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COMPUTER MODELLING OF HEAT AND MASS FLOW IN STEAMING GROUND AT KARAPITI THERMAL AREA, NEW ZEALAND

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ABSTRACT

Heat and mass transfer in steaming ground have been modeled using the TOUGH2 geothermal simulator and the results compared with field data collected by Bromley and Hochstein (2001). They measured temperatures at several sites over periods of 4 to 7 days at the soil surface, and depths of 0.01 m, 0.05 m, 0.10 m, 0.15 m, and 0.20 m. Soil porosities and saturations were also measured. These data sets were processed to extract four key sub-sets of data that were then used to calibrate a TOUGH2 model for each site. Two of these data sets are the steady state temperature and gas saturation versus depth; and the other two involve parameters of the variation with depth of the transient, approximately sinusoidal, diurnal temperature, namely, amplitude decay and phase shift. Calibration of the TOUGH2 models provides information about soil properties and heat and mass flows at each site. Model calibration also indicates a suitable range of parameters for the van Genuchten-Mualem relative permeability and van Genuchten capillary functions (Mualem, 1976; van Genuchten, 1980).

INTRODUCTION

This study uses data from site KP02 at Karapiti, and builds on the experience gained from analytic modeling of the Karapiti data (Newson et al, 2001), and numerical modeling of site KP03 (Newson and O'Sullivan, 2002).

The geothermal simulator TOUGH2 (Pruess, 1991) and the associated inverse modelling package iTOUGH2 (Finisterle, 2000) are used to investigate heat and mass transfer in warm ground at KP02. Firstly, steady state soil temperatures are used to calibrate geothermal heat and mass flows, and the thermal conductivity of the soil. Plots showing the fit of observed data to model results for combinations of heat and mass flows are used to select the parameters giving the best match. A similar process is applied choosing the van Genuchten parameters to give the best match to measured saturations. Particular attention is paid to the model sensitivity and correlation between parameters.

The parameters obtained from calibrating the model with the steady state data are further refined by matching transient, sinusoidal data.

BACKGROUND

Calibration data

Field measurements

The air temperature, and ground temperatures at depths of 1, 5, 10, 15, and 20 cm were measured at 6 sites at Karapiti, in the summer of 2000 by Bromley and Hochstein (Bromley and Hochstein, 2001). This data clearly shows the effect of the diurnal air temperature cycle at all the measured depths. The present study site KP02 has temperatures of around 55 °C at a depth of 20 cm (Figure 1).

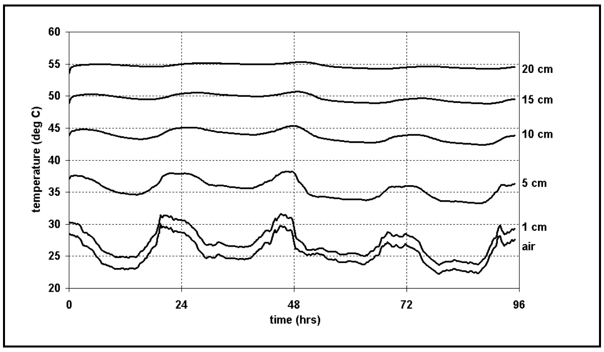

Figure 1. Temperature measurements at site KP02.

At the same time cores from 0 to 15 cm, and 15 to 30 cm depth were retrieved for laboratory determination of water content and porosity.

Laboratory data

The results of the laboratory work by Manfred Hochstein enabled calculation of saturation and porosity for the core samples. The porosity value used for modeling was 0.68. The gas saturations for cores from KP02 is shown in Table 1. The calculated saturation values were interpolated to obtain values at the model block centres.

Table 1 Gas saturation for KP02.

Depth (cm)	Gas saturation	Calibration depth (m)	Interpolated gas saturation
0 – 15	0.55	0.1	0.45
15 – 30	0.33	0.2	0.35

Modelling background

Mathematical models

Newson, et al, (2001) used three simple analytical mathematical models to investigate mass and heat flows, and soil thermal properties, at the Karapiti sites. A purely conductive heat flow model suggested that KP02 heat flows were 149.2 W/m^2, given a thermal conductivity of 1 W m/K. The second model included a heat loss boundary condition, but did not match the measured data and did not yield any useful information. The third model included mass flow, thus allowing both advective and conductive heat transfer in the soil. This last model predicted a deep upflow with a temperature of 72.9 °C.

