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Assessing the calibration of the Sydney Basin thermal structure model – are shallow groundwater bores a good substitute for deeper measurements

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SUMMARY

Estimating subsurface temperature and assessing the thermal structure in numerical models requires a vast database of measured values, a detailed geological model and the ability to identify, incorporate and constrain uncertainty in the parameters to provide a reliable and robust result. Sparse datasets with limited results required additional observables to be gathered. Using groundwater bores temperature in the shallow crust can be measured over a widely distributed area and in depth profiles. Calibration of the Sydney Basin thermal model has shown that using shallow groundwater bores strong constraints on parameters can be made, thus reducing overall model uncertainty. Deep measurements are limited therefore shallow groundwater bores are a good data substitute. The largest sources of uncertainty are the parameters governing temperature dependent thermal conductivity of the basement and Permian Coal Measures, as well as the basal temperature condition and unconstrained heterogeneities in the basement rocks. Variance in these parameters may significantly influence the resulting estimate of subsurface temperature. However through calibration the possible variance is limited due to the large number of available calibration points.

Key words: thermal structure, temperature, calibration, groundwater, numerical simulation, Underworld.

INTRODUCTION

Understanding the shallow crust thermal structure is critical as it is a vital component that underpins many geodynamic processes and the development of key economic resources, such as petroleum, gas and geothermal energy. Multidimensional thermal models, using a combination of geology derived from borehole and mapping and 3D seismic and gravity together with temperature heat flow and thermal conductivity parameters are used to estimate subsurface temperatures. However the uncertainties involved with heat flow model parameters are often under-explored yet necessary to assess the robustness and sensitivity of the model and the anomalies observed.

In any assessment or model of subsurface conditions, the ability to identify and quantify the uncertainties involved will determine the quality and reliability of the results. A robust assessment of model uncertainty is an integral part of any parameter estimation problem (Tarantola and Valette, 1982). Gaining an understanding of parameter uncertainty, non-uniqueness, and correlation is as important as estimating the parameter values themselves (Minsley *et al*. 2012). In this case upper crustal temperatures, uncertainties in thermal measurement, geological architecture, and physical properties, such as thermal conductivities and heat production at depth, all fundamentally affect model outcomes and applicability. As the physical model complexity increases, the ability to sample adequately for formally reliable statistical meaning becomes difficult. The very nature of geological models posed with a relatively small set of observables and non-linear rheology leads to the difficulties in obtaining unique optimum parameters.

Sydney Basin Thermal Model

The Sydney Basin thermal model, developed from the 3D geological model of Danis *et al*. (2011a), exhibited distinct challenges in calibration – the process of tuning unknown model parameters such that the model plausible matches real world observables. Large quantities of reliable observables were essential but often lacking and the standard methods of calibration too time consuming for a large scale forward model. A purely probabilistic approach, where statistical validity or sensitivity analysis is demonstrated through a Monte-Carlo approach with thousands of simulations computed and the resultant output treated statistically was considered simply impractical and not necessary when some of the parameters were known. The most basic approach would be to manually adjust the parameters and visually inspect the agreement between the observables and the computer model. However at hundreds of observation points over many scenarios, this method is tedious, subjective and fails to capitalise on the potential statistical properties of the observation space.

A practical approach was use of model 'ensembles' to determine best-fit parameters and their uncertainty, utilising an objective function which quantifies model misfit with observed measurements followed by optimisation to minimise the misfit (discussed in detail in Danis, 2012). Through simulations in *Underworld* the Sydney Basin thermal model was constrained with down-hole temperature measurements, varying spatially and laterally with depth (Figure 1). This provided good spatial distribution of control points, which possess a strong coverage of shallow (less than 100m) depths and near surface lithologies (depths ranging from 100m to 900m). Through an objective function the fit between the model simulated values and observables was assessed to identify parameters which contribute the largest uncertainty and those most sensitive to change.

