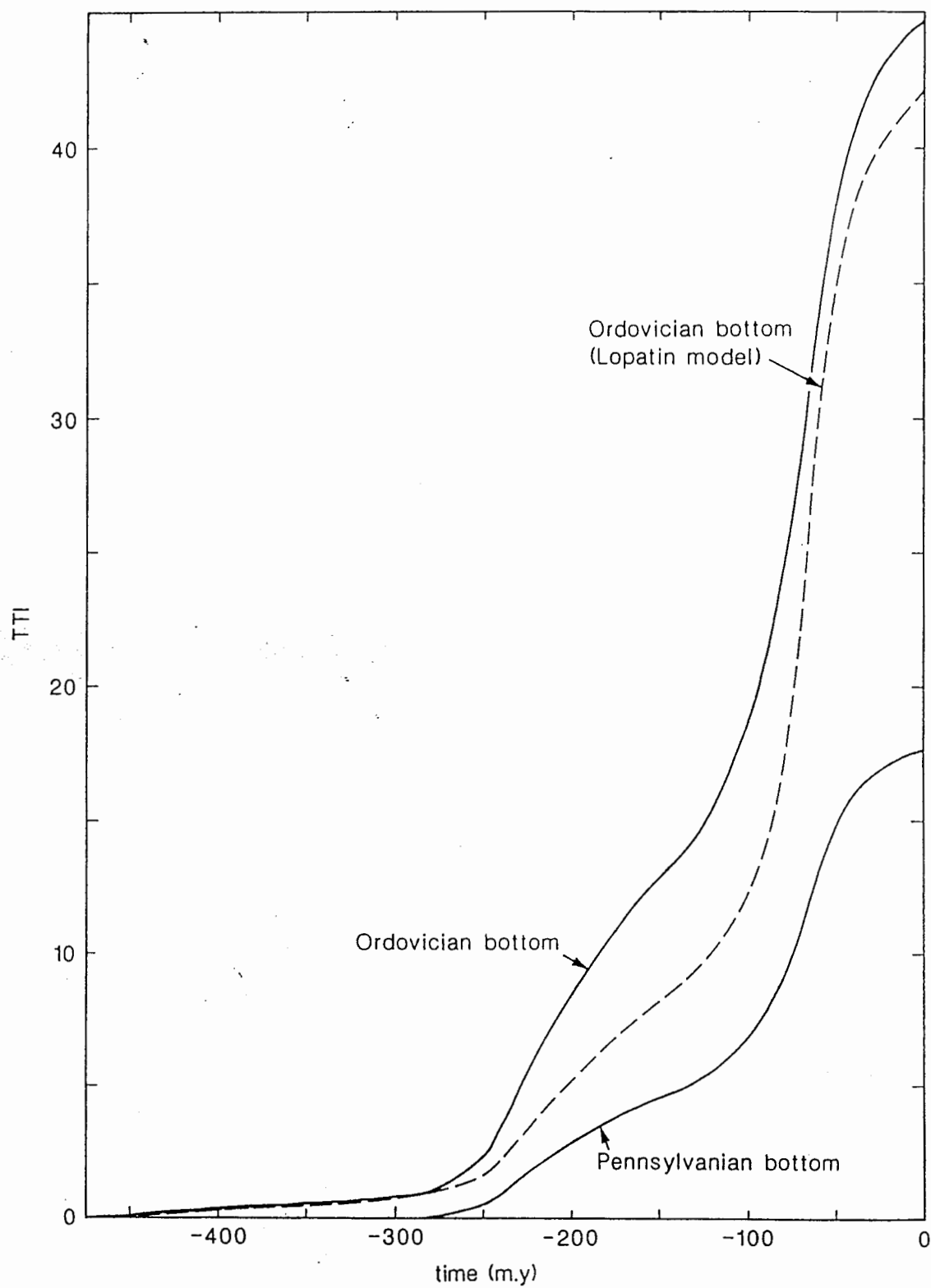


Fig. 15. TTI vs. time for two Salina basin formation bottoms.

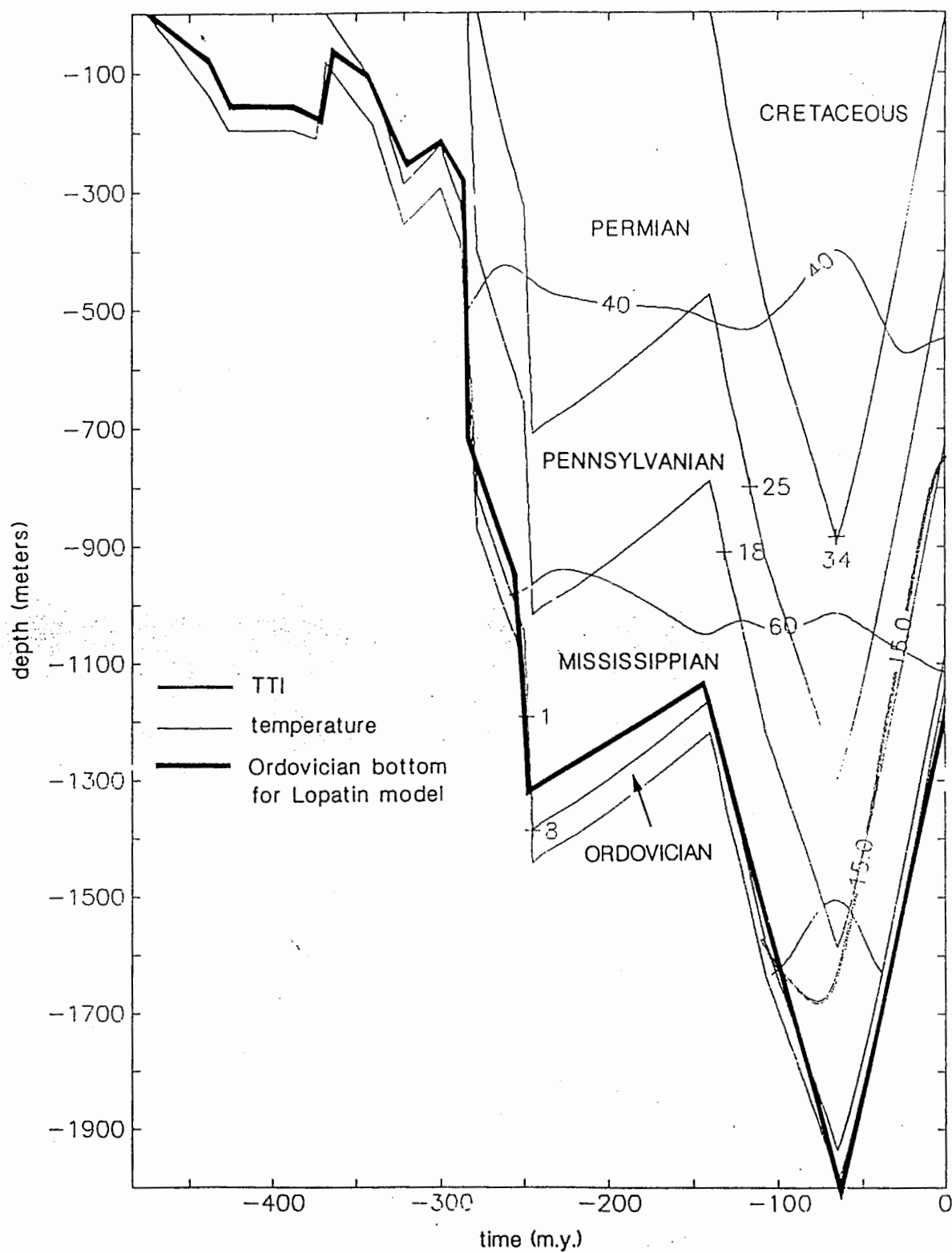


Fig. 16. Burial history with temperature and TTI contours, Salina basin model.

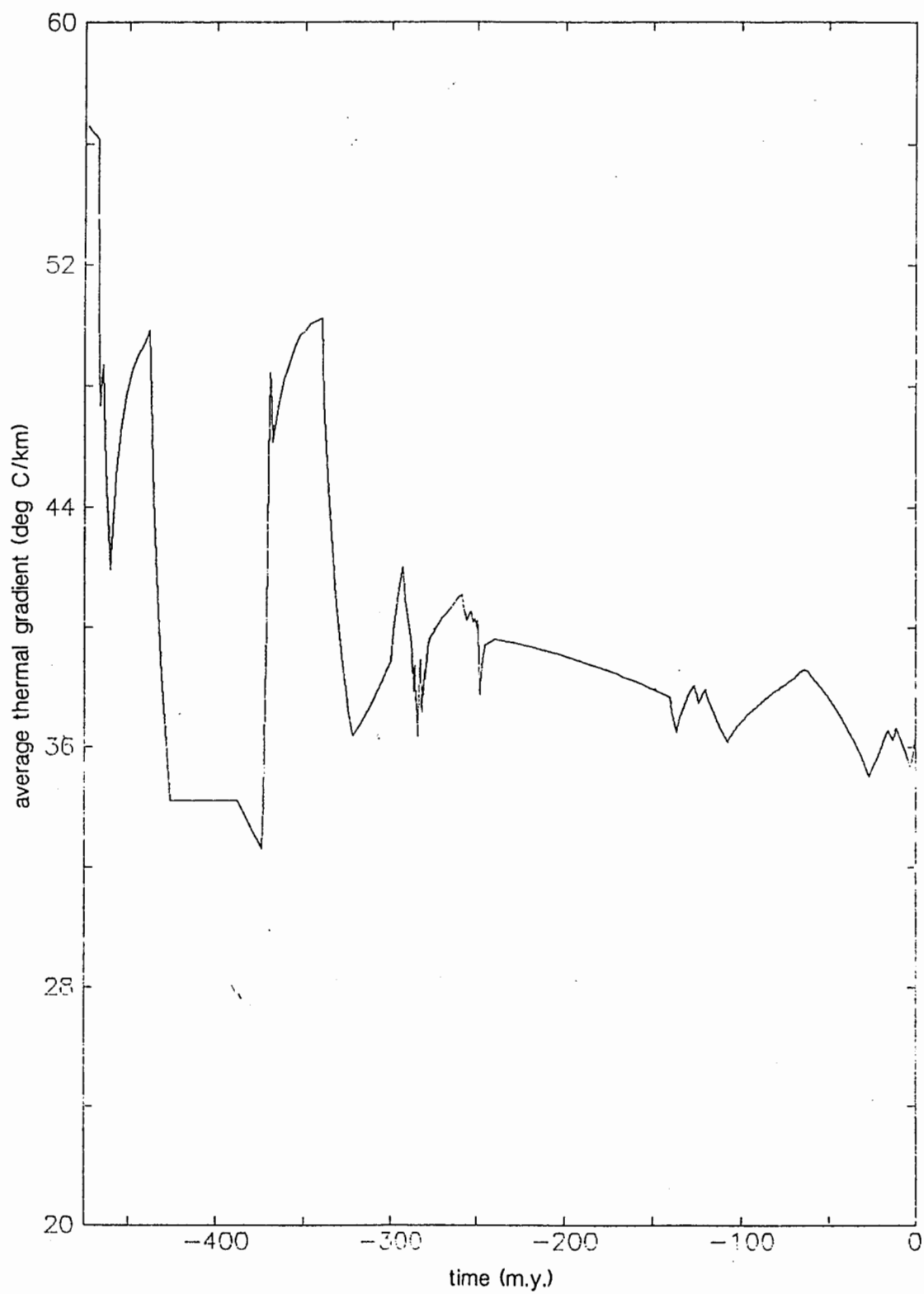


Fig. 17. Thermal gradient vs. time for Salina basin model.

Table 6. Present-day data for Salina basin

FORMATION	DEPTH (M) (CALC.)	DEPTH (M) (OBS.)	TTI (BOTTOM)
ORDOVICIAN	1141.23	1149.1	44.6
MISSISSIPPIAN	1086.65	1094.23	38.3
VIRGILIAN	725.39	728.47	17.6
PERMIAN	427.68	429.77	7.5

From these results one can gather that the Salina Basin is a very immature basin. Only the bottommost formations were predicted to have been exposed to the oil window. This conclusion reinforces that derived from a more coarse model presented previously (ref. 1). The average thermal gradient is plotted in Fig. 17. Notice that the average thermal gradient for this model does not vary as smoothly with time as does the hypothetical Gulf Coast model. The sudden rises in the curve are due to either deposition of a formation with lower thermal conductivity than the current average thermal conductivity (such as a shale) or erosion of a formation with higher than average thermal conductivity. The sudden dips are due to erosions of the former or depositions of the latter. In the complete Gulf Coast model of ref 1 all the rock thermal conductivities were the same and thus all changes in the average thermal gradient were due to smooth changes in the average thermal conductivity resulting from compaction. Notice also that the wide variations in the the average thermal gradient decrease in magnitude as time goes on and the general trend of decreasing average thermal gradient due to compaction becomes more noticeable as depositions and erosions constitute less of a percentage of the column length. The thermal gradients generally ranged between 34 and 40 (DEG. C)/KM., which are relatively high values. Thus from thermal history alone (basement flux was held constant at 40 MW/(m**2)) one expects generally steep exponential increases in the TTI vs. time curves for the formation sediment points. However the sedimentation rates were not generally large and the erosion episodes were relatively many. The last event consisted of a rather lengthy erosion, thus the TTI increase during this period was astronomically smaller than what it would have been had there been a deposition instead (Compare shape of Fig 15 in last time period to that for Fig 8). If the last event were a deposition, the TTI increases would have been rapid and exponential, however since there was an erosion instead, they were less than linear (see Fig.15) Thus erosions, particularly the post-Cretaceous, seem to be the primary factor in causing this basin to be immature.

Figure 16 shows the depth vs. time plot upon which is superimposed the temperature contours and the TTI contour constituting the top (15) of the oil window. From Table 6, the maximum TTI (achieved by the bottommost sediment point was 44.6. Thus none of the formations even came close to the bottom of the oil window (160). In fact, only the Ordovician, Mississippian, and the very bottom of the Pennsylvanian reach the oil window. The shape of the top of the oil window can be explained as follows: During the periods of deposition which follow the third period of erosion the contour rapidly descends. At 107 M.Y.B.P a deposition of a very thick shale occurs until 65 M.Y.B.P causing the TTI=15 contour to gradually increase in slope (shales have the lowest thermal conductivity of any sediment in the basin,

thus their deposition will increase the average thermal gradient and thus increase the slope of the TTI contour (see tables 3,4). At 65 M.Y.B.P the relatively rapid final erosion occurs causing the TTI contour to rise (erosion of the topmost shale also contributes to the rising (table 4). Due to the superposition of the effects of erosion and raising of thermal conductivity, we have the extreme case in which the TTI's of the sediment points (at least those near the Mississippian-Pennsylvanian boundary) begin to approach a constant value (see figure 15).

b. Compaction and water flow in more detail

It had been noted previously (ref 1) that the classical Lopatin model (one with no compaction or water flow may underestimate the TTI in certain situations. The results of the present report may be used to clarify this statement. In the general Gulf Coast model, where there is no erosion, all sediment points (formation barriers, for instance) will be at greater depth than the corresponding sediment points in the classical Lopatin model throughout the period under consideration. Thus from burial history consideration alone, under these conditions the TTI will have a greater rate of exponential increase in the general model than in the classical Lopatin model throughout the entire period. Additionally, since all formations remain at their present day porosities throughout time in the Lopatin model they remain at their maximum thermal conductivities (or close to this). Thus the average thermal gradient in the Lopatin model is lower than that in the general model throughout time. From table 4, this would also contribute to a higher TTI for the general model than for the Lopatin model (actually, some Lopatin-type models use rock thermal conductivities and ignore the presence of water and thus produce the disastrously low values of TTI observed in figs 2-5 where water was ignored to hold thermal conductivity constant in the general model.). However, when erosions are a part of the geologic history of the basin, then the picture is not quite as simple. Table 7 summarizes the present-day data for the Lopatin and general model. Notice that there is a very small difference in the present day TTI's of the formation bottoms in the two models. Somewhere between 107.4 M.Y.B.P and 65 M.Y.B.P the Lopatin model went deeper than the general model and remained below it until the present day (see also fig 16). During this period a very thick shale was deposited until maximum depth was reached, then erosion occurred. Although the thermal gradient for the Lopatin model is generally lower than that for the general model, they are nearly equal at present day and at this point the model is approaching present day. Thus the Lopatin model goes deeper during a period where average thermal gradient is increasing for both models up until

the time of maximum depth. This results in higher temperatures for some of the sediment points in the Lopatin Model than for their counterparts in the general model. The resulting TTI gains for these sediment points in the Lopatin model are greater during this period than for the general model. Table 7. lists these results for the bottom sediment points in both models. Notice that the gain of TTI in the Lopatin model was greater than that of the general model during the time in which it was deeper than the general model (see also fig 16).

The conditions which will lead to a deeper Lopatin model are the following: If the formations descend to a depth which is far enough below their present depth such that the extent of their compaction at the this time is greater than the extent of their compaction at the present day, then the formations will be thinner than at the present day and the Lopatin model will be deeper. This, of coarse requires at least one erosion between the time at which the Lopatin model becomes deeper and the present. In our Salina basin model this time was about 80 M.Y.B.P. (see fig. 16) The Lopatin model remained below the general model from this time to the present.

To clarify the conclusion of (ref. 1) we state the following two rules:

1. If there are no periods of erosion in the geologic history of the basin the Lopatin model will underestimate the TTI.
2. If there are erosions in the geologic history of the basin such that the formations during any time period become thinner than they are at present day (due to compaction, not due to the erosions themselves), then it is quite possible that the Lopatin model may overestimate the TTI or compute a closer TTI (to the general model) due to cancellation of errors. The extent to which the overestimation occurs depends on the thermal parmeter values during the period in which the Lopatin model is deeper and how far deeper the Lopatin model remains and for how long.

C. Ardmore Basin Results

To further develop and test the general model it was also applied to the Ardmore basin of the southern Oklahoma Aulacogen. The lithology, thicknesses, geologic events and times along with the computed thicnesses are listed in Table 8.

Table 7. Comparison of Salina Basin results for General and Lopatin models.

TIME (M.Y.B.P)	DEPTH (GEN.) (M)	DEPTH (LOPATIN) (M)	TEMP. (GEN.) (DEG. C.)	TEMP. (LOPATIN) (DEG. C.)	TTI (GEN.)	TTI (LOPATIN)
107.4	1634	1537.5	79	73	17.3	11.1
65.0	1990.3	2055.7	97	105	31.1	26.3
0.0	1141.2	1141.2	61.4	60.4	44.6	41.6

Table 8. Summary of geologic events, formation lithologies and thicknesses for the Ardmore basin

UNIT	LITHOLOGY	START DEP. (M.Y.B.P)	STOP DEP. (M.Y.B.P)	THICKNESS (M) (OBS.)	THICKNESS (M) (CALC.)
REAGAN	SANDSTONE	525	513	175	190
FORT-SILL	LIMESTONE	513	507	360	374
SIGNAL MTN.	LIMESTONE	507	500	950	987
COOL-CREEK	LIMESTONE	500	492	500	521
KINDBLADE	LIMESTONE	492	486	350	370
W. SPRING CREEK	LIMESTONE	486	475	550	547
OIL CREEK	SANDSTONE	475	473	300	290
MCLISH	LIMESTONE	473	468	190	184
BROMIDE	LIMESTONE	468	460	375	356
VIOLA	LIMESTONE	460	440	300	278
SYLVAN	SHALE	440	435	125	116
HUNTON	LIMESTONE	435	360	100	101
WOODFORD	SHALE	360	345	200	198

a.) Gradual Changes in Flux due to Cooling of Basin

The flux in this application was computed by the method of Turcotte and Ahern in which the asthenosphere (mantle) cools slowly as the lithosphere grows and subsidence takes place. The heat flux from the basement gradually decreases with time and is given by the relationship (ref. 16):

$$(30) \quad Q = k_m(T_m - T_0)((K_m t)^{-.5})$$

where:

k_m = thermal conductivity of the mantle

T_m = temperature of the mantle
at point at which it becomes fluid

T_0 = temperature of the surface

K_m = thermal diffusivity of mantle

t = time since start of subsidence

This yields the basement flux curve of figure 18. To compare our results to those of Feinstein (ref. 15) the thermal conductivity of sediments was set to the constant value of 2.093 W/(M. DEG. C.) throughout the time period under consideration. The values for the other parameters were taken from the references mentioned in sec III.1 (these were the ones used in the Salina Basin and Gulf Coast models.) Since the sediment thermal conductivity was held constant throughout, if the model is correct, the average thermal gradients computed according to eq. (27) from the surface and basin bottom temperatures should be equal (or very close) to that computed from eq.(28) from the flux. If we divide the flux values in fig 18 by 2.093 we find that the resulting curve is (for all practical purposes) the same as the average thermal gradient curve of fig. 19 (computed from eq. (27)).