Previous numerical modelling

TOUGH2 was used to model site KP03 at Karapiti (Newson and O'Sullivan, 2002).

First calibration of the steady state model with the temperature versus depth profile was used to determine the heat inflow, mass inflow and thermal conductivity to within the same multiplicative constant. Then saturation data were used to select the van Genuchten (unsaturated zone) parameters: lambda, alpha, S_{lr}, and P_{max}.

The transient model included the diurnal temperature variation in the atmosphere block of the model. The amplitude decay and phase shift of the daily variations of temperature in the soil depend on the heat and mass flow through the model. A simple optimization of the fit of model results to data for amplitude decay and phase shift was used to determine best-fit values for heat and mass flow

Some problems with the KP03 study are:

1. Each calculation of the objective function required one TOUGH2 run, and extra processing of results. This was a limiting factor in the combinations of parameters that could be used, although it had the advantage of simplicity.

2. Correlation of the van Genuchten parameters, in other words, the uniqueness of the solution was not investigated and so it is possible that more than one combination of parameters will give the same answer.

3. The study did not include the temperature observations in the objective function when considering the best-fit van Genuchten parameters.

The present work uses the inverse modelling package iTOUGH2 in 'grid search' mode to generate objective functions for a wider range, and more combinations, of parameters. Correlation between parameters and the temperature contribution to the objective function for the van Genuchten parameters are also investigated in this study.

Conductivity

TOUGH2 has several options relating thermal conductivity to saturation. The option selected for this study has thermal conductivity K as a function of the square root of saturation (Equation (1))

$$K = KDRY + \sqrt{S_l}\left(KWET - KDRY\right) \qquad (1)$$

Here KWET and KDRY are the wet and dry thermal conductivity, and are specified in the model input. S_l is the liquid saturation. Equation (1) includes porosity implicitly in the measurement or calculation of values of KWET and KDRY. For the present study we calculated a value for KWET and KDRY based on a combination of two permeable media models:

- a parallel plate model of rock and fluid, where the heat flow is parallel to the layers of rock and fluid. The wet and dry thermal conductivities are shown in Equations (2) and (3):

$$KDRY_{PARALLEL} = (1-\phi)K_{ROCK} + \phi\, K_{AIR} \qquad (2)$$

$$KWET_{PARALLEL} = (1-\phi)K_{ROCK} + \phi\, K_{WATER} \tag{3}$$

- and a series model, where the heat flow is across layers of rock and fluid. The wet and dry thermal conductivities are given in equations (4) and (5).

$$KDRY_{SERIES} = \left[\frac{\phi}{K_{AIR}} + \frac{1-\phi}{K_{ROCK}}\right]^{-1} \tag{4}$$

$$KWET_{SERIES} = \left[\frac{\phi}{K_{WATER}} + \frac{1-\phi}{K_{ROCK}}\right]^{-1} \tag{5}$$

Here ϕ is the porosity (0.68 for KP02). The thermal conductivities of air, water and rock are given in Table 2.

Table 2: Values for thermal conductivity.

	air	**water**	**rock**
Symbol	K_{AIR}	K_{WATER}	K_{ROCK}
Thermal conductivity (W.m/K)	0.026	0.6	2.5

The question then arises of how to best combine the parallel and series models. After some experimentation and comparison with laboratory data it was decided to use the arithmetic mean:

$$KWET = 0.5\left[KWET_{SERIES} + KWET_{PARALLEL}\right] \tag{6}$$

$$KDRY = 0.5\left[KDRY_{SERIES} + KDRY_{PARALLEL}\right] \tag{7}$$

The calculated KWET and KDRY values for KP02 are 1.00 W.m/K and 0.43 W.m/K. This study uses these values as an indication of the actual thermal conductivity, and investigates a range of values for KWET from 0.8 to 1.2 W.m/K. The ratio of KWET to KDRY (1:0.428) is retained, which eliminates KDRY as a parameter from the model fitting process. This process is equivalent to varying the porosity.

COMPUTER MODEL

Simulator

The geothermal simulator TOUGH2 and the inverse modelling package iTOUGH2, have been used for all the simulations described in this paper. TOUGH2 can model the transport of energy, water, steam, air and water vapour through porous media. These capabilities are required for modelling the unsaturated zone above the water table.

TOUGH2 allows a choice of relative permeability and capillary functions. The previous KP02 study used the van Genuchten-Mualem relative permeability function, and the van Genuchten capillary function, which were also selected for this study.