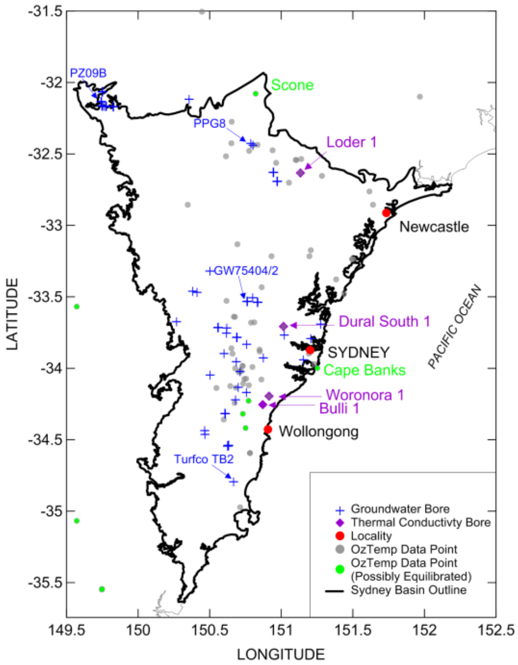

Figure 1. Location of bores in the Sydney Basin. Calibration temperature bores are shown in blue (crosses), thermal conductivity bores in purple (diamonds), OzTemp temperature locations in grey and green (circles).

Limited deep measurements exist and most are contained within the OzTemp 2010 database (Gerner and Holgate, 2010). They are either non-equilibrated or have been analytically corrected using Horner Plots thus are not likely to truly represent the subsurface conditions and were not be used in calibration. Down-hole temperature measurements gathered by Danis *et al*. (2011b), primarily from groundwater bores, all constrain the near surface lithologies. Using a multitude of points in a profile provides vertical spatial distribution over the model domain and helps to overcome the problem of limited deep calibration points. The uncertainty and sensitivity analysis and parameter optimisation suggests that deeper temperature measurements, if not practical to obtain, may not be necessary to adequately assess subsurface temperature in thermal models.

To validate the optimised model of the Sydney Basin as representative of geological reality both temperature and model thermal conductivity profiles were compared to thermal conductivity results from drill-core measured by Granite Power Pty Ltd and temperature measured in bores not used in the calibration. In general there is good correlation with the data but the results do clearly highlight the effects of heterogeneity and the limitations associated with inherent model assumptions (i.e. homogenous layers, conductive heat flow, model geometry). The existing levels of uncertainty during model development compound into the results of uncertainty and sensitivity in the model analysis.

METHOD AND RESULTS

The down-hole temperature points were collected from over 40 bore-hole locations in the Sydney Basin (Figure 1) were assigned a qualitative confidence level; either ‘well trusted’ (i.e. high confidence in the quality of the measurement and generally measured by us) and ‘possibly ok’ (i.e. measurement is assessed as equilibrated but not measured by us directly). Parameters in the thermal model (Table 1) representing the thermal conductivity and heat flow of each model layer were varied, within their known physical bounds (i.e. the thermal conductivity of sediments was not varied to outside that of published experimental data), and the resulting temperature output compared to the observables via the objective function.

Table 1. Initial properties of each model material, using temperature dependent conductivity

Model Material	K_0 (W/m-K)	K_{crit} (W/m-K)	T_{crit} (°C)	Heat Production (μW/m^3)
Sediments	2.00	1.50	300	1.25
Coal Measures (Jurassic, Greta, Reid Dome, Maules Creek	0.30	0.20	300	1.25
Permian Coal Measures (PCM)	1.20	0.20	300	1.25
Basal Volcanics	3.00	2.25	300	0.50
Basement (under fault)	3.00	2.25	300	2.00
Lachlan Basement	3.00	1.50	300	2.00

The objective function (Eq1.) is more complicated than a simple temperature difference used in computational assessment.

$$obj = \frac{1}{4} \cdot \left[\frac{ave_T}{C_{aveT}} + \frac{stdev_T}{C_{stdevT}} + \frac{ave_P}{C_{aveP}} + \frac{stdev_P}{C_{stdevP}} \right] \text{Eq. 1}$$

Here aveT and stdevT is the average and standard deviation of temperature misfits between the model and the observed for all ‘Well trusted’ observation points. Similarly, aveP and stdevP are for all ‘Possibly ok’ observation points. Here we are giving the trusted bore-holes just as much weighting as the possibly ok because we know there are not enough trusted ones to use solely. To avoid bias from outlying points the standard deviation is also considered in the objective function. For example, where a down-hole profile has a different gradient to the modelled the outliers bias the results when just using an average, compared to a gradient that matches the model. This objection function exposes more information than the raw average and relates to the shape of the bore-hole profile. Figure 2 presents the measured (observed) temperature compared to the model estimated temperature for four bore-holes, two in the Hawkesbury Sandstone lithology and two in the Permian Coal Measures lithology for the optimised thermal model results.