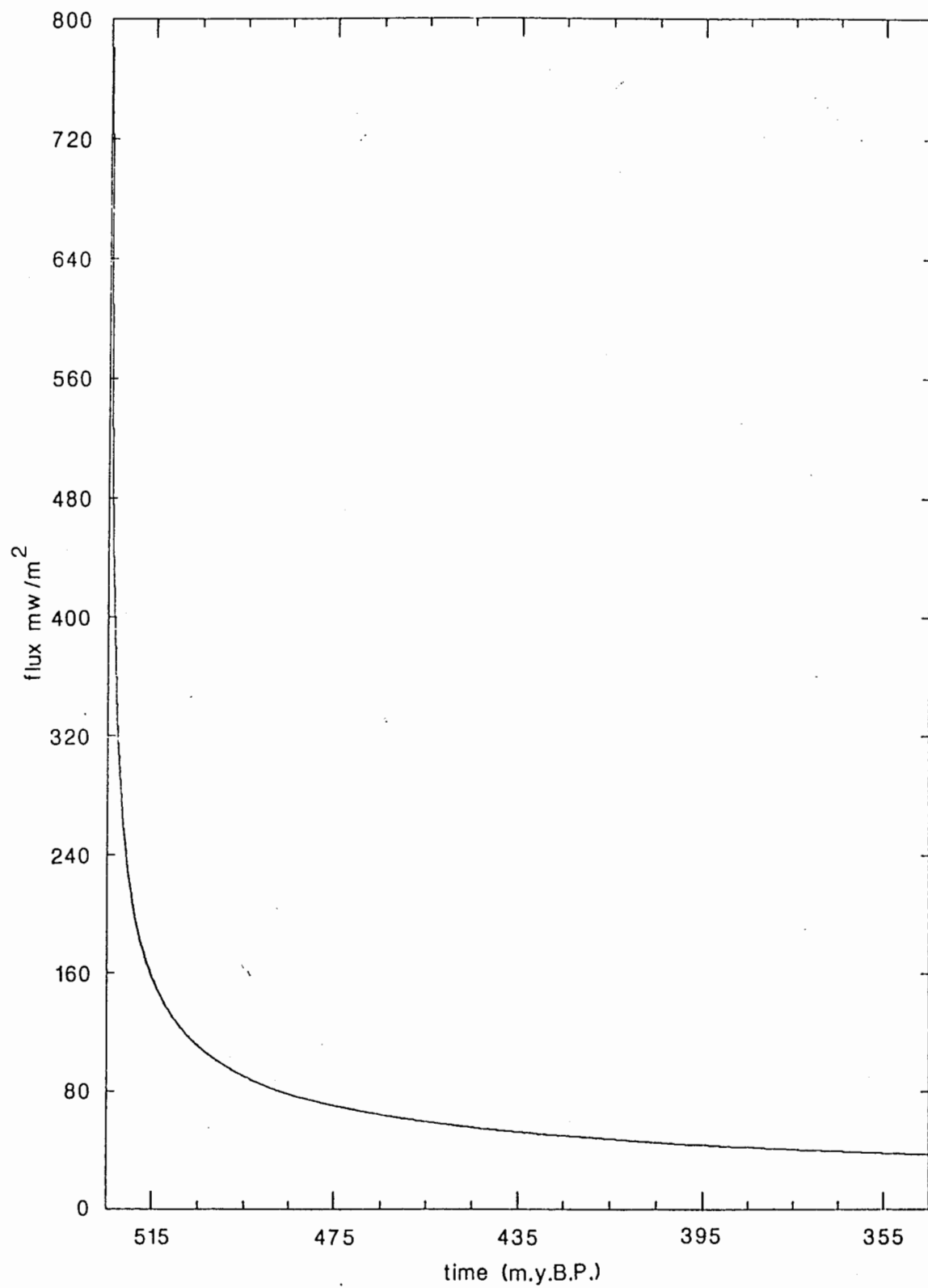


Fig. 18. Basement flux from isostatic subsidence model (eq. 30).

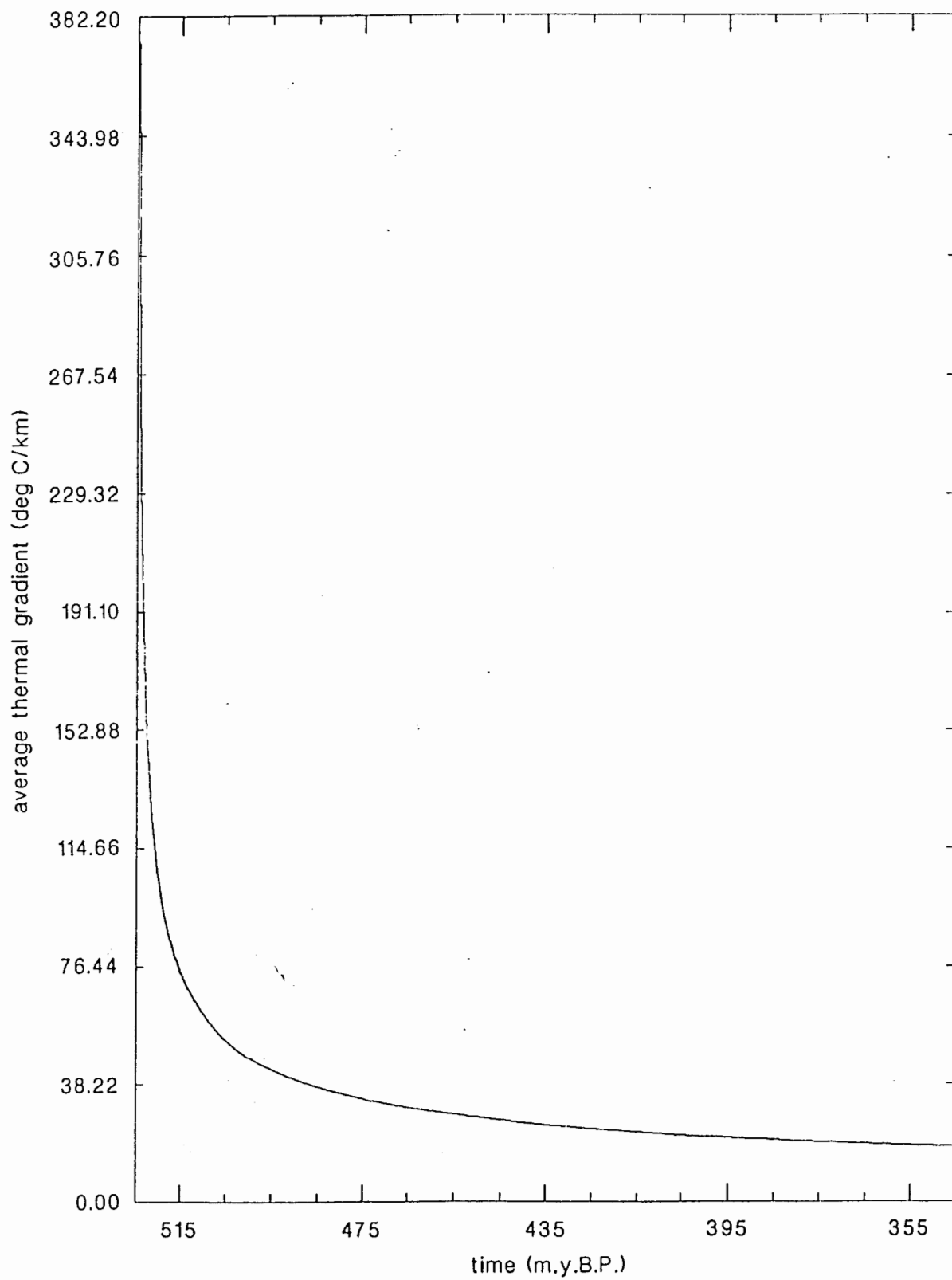


Fig. 19. Average thermal gradient vs. time (Ardmore basin model).

Fig. 20 shows the burial history graph upon which are superimposed the iso-temperature contours and the iso-TTI contours which mark the top (15) and bottom (160) of the oil window. Despite the differences in the two models, our results (depth of burial and iso-temperature contours) are in remarkable agreement with those of Feinstein (ref. 15). The slope changes of the top and bottom of the oil window reflect the changes in the sedimentation rate throughout time but any slope increases are retarded more and more by the gradually decreasing flux and thermal gradient (see table 4). Slope decreases are likewise enhanced. Note that whenever the sedimentation rate decreases the slopes of the two TTI contours increase but at a seemingly slow rate. Note that in a period of nearly constant sedimentation rate the slopes very gradually decrease reflecting the decreasing thermal gradient.

According to our results all formations from the bottom region of the Kindblade formation downward have entered the oil window. At the end of the time period under consideration (345 M. Y. B. P) the oil window was between 2300 meters and 3600 meters below the surface. The onset of oil generation occurred at about 493 M.Y.B.P at a depth of about 2200 meters.

b. Intrusions of Magma

Because of the enormous fluxes produced by intrusions of magma and the magnitude of the effect of basement flux on the TTI (see section III.2.A.d), one might expect that the ability to include intrusions as part of the general model would be very important. In the model that we are presenting, intrusions are described in a very simple way. They are described as a rectangular volume of magma with finite thickness at a certain depth below the basin bottom. The flux coming in from the basement is approximated as the sum of two components: 1) the flux resulting from cooling of the intrusive magma and 2) a background flux from below the intrusive layer. The Total flux at each time step is calculated from the following relationships:

$$(31) \quad Q_{Ti} = \bar{k}_B(T_{mi} - T_{Bi})/L_B$$

$$(32) \quad Q_{mi} = Q_{Ti} - Q_{bi}$$

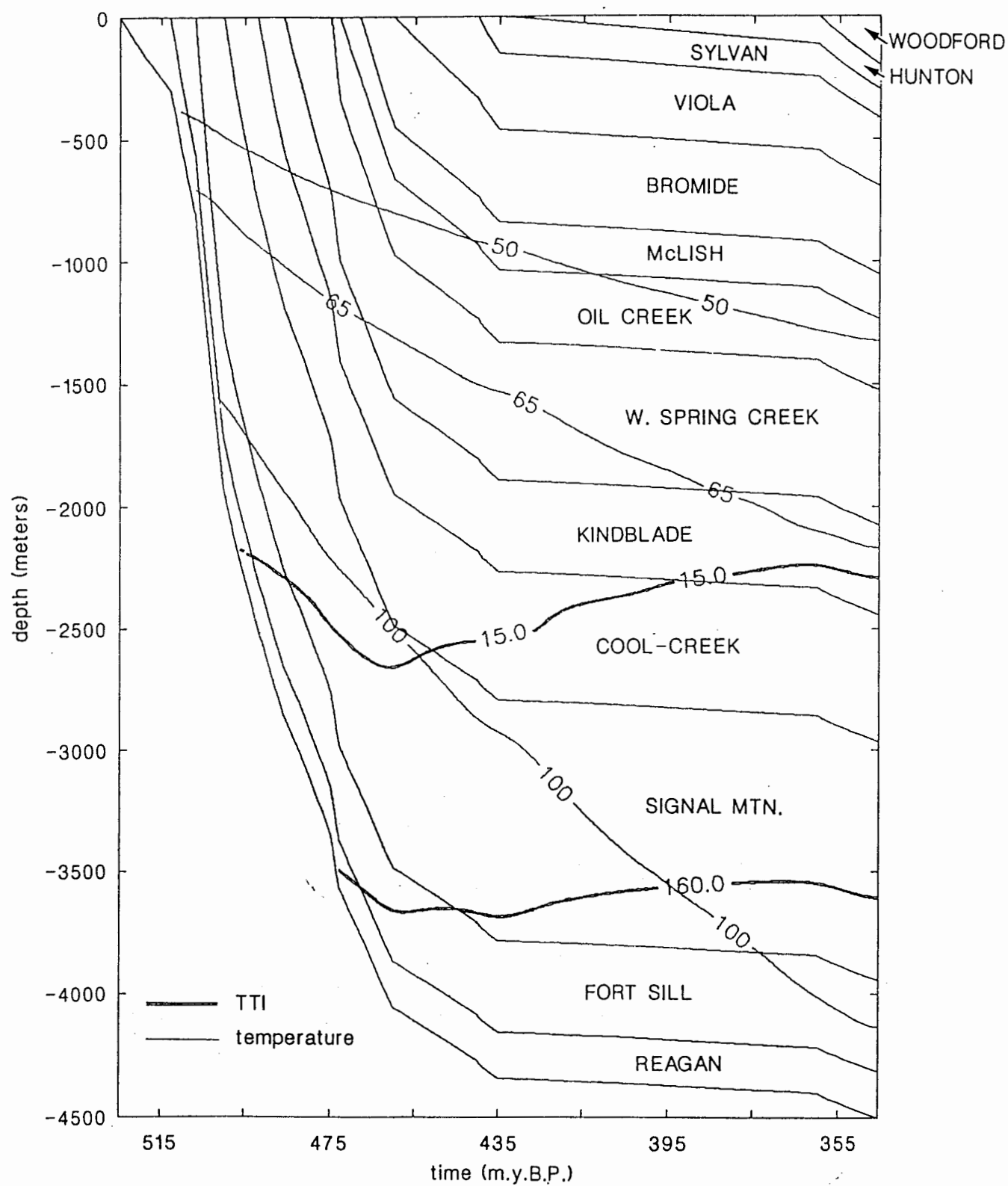


Fig. 20. Burial history with temperature and TTI contours (Ardmore basin).

$$(33) \quad T_{mi+1} = Q_m(\text{delt}/(ch)) + T_{mi}$$

where: Q_{Ti} = total flux at time step i

$\overline{k_B}$ = thermal conductivity of basement layer

T_{mi} = magma temperature at time step i

T_B = temperature of basin bottom at time step i

L_B = thickness of basement layer above magma

T_{mi} = magma temperature at the current time step

Q_{mi} = flux due to intrusive magma at time step i

Q_{bi} = background flux

delt= size of time step

= magma density

c = magma specific heat

h = magma thickness

As the intrusive magma cools, its flux component and its temperature drop until the magma is at equilibrium with the basement rock and ceases to release heat (and flux). At this point the total flux is equal to the background flux.

The time period in which the total flux decays from its initial, enormous value to the value of the background flux is relatively short (under 3 M. Y. for a magma thickness of 5000 meters) but increases with the thickness of the magma.

In fig. 21 the average thermal gradient for the Ardmore basin model with flux calculated according to eqs. (31) - (33) is plotted against time. Note the enormous drop in thermal gradient (from its initial value (about 800 deg/KM)) in the first 3 M.Y. of deposition. Since the background flux is constant, from this point on changes in average thermal gradient are due primarily to changes in thermal conductivity of the rock matrix and changes in thermal conductivity due to compaction. Comparison of Fig 21 to table 8 verifies that the changes in thermal conductivity are consistent with the type of sediment being deposited at time t .

Although the initial flux generated in this application was rather enormous (816 MW/M**2), because the flux decayed so rapidly, the column had not grown to appreciable length by the time the flux degenerated to nearly the value of the background flux. Since the temperatures throughout the time of decay were then rather low (under 35 degrees C) the contributions to the TTI at this point were very very small. Thus if intrusions occur at the beginning of deposition, when the column has not gained appreciable length (and thus Temperatures approaching $T_r=105$ Deg C have not been reached), they make little difference in the TTI summ regardless of the high fluxes generated. But if intrusions were to occur much later, say 435 M.Y.B.P, the enormous flux, occurring even for a short time would produce an enormous thermal gradient which for a 3500 meter column would produce an enormous bottom temperature. The irreversible contributions to the TTI would be astronomical.

D. Conclusions

Examination of eq. (14) shows that the TTI of a sediment point is exponentially dependent upon, and thus **extremely** sensitive to sediment point temperature. Thus in order to obtain a realistic assesment of the maturity of a basin using the TTI, one must be able to describe the thermal and geologic history of the basin as accurately as possible in the basin model. This involves obtaining realistic thermal parameters, sedimentation rates, compressibilities and porosities for the sediments in the basin (assuming thr lithology is precisely known). Examination of figures 2 through 13 demonstrates the extreme importance of thermal conductivity, basement flux, and sedimentation rate in describing the TTI function. We believe that the general model provides the opportunity to describe these properties well. One might argue that the (variable thermal conductivity) classical Lopatin model also provides this opportunity. But this model does not include compaction and fluid flow. We have demonstrated here (see figs. 4,5,8,9,12,14 and eq. 26) that compaction and fluid flow are vital to accurate computation of the thermal conductivity and thus the TTI function. Furthermore it is necessary to include compaction of sediments in order to

accurately compute the depth of a sediment point vs. time (sedimentation rate and compressibility essentially determine the grain velocity as a function of depth, see eq. (4)). This is also essential in computing the TTI function. One might also argue that the model requires more data than is realistically obtainable. But the present general model offers the flexibility to describe sedimentary basin maturity to a level of complexity which matches the available data and is more easily modified (than is the classical Lopatin model) should data become available.

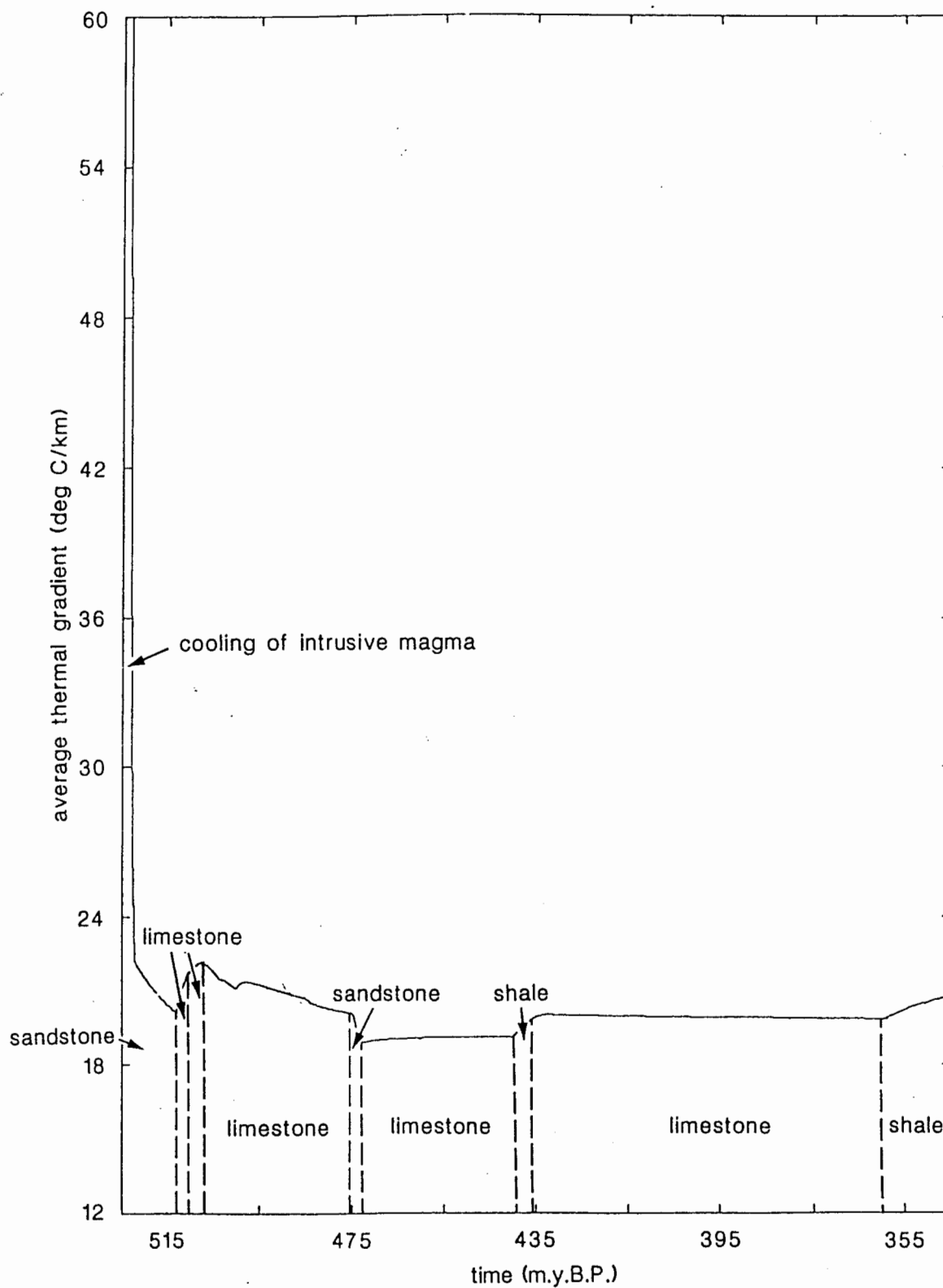


Fig. 21. Average thermal gradient vs. time for Ardmore basin (constant background flux with intrusion at deposition onset).

