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Use of Modified Tikhonov Regularization in Analysis of Ground Surface Temperature Variations

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Abstract

Inversion techniques employed in geothermal studies of ground surface temperature (GST) changes are known to have problems of instability and non-uniqueness in numerical solutions. In the present work it is pointed out that some of these difficulties can be overcome through the use of a method based on Tikhonov regularization of order one which imposes smoothing of main parameters. A major disadvantage of this approach is obliteration of weak thermal signals usually present at larger depths at the expense of strong ones present at relatively shallow depths. In the present work we consider a convenient way of minimizing this problem using a method based on Tikhonov regularization of order one. In this approach residuals of observational data are minimized by imposing constraints on the variations of smoothing parameters, that is controlled by the magnitude of regularization coefficients. This is accomplished in two stages of inversion. In the first stage we seek an estimation of the dates of climate events derived from results of temperature logs. Inversion of the second stage allows estimation of the magnitudes of GST variations that are compatible with the ages of climate events of the first stage. The advantage is in finding better solutions without introducing other artefacts on the climate history. Such two-stage Tikhonov regularization procedures has been employed for extracting complementary information on GST history in continental regions of Brazil. The results reveal that the main warming event of the last century has been preceded by several secondary events during the time period of 1400 to the 2000 A.D.

1. Introduction

Geothermal methods have been widely used over the last few decades in studies surface temperature changes of the recent past (Birch, 1948; Cermak, 1971; Lachenbruch et al, 1986; Hamza, 1991; Shen and Beck, 1983; Hamza et al, 2007; Hamza and Vieira, 2011). The main events identified as having affected ground surface temperatures (GST) on global scale include those associated with the warming event of the of the last two centuries, the cooling event associated with the little ice age of the 15th and 16th centuries and the thermal effects of glaciations since the Holocene times. The periods associated with such changes range from hundreds to thousands of years. Inversion schemes (such as the functional space inversion – FSI) employed for extracting ground surface temperature history from borehole temperature profiles are widely considered as reliable. In such model studies temperature history that best fit the data set is obtained as a posteriori result (see for example Shen and Beck, 1983; Beltrami and Mareschal, 1995; Beltrami, 2001). The results of FSI method for some selected sites in Brazil, illustrated in

Figure (1), reveal characteristic features in the GST history. Foremost among these are indications of increase in surface temperatures by as much as 1 to 4°C, over the last century.

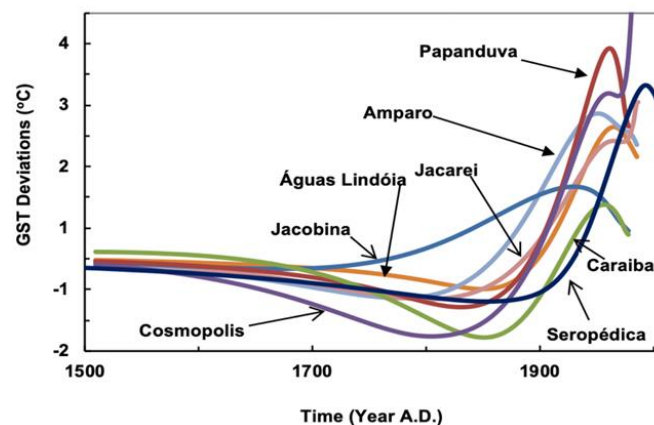


Figure 1 – Functional space inversion models of borehole temperature profiles, for selected localities in Brazil (Adapted with modifications from Hamza et al., 2007).

The Paleocene–Eocene thermal maximum (PETM), alternatively "Eocene thermal maximum 1" (ETM1), and formerly known as the "Initial Eocene" or "Late Paleocene thermal maximum", was a time period with a more than 5–8°C global average temperature rise across the event. This climate event occurred at the time boundary of the Paleocene and Eocene geological epochs. The exact age and duration of the event is uncertain, but it is estimated to have occurred around 55.5 million years ago.