Model grid and boundaries

The model grid is a 1 m x 1 m vertical column, divided into 35 layers. The layer structure is very fine at the top of the model to provide the definition required to match the field data. The layer thickness increases with depth and the lowest layer, at 50 m depth, is 5 m thick. The top block of the model is connected to a very large ‘atmosphere’ block, which is large enough for specified atmospheric conditions to remain unchanged despite flows into and out of the model. The atmospheric temperature is derived from the Fourier analysis of the measured data, and a humidity of 85 % is used.

The side boundaries of the model are closed. There is a specified heat and mass input to the base of the model.

Modelling approach and calibration data

Fourier analysis of the field data gives a simplified representation of surface temperature, and soil temperature, in terms of a single Fourier component and the mean. This allows us to separate the calibration data into steady state (average values) and transient data. Steady state saturation data are also available.

Thus the steady state data consists of:

- stable, or average, temperature profiles with depth;
- saturation values at 0.1 m and 0.2 m depth.

The transient data are:

- the amplitude decay and phase shift of the diurnal temperature variation with depth.

The approach used in this study is to first calibrate the steady state model, and then use the information from this process in the calibration of the transient model.

The main difference between the present study and the previous KP03 study (Newson and O’Sullivan, 2002) is that this work uses iTOUGH2 to investigate model behaviour, and the correlation, or otherwise, of parameters.

Calibration parameters

The input parameters required for the model are shown in Table 3. Permeability is not a calibration parameter in this model because the results depend on the ratios of mass, energy, and thermal conductivity divided by permeability. Thus it was decided to fix the value of permeability and treat the others as calibration parameters. Some parameters have been assigned a fixed value, shown in the table, while the others are determined by the calibration process.

Table 3. Input parameters.

Parameter name	Symbol	Unit	Fixed value
Lambda	λ		calibration
Residual saturation	S_{lr}		calibration
Fully mobile liquid saturation	S_{ls}		1.0
Residual gas saturation	S_{gr}		0.0
Maximum capillary suction	P_{max}	Pa	1E6
Alpha	α	1/Pa	calibration
Mass flow	q_m	kg/s	calibration
Enthalpy of the mass flow	h	(J/kg)	83.9
Heat flow	q_e	W	calibration
Saturated thermal conductivity	KWET	W m/K	Range from 0.8 to 1.2
Dry thermal conductivity	KDRY	W m/K	0.428*KWET
Porosity			0.68
permeability		m^2	1E-13

MODELLING PROCESS AND RESULTS

Steady state model

The steady state temperatures and steady state saturations are investigated separately. This is mainly because they are sensitive to different parameters. The temperatures are most sensitive to heat and mass flow, and the saturations are most sensitive to the unsaturated zone parameters. The other reason is because visualization of the results is easier for a smaller number of parameters.

Temperature versus depth profile

iTOUGH was used in 'grid search' mode to generate the objective function for a range of heat and mass inputs to the base of the model. This method was used in order to understand the behavior of the objective function over the selected range of model heat and mass inputs, and evaluate whether a unique solution is possible for each thermal conductivity.

Each grid search run used a different thermal conductivity (with KDRY = 0.428KWET). Other than this the models used for each grid search were identical. Table 4 shows the thermal conductivity values used. The observation data for the grid search were the average temperature for depth profiles.

Table 4. Thermal conductivity values.

KWET	KDRY
0.8	0.342
1.0	0.428
1.2	0.513

The objective function values, for temperature observations only, with KWET = 0.8, 1.0, and 1.2 are shown in Figure 2. Because of the diagonal orientation of the valley in the objective function surface, the objective function surface is difficult to contour. Hence the lowest objective function values are represented by shaded squares, with the darkest squares being the lowest value of the function (< 110 in all cases). The grid search results show a region in each valley that contains the lowest values of the objective function. However, the long valley in each objective function surface shows this would be a difficult optimization problem to solve with iTOUGH2.

All the heat/mass combinations represented by the black squares in Figure 2 are shown in Figure 3. All three clusters in Figure 3 lie on a straight line, as hypothesized from previous results. At this point we can say that the best-fit heat and mass flows lie somewhere on the trend line shown in Figure 3, but the precise location depends on the value of thermal conductivity. A representative temperature profile from these results is shown in Figure 4.