IV. Use of Computer Program.

Program NL.TTI, the program which simulates the basin development, is very general. Both Lopatin-type and general models may be implemented depending on the input. There are, in addition, a multitude of calculation, input and plotting options available. The input data file is quite complex. All data input, output, options and suggestions are discussed in the subsections which follow. The content of these subsections will center on the main input file. Optional input items will be indicated as such. For more information concerning program NL.TTI see the documentation in the source listing. One may, if desired, proceed to one of the complete examples starting on p. 113 and refer to the appropriate item(s) for explanation. The item numbers are listed to the right of each line in the examples and in the table of contents.

1) Input File

The following is a step by step discussion of the required input in the input file. This (input) file must be named **NL.TTI.IN**. The input data are grouped into numbered sets of one or more **items** for discussion.

ITEM #	DESCRIPTION
--------	-------------

- | | |
|-----|----------------------------------------------------------------------------------------|
| 1a. | (1 LINE, "A" FORMAT) name of main output file.
This is described in section IV.2.B. |
|-----|----------------------------------------------------------------------------------------|

POSSIBLE VALUES: Any legal system file
name up to 30 characters
long. This item must
NEVER BE IDENTICAL TO
ANY OTHER FILE NAME

example: :SI20:GGTEMP:NL.TTI.OUT

note: This is the main output file for the
program. See sec.IV.2.B and fig. 22

- | | |
|-----|-------------------------------------------|
| 1b. | (1 LINE, "A" FORMAT) title of calculation |
|-----|-------------------------------------------|

example: GULF COAST 3

POSSIBLE VALUES: Any character string up to 20
characters in length.

2. (1 LINE, "A" FORMAT) formation thickness input
units switch

POSSIBLE VALUES:

M requires input formation thicknesses
to be in meters

F requires the above to be in feet

example: M

3. (1 LINE, A FORMAT) magma intrusion switch

POSSIBLE VALUES:

Y If switch is set to this value
an intrusion of magma will begin
at the onset of deposition and
the flux will be calculated
according to eqs. (31) - (33) of
section III.2.C.a.

N No such intrusion will be
considered when the flux is
calculated.

example: N

4. Decompaction switch (1 LINE, "A" FORMAT, 1 ITEM)

POSSIBLE VALUES:

- | | |
|---|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Y | If switch has this value, then during an erosion (or uplift) the compressibility at a sediment point will be held at the value the value it had at the end of the last deposition. |
| N | If it has this value then the compressibility will be set to zero during the erosion and no decompaction will occur. |

example: Y

5. (1 LINE, FREE FORMAT) onset time for deposition
(in million years before the present (M. Y. B. P))

POSSIBLE VALUES: any FORTRAN real or
double precision number
> 0

UNITS: M. Y. B. P.

examples: 476
476.0

6. NOTE: FOR ITEMS 6 AND 7 THERE MUST BE F OCCURENCES OF A LINE CONTAINING ITEMS 6 AND A LINE CONTAINING ITEMS 7 WHERE F IS THE TOTAL NUMBER OF FORMATIONS. SEE EXAMPLES THAT FOLLOW. A LINE CONTAINING ITEMS 6 IS NECESSARY FOR AN EROSION OR A HIATUS BUT NO ITEMS 7 ARE NECESSARY FOR THESE EVENTS.

ITEMS 6: (1 LINE, FREE FORMAT) end time, thickness for a geological event

POSSIBLE VALUES: End time must be a positive, FORTRAN real or double precision number. Each successive end time must be less than the previous one and the last one must be zero.

For depositional events thicknesses are the **estimated present-day thicknesses neglecting erosion**.

Thickness may be any any fortran double precision or real number where:

Thickness > 0 indicates a deposition.

Zero thickness indicates hiatus.

Negative thickness indicates an erosion episode.

UNITS: end time---
M. Y. B. P.

thickness---
the units were
chosen as item 2.

example: 0,-300 corresponds to an erosion of 300 meters ending at the present day.

example: 150, 450 corresponds to a deposition of a unit with estimated present day thickness of 450 meters ending at 150 (M. Y. B. P.)

7. (1 LINE, FREE FORMAT) formation name, present porosity, initial porosity, final output switch

NOTE: a line containing items 7 is necessary for each deposition in the model but no such line exists for a hiatus or an erosion.

POSSIBLE VALUES: formation name-- any string of characters (up to length 15) enclosed in quotes

present porosity--any FORTRAN real number between zero and one exclusive. This is the estimate of the formation's porosity at present day

initial porosity--same as above except that this is the estimate of the formation's porosity at the at the start of it's deposition.

output switch---

"Y" indicates that burial history, temperature history, and TTI history will be printed for this formation.

"N" indicates that
the above information
will not be printed
(for this formation)

UNITS: porosity--dimensionless

examples:

example: "SIMPSON", .11, .55, "Y"

example of items 6 and 7 for 3 formations,
an erosion and a hiatus:

```
59, 7140
"CRETACEOUS", 0.1, 0.45, "Y"
39, -100
29, 0
1, 2223
"TERTIARY", 0.14, 0.45, "Y"
0, 666
"QUATERNARY", 0.32, 0.45, "N"
```

The above example of a portion of the input file contains 1 line of items 6 followed by 1 line of items 7 for the CRETACEOUS formation. These two lines are followed by 1 line of items 6 for an episode of erosion and one line of items 6 for a hiatus. Following these lines are 1 line of items 6 and 1 line of items 7 for deposition of the TERTIARY formation followed by 1 line of items 6 and 1 line of items 7 for deposition of the QUATERNARY formation.

Thermal History input

8. (MM LINES, WHERE MM IS THE NUMBER OF SURFACE TEMPERATURE VALUES THROUGHOUT THE BASIN'S GEOLOGIC HISTORY. FREE FORMAT) surface temperature, end time of temperature period:

example: 25.0, 140
20.0, 0

In this example the surface temperature is held fixed at 25.0 degrees Celcius from the onset of deposition until 140 M.Y.B.P and held fixed at 20.0 degrees Celcius from 140 M.Y.B.P until the present day.

POSSIBLE VALUES: temperature, end time-
any positive real
or double precision
FORTRAN number. Each
end time must be less
than the previous one
and the last one must
be zero.

UNITS: temperature-- DEG.
CELSIUS

end time-- M. Y. B. P.

The number of temperature periods in the above example is two. There may be as many temperature periods as one wishes. The only upper bound is the dimension of the arrays involved (see program documentation). Each line of items 8 in the file will indicate another temperature period.

9a. (1 LINE, A FORMAT) FLUX CHOICE

POSSIBLE VALUES: F indicates that flux
will be read in as
different time periods
of constant flux
(background flux if
magma intrusion switch
is set to Y). The
flux input in this
case is similar to
the surface
temperature input
(items 8).

T indicates that the flux will be estimated from the average present day thermal gradient using eqs. (12), (13), (27) and (28) and held constant (background flux held constant if magma intrusion switch is set to Y) throughout the calculation.

The value of the flux choice switch determines the input items that immediately follow.

IF ITEM 9a HAS BEEN SET TO F:

(the following item(s) must be read:

9b. (1 LINE, A FORMAT) Isostatic cooling switch.

POSSIBLE VALUES:

- Y if this switch is set to Y then the flux is computed by the method of Turcotte and Ahern (eq. (30)). No values for the basement flux are directly read.
- N if set to N then the flux values are read in the form of periods of constant flux as explained in item 9 above (see items 9b1 below).

IF ITEM 9b HAS BEEN SET TO N:

(the following items must be read:)

9b1. basement flux, end time (LL LINES, WHERE LL IS THE NUMBER OF PERIODS OF CONSTANT FLUX)

The format and possible values for these items are identical to items 8 (possible legal values, that is. The actual values for basement flux and surface temperature will seldom be identical and neither will the end times of the time periods (see

examples that follow).

IF ITEM 9a HAS BEEN SET TO T:

(The following items must be read:)

9c. Thermal Gradient Input Switch:
(1 LINE, A FORMAT)

POSSIBLE VALUES:

- T indicates that the bottom hole temperature and bottom hole depth will be read and the average present-day thermal gradient will be computed using these values (eq.(27)). The flux will be computed from the average thermal gradient and will remain constant.
- G indicates that the average thermal gradient will be read in directly. The flux will be computed as described above.

IF ITEM 9c HAS BEEN SET TO T:

(the following items must be read in:)

9c1. Bottom hole temperature, bottom hole depth
(1 LINE, FREE FORMAT)

POSSIBLE VALUES: for both items, any positive real or double precision FORTRAN number.

UNITS: bottom-hole temperature-
DEGREES CELSIUS

bottom-hole depth-
METERS

example: 226, 10442

In the above example the average present-day thermal gradient will be computed from a bottom-hole temperature of 226 DEG. C and a bottom depth of 10442 meters (assuming M was chosen as the value for item 2).

IF ITEM 9c HAS BEEN SET TO G:

9c2: Average Present-day Thermal Gradient:
(1 LINE, FREE FORMAT)

POSSIBLE VALUES: any positive FORTRAN real
or double precision number.

UNITS: (DEGREES/KILOMETER)

example: 20.

9d: (needed only if item 9a has been set to T) Topmost
present-day formation (1 LINE, A FORMAT UP TO 15
CHARACTERS)

POSSIBLE VALUES: any character string up to
15 characters in length.
longer ones will be truncated.

example: PERMIAN

warning: This item is case-sensitive,
i.e. PERMIAN is not the same
as permian or Permian etc..
This item must be identical
(in case as well as
spelling) to one of the
formation names in items 7
(without the quotes).

- 9e. (needed only if item 9a has been set to T) Name of totally or partially eroded formation, Its present-day thickness (a total of FERODE lines where FERODE is the number of the totally or partially eroded formations. The input format for these lines of two items each is free format (up to 15 chars.).

example: "PERMIAN", 154.0
"VIRGILIAN", 226.0
"HUNTON-SIL.", 0.0
"HUNTON-DEL", 0.0
"END", 0.0

Note that a formation name of "END" acts as a sentinel for the input list (signals the end of the input list). The thickness corresponding to the sentinel line is zero.

In this example, since T was chosen in response to item 9a, the flux will be computed from an estimate of the thermal gradient (eqs. (12), (13) and thus the actual present day thicknesses of all formations must be known. In item 7 the input thicknesses for these formations were the estimated present-day thicknesses neglecting erosion, not the actual present-day thicknesses.

POSSIBLE VALUES: eroded formation---any character string up to 15 characters long enclosed in quotes. Each character string must be identical to one of the formation names in items 7 (including the quotes).

present-day thickness---any FORTRAN real or double precision number > 0.

UNITS: (thickness) chosen in item 2.

- 10a. (needed only if item 3 was set to Y) intrusive magma temperature, intrusive magma thickness, basement rock thickness) (1 LINE, FREE FORMAT)

POSSIBLE VALUES: (both items) any positive
FORTRAN double precision or
real constant.

UNITS: temperature---DEG. CELSIUS
thicknesses--- METERS

examples: 1200., 5000., 1500.

- 10b. (needed only if item 9b has been set to Y, i. e. basement flux will be computed by the method of Turcotte and Ahern) mantle thermal conductivity, mantle thermal diffusivity, mantle temperature (1 LINE, FREE FORMAT, 3 ITEMS)

POSSIBLE VALUES: any positive, real
FORTRAN real or
double precision
number

UNITS: mantle thermal
conductivity--
(WATT/(METER DEG. C.)

mantle thermal
diffusivity--
METER²/SEC.

mantle temperature--
DEGREES CELSIUS

example: 2.093, 1.0e-6, 1200.

11. Thermal Parameters for Intrusive Magma and Basement Rock. (Items 11a-11f2 are needed only if item#3 has been set to Y (intrusion of magma is to occur at the onset of deposition.))

11 a. Number of magma specific heat values (1 LINE, FREE FORMAT).

POSSIBLE VALUES: any FORTRAN integer
> 0.

example: 5

11b. Magma Specific Heat Table. The magma specific heat table contains the values of the magma specific heat at various temperatures. It is a one-dimensional table whose input consists of the items discussed below.

11b1. Table temperatures. (NHEAT items where NHEAT is item #11a, the number of magma specific heat values, free format)

POSSIBLE VALUES: any positive, FORTRAN double precision or real number.
Each successive temperature must be greater than the previous one.

UNITS: DEGREES CELSIUS

example: 0.,25.0, 100.0, 125.0, 150.0

In the above example, the five temperatures corresponding to the five magma specific heat values (see item 11a) will be read in on one line (more lines may be used for the temperature input if needed).

- 11b2. Magma Specific heat values. (NHEAT items where NHEAT is item #11a. All of these items are input in free format (see examples).

POSSIBLE VALUES: any positive FORTRAN real or double precision number

UNITS: (CAL/(GRAM DEG. C))

example: .208, .210, .214, .220, .222

In the above example, the input line contains the five specific heat values corresponding to the five temperatures in item #11b1.

- 11c. Number of basement rock thermal conductivity values (FORMAT IDENTICAL TO THAT OF ITEM 11a).

POSSIBLE VALUES: same as item 11a.
example: 4

In the example above the user has indicated that there will be 4 basement thermal conductivity values. These are items 11d1 (see below).

- 11d. (11d1 and 11d2) Basement rock thermal conductivity table. Similar to items 11b except applies to basement rock thermal conductivity. The items which constitute the table are items 11d1 and 11d2 below.

- 11d1. Basement rock thermal conductivity temperatures (AS MANY LINES AS NEEDED, FREE FORMAT. THE NUMBER OF THESE ITEMS IS ITEM 11c.)

POSSIBLE VALUES: Same as items 11b1.

example: 0., 50., 100., 200

- 11d2. Basement rock thermal conductivity values (FORMAT IDENTICAL TO THAT OF ITEMS 11b2)

POSSIBLE VALUES: Same as items 11b2

example: 2.34, 2.17, 2.08, 1.96

The example above lists the values of the basement rock thermal conductivity corresponding to the temperatures which are items 11d1.

- 11e. Number of magma density values (FORMAT AND POSSIBLE VALUES ARE IDENTICAL TO THOSE OF ITEMS 11a AND 11c).

example: 1

The example above indicates that there will be one magma density value.

- 11f1. Magma density table temperatures (FORMAT AND POSSIBLE VALUES ARE IDENTICAL TO THOSE OF ITEMS 11b1 AND 11d1).

example: 0.0

The example above lists the single magma density table temperature of zero degrees Celsius.

- 11f2. Magma density table values (FORMAT AND POSSIBLE VALUES ARE IDENTICAL TO THOSE OF ITEMS 11b2 AND 11d2).

example: 2.9

In the above example the user has indicated that the magma density value at zero degrees Celsius is to be 2.9 grams per cubic centimeter.

12. Rock and Water Parameter Input

The following items are those necessary for input of the rock and water parameter values. These are read in the following manner:

1.) The parameter name is read
- 2.) The parameter values are read in tabular form (except for compressibility and permeability (see below). There may be as many tables of parameter values as the number of formations plus one. The required input (items 12) has the general organization sketched below:

```
PARAMETER NAME
NUMBER OF FORMATIONS TO WHICH DATA IS TO APPLY
LIST OF THESE FORMATIONS
PARAMETER TABLE DATA OR SET OF REFERENCE VALUES
(NEXT) NUMBER OF FORMATIONS TO WHICH DATA IS TO APPLY
(NEXT) LIST OF THESE FORMATIONS
(NEXT) PARAMETER TABLE OR SET OF REFERENCE VALUES
      .
      .
      .
      (etc.)
(NEXT) PARAMETER NAME
      .
      .
      .
      (etc.)
ENDPARAM
```

For the general model there must be one set of items 12 for each of the five water and rock parameters. These are (SPELLING MUST BE EXACTLY AS SHOWN):

```
CONDUCTIVITY          (thermal conductivity)
COMPRESSIBILITY
DENSITY
SPECIFIC HEAT
PERMEABILITY
```

For a linear (Lopatin-type) calculation one must enter items 12 for CONDUCTIVITY only. A parameter name of ENDPARAM indicates then end of items 12. Input items 12 are discussed in detail below:

12a. Parameter Name (1 line, A FORMAT)

POSSIBLE VALUES: See parameter list
above. ENDPARAM is
also allowed.

example: CONDUCTIVITY

warning: This input item is
case-sensitive. The
spelling of any
parameter name must be
exactly as shown
above. (all letters
must be in upper case)

12b. Number of formations to which the parameter table is
to apply (1 LINE, FREE FORMAT).

POSSIBLE VALUES: any positive FORTRAN
integer.

example: 2

In the example above, the first parameter table for
thermal conductivity (items 12d) is to apply to 2
formations. The formation names are items 12c.

If item 12b is equal to the total number of
formations plus one, then the table or set of reference
values for the current parameter will apply to all
formations including WATER. Items 12c in this case must
be omitted for this parameter.

12c. Formation names of those formations to which the parameter table is to apply. (EACH LINE IS "A" FORMAT, 1 NAME TO A LINE. THE NUMBER OF LINES IS ITEM 12b).

POSSIBLE VALUES: (each line) a
character string up
to 15 characters in
length. The character
string must be
identical to
one of the formation
names of items 7.
(without quotes, of
course)

example: CRETACEOUS
TERTIARY

The above example implies that the following table for the current parameter (thermal conductivity) will apply to 2 formations: Cretaceous and Tertiary.

NOTE: Items 12d (parameter table input) are needed only if the current parameter (item 12a) is NEITHER PERMEABILITY OR COMPRESSIBILITY

12d. Parameter Table. Three sets of items are required for each parameter table. This table contains the values for the parameter which corresponds to item 12a. It applies to the formations enumerated in item 12b and listed in items 12c. The input is described as follows:

12d1. number of temperatures (in table), number of pressures. (1 LINE, FREE FORMAT)

POSSIBLE VALUES: (both items) any FORTRAN integer
> 0

This line defines the dimensions of the table. (temperature is column index, pressure is the row index.

example: 3, 2

The above example implies that the table will have three temperatures and two pressures.

12d2. Table temperatures. (FREE FORMAT, AS MANY LINES AS NEEDED. THE NUMBER OF TEMPERATURES MUST BE EQUAL TO THE FIRST ITEM OF ITEMS 12d1 (in the example above, this is 3).

POSSIBLE VALUES: (each temperature) a positive, real or double precision FORTRAN number with the following restriction:

Each successive temperature must be greater than the previous one

These temperatures are limiting values for temperature ranges.

12d3. Table rows: row pressure followed by parameter values at each temperature for that pressure

POSSIBLE VALUES: pressure value---
must be greater than
that of the previous
row. It must
be a FORTRAN real or
double precision number
greater than or equal to
zero.

parameter values---
must be nonnegative
FORTRAN real or double
precision numbers

UNITS: Pressure: MPa

Parameters:

CONDUCTIVITY: W/(M DEG.C)

DENSITY: G./CM³

SPECIFIC HEAT:

KJ/(KG. DEG. C.)

examples of items

12d2 and 12d3: 0.0, 20.0., 40.0
 0.0, .88, .91, .94
 1.0, .88 .93, .96

The example above illustrates typical input of items 12d2 and 12d3, (parameter table). In this case the parameter is thermal conductivity. The first line contains the table temperatures. The remaining lines each contain a single pressure value followed by the thermal conductivity values at that pressure and each column temperature.