However, in all localities the warming events seem to be preceded by cooling episodes occurring over the time period extending to an additional cooling event occurring over the last few decades. The amplitudes of these cooling events are relatively less, falling generally in the range of 0.5 to 1 °C. For time periods prior to the 17th century the resolving power of the inversion method is poor, a consequence of the limitations in sensitivity and precision of sensors used for temperature measurements in boreholes. Hence FSI model calculations for periods prior to 1700 may not necessarily be representative of true climate history. Also, the estimates of the depth at which the thermal regime is supposedly affected by GST variations and the time limit beyond which such variations cannot be recovered from the given temperature log are chosen in accordance with the depth extent of the available temperature log data. In particular, the depth estimate is set to be greater than the deepest data point because the calculated data are projected (interpolated) from the finite element solution. As for the time limit there is no harm in setting a value compatible with or greater than the depth extent of the borehole (Shen and Beck, 1992). On the other hand, use of a shorter-than-necessary time span would end up in restricting extraction of complete GST history. Unless there are independent evidences indicating a rapid return to unperturbed conditions it seems prudent to assume that this return take place gradually. Use of shorter time spans leads to slight reductions in the magnitude and duration of the cooling events of earlier periods. As pointed out by Shen and Beck (1991; 1992) the results of GST history, determined by functional space inversion, is sensitive to a priori standard deviations of thermal conductivity. The preferred values for the standard deviations are based on considerations of the trade-off between consistency of the solution and data resolution.

A major weakness of inverse methods employed, such as FSI, is the implicit assumption that the degree of uncertainty in parameter estimates are uniform over the entire time period considered. The nature of this limitation can be understood by considering the interrelations between data and estimated parameters in the inversion process. There are other problems in FSI inversion methods related to numerical stability in reaching solutions. For example, the procedure suggested by Shen and Beck (1993) makes use of a criterion that minimizes uncertainties in data and model results. This approach in turn is known to preserve mainly large amplitude thermal signals of recent periods but smear out weak signals associated with older signals that usually occur at larger depths. As a result, model results of FSI inversion leads to a simplified GST history which enhances the importance of recent warming event at the expense of older events which are associated. With earlier events. Clearly there is need for a new model that can also identify weak signals of earlier climate events. In the present work we employ a method based on Tikhonov regularization but with a differential weighting scheme. It has the potential for identifying low amplitude events in GST

history, relative to FSI inversion. A brief discussion of the theoretical background is presented first, followed by examples illustrating the procedures and advantages of this approach.

2. Theoretical Background

Consider an m-dimensional vector $\bar{\mathbf{S}}_{\Delta}$ of the corrections for one a priori assumed theoretical local ground temperature S_{theor} . Let $\bar{\mathbf{W}}_s^{1/2}$ be a positive diagonal matrix with dimensions $(m - 1) \times (m - 1)$ of weights attributed to adjacent intervals of the estimated parameters $\{s_{\Delta_i}\}$ and $\bar{\mathbf{R}}$ a matrix of $(n - 1) \times m$ dimensions representing a regularization functional of order one (Tikhonov, 1963; Tikhonov, et al,1977). This is a first order discrete differential operator (Toomey, 1963; Constable et al., 1987; Silva Dias et al, 2007) relative to the parameters $\{s_{\Delta_i}\}$. Note that the use of this regularization will impose a uniform degree of uncertainty smoothness in variations of estimated parameters $\{s_{\Delta_i}\}$ for the selected time interval.