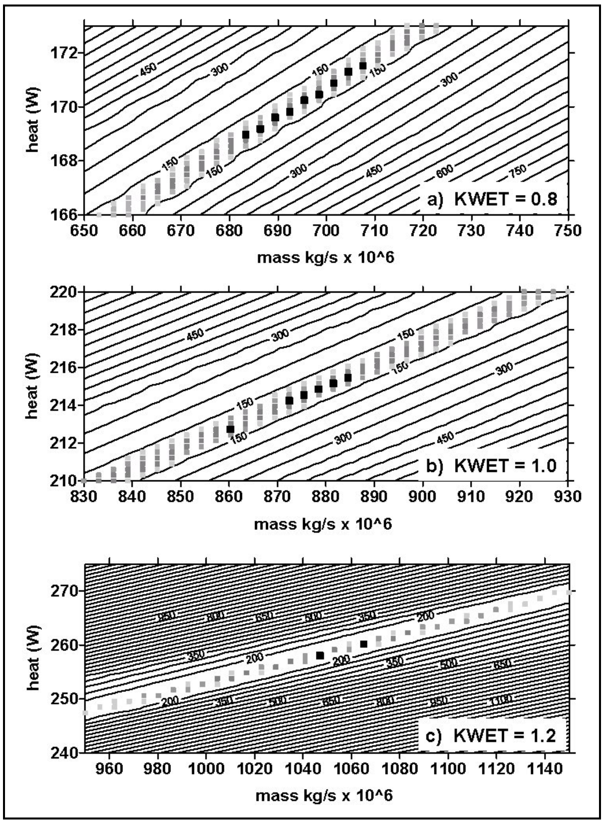

Figure 2. Objective function contours for the steady state temperature calibration (note that the mass flow values are multiplied by 10^6).

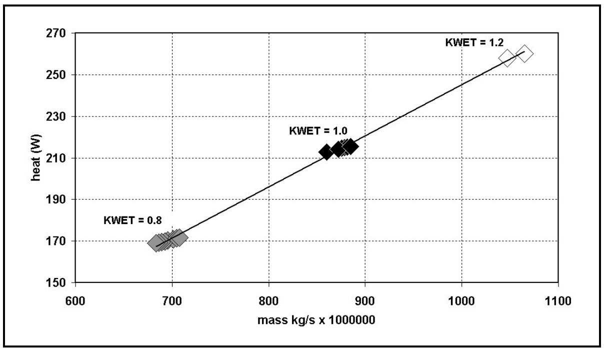

Figure 3. Heat and mass combinations with an objective function value of less than 110.

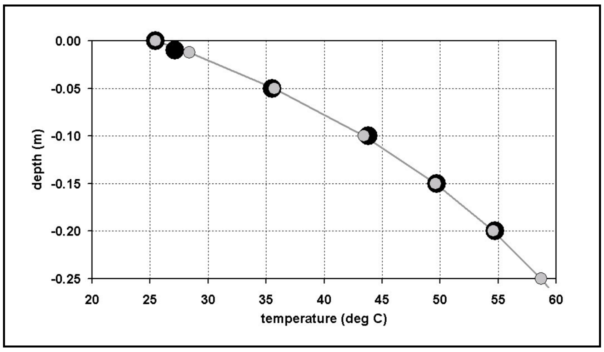

Figure 4. KP02 average ground temperatures (large black dots) and modelled temperature (Grey dots and line).

This work has determined the values of heat flow, mass flow and thermal conductivity only to within a multiplicative constant. Although this process still does not provide a precise value for any of these parameters, it has reduced the number of parameters to a single constant.

Saturation versus depth profiles

Unfortunately there are only two data points for the saturation versus depth profile. This lack of detail makes it difficult to determine accurate values for the unsaturated zone parameters. A grid search technique is used to address questions resulting from the previous KP03 study, namely:

1. How sensitive is the temperature response of the model to the van Genuchten parameters?

2. Is there a correlation between the parameters?

iTOUGH2 is used to generate a grid of objective function values for combinations of the van Genuchten parameters α and λ. Grids were generated for residual liquid saturation values of 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, and 0.40. The range of α and λ was $6.31*10^{-5}$ to $1*10^{-5}$, and 0.5 to 0.9, respectively. This entire process was carried out three times for models with KWET values of 0.8, 1.0, and 1.2. The heat and mass flows were determined from the trend line in Figure 3, using the values at the centre of each cluster of points.