NOTE: The following input items are needed only if the current parameter is either COMPRESSIBILITY or PERMEABILITY. There is no table input (items 12d) for these parameters.

12e. parameter reference value 1, porosity value 1,
parameter reference value 2, porosity value 2
(1 LINE, FREE FORMAT, 4 INPUT ITEMS)

If the current parameter whose data is being read is COMPRESSIBILITY or PERMEABILITY two reference values of these parameters at two different porosities are needed to compute these parameters. These values are read in the order shown above.

***** NOTES ON WATER:

- 1) Water has no permeability and therefore no permeability input is needed (or allowed) for water.
- 2) The compressibility input for WATER is not in the format of items 12e. There are two options for WATER compressibility input. These generally follow the format of items 12d:
 - a.) If the table dimensions (items 12d1) are both greater than zero, then the water compressibility data is read in the tabular format of items 12d.

- b.) If the table dimensions are both zero, then the water compressibility table is computed from the table of water densities. There must be at least two water density values or else the water compressibility cannot be computed. These must correspond to two different pressure values.

Note that for water compressibility both of items 12d1 must be either positive or zero.

POSSIBLE VALUES: compressibilities and permeabilities--
any positive, double precision or real FORTRAN number.

porosities--
any positive real or double precision FORTRAN number less than 1 and greater than 0.

UNITS:

PERMEABILITY: 10^{-10} CM²

COMPRESSIBILITY:

10^{-10} M²/NEWTON

In the following example all of the (needed) items 12 are shown for COMPRESSIBILITY and PERMEABILITY for a 3-formation basin. Item numbers are shown to the right in boldface for reference. See also the discussion following.

example: (items 12 for other rock and
water parameters may precede)

```

.
.
.
.

COMPRESSIBILITY      (12a)
2                    (12b)
CRETACEOUS           (12c)
TERTIARY
1200, .5, 1, .05     (12e)
1                    (12b)
QUATERNARY           (12c)
600, .5, 1, .05     (12e)
1                    (12b)
WATER                (12c)
0,0                  (12d1)
PERMEABILITY         (12a)
1                    (12b)
CRETACEOUS           (12c)
.000001, 0.5,.000001, .05 (12e)
2                    (12b)
QUATERNARY           (12c)
TERTIARY
.00001,0.5, .000001, 0.05 (12e)
.
.
.
(items 12 for any remaining rock
and water parameters follow)

```

Item 12a is the parameter name and thus occurs only once per parameter. For each parameter, there must be as many occurrences of item 12b as there are sets of reference values (PERMEABILITY or COMPRESSIBILITY) or tables (all other rock and water parameters). Lists of items 12c (formation names) occur as many times for each parameter as does item 12b. The example above shows the input for COMPRESSIBILITY and PERMEABILITY, thus for all formations except WATER items 12e (not 12d) are required for these two parameters. In the example above CRETACEOUS and TERTIARY will share the same set of reference values for the computation of COMPRESSIBILITY while QUATERNARY will use a different set. For PERMEABILITY one set of reference values will be used solely for the CRETACEOUS formation while the TERTIARY and QUATERNARY formations will share the same set of reference values. Note that there are no items 12e for WATER. Instead, items 12d1 (table dimensions) are required. Since these are

both zero in the example, the WATER compressibility table will be computed from the WATER density table (DENSITY data for all formations and WATER are items 12 for DENSITY and may be read in before or after items 12 for COMPRESSIBILITY and PERMEABILITY). Tables of water compressibility (12d2, 12d3) are thus not required in the example. Had the table dimensions been positive, items 12d2 and 12d3 would have been required for water compressibility.

The following example shows all of the item 12 input needed for a 3-formation general model simulation.

```

example: .
          .
          (data items 1-11)           item #
          .
          .
          CONDUCTIVITY                (12a)
          2                           (12b)
          CRETACEOUS                   (12c)
          TERTIARY
          1,1                           (12d1)
              0                        (12d2)
          0, 2.0                       (12d3)
          1                           (12b)
          QUATERNARY                  (12c)
          2,1                           (12d1)
              0, 50.0                 (12d2)
          0, .88, .91                 (12d3)
          1                           (12b)
          WATER                        (12c)
          3,3                           (12d1)
              0, 25.0, 100.0          (12d2)
          0, .56, .61, .664           (12d3)
          9.9, .57, .615, .67
          98.7, .61, .65, .69
          COMPRESSIBILITY              (12a)
          2                           (12b)
          CRETACEOUS                   (12c)
          TERTIARY
          1200, .5, 1, .05             (12e)
          1                           (12b)
          QUATERNARY                  (12c)
          600, .5, 1, .05             (12e)
          1                           (12b)
          WATER                        (12c)
          0,0                          (12d1)
          PERMEABILITY                (12a)
          1                           (12b)
          CRETACEOUS                   (12c)
          1.0E-6, .5, 1.0E-7, .05     (12e)

```

2		(12b)
QUATERNARY		(12c)
TERTIARY		
1.0E-5, .5, 1.0E-6, 0.05		(12e)
DENSITY		(12a)
3		(12b)
CRETACEOUS		(12c)
TERTIARY		
QUATERNARY		
1, 1		(12d1)
0		(12d2)
0 2.65		(12d3)
1		(12b)
WATER		(12c)
3, 2		(12d1)
15., 25., 50		(12d2)
.099, .999, .998, .997		(12d3)
1.19, 1.0, .999, .998		
SPECIFIC HEAT		(12a)
1		.
CRETACEOUS		.
2, 1		etc.
20.0 50.0		
0.0, .855, .825		
1		
TERTIARY		
2, 1		
20.0, 50.0		
0.0, 1.1, 0.99		
1		
QUATERNARY		
2, 1		
20.0, 75.0		
0.0, .758, .805		
1		(12b)
WATER		(12c)
4, 4		(12d1)
0.0, 50., 100., 120.		(12d2)
099, 4.217, 4.181, 2.026, 2.005		(12d3)
2.47, 4.204, 4.175, 4.239, 4.304		(12d3)
5.92, 4.186, 4.167, 4.203, 4.230		(12d3)
8.88, 4.17, 4.161, 4.196, 4.223		(12d3)
ENDPARAM		
.		
.		

(remaining data items)

13. NN, TT, ERR, OPN, DEBUG, PINT, IBN (1 LINE, FREE FORMAT, 7 ITEMS)

where: NN+1 = Maximum number of sediment points used to define a column.

TT = Time steps per per sediment point deposition. The time required for deposition of a portion of sediment which is between two sediment points is further divided into TT time steps. This yields the smallest indivisible time step in the model.

ERR = Convergence criterion for the approximate solution of the pressure, temperature, and grain velocity equations.

OPN = Number of sediment points (nodes) per output interval. For example, if OPN=5, the depth, temperature, and TTI history of all formation barriers will be printed after the deposition of every fifth node at the onset of deposition and at the end of every major event. if OPN is greater than the total number of node-depositional time steps (those corresponding to the deposition of a single node, the erosion of a single node, or a similar period during hiatus) then this output will be printed only at the onset of deposition and at the end of every major event (deposition of a formation, erosion or hiatus.)

DEBUG = switch controlling diagnostic output for the first six node depositional time steps.

PINT = the average spacing between nodes for which values of temperature, pressure, Darcy velocity and porosity will be output at the end of each event in the depositional history of the basin.

IBN = If this switch has the value 1, the bottom-node pressure, porosity and compressibility will be printed at each node-depositional time step (see above).
If this switch has any other value this output will not be printed.

example: 500, 5, 0.01, 10, "OFF", 5, 0

See figure 22 for an example of the output of program NL.TTI.

The example above indicates that the maximum number of nodes (sediment points) describing the column will be 501. Each node-depositional time step will be divided into 5 time steps. The relative error tolerated in the iterative solution to the pressure, temperature and grain velocity equations will be 0.01.

POSSIBLE VALUES:

NN-- any positive integer subject to the dimensional limits of the program

TT-- any positive integer. suggested range: 5-10. The larger the value the longer will be the execution time

ERR-- any positive
FORTRAN real or double
precision number less
than 1. Suggested
value: 0.01.

OPN-- any positive
FORTRAN integer

DEBUG-- "YES" or "NO"
**quotes must be
included!**

PINT-- any nonegative
FORTRAN integer. A
value of 0 will cause
the output not to be
printed

IBN -- any positive
integer

For more output information see sample output (figs. 22).

Plotting input (items 14-21).

14. Plotting Option (1 LINE, "A" FORMAT).

POSSIBLE VALUES: S Plots are to be
 created using the
 SURFACE II graphics
 system

N No plots are to be
 made.

**NOTE: If item 14
has this value (N)
NO MORE INPUT DATA
IS REQUIRED FOR
THE PROGRAM. (ITEMS
15-21 ARE NOT
NEEDED)**

15. Plotting Switches:

Formation-plot, temperature-contour-plot,
TTI-contour-plot, TTI vs. TIME plot,
thermal gradient plot, Flux plot

(1 LINE, 5(A, 1X), A FORMAT, 6 ITEMS)

example: Y Y Y N N N

**NOTE: THIS LINE MUST START IN COLUMN 1 AND THERE
MUST BE AT LEAST ONE SPACE BETWEEN EACH
ITEM.**

POSSIBLE VALUES:

A value of Y for any of these switches
indicates that the corresponding plotting
option has been chosen. A value of N
indicates that the option has not been
chosen. All plotting options are
explained on the following page.

Formation-plot:

If this item has the value Y then
then the program will create and
write to three Formation plotting files:
(See items 16c.)

- a. A file containing all formation
bottom points for those formations
which are chosen to be plotted.
- b. A file containing numeric labels
of all formations.

c. A file containing formation barrier points for the oldest (deepest) formation along with the (0,0) point. (These will define the border of the plot).

in addition, items 16 must be read.

Temperature-contour-plot:

If this item has the value Y then the program will create a temperature contour plotting file which will contain the temperatures corresponding to times and depths determined using items 17.

In addition, all of items 17 must be read.

TTI-contour-plot:

If this item has the value Y then the program will create a TTI contour plotting file which will contain the TTI's corresponding to the times and depths determined using items 18.

TTI vs. time plot:

If this item has the value Y then the program will create a file containing TTI points as a function of time for all formations chosen in items 19.

Thermal-gradient-plot:

If this item has the value Y then the program will create a file containing the thermal gradient values at each node-depositional time step starting at a time which is item 20a. In addition, items 20 must be read.

Flux-plot:

If this item has the value Y then the program will create a file containing the basement flux values at each node-depositional time step (Items 21 must be

read).

16. Formation Barrier Plotting Input.

(NEEDED ONLY IF FORMATION-PLOT SWITCH WAS SET TO Y)

16a. Number of formations to be plotted (1 LINE, FREE
FORMAT).

POSSIBLE VALUES: Any positive number less
than or equal to the
total number of
formations.

example: 3

In the above example the depth of the bottom sediment
point of three formations is to be plotted as a function
of time.

16b. Names of formations whose bottom sediment point is to be
plotted against time (x LINES, WHERE x IS ITEM 16a.,
EACH LINE CONTAINS 1 ITEM IN "A" FORMAT).

POSSIBLE VALUES: A character string
of 15 characters or
less. Each string
must be identical
to one of the formation
names (items 7) without
the quotes.

example: CRETACEOUS
TERTIARY
QUATERNARY

16c. Names of formation plotting files (3 LINES, EACH IN "A"
FORMAT, 1 ITEM EACH).

POSSIBLE VALUES: Any character string of
30 characters or less in
length. String must
be a legal file name.

example: NL.TTI.BOUND
NL.TTI.POST
NL.TTI.BORD

The first file name will be that of the file which will contain the formation barrier points (bottom sediment points) of the formations corresponding to items 16b.

The second filename will be that of the file containing the numerical formation labels (these are numbered from one to the total number of formations starting with the oldest and are in order of age. The third file name contains the border of the plot (bottom formation barrier plus surface plus right edge.

17. Point Distribution Parameters for Temperature Contour Plot.

(ITEMS 17 NEEDED ONLY IF TEMPERATURE-CONTOUR-PLOT SWITCH HAS VALUE Y)

17a. Time-step, depth-step, end-time (M LINES, FREE FORMAT, WHERE M CAN BE ANY POSITIVE INTEGER).

POSSIBLE VALUES: time-step, depth-step--
any positive integer.

If depth-step has value:

- | | |
|---|-------------------------------------------------------------------------------------------------------|
| 1 | At a given time, temperatures at every node point will be written to a temperature output file. |
| 2 | At a given time, temperatures at every other node point will be written to a temperature output file. |

3 At a given time,
 temperatures at every
 third node point will
 will be written to a
 temperature output
 file.

.
.
etc.

If time-step has value:

1 Nodal temperatures
 (at the nodes
 determined by item
 17a.) will be written
 to the temperature
 output file at every
 node-depositional time
 step.

2 Nodal temperatures
 at every other such
 time step will be
 written to this file.

.
.
etc.

end-time: May be any positive
 FORTRAN real or double
 precision number less
 than the start time for
 deposition (item 5).
 Each successive end
 time must be less than
 the previous.

example: 1,1, 160.
 2,2 60.
 1,2, 0.

Items 17a define a temperature grid whose independent variables are depth and time. In the example above, temperatures at every node-depositional time step at every node point from the onset of deposition until 160 M.Y.B.P will be written to the temperature output file. From this time until 60 M.Y.B.P temperatures at every other node-depositional time step at every other node point will be written to the temperature output file. From this time to the present, temperatures at every node depositional time step at every other node point will be written to the temperature output file.

- 17b. Name of output file containing temperature points.
(1 LINE, "A" FORMAT, 1 ITEM)

POSSIBLE VALUES: any legal file name up
to 30 characters in
length.

example: :SI20:GGTEMP:NL.TTI.TEMPS

18. TTI Contour Plotting Input.

(NEEDED ONLY IF TTI-CONTOUR-PLOT SWITCH WAS SET TO Y (ITEMS
15))

- 18a. Time-step, Depth step, end-time. (M LINES, FREE FORMAT,
3 ITEMS PER LINE, M MAY BE ANY POSITIVE INTEGER)

The format and possible values are identical to
items 17a. (see Items 17a. but replace "temperature"
with "TTI" when you read the explanations.)

- 18b. Name of output file containing TTI points.
(1 LINE, "A" FORMAT, 1 ITEM)

Everything here is the same as item 17b. except

MAKE SURE THAT THE ACTUAL FILENAMES CHOSEN FOR

ITEMS 18b AND 17b ARE NOT THE SAME

18c. Number of contour lines to be plotted. (1 LINE, FREE
FORMAT, 1 ITEM)

POSSIBLE VALUES: Any positive FORTRAN
integer.

example: 2

The example above indicates that two TTI contours
will be plotted.

18d. Values of the TTI contours to be plotted (Y ITEMS,
WHERE Y IS ITEM 18c. AS MANY LINES AS NEEDED)

POSSIBLE VALUES: Any non-negative FORTRAN
real or double precision
number.

example: 15., 160.

In the example above, the iso-TTI contour values 15
160 will be written to the an output file (whose name
is the next item). This output file may be used by
SURFACE II in plotting the TTI contours.

This file also contains the depth and time points
at which the contours intersect the basin bottom.

18e. Name of file containing the values of the TTI contours
to be plotted. (1 LINE, A FORMAT)

Format is the same as that of items 17b and 18b but
again, **MAKE SURE THAT THERE ARE NO DUPLICATE FILE
NAMES.**

19. TTI vs. time x-y plot input.

(NEEDED ONLY IF TTI VS TIME SWITCH WAS SET TO Y (SEE ITEMS 15))

- 19a. Number of formations whose Bottom-node TTI vs. time dependence is to be plotted. (1 LINE, FREE FORMAT, 1 ITEM)

POSSIBLE VALUES: Any positive integer less than or equal to F, the number of formations.

example: 2

The example above indicates that there will be two formations whose bottom-node TTI vs. time dependence will be plotted.

- 19b. Formations whose TTI's are to be plotted. (Z LINES, WHERE Z IS ITEM 19a., Z ITEMS, (1 ITEM TO A LINE), EACH LINE IS "A" FORMAT)

POSSIBLE VALUES: Character strings must correspond exactly to one of the formations corresponding to items 7 without the quotes.

example: CRETACEOUS
TERTIARY

In the example above the the bottom-node TTI's of the CRETACEOUS and TERTIARY formations are to be plotted against time. These points will be written to a file whose name is item 19c.

19c. TTI vs. time plotting file. (1 LINE, "A" FORMAT, 1 ITEM).

POSSIBLE VALUES: Any character string
which is a legal file
name.

example: :SI20:GGTEMP:TTIXY

In the example above the user has chosen a legal AOS/CLI file name for the TTI vs. time plotting file. TTI vs. time points will be written to this file at every node-depositional time step.

20. Thermal gradient plotting input.

(NOT NEEDED IF THERMAL-GRADIENT-PLOT SWITCH HAS BEEN SET TO Y)

20.a Start time for thermal gradient plot (1 LINE, FREE FORMAT, 1 ITEM)

POSSIBLE VALUES: Any positive FORTRAN
real or double precision
number less than or
equal to item 5, the
onset time for
deposition.

UNITS: M. Y. B. P.

example: 138.0

In the example above, the user has indicated that Thermal gradient vs. time points are to be written to the thermal gradient plotting file starting at 138 M.Y.B.P (and finishing at the present day).

- 20b. Name of output file which is to contain the thermal gradient vs. time points. (1 LINE, "A" FORMAT)

POSSIBLE VALUES: Any character string
which is a legal file
name and is less than
or equal to thirty
characters in length.

example: :SI20:GGTEMP:TGVT

The example above indicates that the thermal gradient vs. time points are to be written to a file named :SI20:GGTEMP:TGVT, a legal AOS/CLI file name. Points will be written at each node depositional time step. This file will be used by the SURFACE II plotting package to create a file which can be used to make the actual plot.

21. Basement flux plotting input.

(NEEDED ONLY IF BASEMENT-FLUX-PLOT SWITCH HAS VALUE Y)

- 21a. Start time for basement flux vs. time plot (1 LINE, FREE FORMAT, 1 ITEM)

Identical format to that of item 20a.

- 21b. Basement flux plotting file (1 LINE, "A" FORMAT, 1 ITEM).