In the conventional approach, the inverse problem proposed for estimating GST minimizes the function:

$$\|\bar{\mathbf{W}}_s^{1/2} \bar{\mathbf{R}} \bar{\mathbf{S}}_{\Delta}\|_2^2 \quad (1)$$

subject to:

$$\|\bar{\mathbf{W}}_r^{1/2} (\bar{\mathbf{P}} - \bar{\mathbf{J}} \bar{\mathbf{S}}_{\Delta})\|_2^2 = \epsilon^2 \quad (2)$$

and

$$\bar{\mathbf{P}} = \bar{\mathbf{P}}_{obs} - \bar{\mathbf{P}}_{grad} \quad (3)$$

and

$$\bar{\mathbf{S}} = \bar{\mathbf{S}}_{theor} + \hat{\mathbf{S}}_{\Delta} \quad (4)$$

In equations (2) and (3) $\bar{\mathbf{P}}$ represents the n-dimensional vector of GST measured signal to be inverted and $\bar{\mathbf{P}}_{grad}$ is composite for corresponding linear interpolation values of the $\bar{\mathbf{P}}_{obs}$ components. The scalar ϵ of is the observational mean quadratic errors associated with the observations $\bar{\mathbf{P}}_{obs}$. Note that $\bar{\mathbf{W}}_r^{1/2}$ represents the diagonal weight matrix of dimensions $(m - 1) \times (m - 1)$, and is used as a relative indicator imposing balance for the approximation between the geothermal signal $\bar{\mathbf{P}}$ and the “forward model” $\bar{\mathbf{J}} \bar{\mathbf{S}}_{\Delta}$ values. The matrix $\bar{\mathbf{J}}$ of dimension $n \times m$ in equation (2) is the Jacobian of the physical functional described in equation (3) which relates a the data on surface temperatures variation s_{Δ_i} with estimates of the perturbation temperatures $\bar{\mathbf{P}} = \{p_i\}$. The $\bar{\mathbf{S}}_{theor}$ vector have one same value for all component, s_{theor_i} , whose value results of a previous linear adjust of the $\{p_{obs_i}\}$ components to fix one feasible ground temperature initial value.

It is usual practice to make use of the following In solving the problem of conditional minimization proposed in with the equations (1), (2), (3) and (4), whose estimated parameters explain the observational data set in the minimal square method sense, the cost function Φ is:

$$\Phi = \|\bar{\mathbf{W}}_r^{1/2} (\bar{\mathbf{P}} - \bar{\mathbf{J}} \bar{\mathbf{S}}_{\Delta})\|_2^2 + \epsilon^2 + \lambda \|\bar{\mathbf{W}}_s^{1/2} \bar{\mathbf{R}} \bar{\mathbf{S}}_{\Delta}\|_2^2 \quad (5)$$

where the scalar λ is the regularization factor. It is usual practice to attribute a sufficiently small value to this

regularization factor, in obtaining a unique solution that is stable and realistic from a geophysical point of view.

Equating to zero the first derivative of this cost function Φ relative to the parameters $\bar{S}_\Delta = \{s_{\Delta i}\}$, we have:

$$\nabla_s \Phi = \nabla_s \left\{ [\bar{P} - \bar{J} \bar{S}_\Delta]^T \bar{W}_r [\bar{P} - \bar{J} \bar{S}_\Delta] - \epsilon^2 + \left\{ [\bar{P} - \bar{J} \bar{S}_\Delta]^T \bar{W}_r [\bar{P} - \bar{J} \bar{S}_\Delta] - \epsilon^2 + \lambda [\bar{R} \bar{S}_\Delta]^T \bar{W}_s [\bar{R} \bar{S}_\Delta] \right\} \right\} \quad (6)$$

On solving equation (6) with respect to the parameters $\{s_{\Delta i}\}$ we have:

$$2\bar{J}^T \bar{W}_r \bar{J} \bar{S}_\Delta - 2\bar{W}_r \bar{J}^T \bar{P} + 2\lambda \bar{R}^T \bar{W}_s \bar{R} \bar{S}_\Delta = \bar{0} \quad (7)$$

Equation (7) leads to the inverse operator allowing the estimated GST parameter \hat{S}_Δ to be derived directly from the GST well signal \bar{P} :

$$\hat{S}_\Delta = \left\{ (\bar{J}^T \bar{W}_r \bar{J} + \lambda \bar{R}^T \bar{W}_s \bar{R})^{-1} \bar{J}^T \bar{W}_r \right\} \bar{P}. \quad (8)$$

In other words:

$$\bar{P} = \{(p_{obs} - p_{teórico})_i\} \quad (8)$$

corresponds to the vector of perturbed values relative to an expected vertical distribution of temperatures arising from a stationary geothermal event $\bar{P}_{theoretical}$.