Sensitivity: Figure 5 shows the range of values for the two objective functions, for saturation and for temperature, for each grid search. Sensitivity of the fit to temperature observations was quite high at low Slr values, although it was never as high as the sensitivity to saturation data. Because of the sensitivity of model temperatures to α, λ, and Slr, the objective function used to determine the best-fit behaviour of the van Genuchten parameters is the sum of the objective functions for temperature and saturation.

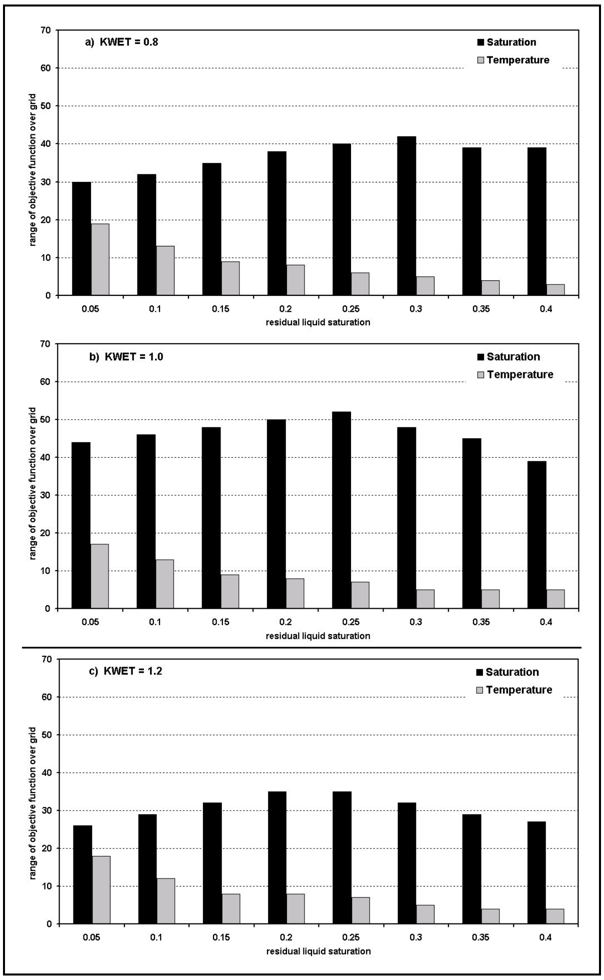

Figure 5. Range of the objective function over the entire log(alpha) vs lambda grid.

Correlation: Each plot in Figure 6. shows contours of the combined objective function including temperature and saturation data. In all cases the contour shown is for the same numerical value. The lowest value of the objective function occurs at two points for the case KWET = 1.2, within the contour for Slr = 0.20. These points are shown as black dots in Figure 6. The figure shows that non-uniqeness is a problem as there are two combinations of α, λ and Slr that will produce a good fit to the observation data. Also the elongated nature of the contours in Figure 6 indicates correlation between the parameters. Therefore although the parameter range has been considerably narrowed, more saturation data are be required to identify a unique solution. Based on Figure 6 we chose representative "good" parameters: KWET =1.2, Slr=0.2, log(α) = -4.86 and λ = 0.85. The modeled saturation for this case is shown in Figure 7.

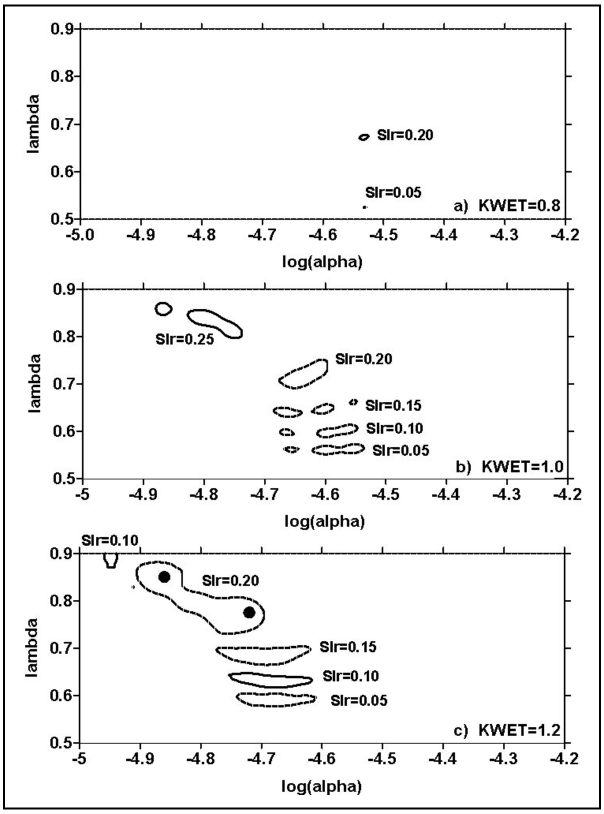

Figure 6. Contours of the objective function for temperature and saturation.