Identical format to that of item 20b.

complete example 1:

The following is an example of a complete input file which, if used as input to program NL.TTI, would result in a simulation using the general model. Item numbers are provided to the right of each line in **boldface** for reference.

	item number
:SI20:GGTEMP:NL.TTI.OUTPUT	(1a)
GULF COAST 3	(1b)
M	(2)
N	(3)
Y	(4)
138	(5)
59, 2221	(6)
"CRETACEOUS",0.1,0.45,"Y"	(7)
1, 7178	(6)
"TERTIARY", 0.2,0.45,"Y"	(7)
0, 652	(6)
"QUATERNARY",0.35,0.45,"Y"	(7)
20, 0.0	(8)
F	(9a)
N	(9b)
40.0, 0.0	(9b1)
CONDUCTIVITY	(12a)
2	(12b)
CRETACEOUS	(12c)
TERTIARY	(12c)
2,1	(12d1)
0.0, 25.0	(12d2)
0.0, 2.0, 2.04	(12d3)
1	(12b)
QUATERNARY	(12c)
1,1	(12d1)
0.0, 25.0	(12d2)
0.0, 1.8, 1.88	(12d3)
1	(12b)
WATER	(12c)
4,3	(12d1)
0, 25., 50., 75.	(12d2)
4.93, .567, .613, .645, .667	(12d3)
14.8, .573, .617, .650, .673	(12d3)
28.0, .579, .621, .655, .677	(12d3)
COMPRESSIBILITY	(12a)
2	(12b)
CRETACEOUS	(12c)
TERTIARY	(12c)
1200, .5, 1, .05	(12e)
1	(12b)

QUATERNARY	(12c)
600, .5, 1, .05	(12e)
1	(12b)
WATER	(12c)
0,0	(12d1)
PERMEABILITY	(12a)
1	(12b)
CRETACEOUS	(12c)
1.0E-5, .5, 1.0e-7, .05	(12e)
2	(12b)
QUATERNARY	(12c)
TERTIARY	(12c)
1.0E-5, .5, 1.0E-6, 0.05	(12e)
DENSITY	(12a)
3	(12b)
CRETACEOUS	(12c)
TERTIARY	(12c)
QUATERNARY	(12c)
1,1	(12d1)
0	(12d2)
0 2.65	(12d3)
1	(12b)
WATER	(12c)
3,2	(12d1)
15., 25., 50.	(12d2)
.099, .999, .998, .997	(12d3)
1.19, 1.0, .999, .998	(12d3)
SPECIFIC HEAT	(12a)
1	(12b)
CRETACEOUS	(12c)
2,1	(12d1)
20.0, 50.0	(12d2)
0.0, .855, .825	(12d3)
1	(12b)
TERTIARY	(12c)
2,1	(12d1)
20.0, 50.0	(12d2)
0.0, 1.1, 0.99	(12d3)
1	(12b)
QUATERNARY	(12c)
2, 1	(12d1)
20.0, 75.0	(12d2)
0.0, .758, .805	(12d3)
1	(12b)
WATER	(12c)
4,4	(12d1)
0.0, 50., 100., 120.	(12d2)
.099, 4.217, 4.181, 2.026, 2.005	(12d3)
2.47, 4.204, 4.175, 4.239, 4.304	(12d3)
5.92, 4.186, 4.167, 4.203, 4.230	(12d3)
8.88, 4.17, 4.161, 4.196, 4.223	(12d3)
ENDPARAM	(12a)

500, 5, 0.01, 1, "OFF",200,0	(13)
S	(14)
Y Y Y Y Y N	(15)
3	(16a)
CRETACEOUS	(16b)
TERTIARY	(16b)
QUATERNARY	(16b)
NL.TTI.BOUND	(16c)
NL.TTI.POST	(16c)
NL.TTI.BORD	(16c)
2,2, 3.0	(17a)
2,1, 0.	(17a)
:SI20:GGTEMP:NL.TTI.TEMPS	(17b)
3,2,120.0	(18a)
2,2,30.0	(18a)
2,2,15.0	(18a)
2,2,4.0	(18a)
2,1,0.0	(18a)
:SI20:GGTEMP:NL.TTI.TTIF	(18b)
2	(18c)
15.0, 160.0	(18d)
nl.tti.ledge	(18e)
2	(19a)
CRETACEOUS	(19b)
TERTIARY	(19b)
:SI20:GGTEMP:NL.TTI.TTIXY	(19c)
138	(20a)
:si20:ggtemp:NL.TTI.TG	(20b)

complete example 2:

In the following example, an intrusion of magma is to occur at the onset of deposition. The constant background flux is to be computed from an input thermal gradient.

:SI20:GGTEMP:ARDOUT	(1a)
ARDMORE BASIN 1	(1b)
M	(2)
Y	(3)
Y	(4)
180	(5)
168, 175.	(6)
"REAGAN",.10,.55, "Y"	(7)
162, 360.0	(6)
"FORT-SILL",0.8,.50,"Y"	(7)
155, 950.	(6)
"SIGNAL-MTN.",.10,.50,"Y"	(7)
147.,500.	(6)
"COOL-CREEK",.12,.57,"Y"	(7)
141.,350	(6)

"KINDBLADE",.13,.57,"Y"	(7)
130, 550.	(6)
"WEST-SPR.-CR.",.21,.50,"Y"	(7)
128,300.	(6)
"OIL-CREEK",.29,0.40,"Y"	(7)
123.,190.	(6)
"MCLISH",.28, .50, "Y"	(7)
115, 375	(6)
"BROMIDE", .32, .50 "Y"	(7)
95., 300.	(6)
"VIOLA", .38, .50, "Y"	(7)
90.0, 125.0	(6)
"SYLVAN", .36, .58, "Y"	(7)
15.0, 100.0	(6)
"HUNTON",.40,.50,"Y"	(7)
0.0, 200.0	(6)
"WOODFORD", .46, .58, "Y"	(7)
20.0, 0.0	(8)
T	(9a)
G	(9c)
22.0	(9c2)
WOODFORD	(9d)
"END",0	(9e)
1200., 5000., 1500	(10a)
4	(11a)
0., 100., 300., 400.	(11b1)
.858, .963, 1.1, 1.14	(11b2)
4	(11c)
0, 50, 100, 200	(11d1)
2.34, 2.00, 1.70, 1.37	(11d2)
1	(11e)
0.	(11f1)
2.9	(11f2)
CONDUCTIVITY	(12a)
2	(12b)
REAGAN	(12c)
OIL-CREEK	(12c)
4,1	(12d1)
0., 50., 100., 200.	(12d2)
0., 5.49, 4.78,4.31, 3.62	(12d3)
9	(12b)
FORT-SILL	(12c)
SIGNAL-MTN.	(12c)
COOL-CREEK	(12c)
KINDBLADE	(12c)
WEST-SPR.-CR.	(12c)
MCLISH	(12c)
BROMIDE	(12c)
VIOLA	(12c)
HUNTON	(12c)
6,1	(12d1)
0., 25., 50., 100., 200.,300.	(12d2)

0., 3.0,2.77,2.57,2.3, 2.01, 1.4	(12d3)
2	(12b)
SYLVAN	(12c)
WOODFORD	(12c)
6,1	(12d1)
0., 25., 100.,200.,300., 400.	(12d2)
0.,0.88,0.91, 0.94,1., 1.06, 1.12	(12d3)
1	(12b)
WATER	(12c)
4, 3	(12d1)
0, 50., 100., 150.	(12d2)
0.99,.563,.61, .664, .025	(12d3)
.493,.563,.611,.6643,.6803	(12d3)
9.87,.571,.615, .6693,.6862	(12d3)
COMPRESSIBILITY	(12a)
2	(12b)
REAGAN	(12c)
OIL-CREEK	(12c)
900, .5, .1, 0.05	(12e)
9	(12a)
FORT-SILL	(12c)
SIGNAL-MTN.	(12c)
COOL-CREEK	(12c)
KINDBLADE	(12c)
WEST-SPR.-CR.	(12c)
MCLISH	(12c)
BROMIDE	(12c)
VIOLA	(12c)
HUNTON	(12c)
850,.5,1.0,0.05	(12e)
2	(12b)
SYLVAN	(12c)
WOODFORD	(12c)
2200,.5,1.0,0.05	(12e)
1	(12a)
WATER	(12b)
0,0	(12d1)
PERMEABILITY	(12a)
2	(12b)
REAGAN	(12c)
OIL-CREEK	(12c)
100., .5, .001, .05	(12e)
9	(12b)
FORT-SIL	(12c)
SIGNAL-MTN.	(12c)
COOL-CREEK	(12c)
KINDBLADE	(12c)
WEST-SPR.CR.	(12c)
MCLISH	(12c)
BROMIDE	(12c)
VIOLA	(12c)
HUNTON	(12c)

50., .5, .0001, .05	(12e)
2	(12b)
SYLVAN	(12c)
WOODFORD	(12c)
.001, .5, .00000001, .05	(12e)
SPECIFIC HEAT	(12a)
2	(12b)
SYLVAN	(12c)
WOODFORD	(12c)
5, 1	(12d1)
0., 50., 100., 200., 300.	(12d2)
0., 0.8, 0.84, .871, 1.0, 1.01	(12d3)
9	(12b)
FORT-SILL	(12c)
SIGNAL-MTN.	(12c)
COOL-CREEK	(12c)
KINDBLADE	(12c)
WEST-SPR.-CR.	(12c)
MCLISH	(12c)
BROMIDE	(12c)
VIOLA	(12c)
HUNTON	(12c)
1, 1	(12d1)
0.	(12d2)
0, .855	(12d3)
2	(12b)
REAGAN	(12c)
OIL-CREEK	(12c)
2, 1	(12d1)
0.0, 100.0	(12d2)
0., .825, 1.1	(12d3)
1	(12b)
WATER	(12c)
4, 4	(12d1)
0.0, 50., 100., 120.	(12d2)
.099, 4.217, 4.181, 2.026, 2.005	(12d3)
2.47, 4.204, 4.175, 4.239, 4.304	(12d3)
5.92, 4.186, 4.167, 4.203, 4.230	(12d3)
8.88, 4.17, 4.161, 4.196, 4.223	(12d3)
DENSITY	(12a)
2	(12b)
SYLVAN	(12c)
WOODWARD	(12c)
1, 1	(12d1)
0.	(12d2)
0., 2.87	(12d3)
9	(12b)
FORT-SILL	(12c)
SIGNAL-MTN.	(12c)
COOL-CREEK	(12c)
KINDBLADE	(12c)
WEST-SPR.-CR.	(12c)

MCLISH	(12c)
BROMIDE	(12c)
VIOLA	(12c)
HUNTON	(12c)
3,1	(12d1)
0.0, 25., 50.	(12d2)
0., 2.65, 2.6, 2.55	(12d3)
2	(12b)
REAGAN	(12c)
OIL-CREEK	(12c)
1,1	(12d1)
0	(12d2)
0.,2.61	(12d3)
1	(12b)
WATER	(12c)
4,4	(12d1)
15., 20., 30., 35.	(12d2)
.0987, .9991,.9982,.9997,.9957	(12d3)
2.47, 1.0003,.9993,..9981,.9967	(12d3)
4.74, 1.0013, 1.0004,.9992,.9977	(12d3)
7.5, 1.0026, 1.0016, 1.0004,.9990	(12d3)
ENDPARAM	(12a)
350, 5, .01, 10 "ON", 30.0, 0	(13)
S	(14)
Y Y Y Y Y Y	(15)
13	(16a)
REAGAN	(16b)
FORT-SILL	(16b)
SIGNAL-MTN.	(16b)
COOL-CREEK	(16b)
KINDBLADE	(16b)
WEST-SPR.-CR.	(16b)
OIL-CREEK	(16b)
MCLISH	(16b)
BROMIDE	(16b)
VIOLA	(16b)
SYLVAN	(16b)
HUNTON	(16b)
WOODFORD	(16b)
NL.TTI.PLOT13	(16c)
NL.TTI.POST	(16c)
NL.TTI.BORD	(16c)
1,1,160.	(17a)
2,2, 60.0	(17a)
1,2, 0.0	(17a)
:SI20:GGTEMP:NL.TTI.TEMPS	(17b)
3,3,120.	(18a)
2,2,110.0	(18a)
1,2,0.0	(18a)
:SI20:GGTEMP:NL.TTI.TTIF	(18b)
2	(18c)
15, 160	(18d)

NL.TTI.LEDGE	(18e)
2	(19a)
REAGAN	(19b)
KINDBLADE	(19b)
:SI20:GGTEMP:NL.TTI.TTIXY	(19c)
180.0	(20a)
NL.TTI.TG	(20b)
180.0	(21a)
NL.TTI.Q	(21b)

Note that items 9e consist only of the sentinel line "END",0. This means that there are no eroded or partially eroded formations.

Complete example 3: Lopatin- type (linear) calculation.

Note that in this example the only rock and water parameter needed (if there is no intrusion and isostatic cooling is not in effect) is THERMAL CONDUCTIVITY. COMPRESSIBILITY, PERMEABILITY, SPECIFIC HEAT, and DENSITY are all set to zero in a linear calculation. Omitting all rock and water parameters except THERMAL CONDUCTIVITY causes the program to use the linear rather than the general model (see complete example 3).

:SI20:GGTEMP:LINOUT	(1a)
GULF COAST LIN.	(1b)
M	(2)
N	(3)
Y	(4)
138	(5)
59, 2221	(6)
"CRETACEOUS",0.1,0.1,"Y"	(7)
1,7178	(6)
"TERTIARY",0.2,0.2,"Y"	(7)
0, 652	(6)
"QUATERNARY",0.35,0.35,"Y"	(7)
20.0, 0.0	(8)
F	(9a)
N	(9b)
40, 0.0	(9b1)
CONDUCTIVITY	(12a)
3	(12b)
CRETACEOUS	(12c)
TERTIARY	(12c)
QUATERNARY	(12c)
1,1	(12d1)
0	(12d2)
0, 2.0	(12d3)
1	(12b)
WATER	(12c)
1,1	(12d1)

0	(12d2)
0., .63	(12d3)
ENDPARAM	(12a)
500, 5, 0.01, 1, "OFF", 200,0	(13)
N	(14)

A flow chart describing the input is shown in fig 24.

2) Output files (all are required except where indicated).

A.) **Main Output File.** This file contains all principal output information. An example of this output file is shown on the following pages (fig. 22). This output file is controlled by items 13. The contents of the input file used to produce this output file are listed on the pages immediately following fig. 22.

B.) **SURFACE II Plotting Files (optional).** Discussed along with items 16-21 above.

C.) **Present-day Summary File.** Contains a table with the formation names, present-day depths, present-day thicknesses, present-day bottom sediment point temperatures, and formation barrier TTI's of all formations existing at the present day. Fig. 23 is an example of the output to this file. The name of this file is NL.TTI.SUMM.

D.) **Batch output file.** The batch output file contains a listing of quantities related to computation of the (vertical) Darcy velocity. These are:

DEPTH
WATER VISCOSITY
ROCK PERMEABILITY
WATER DENSITY
TERM1
TERM2

Where TERM1 and TERM2 are elevation and pressure force (per unit volume) terms.

$$\begin{aligned}
 (34) \quad \text{TERM1} &= \rho * G \\
 (35) \quad \text{TERM2} &= \frac{\partial p}{\partial z}
 \end{aligned}$$

WELL: GULF COAST TEST

Fig. 22, Sample Output.

THE DECIMAL ERROR CRITERION FOR CONVERGENCE WAS .01000.

SURFACE TEMPERATURE (C) END TIME (M.Y.B.P.)
20.00 .0

FLUX (mW/M**2) END TIME (M.Y.B.P.)
40.00 .0

SED. RATE (M/M.Y.) END TIME (M.Y.B.P.)
46.00 59.0
180.01 1.0
770.55 .0

TIME = 59.0

DEPTH (M)	TEMP. (C)	PRESS. (MPa)	DARCY V (M/S)	POROSITY
.000000	20.0	.1000000	.2317E-12	.450E+00
383.502436	32.7	4.9761387	.2110E-12	.440E+00
759.724036	45.0	9.4558981	.1847E-12	.429E+00
1128.143209	56.9	13.6475460	.1578E-12	.416E+00
1488.549162	68.4	17.6121840	.1309E-12	.403E+00
1840.924941	79.4	21.3875501	.1046E-12	.389E+00
2185.375239	90.1	24.9985913	.7918E-13	.375E+00
2522.086706	100.4	28.4626777	.5471E-13	.361E+00
2851.293590	110.3	31.7923801	.3133E-13	.346E+00
3173.254453	119.8	34.9970439	.9072E-14	.332E+00
3295.220109	123.3	36.1978599	.0000E+00	.326E+00

CPU TIME = 0: 1:41

TIME = 1.0

DEPTH (M)	TEMP. (C)	PRESS. (MPa)	DARCY V (M/S)	POROSITY
.000000	20.0	.1000000	.2489E-11	.450E+00
380.956146	32.0	5.0743884	.2369E-11	.435E+00
751.215776	43.6	9.6684745	.2209E-11	.418E+00
1110.435236	54.5	13.9790751	.2049E-11	.400E+00
1458.722327	65.0	18.0637917	.1892E-11	.381E+00
1796.453004	75.0	21.9605773	.1742E-11	.362E+00
2124.174094	84.5	25.6973401	.1601E-11	.343E+00
2442.473670	93.5	29.2952588	.1469E-11	.324E+00
2752.012666	102.1	32.7714558	.1346E-11	.305E+00
3053.411346	110.4	36.1401685	.1233E-11	.287E+00
3347.298043	118.2	39.4135124	.1128E-11	.269E+00
3634.263996	125.8	42.6619705	.1032E-11	.252E+00
3914.263505	133.1	45.7147250	.9442E-12	.235E+00
4189.633736	140.1	48.7598944	.8633E-12	.220E+00
4459.044664	146.8	51.7447088	.7892E-12	.205E+00
4723.543516	153.3	54.6756463	.7214E-12	.191E+00
4983.561397	159.6	57.5585408	.6593E-12	.177E+00
5239.460078	165.8	60.3986703	.6025E-12	.165E+00
5491.594145	171.7	63.2008303	.5506E-12	.153E+00
5740.283220	177.5	65.9693987	.5031E-12	.141E+00
5985.820132	183.2	68.7083840	.4597E-12	.131E+00
6228.473344	188.7	71.4214777	.4200E-12	.121E+00
6468.483553	194.2	74.1120321	.3837E-12	.112E+00
6706.091246	199.5	76.7833956	.3506E-12	.103E+00
6941.483106	204.7	79.4383399	.3203E-12	.948E-01
7174.871367	209.9	82.0796731	.2926E-12	.873E-01
7406.417326	214.9	84.7099204	.2673E-12	.804E-01
7636.297336	219.9	87.3312948	.2430E-12	.740E-01

7877.973379	225.4	91.1488899	.2118E-12	.119E+00
8118.443788	230.9	94.9031141	.1808E-12	.113E+00
8357.262396	236.3	98.5084245	.1514E-12	.106E+00
8594.455249	241.6	101.9595767	.1237E-12	.100E+00
8830.048499	246.8	105.2489844	.9749E-13	.942E-01
9064.066339	252.0	108.3658004	.7290E-13	.882E-01
9296.538020	257.1	111.2950435	.4982E-13	.821E-01
9527.492852	262.2	114.0163837	.2824E-13	.761E-01
9756.961696	267.2	116.5023422	.8095E-14	.702E-01
9844.827893	269.1	117.3883015	.0000E+00	.679E-01

CPU TIME = 0:25:10

TIME = .0

DEPTH (M)	TEMP. (C)	PRESS. (MPa)	DARCY V (M/S)	POROSITY
.000000	20.0	.1000000	.1131E-10	.450E+00
368.425058	30.1	4.3148129	.8093E-11	.365E+00
670.373441	37.8	7.7671181	.6314E-11	.303E+00
695.710475	38.4	8.0839525	.4189E-11	.406E+00
1050.392297	48.5	14.0172333	.5386E-11	.397E+00
1399.124765	58.0	19.3271290	.4676E-11	.385E+00
1740.698000	67.6	24.1779344	.4049E-11	.371E+00
2074.383641	76.6	28.6763745	.3502E-11	.356E+00
2399.923644	85.6	32.8947361	.3030E-11	.340E+00
2717.359268	94.1	36.8843400	.2626E-11	.323E+00
3026.909088	102.5	40.6831688	.2280E-11	.306E+00
3328.927177	110.2	44.3203539	.1985E-11	.289E+00
3623.827222	117.9	47.8189198	.1733E-11	.272E+00
3912.054241	125.2	51.1975264	.1517E-11	.256E+00
4194.062041	132.3	54.4716135	.1333E-11	.240E+00
4470.293613	139.2	57.6541786	.1174E-11	.224E+00
4741.196941	145.8	60.7563196	.1038E-11	.209E+00
5007.169490	152.2	63.7876264	.9197E-12	.195E+00
5268.605137	158.6	66.7564701	.8177E-12	.182E+00
5505.863083	164.6	69.6702205	.7290E-12	.169E+00
5779.297122	170.6	72.5354158	.6517E-12	.157E+00
6029.206641	176.2	75.3578946	.5841E-12	.145E+00
6275.887320	181.9	78.1429029	.5247E-12	.135E+00
6519.607414	187.4	80.8951806	.4723E-12	.125E+00
6760.614144	192.8	83.6190325	.4260E-12	.115E+00
6999.135133	198.1	86.3183871	.3849E-12	.106E+00
7235.380211	203.3	88.9968450	.3483E-12	.980E-01
7469.542536	208.4	91.6577137	.3156E-12	.903E-01
7701.801348	213.4	94.3040235	.2862E-12	.831E-01
7932.324128	218.4	96.9385012	.2599E-12	.765E-01
8143.713279	222.9	99.3618305	.3093E-12	.708E-01
8161.804663	223.3	99.5874786	.1659E-12	.120E+00
8402.709443	228.8	103.4865778	.2028E-12	.114E+00
8641.957726	234.2	107.2374416	.1724E-12	.108E+00
8879.613785	239.6	110.8374201	.1440E-12	.102E+00
9115.704202	244.7	114.2824055	.1173E-12	.962E-01
9350.252376	249.9	117.5648108	.9221E-13	.903E-01
9583.284191	255.1	120.6731557	.6861E-13	.844E-01
9814.826783	260.1	123.5913814	.4648E-13	.786E-01
10044.908031	265.1	126.2976283	.2575E-13	.727E-01
10273.556360	270.1	128.7522740	.6390E-14	.669E-01
10343.625663	271.6	129.4661246	.0000E+00	.652E-01

CPU TIME = 0:23:1

THERE WERE 4980 ITERATIONS IN 2490 TIME STEPS.