It is clear from equation (6) and (7) that the final solution depends on the magnitude of λ . In practice value of this parameter is adjusted with a new fit. It is common practice to make use of inversion schemes that construct GST history from superposition of error function solutions (Carslaw and Jaeger, 1959; Beltrami et al, 1997; Mareschal et al., 1999; Rimi, 2000). In such cases, the perturbation temperatures are given by:

$$p_k = \sum_{k=1}^{\ell} \left\{ \sum_{i=1}^m s_i \left(\operatorname{erf} \left(\frac{z_k}{\sqrt{k}(s_i-1)} \right) - \operatorname{erf} \left(\frac{z_k}{\sqrt{k}s_i} \right) \right) \right\} \quad (8)$$

The essence of this inversion method may be understood by considering the kernel (Jacobian matrix) employed in computational schemes:

$$j_{ki} = \frac{\partial}{\partial s_i} p_k = \sum_{k=1}^{\ell} \left\{ \sum_{i=1}^m \left(\operatorname{erf} \left(\frac{z_k}{\sqrt{k}(s_i-1)} \right) - \operatorname{erf} \left(\frac{z_k}{\sqrt{k}s_i} \right) \right) \right\} \quad (9)$$

A careful examination of the solution determined by equation (9) reveal that large-amplitude changes are intercalated with low amplitude variations in GST. In such cases there is apparent conflict between the selected scheme for regularization and the premise that smooth variations in temperatures contain transient changes. In fact, dealing simultaneously with short-term and long-term variations requires modifications in the inversion process for minimizing problems of instability and non-uniqueness. In such cases, incorporation of additional information that is present in observational data is necessary.

3. Inversion with Differential Weighting

The methodology employed in numerical simulations with differential weighting is based on following considerations in which the climate changes are considered as transient events of short periods. Also, the thermal properties of the medium (thermal conductivity and thermal diffusivity) are considered constants and independent of temperatures. For the periods

between transient changes climate is characterized by stable values.

3.1 First stage of Inversion

In the first stage of inversion we seek a simple solution for thermal signals which induced main surface temperature variations. It is not necessary at this stage to specify accurately the ages of these variations.

The inversion is carried out with unit weight matrix, in other words, $W_s = W_r = 1$. Thus, an initial guess of the dates of as to the elapsed times since the occurrence of transient changes in surface temperatures over the period is considered.

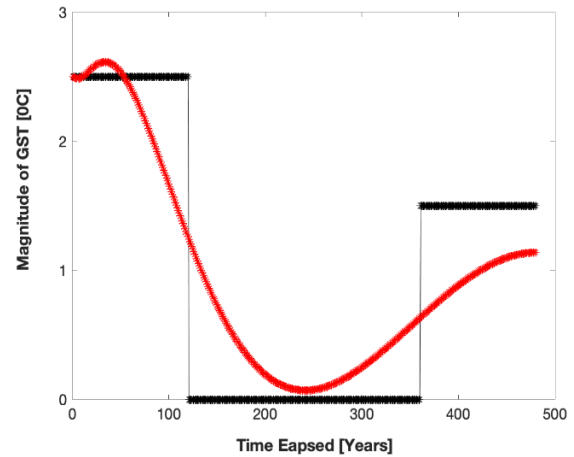


Figure 2 – The black line in this figure is the synthetic surface temperature history, with two transient variations around 125 and 375 years. The red line is the estimate obtained in the inversion process.