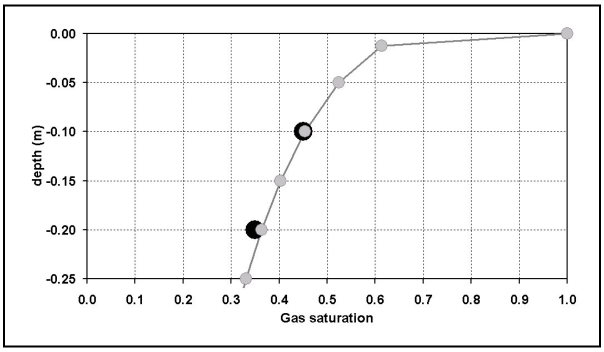

Figure 7. KP02 saturations (large black dots) and modelled saturation (grey dots and line).

Summary of the steady state model

So far the steady state modelling has given us three clusters of values for heat flow, mass flow, and thermal conductivity through which we can put a trend line. Any point on this trend line will result in a good fit to the temperature vs depth calibration data. This means that for one known point on the trend line, the mass flow, heat flow, and thermal conductivity can be multiplied by a constant, and will give the same goodness of fit for the temperature vs depth profile. This has effectively reduced the number of parameters from three to one. The following transient analysis is used to optimize this parameter.

The best-fit van Genuchten parameters (in the form of (log(α), λ)) occur around (-4.7, 0.775), and (-4.85, 0.85). These values occur at KWET=1.2, but because of the coarse sampling of KWET values, we decided at this stage to only assume that the best fit will be for KWET> 1.0.

Transient model

In addition to the steady state observation data described in the preceding sections, there is also transient information (shown in Figure 1) with over 1200 data points for ground temperatures. The original data has been subject to a Fourier analysis, which characterizes the amplitude decay and phase shift of the diurnal temperature wave with depth. The sinusoidal function, representing the daily component of the atmospheric temperature, is used as an atmospheric boundary condition for the transient model, and the steady state model provides the initial conditions. The temperature amplitude decay and phase shift in the model are compared with the observation data for model calibration.

Because of the nature of the data (temperature), the model response will be most sensitive to the heat and mass flows in the model, and less sensitive to the unsaturated zone parameters. Therefore the van Genuchten parameters are fixed at the first estimates of the optimal values derived previously: log(α)=-4.86, λ = 0.85, and Slr = 0.20.

The transient model amplitude and phase shift behaviour with depth are strongly affected by the mass flow, heat flow and conductivity parameter, which as discussed above have been determined to within a multiplicative constant. The calibration of the transient model can now be used to choose this multiplicative constant.

The transient models were run and a simple objective function (based on the sum of squares of errors) was calculated for the amplitude decay and phase shift, at various depths (see Figure 8). For increasing mass flow through the model the match to the temperature amplitude decay improves, while the reverse is true for the phase shift (Figure 8). The crossover point, where the two objective functions are equal, is at mass flow = 1.004E-3 kg/s, and heat flow = 247 kg/s, wet thermal conductivity (KWET) = 1.15, and dry thermal conductivity (KDRY) = 0.49. We use these values for the best-fit model. The corresponding model results and calibration data for the amplitude and phase shift with depth are shown in Figure 9 and Figure 10, respectively. The detailed model temperature response and the measured ground temperatures are shown in Figure 11.

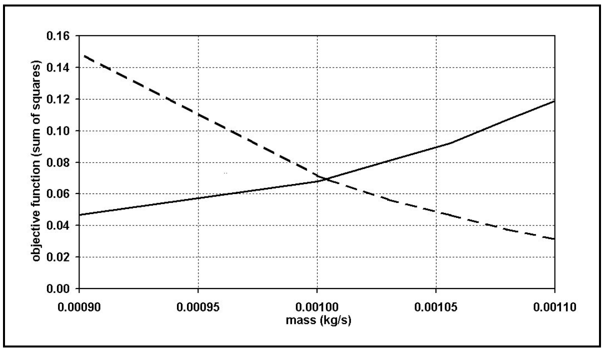

Figure 8. Objective functions for the amplitude decay(solid line), and phase shift(dotted line) for the transient model.