THE MAX. NO. OF NODES (INC. NODE 0) WAS 499 AT .0 M.Y.B.P.

FORMATION	M.Y.B.P.	DEPTH (M)	THICKNESS	TEMP. (C)	TTI (BOTTOM\TOP)
CRETACEOUS	138.0	.00	.00	20.0	.0\ .0
CRETACEOUS	131.5	294.70	294.70	29.8	.0\ .0
CRETACEOUS	125.0	583.94	583.94	39.4	.1\ .0
CRETACEOUS	118.6	863.20	863.20	48.6	.2\ .0
CRETACEOUS	112.1	1147.82	1147.82	57.6	.4\ .0
CRETACEOUS	105.6	1423.10	1423.10	66.4	.7\ .0
CRETACEOUS	97.1	1694.29	1694.29	74.9	1.3\ .0
CRETACEOUS	92.7	1961.58	1961.58	83.2	2.4\ .0
CRETACEOUS	86.2	2225.17	2225.17	91.3	4.3\ .0
CRETACEOUS	79.7	2485.22	2485.22	99.2	7.6\ .0
CRETACEOUS	73.2	2741.88	2741.88	106.9	13.4\ .0
CRETACEOUS	66.8	2995.27	2995.27	114.5	23.1\ .0
CRETACEOUS	60.3	3245.53	3245.53	121.9	39.4\ .0
CRETACEOUS	59.0	3295.22	3295.22	123.3	43.8\ .0
CRETACEOUS	57.7	3310.73	3275.92	127.9	49.2\ .0
CRETACEOUS	56.0	3754.99	3243.80	135.3	59.8\ .0
CRETACEOUS	54.4	4005.85	3205.30	142.1	77.1\ .0
CRETACEOUS	52.7	4235.53	3162.05	148.4	104.3\ .1
CRETACEOUS	51.1	4455.35	3115.53	154.2	145.6\ .1
CRETACEOUS	49.4	4663.44	3067.10	159.6	206.4\ .2
CRETACEOUS	47.8	4874.65	3017.97	164.7	293.8\ .4
CRETACEOUS	46.1	5075.63	2969.06	169.5	417.1\ .7
CRETACEOUS	44.5	5272.29	2921.09	174.2	588.0\ 1.2
CRETACEOUS	42.8	5465.35	2874.51	178.6	821.9\ 2.0
CRETACEOUS	41.2	5655.36	2829.54	182.9	1138.4\ 3.3
CRETACEOUS	39.5	5842.77	2785.54	187.1	1562.7\ 5.2
CRETACEOUS	37.8	6027.89	2745.56	191.1	2127.4\ 8.2
CRETACEOUS	36.2	6210.93	2705.42	195.1	2873.7\ 12.8
CRETACEOUS	34.5	6392.26	2669.16	199.0	3854.4\ 19.6
CRETACEOUS	32.9	6571.88	2633.72	202.9	5135.5\ 29.7
CRETACEOUS	31.2	6749.99	2600.03	206.6	6805.0\ 44.3
CRETACEOUS	29.6	6926.70	2568.00	210.4	8967.3\ 65.6
CRETACEOUS	27.9	7102.13	2537.55	214.0	11759.0\ 96.0
CRETACEOUS	26.3	7275.37	2508.50	217.6	15351.0\ 139.2
CRETACEOUS	24.6	7449.51	2481.09	221.2	19957.9\ 199.9
CRETACEOUS	23.0	7621.62	2454.92	224.7	25849.6\ 284.8
CRETACEOUS	21.3	7792.30	2430.05	228.2	33354.1\ 402.5
CRETACEOUS	19.7	7963.10	2406.40	231.7	42925.0\ 564.5
CRETACEOUS	18.0	8132.60	2383.92	235.1	55062.0\ 786.1
CRETACEOUS	16.4	8301.35	2362.55	238.5	70437.2\ 1087.5
CRETACEOUS	14.7	8462.43	2342.24	241.9	89877.4\ 1495.0
CRETACEOUS	13.1	8636.88	2322.93	245.2	114414.2\ 2043.1
CRETACEOUS	11.4	8803.76	2304.59	248.5	145333.9\ 2776.5
CRETACEOUS	9.8	8970.12	2287.17	251.9	184239.7\ 3753.6
CRETACEOUS	8.1	9135.00	2270.62	255.1	233128.0\ 5049.4
CRETACEOUS	6.5	9301.45	2254.91	258.4	294484.5\ 6760.7
CRETACEOUS	4.8	9466.50	2240.00	261.7	371402.5\ 9012.3
CRETACEOUS	3.1	9631.20	2225.85	264.9	467729.7\ 11964.0
CRETACEOUS	1.5	9795.57	2212.42	268.1	588251.3\ 15820.1
CRETACEOUS	1.0	9844.33	2208.53	269.1	629980.0\ 17190.6
CRETACEOUS	.7	10010.35	2206.09	269.6	654805.5\ 18014.0
CRETACEOUS	.3	10207.50	2202.64	270.5	692025.5\ 19263.1
CRETACEOUS	.0	10345.63	2199.91	271.6	723920.9\ 20350.6
TERTIARY	39.0	.00	.00	.0	.0\ .0
TERTIARY	57.7	234.81	234.81	27.4	.0\ .0

TERTIARY	56.6	521.19	521.19	36.4	.0\	.0
TERTIARY	54.4	800.55	800.55	45.0	.0\	.0
TERTIARY	52.7	1073.48	1073.48	53.4	.1\	.0
TERTIARY	51.1	1340.33	1340.33	61.4	.1\	.0
TERTIARY	49.4	1601.33	1601.33	69.2	.2\	.0
TERTIARY	47.8	1856.68	1856.68	76.7	.4\	.0
TERTIARY	46.1	2106.56	2106.56	84.0	.7\	.0
TERTIARY	44.5	2351.20	2351.20	90.9	1.2\	.0
TERTIARY	42.8	2590.83	2590.83	97.7	2.0\	.0
TERTIARY	41.2	2825.72	2825.72	104.2	3.3\	.0
TERTIARY	39.5	3056.13	3056.13	110.5	5.2\	.0
TERTIARY	37.8	3282.32	3282.32	116.6	8.2\	.0
TERTIARY	36.2	3504.57	3504.57	122.5	12.8\	.0
TERTIARY	34.5	3723.10	3723.10	128.2	19.6\	.0
TERTIARY	32.9	3938.16	3938.16	133.7	29.7\	.0
TERTIARY	31.2	4149.96	4149.96	139.1	44.3\	.0
TERTIARY	29.6	4358.71	4358.71	144.4	65.6\	.0
TERTIARY	27.9	4564.58	4564.58	149.5	96.0\	.0
TERTIARY	26.3	4767.77	4767.77	154.5	139.2\	.0
TERTIARY	24.6	4968.42	4968.42	159.4	197.9\	.0
TERTIARY	23.0	5166.70	5166.70	164.1	284.8\	.0
TERTIARY	21.3	5362.75	5362.75	168.8	402.5\	.0
TERTIARY	19.7	5556.70	5556.70	173.4	564.5\	.0
TERTIARY	18.0	5748.68	5748.68	177.8	786.1\	.0
TERTIARY	16.4	5938.81	5938.81	182.2	1087.5\	.0
TERTIARY	14.7	6127.19	6127.19	186.6	1495.0\	.0
TERTIARY	13.1	6313.95	6313.95	190.8	2043.1\	.0
TERTIARY	11.4	6499.17	6499.17	195.0	2776.5\	.0
TERTIARY	9.8	6682.95	6682.95	199.1	3753.6\	.0
TERTIARY	8.1	6865.38	6865.38	203.1	5049.4\	.0
TERTIARY	6.5	7046.54	7046.54	207.1	6766.7\	.0
TERTIARY	4.8	7226.50	7226.50	211.0	9012.3\	.0
TERTIARY	3.1	7405.35	7405.35	214.9	11964.0\	.0
TERTIARY	1.5	7583.15	7583.15	218.8	15320.1\	.0
TERTIARY	1.0	7636.30	7636.30	219.9	17190.6\	.0
TERTIARY	.7	7804.28	7599.97	220.5	18014.0\	.0
TERTIARY	.3	8004.96	7533.74	221.7	19263.1\	.0
TERTIARY	.0	8143.71	7473.33	222.9	20350.6\	.0
QUATERNARY	1.0	.00	.00	.0	.0\	.0
QUATERNARY	.7	204.30	204.30	25.8	.0\	.0
QUATERNARY	.3	471.22	471.22	32.7	.0\	.0
QUATERNARY	.0	670.38	670.38	37.8	.0\	.0

CPU TIME = 0:28: 3

:si20:qatemp:nl.tti.out.gctest

GULF COAST TEST

M

N

Y

138

59, 2221

"CRETACEOUS",0.1,0.45,"Y"

1,7178

"TERTIARY",0.2,0.45,"Y"

0, 652

"QUATERNARY",0.35,0.45,"Y"

20, 0.0

F

N

40, 0.0

CONDUCTIVITY

3

CRETACEOUS

TERTIARY

QUATERNARY

1,1

0

0, 2.0

1

WATER

1,1

0

0, 0.63

COMPRESSIBILITY

1

CRETACEOUS

90, 0.5, 10, 0.05

1

TERTIARY

150, 0.5, 10, 0.05

1

QUATERNARY

800, 0.5, 10, 0.05

1

WATER

0,0

PERMEABILITY

1

CRETACEOUS

0.00001, 0.5, 0.0000001, 0.05

1

TERTIARY

0.0001, 0.5, 0.000001, 0.05

1

QUATERNARY

0.001, 0.5, 0.00001, 0.05

SPECIFIC HEAT

3

CRETACEOUS

TERTIARY

QUATERNARY

1,1

0

0, 0.5

1

WATER

1,1

```

      0
      0.0, 4.4
DENSITY
3
CRETACEOUS
TERTIARY
QUATERNARY
1.1
      0
0, 2.65
1
WATER
1.1
      0.
0..1.0
ENDPARAM
500, 5, 0.01, 10, "OFF", 100, 0
S
Y Y Y Y Y Y
3
CRETACEOUS
TERTIARY
QUATERNARY
NL.TTI.PLOT3
NL.TTI.POST
NL.TTI.BORD
2,2,10.0
2,2, 2.0
2,1, 0.0
:SI20:GGTEMP:NL.TTI.TEMPS
3,2,120.0
2,2,30.0
2,2,10.0
2,2,2.0
2,1,0.0
:SI20:GGTEMP:NL.TTI.TTIF
2
15.0,160.0
nl.tti.Ledge
3
CRETACEOUS
TERTIARY
QUATERNARY
:SI20:GGTEMP:NL.TTI.TTIXY
138.0
:SI20:GGTEMP:NL.TTI.TG
138.0
:SI20:GGTEMP:NL.TTI.Q

```

PRESENT DAY SUMMARY:

FORMATION	DEPTH (M)	THICKNESS	TEMP. (C)	TTI (BOTTOM\TOP)	
CRETACEOUS	10343.63	2199.91	271.6	723920.9\	20350.6
TERTIARY	8143.71	7473.33	222.9	20350.6\	.0
QUATERNARY	670.38	670.38	37.8	.0\	.0

Fig. 23. Output file NL. TTI. SUMM.

where:

ρ_w = water density
G = acceleration of gravity
P = pressure
Z = altitude (- depth)

The (vertical) Darcy velocity is given by:

$$(36) \quad V_D = -(k/u) * (TERM1 + TERM2)$$

where:

k = rock permeability
u = water viscosity

These quantities are printed at the end of every major event in the geological history of the basin.

This output file also may contain the number of Temperature and/or TTI grid points depending on the plotting option chosen.

3) Suggestions for Use of SURFACE II for Plotting Results.

SURFACE II is a graphics system developed by R. J. Sampson. It uses command files to perform operations (contour plotting, x-y plotting, posting, etc.) on sample data (existing on files). The SURFACE II graphics system and all of its commands are explained in the SURFACE II manual (ref. 17).

We are primarily interested in two kinds of plots:

- a. A depth vs. time plot of the formation barriers upon which is superimposed the contour plots of the temperatures and TTI's vs. depth and time (see fig 9 for example). An example of a SURFACE II command file which does this is shown below (example 1). A brief explanation of each command used is given following the example. For further explanation consult the SURFACE II manual.

b. Various two-dimensional (x-y) plots:

Average thermal gradient vs. time (see fig. 12)

Average basement flux vs. time (see fig. 21)

TTI of a (bottom) sediment point vs. time
(may be more than one such curve on a plot,
see fig. 8).

Examples of SURFACE II command
files which are used in creating an Average thermal
gradient vs. time plot and a TTI vs. time plot
(3 formations are shown below (examples 2 and 3
respectively)).

Surface II produces an output plotting file which is
used to make the actual plots.

example 1. SURFACE II command file used to produce a
plot similar to figure 9.

```
TITL      Gulf Coast 3 Formation TTI, TEMP. Contours
DEVI      6, 'WOODS'
IDXY 35238,14,3,1,2,3,-1,0,0,, '(2(1X,F12.3),1X,F13.3)'
GRID      1,1.50,100.,0,4,0,0
NEAR      2,8,240.0,300.0
EXTR      -138.0,-.2,-10418.00,-.5
BOX        20.,1,500,2,0,-160.,-11000,2,.1
BXEX      -140.,0., -10420,0.0,1.65,1.65,1.75,1.75
SIZC      1, 5.2, 7.5
ROUT      15,1,'(2(1X,F10.3))'
BLANK
MSMO      1,2,1,2,2
CONT      1,0,.05,0.0,1, ,
CINT      0, 40., 20., 0, 1, .1, 0, .8,0
PERF
OVER
IDXY 35682,16,3,1,2,3,-1,0,0,, '(2(1X,F12.3),1X,F13.3)'
GRID      1, 1.38, 100.0,0,3,0,0
NEAR      2,8, 80.0, 140.0
BLANK
MSMO      7,2,1,2,2
CONT      1,0,0.0,1, ,
LEVE      17,5,'(F6.1,I2)'
CINT      2,,,1,.1,1,0.4,1
PERF
OVER
IDXY      3, 13, 3, 1, 2, 3, -1, 0, 0,, '(3(1X,F10.3))'
```

```

POST      0,0,0.1,0.1,1
ROUT      12,3,'(2(1X,F10.3))'
POUT
PERF
STOP
END

```

SURFACE II commands are executed in an order determined by SURFACE II and not the order of appearance in the command file. Additionally, no command is executed until a PERFORM statement is encountered. When a PERFORM statement is encountered, all commands between the most previous (if any) PERFORM statement and the current PERFORM statement are executed. If the current PERFORM statement is the first perform statement in the file, then all commands between the beginning of the command file and this PERFORM statement are executed. Execution terminates when the STOP statement is executed. Brief explanations of the commands are given below.

TITL	Accepts labeling message (up to 60 chars.long)
DEVI	Parameters for plotting device. Device code is 6 for both the Versatec V-80 plotter and the plotters at Automated Cartography.
EXTR	Defines the X (time) and Y (- depth) limits of the grid matrix (column of temperatures (or TTI's) at node-depositional time steps determined using items 17 (or 18)).
BOX	Draws and labels index or tic marks around the plot.
SIZC	Specifies the physical size of a plot created on a plotter.
ROUT	Reads in X (time) and Y (-depth) coordinates of points to be connected by straight lines, forming an outline within the map area. In the example above, the outline is read from the file whose name is the third of items 16c. Thus the outline consists of the bottom formation barrier, the right edge of the plot, and the surface. The format statement for the data on the file whose name is the third of items 16c must be exactly as that shown in the

example.

IDXY	<p>Reads sample data points (time, depth, temperature (or TTI)) and/or posting symbols into memory. For the contour plots in this report, 20000-37500 sample points were needed (the maximum number of points allowed is very close to 38000). The number of points generated is controlled by items 17 and 18. One should choose the optimum point distribution (often by trial and error) which will result in the smoothest and most accurate contours without exceeding the point limit. For temperature contour plots the sample data points are read from the file whose name is item 17b. For TTI contour plots the sample data points are read from the file whose name is item 18b. Formats for these files are exactly as shown in the first IDXY statement (for temperature data) and in the second IDXY statement (for TTI data) in example 1.</p>
GRID	<p>Creates a grid matrix of new Z (TTI or temperature values) at evenly-spaced intervals of X (time) and Y (- depth). The contours are computed using this grid. Parameter 4 of the GRID command was set to zero in all examples since other settings resulted in jagged contours (see SURFACE II manual). Parameter 5 was set to either 2 or 3 (see SURFACE II manual for a full explanation of all commands and command parameters).</p>
NEAR	<p>Specifies to SURFACE II that the sample points used to compute the grid matrix points will be "found" by a nearest-neighbor search (again, see SUFACE II manual).</p>
BLANK	<p>Blanks out all grid points between the outline defined by the previous ROUT command and the (rectangular) map border making the outline into a "pseudo-border" (see fig. 9, for example). Thus all points below and to the left of the bottom-most formation barrier are blank.</p>
MSMO	<p>Removes unwanted "noise" from grid matrix so that contours will have a smooth appearance. Must be used with a bit of caution since abuse of this command may remove important features of the contours.</p>

CONT Generates the instructions used by the plotting device to make a contour map from the grid matrix. The parameter values used in example 1 are quite adequate. Parameter 4 may be adjusted for clarity.

LEVE allows the user to specify unequal contour intervals. This is the most flexible way to specify contour values. The contours are read in from a data file created by the user. The Format in quotes must correspond to the format of the data on the user-created file.

CINT specifies spacing, annotation, and labeling of contour lines. Notice that in the example, parameters 2, 3 and 4 have been omitted. parameters 2, 3 and 4 control the number and values of regularly-spaced contours. In example 1, contours are not to be regularly spaced. This is indicated by parameter 1. The contour values are to be read in using the LEVE (LEVELS) command.

PERF (PERFORM) discussed previously.

OVER allows superposition of two or more plots. In example 1 the OVER command indicates that the plot created by the following group of commands is to be superimposed on that created by the first group of commands (those before the first PERF). In this example, the second group of commands is similar to the first. It creates the TTI contour plots which will be superimposed on the temperature contour plots created by the first group of commands. The final group of commands creates the formation barrier depth vs. time plots. The names of the formations whose barriers are to be plotted are items 16b.

POST This command causes labeling of sample data points with their Z (formation barrier number, starting from the deepest) values at the location on the plot defined by their middle X (time) and Y (-depth) coordinates. The formation barrier numbers are read in by use of the IDXY command from the file created by program NL.TTI whose name was the second of items 16c.

In this group of commands the ROUT command is used to define the outlines which are to be the formation barriers. These are read from a file whose name was the first of items 16c.

POUT The POUT command causes the outlines (barriers) to be drawn.

example 2. Surface II command file used to plot thermal gradient vs. time.

```
TITL      Thermal gradient vs. time (Salina Basin)
DEVI      6, 'Woods'
IDXY      3, 18, 3, 1, 2, 3, -1, 0, 0, , '(3F5.0)'
POST      2, , .1, , 1
BOX       50., 2, 4.0, 2, 0, -500., 20., 2, 0.1
BXEX      -480, 0, 20.0, 60., 0, 0, 0, 0
SIZC      1, 5.2, 7.5
ROUT      17, 1, '(1X, F8.3, 1X, E12.4)'
POUT
PERF
STOP
END
```

IDXY	General use of this command is discussed in example 1 above and in the SURFACE II manual. It is used here to read in a set of (3) dummy sample data points to define a plot. We are only interested in the "outline" (thermal gradient vs. time curve) defined by the ROUT command and "drawn" by the POUT command.
POST	General use of this command is explained in example 1 and in the SURFACE II manual. It is used in this file to post the dummy sample data points. These points must be read from a file created by the user using the IDXY command. The dummy points are usually all (0,0,0).
BXEX	Defines X (time) and Y (thermal gradient) limits of the map border. This is used in absence of the EXTR command since there is no grid whose contours are to be plotted in this example.
ROUT	reads in the X (time) and Y (thermal gradient) coordinates of the points defining the outline (curve). The format statement in quotes must be exactly the one shown in example 2.
POUT	causes the outline (curve) to be plotted.

example 3. SURFACE II command file used in plotting
the TTI vs. time for 2 formations
(See fig. 15).

```
TITL      TTI VS TIME XY PLOT (SALINA BASIN)
DEVI      6, 'Woods'
IDXY      3, 18, 3, 1, 2, 3, -1, 0, 0, , '(3F5.0)'
POST      2, , .1, , 1
BOX        50., 2, 5., 2, 0, -500., 0., 2, 0.1
BXEX      -480, 0, 0.0, 45., 0, 0, 0, 0
SIZC      1, 5.2, 7.5
ROUT      17, 2, '(1X, F12.3, 1X, F13.3)'
POUT
PERF
STOP
END
```

The number of curves to be plotted is specified
by the second parameter of the ROUT command.
In this example it is two (as in fig. 15).