Note that there is considerable imprecision in the values of initial and final times and also in the magnitudes of such variations, but this does not constitute a serious obstacle in obtaining convenient solution

3.2 Second stage of inversion

Following this, restrictions are imposed on the plausible range of relevant parameters through choice of an appropriate regularization functional. This is done by selecting suitable values for the diagonal elements of the weight matrix \bar{W}_s . For this purpose, the weight matrix is considered as unitary and a minimum value is elected for the regularization factor λ that is capable of producing a stable and physically realistic solution.

In the second stage, the age values of GST change and its associated uncertainties are introduced into the inversion process. This is achieved by modifying the set of values in diagonal elements of the weight matrix \bar{W}_s that correspond to the time interval for the chosen GST variation. Large values of λ imply strong smoothing while small values lead to weak smoothing. In other words, the procedure allows improvements in the imposed variable degree of smoothing on the estimated parameters $\hat{S}_{\Delta i}$.

Consider now an example of application of the inversion process based on synthetic model, as per the theoretical foundations of which presented in item 2 of this work. The parameters in this model specify values for the beginning and end of the climate event as well as thermal properties of the

subsurface medium. The chosen values of the parameter are given in Table (1).

Table 1 – Parameter values assumed in the numerical model.

Parameter	Numerical Value	Unit
Depth of perturbed layer	500	m
Number of perturb. cycles	480	-
Perturb. period	1	s
Surface temperature	20	°C
Stable thermal gradient	30	°C/km
Thermal diffusivity	$4.3 \cdot 10^{-7}$	m^2/s
Regularization Constant	$1 \cdot 10^{-6}$	-

The corresponding subsurface temperature distribution specified in the model is illustrated.

Test 1: The case considered here refers to a transient change in GST from 2.5°C to 0.5°C over the last 50 years. The results obtained for the case of an underestimate of elapsed time of 25 years is illustrated in upper panel of Figure (3). The solution has the form of a spike with a magnitude of 4.5 °C at about 25 years, followed by a gradual oscillatory decay extending to the entire period considered of 500 years.

The results presented in the middle panel of Figure (3) indicate the case for overestimations of elapsed times of 75 years. The inversion process points to rapid decay in the magnitudes of GST variation with spikes occurring at the age values specified. For larger age values the inversion recovers the true value of 0.5°C.

The results obtained for the correct premise for the elapsed time of 50 years is illustrated in the bottom panel of Figure (3). Note that in this case the solution obtained by the inversion process, indicated by the red colored dashed line, has reproduced the nearly the exact magnitude, shape and time of occurrence of the GST variation.

In the example considered admit initially the case of two transients in GST, with age values around 125 and 375 years and with magnitudes of 2.5°C and 1.5°C respectively. The sampling interval is one year, and the durations of GST changes are 8 years. Initially all diagonal elements of the matrix \overline{W}_s are assigned an arbitrarily selected weight factor of 1000. Following this, information about times of temperature changes are introduced into the inversion process through modification of the diagonal elements of the weight matrix \overline{W}_s corresponding to the specific time periods for the two transient variations. For the case considered the diagonal elements of the matrix \overline{W}_s corresponding to periods of 121 to 129 years and 379 o 379 years have been assigned arbitrarily chosen value of one ($w_{s,jj} = 1$). This constitutes a relatively weak restriction for the 8-year period centered at times of 125 and 375 years. The age values of 125 and 375 years correspond to times of changes in GST in the true solution of the synthetic signal. The signal and the vertical distribution of residuals produced by the model considered are indicated in Figure (2). The black line in this figure is the synthetic surface temperature history, with two transient variations around 125 and 375 years. The red line in this figure is the estimate obtained in the inversion process corresponding to the GST signal $\overline{W}_s \equiv \{w_{ii} = 1\}$. It reveals substantial variations in GST for time intervals corresponding to the age values of the two signals.

Consider now some simple cases that illustrate the procedures employed in inversion of synthetic data. Numerical simulations were carried out for determining the sensitivity characteristics of the procedure suggested, for GST event with total time of 500 years.