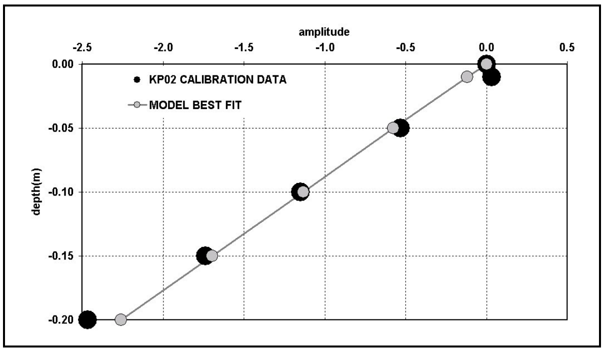

Figure 9. Amplitude decay with depth: the transient model results and calibration data for a model input of 1.004E-3 kg/s.

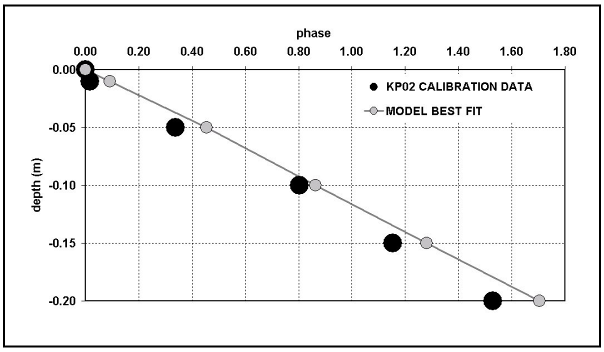

Figure 10. Phase shift with depth: the transient model results and calibration data for a model input of 1.004E-3 kg/s.

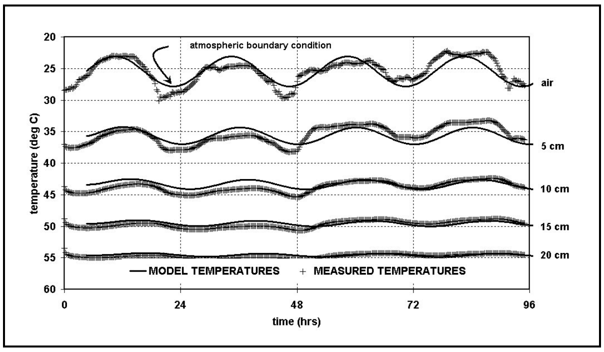

Figure 11. Measured and modelled temperature response.

DISCUSSION

This study has used iTOUGH2 to generate objective function surfaces to further investigate a calibration process for a model of the subsurface temperatures and saturations near the KP02 site at Karapiti.

The study has shown that from the matching of steady state data it is only possible to obtain estimates of heat flow and mass flow and thermal conductivity to within a multiplicative constant. Even this process is difficult because of the valley-like shape of the objective function.

Only two observation data points for soil saturation were available but by using them and the steady state temperature data it was possible to make some progress on choosing best-fit values for the unsaturated zone parameters. However there are difficulties with the non-uniqueness and correlation of parameter values. Greater detail in the soil saturation with depth observation data may resolve some of these problems.

Calibration of the transient behaviour of the model resulted in best-fit values for the mass flow and heat flow through the soil of 1.004E-3 kg/s/m^2 and 246 W/m^2. The thermal conductivities are KWET = 1.15 and KDRY = 0.49. The calibration of the transient model is a fairly simple optimization problem since it involves choosing only one parameter, i.e. the multiplicative constant for mass flow, heat flow and thermal conductivity.

CONCLUSION

A simple computer model has shown that geothermal heat and mass upflow through the soil are a major influence on the way the diurnal temperature variation spreads into the ground. The model geometry, and calibration technique has been tested on two Karapiti sites, and yielded useful information on heat and mass transfer in warm ground. This study has also given information on model sensitivity and parameter correlations.

Future work will involve further automation of the parameter optimization process using iTOUGH2, and the investigation of more complex boundary conditions, including atmospheric pressure fluctuation and the use of the actual air temperature instead of a representative sinusoidal function.

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