SURFACE II may be executed by typing the SURF2 command in response to the AOS/CLI prompt. The SURF2 command has the following general form:

```
SURF2 <command file> <execution report file>
      <command report file> [<plotfile/fc=09>
      <datafile1/fc=x1> <datafile2/fc=x2> ....
      <savefile/fc=21> ...]
```

where:

<command file>	= SURFACE II command file (see examples 1, 2 and 3 above)
<execution report file>	= contains numerical results of calculations and error messages.
<command report file>	= contains sequential breakdown of commands executed along with error messages.
<plotfile/fc=09>	= SURFACE II output plotfile the file code (fc) specified for this file must be 9.
<datafile1/fc=x1>	= Input data files. File codes (xn) for specified for these files should be in the range 10-19 inclusive.
<savefile/fc=21>	= Output grid save file. needed if option to save a grid was chosen in the GRID command.

The square brackets in the general form indicated that the files whose names are enclosed are optional. All others indicated are required.

```
example: SURF2 SURF2.COMM  execrep commrep surf2.plt/fc=9
        nl.tti.plot13/fc=12 :si20:ggtemp:nl.tti.temps/fc=14
        nl.tti.bord/fc=15  :si20:ggtemp:nl.tti.ttif/fc=16
        lvls/fc=17 nl.tti.post/fc=13
```

The above example shows the command necessary to execute the creation of a SURFACE II output plotting file (surf2.plt) which when plotted would produce a plot of temperature contours for the temperature vs. depth and time data residing on file :si20:ggtemp:nl.tti.temps. This plot would include TTI contours whose values reside on file lvls. The TTI contours would be computed from the TTI vs. time and depth data residing on file :si20:ggtemp:nl.tti.ttif. This plot would also include a plot of the formation barrier depths vs. time using the data on files nl.tti.plot13 and nl.tti.post. The border of the plot is determined using the data on file nl.tti.bord. The SURFACE II command file, named SURF2.COMM by the user, would contain the SURFACE II commands listed in example 1 of this section. The Input file to program NL.TTI necessary to create the data files (except lvls, which must be created by the user) would be similar to complete example 2 of section IV.1. The plot would essentially be that of figure 20.

```
example: surf2 surf2.comm.tg execrep commrep sf2.plt/fc=9
        nl.tti.post.tg/fc=18 :si20:ggtemp:nl.tti.tg/fc=17
```

This is an example of the SURFACE II command necessary to create the output plotting file (sf2.plt) which will be used to create a plot of the thermal gradient vs. time points which are in file :si20:ggtemp:nl.tti.tg. The SURFACE II command file is file surf2.comm.tg. The command file shown in example 2 in this section is an example of such a command file. File nl.tti.post.tg contains the dummy points necessary to create the plot (which is really the outline in this example. Figure 17 is an example of such a plot.

4) Procedures to Produce Plots from the SURFACE II Output Plotting File.

A. Use of Program RASTER and the Versatec V-80 Plotter.

This is, by far, the simplest, easiest, and quickest way to produce a plot from a SURFACE II output file. The drawback is minimal flexibility as to coloring and size of plot. Program RASTER uses the SURFACE II output plotting file as an input file and produces an output file which is plotted by program VPLOT (you must log on with userid VPLOT and password VPLOT to execute program VPLOT. Program VPLOT executes immediately.).

The necessary commands are (using the SURFACE II output file in the most recent example):

```
RASTER/V=:SI20:GGTEMP:RASTEROUT SURF2.PLT
```

You may, of course, use any legal system file name as the name of the RASTER output file. The directory GGTEMP (temporary directory available to all users) is recommended because of the large size of RASTER output files.

You must then log on with userid VPLOT and password VPLOT. VPLOT will then execute with the following prompt (user response is in boldface):

```
ENTER FILENAME OF RASTER FILE TO BE PLOTTED:  
:SI20:GGTEMP:RASTEROUT
```

The Versatec V-80 should begin the plot immediately.

B. Making plots using Automated Cartography.

This usually takes a full day but the color and size flexibility is much greater than for option A. The SURFACE II output plotting file must be copied into directory :SI32:PLOT:WK and access to this file must be granted to Automated Cartography by the user. These may be done by executing the following commands:

```
copy :SI32:PLOT:WK.SURF2.PLT SURF2.PLT
.ACL :SI32:PLOT:WK.SURF2.PLT +,OWARE
```

A form must be filled out at Automated Cartography and the plot is picked up at Automated Cartography.

C. Plotting Procedure Summary

The following statements summarize the general procedures necessary to produce contour, average thermal gradient, basement flux and TTI vs.time plots from well (formation thicknesses and possibly present-day average thermal gradients) and (rock and water) parameter data:

1. Make a trial run of program NL.TTI with the input data file (NL.TTI.IN) constructed as shown in this section.
2. If any of the final thicknesses (see fig. 23) calculated for the formations differ from their corresponding measured (well) thicknesses by more than 8%, rerun the program with increased compressibilities for formations whose thicknesses are too large and decreased compressibilities for those formations whose thicknesses are too small. If there were no such formations, proceed to step 3.

3. If the final average (over depth) porosities obtained from the calculation differ from the estimated final porosities (see items 7) for any formations by more than about .04 for shales, .10 for limestones and .20 for sandstones, the estimated final porosities and the compressibilities for these formations must be adjusted (rerunning the program as necessary) until all formation thicknesses agree with their observed values as mentioned in step 2 and all formation average final porosities agree with the estimated final porosities used as input. If such agreement is achieved the model has been "calibrated", proceed to step 4.
4. If the thicknesses and porosities are calibrated, create the SURFACE II command file which is necessary to create the desired plot.
5. Run SURFACE II using the appropriate files in command SURF2
6. Using the SURFACE II output plotting file, make the plots using the procedures outlined in section IV.4.A or IV.4.B.

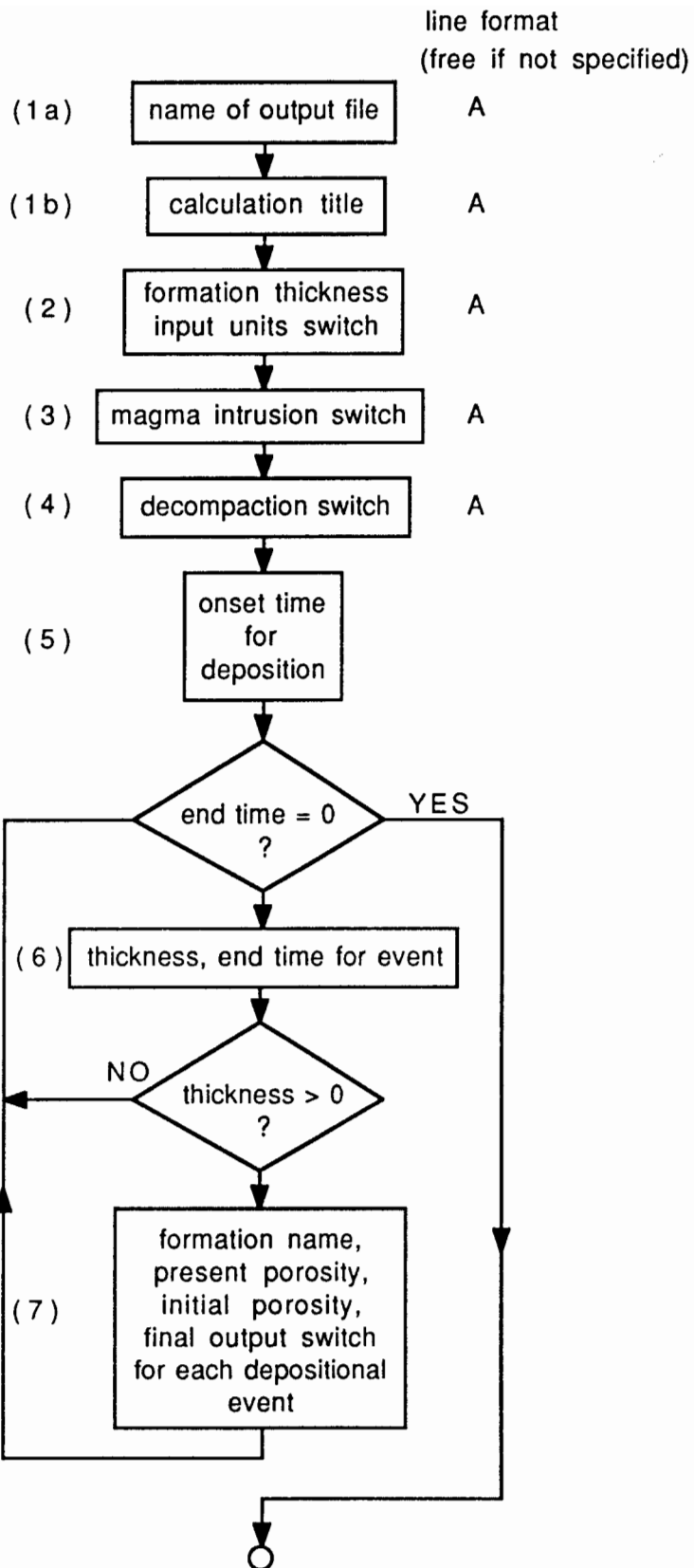
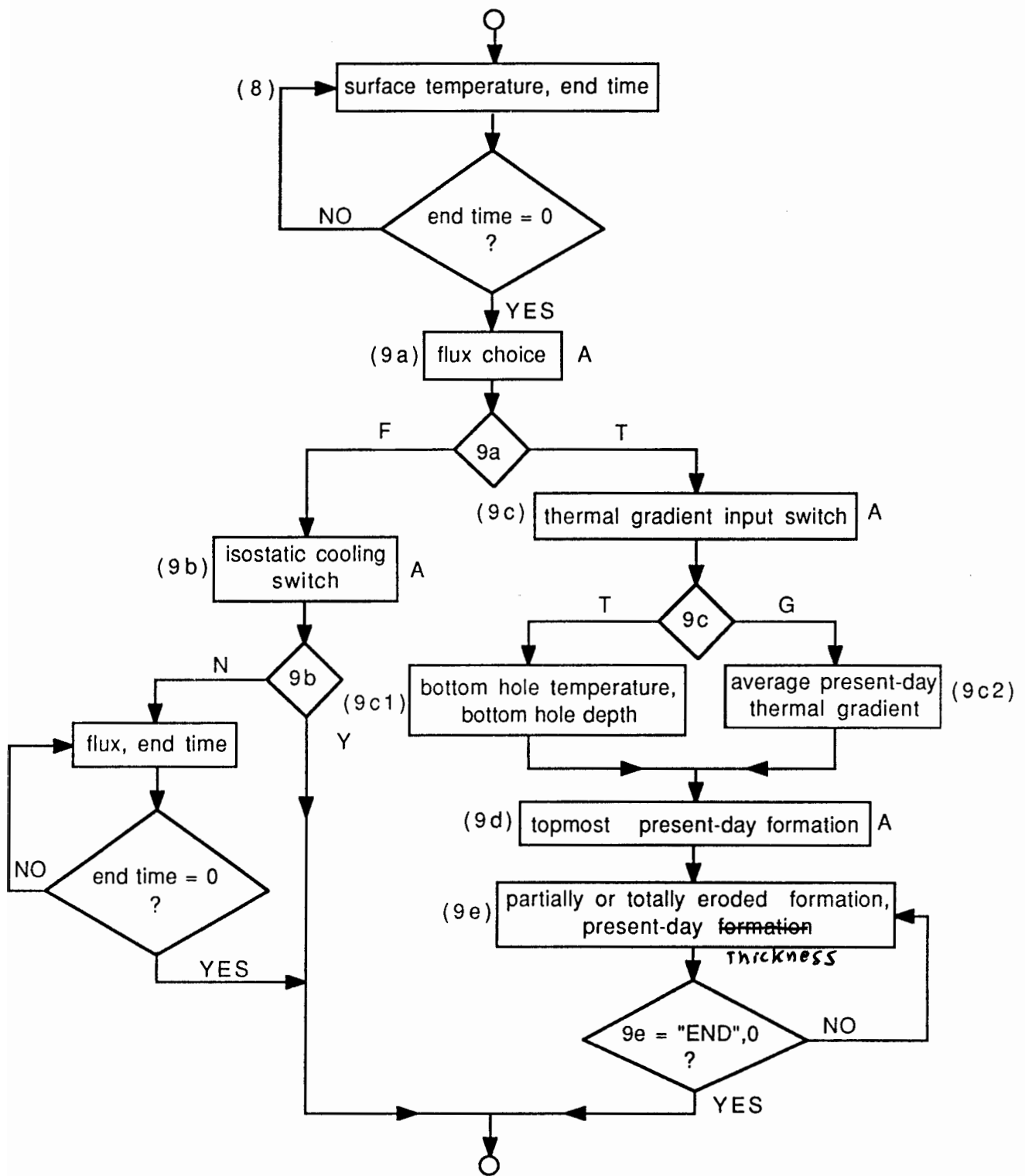
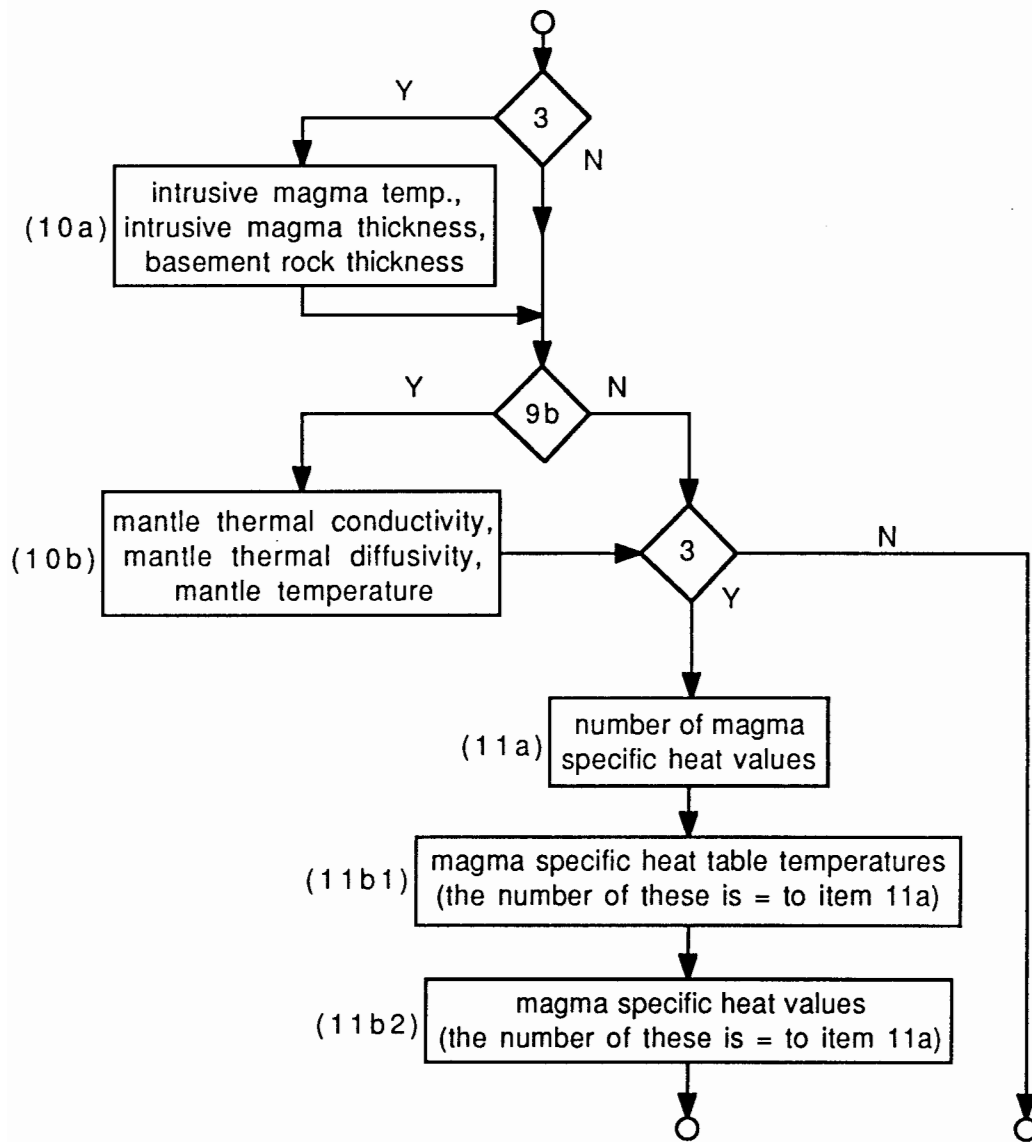
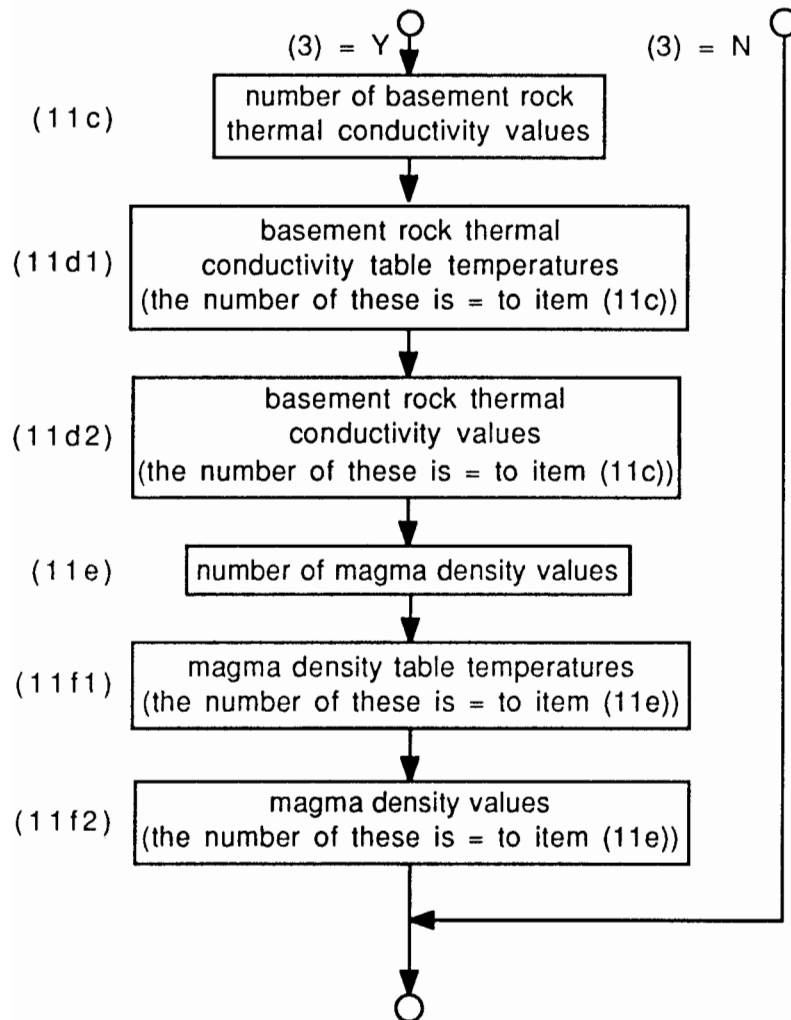
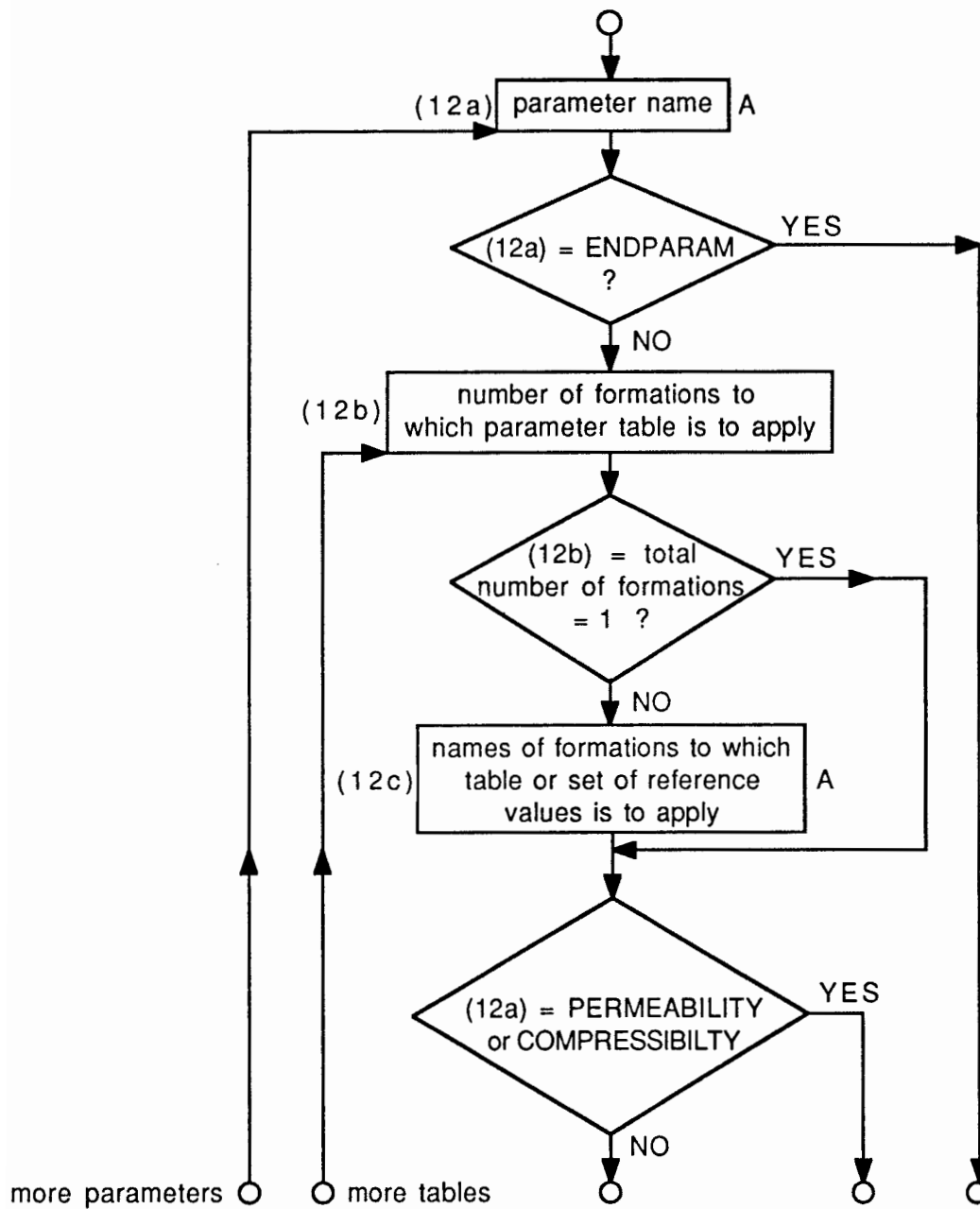