Test 2: The case considered here refers to transient changes with elapsed times of 225, 250 and 275 years, illustrated in Figure (4). In the case of 225 years (top panel) the solution overestimates the GST signal. In the case of 275 years (bottom panel) the solution underestimates the GST signal. The middle panel illustrates the case for the correct estimate of 250 years, for which the solution obtained by the inversion scheme coincides with the stipulated GST variation within the error limits.

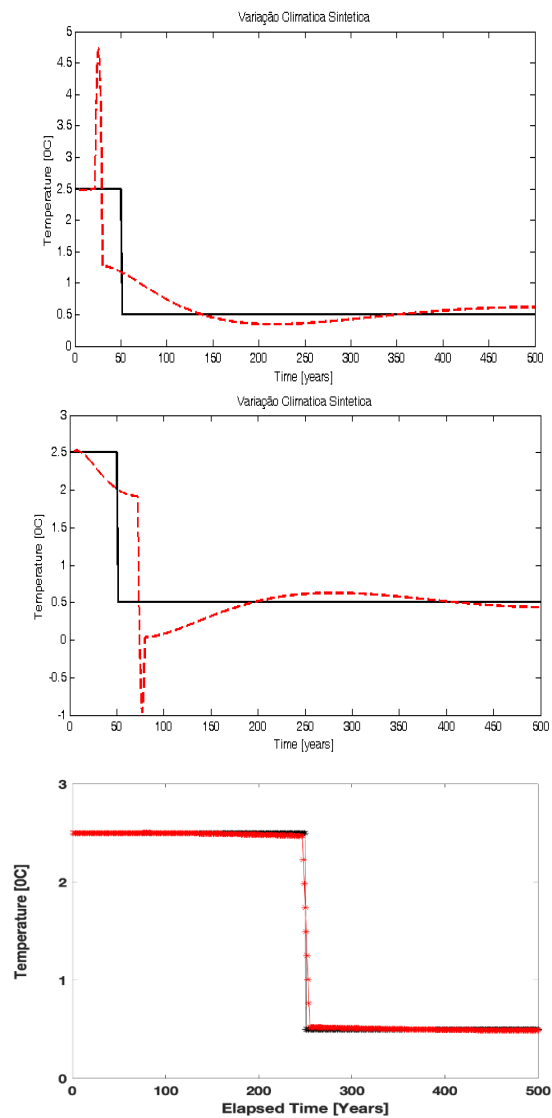


Figure 3 – The upper panel Illustration of the results obtained for an underestimate of the elapsed time. The dashed line in red color is the estimate obtained in the inversion process for the false premise that age of the GST event is 25 ± 4 years. The black line represents the synthetic data. The middle panel refers to results obtained for overestimate of elapsed time. The lower panel refers to results obtained for the correct estimate of the elapsed time. The dashed line in red color is the estimate obtained in the inversion process for the premise that age of the GST event is 50 ± 4 years. The black line represents the synthetic data.

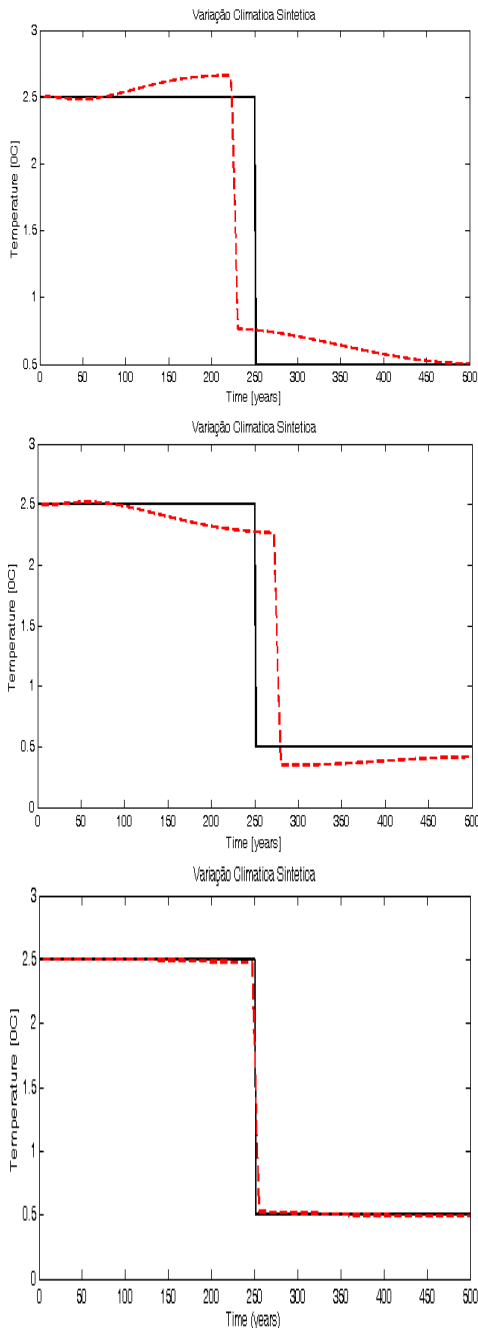


Figure 4 – The illustrations of the results obtained for three estimates of the elapsed time. The top, middle and bottom panels refer to results obtained for elapsed times of 225, 250 and 275 years. The dashed lines in red color indicates results obtained in the inversion process. The black lines represent the synthetic data.

4. Use of Synthetic Data

The first example considered refers to synthetic data set 1. The details of the synthetic log is illustrated in the top panel of Figure (5). Model simulation of this synthetic log is illustrated in the lower panel of this figure. It indicates that there has been a warming event between 30 and 50 years followed by a cooling event between 50 and 170 years. Note that magnitude of GST remains constant in these intervals. Beyond times of 170 years model values of GST remains constant.

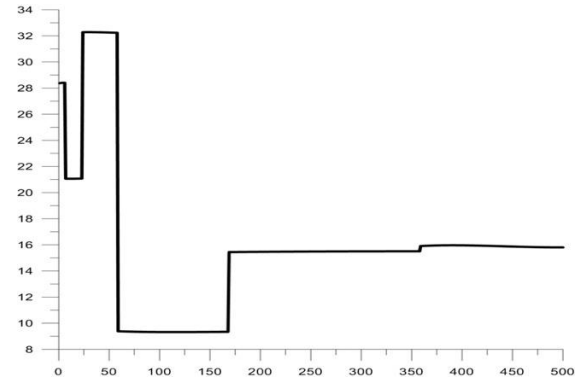


Figure 5 – Illustration of GST changes extracted for the synthetic log 1. The top panel is the observed temperature log and the bottom panel is result of model simulation using the method of Tikhonov regularization with differential weighting schemes.

The second example considered refers to synthetic log 2. The details of the log are illustrated in the top panel of Figure (6). Model simulation of this temperature log is illustrated in the lower panel of this figure. It indicates that there have been three warming events during the period of 1600 years. These warming events are followed by cooling episodes. Note that magnitudes of GST remain constant during both warming and cooling events. these intervals.

4. Conclusions

We conclude that a convenient way of minimizing uncertainty in geothermal climate change problem is using the method based on Tikhonov regularization of order one. In this approach residuals of observational data are minimized by imposing constraints on the variations of smoothing parameters, that is controlled by the magnitude of regularization coefficients. This is accomplished in two stages of inversion. In the first stage we seek an estimation of the dates of climate events derived from results of temperature logs. Inversion of the second stage allows estimation of the magnitudes of GST variations that are compatible with the ages of climate events of the first stage. The advantage is in finding better solutions without introducing other artefacts on the climate history. Such two-stage Tikhonov regularization procedures has been employed for extracting complementary information on GST history in continental regions of Brazil. The results reveal that the main warming event of the last century has been preceded by several secondary events during the time period of 1400 to the 2000 A.D.

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