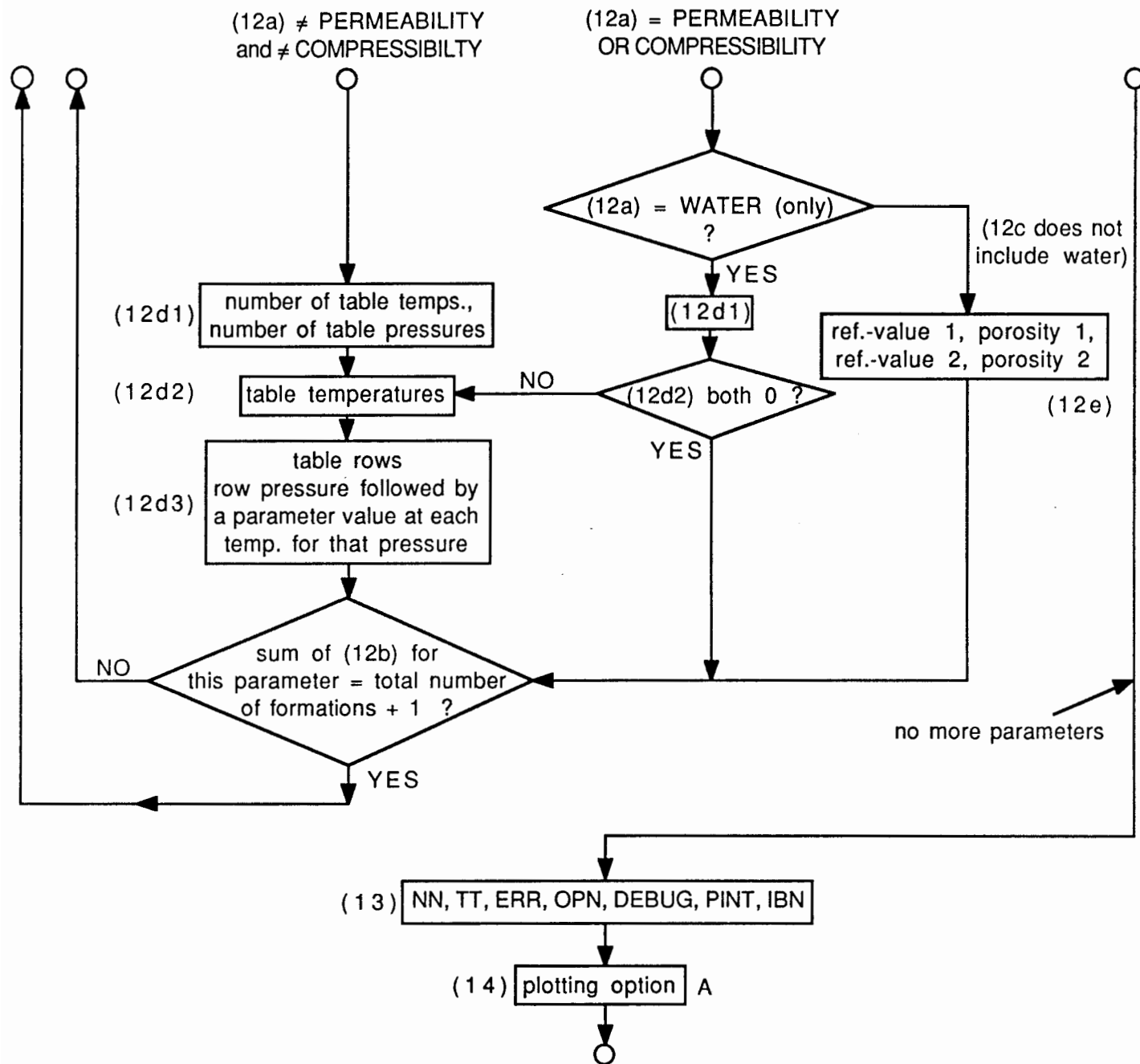
Fig 24 Flow chart describing input file to program NL. TTI (nine pages long)

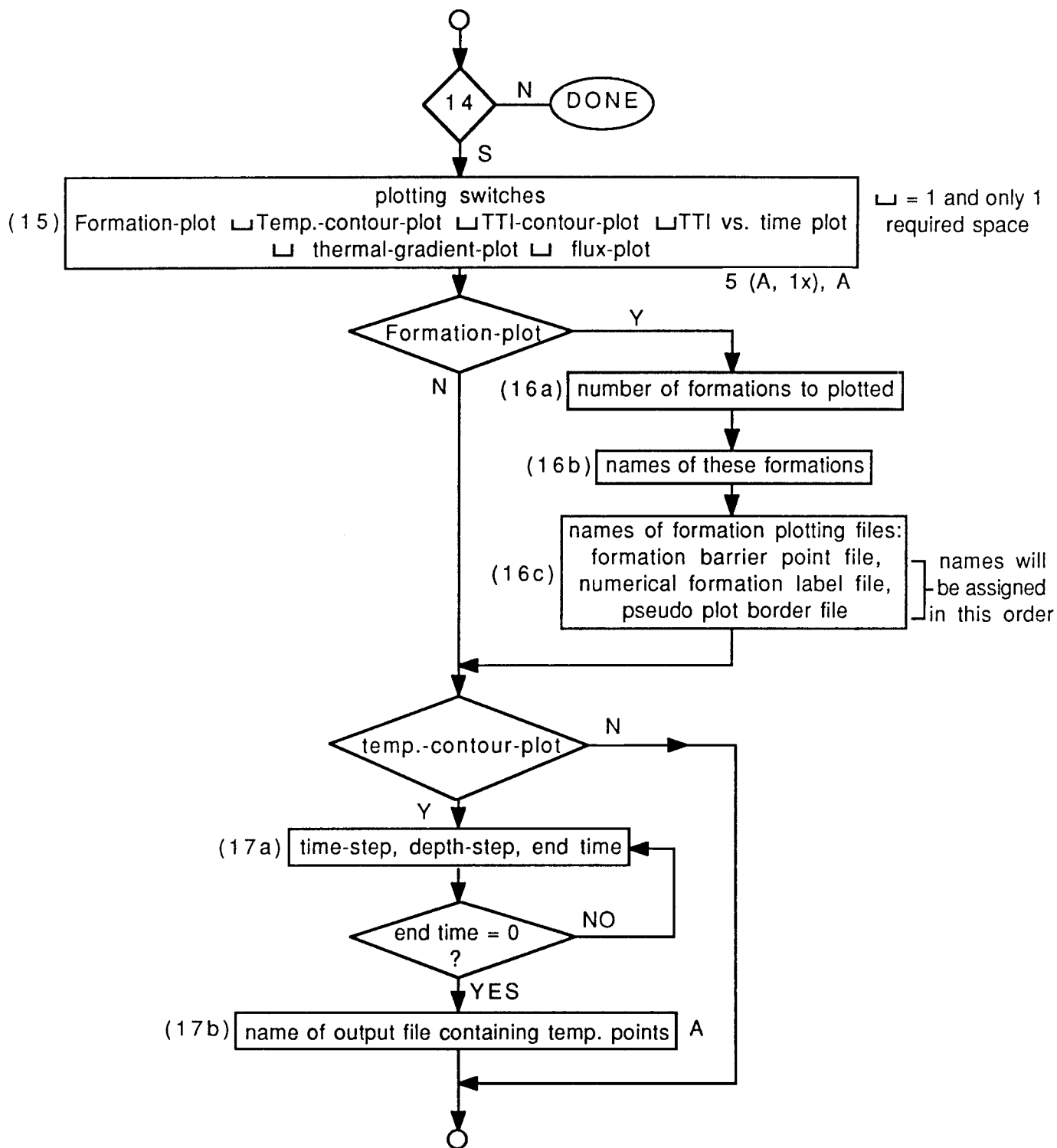


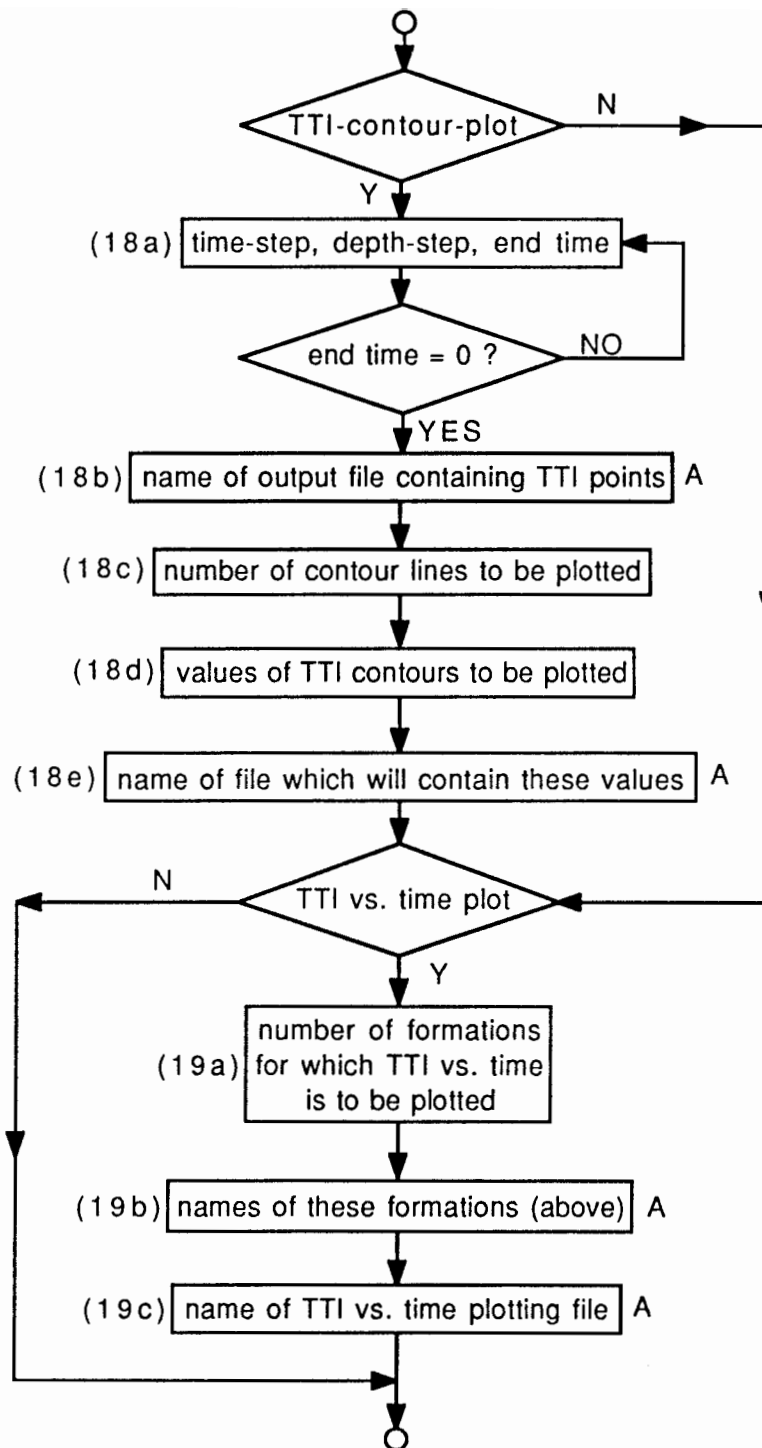


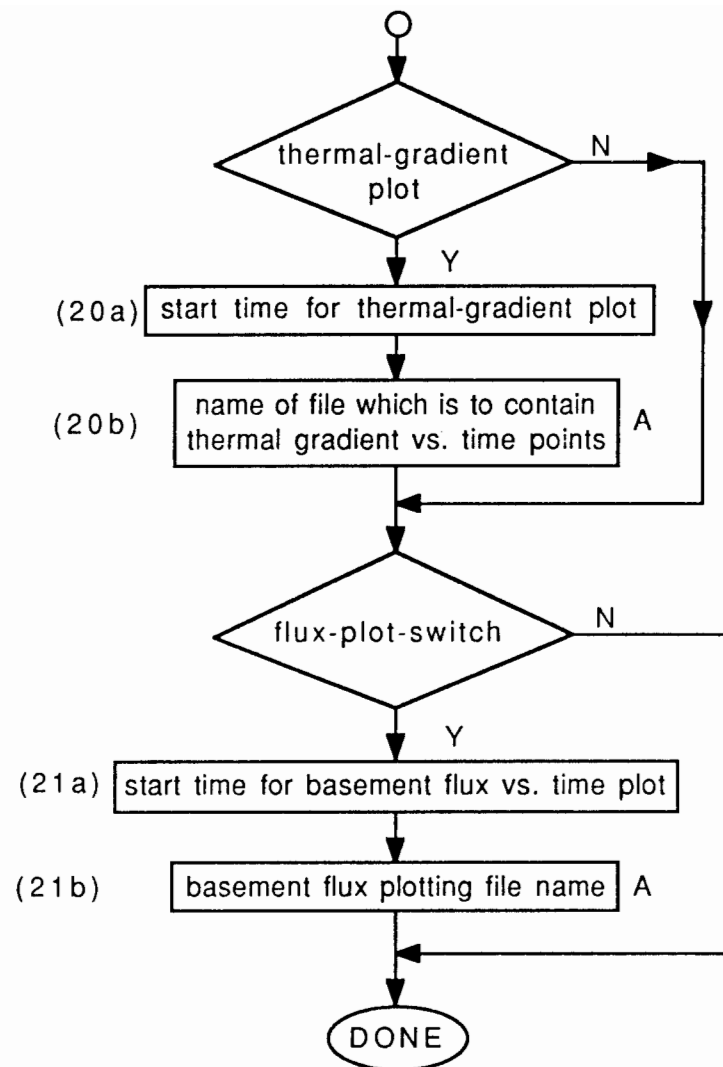












V. REFERENCES

1. McElwee, C. D., and G. C. Bohling, 1987, Thermal Basin Modeling Including Compaction and Fluid Flow:Kansas Geological Survey, Open File Report 86-21.
2. Waples, D. W., 1980, Time and Temperature in Petroleum Formation: Application of Lopatin's Method to Petroleum Exploration:AAPG Bull., 64(6):153-163.
3. Waples, D. W., 1984, Thermal Models for Oil Generation, 1984, in Brooks, J., and Dietrich Welte, ed., Advances in Petroleum Geology, vol. 1:London, Academic Press, pp. 7-67.
4. Kappelmeyer, O., and R. Haenel, 1974, Geothermics with Special Reference to Application:Berlin, Gebruder Borntraeger, pp.203-235.
5. Touloukian, Y. S., Liley, P.E., and S. C. Saxena, 1970, Thermophysical Properties of Matter:vols. 2-6:New York, IF/Plenum.
6. Moinseko, U. I., 1968, Wärmeleitfähigkeit der Gesteine bei Hohen Temperaturen:Freiberger Forsch. H. C. 238 Geophysik:89-94 Leipzig.
7. Haar, L., Gallagher, J. S., and G. S. Kall, 1984, NBS/NRC Steam Tables:Washington, Hemisphere, pp.34-166
8. Schmidt, E., and Ulrich Gringull, 1981, Properties of Water and Steam in S.I.-Units:Berlin, Springer-Verlag:125-145, 156-161.
9. Freeze, R. A., and J. A. Cherry, 1979, Groundwater:Englewood Cliffs, Prentice-Hall:29, 55
10. Pirson, S. J., 1963, Well Log Analysis:Englewood Cliffs, Prentice-Hall, P.6.
11. Tissot, B. P., and D. H. Welte, 1984, Petroleum Formation and Occurrence:Berlin, Springer-Verlag, p.359.
12. Weast, R. C., Selby, S. M., and C.D. Hodgman, ed., 1964, Handbook of Chemistry and Physics:Cleveland, The Chemical Rubber Co., pp. F10-F11.
13. Perrier, R. P., and J. Quibler, 1974, Thickness Changes in Sedimentary Layers During Compaction History:Methods for Quantitative Evaluation:AAPG Bull., 58(3):507-520.

14. Scholle, P. A., and Robert A. Halley, ,Burial Diagenesis:Out of Sight, Out of Mind!:in Schneiderman, N. and Harris, P. M. (eds.), Carbonate Cements, Society of Economic Paleontologists and Minerologists Special Pub. No. 26, pp. 309-334.
15. Feinstein, S., 1981, Subsidence History of Southern Oklahoma Aulacogen:Implications for Petroleum Exploration:AAPG Bull., 65(12):2521-2533.
16. Turcotte, D. L., and J. L. Ahern, 1977, On the Thermal and Subsidence History of Sedimentary Basins:J. Geophys. Rsch., 86(26):3762-3766.
17. Sampson, R. J., 1984, SURFACE II Graphics System:Lawrence, Ks.:Kansas Geological Survey.