Whilst a great many temperature measurements may exist for the shallow profile (0m to 70m) a representative numerical model simulation for the shallow zone, where there are diurnal, seasonal and palaeo climatic effects coupled with groundwater aquifers, would be very complex. An integrated surface and groundwater flow model coupled with heat flow would be necessary and details on aquifer storage and heat flux parameters, groundwater flow direction, recharge and discharge zones, on a regional scale would be required and at present are extremely limited.

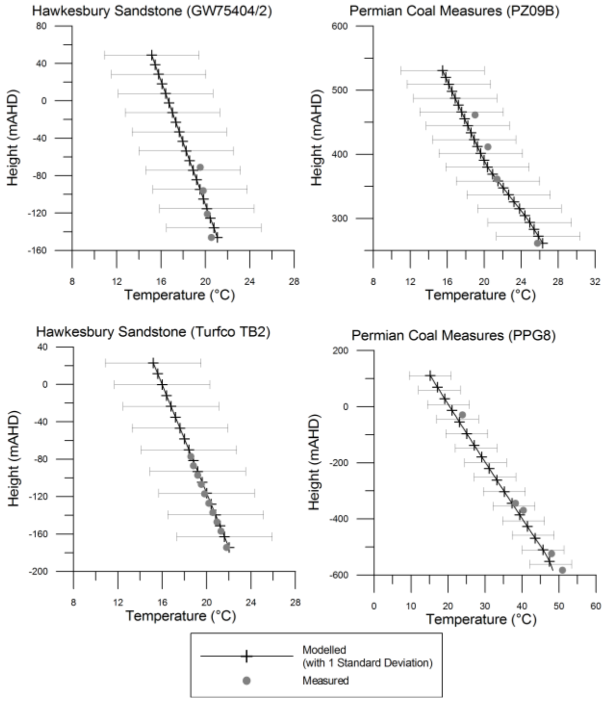

Figure 2. Comparison of modelled temperature (crosses) and measured temperature (grey circles) profiles from bores in the Hawkesbury Sandstone and Permian Coal Measures in the Sydney Basin with one standard deviation error on the modelled values.

However the Sydney Basin thermal model is primarily concerned with the deeper thermal structure and there is good agreement with the deeper part of the measured profiles with the modelled data. For comparison the measured temperature profile at borehole Cape Banks and Scone was compared to model estimated temperatures at these locations as shown in Figure 3. It should be noted that the data from these boreholes is from the OzTemp database and have been listed as have an equilibrium measurement.

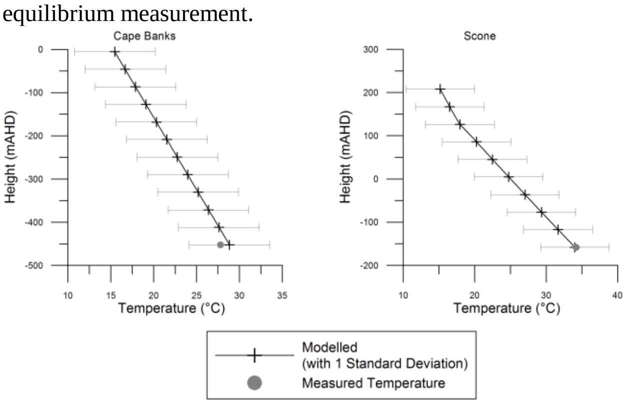

Figure 3. Comparison of modelled temperature (crosses) and measured temperature (grey circles) profiles Cape Banks and Scone with one standard deviation error on the modelled values.

In Figure 3 the measured temperature fit well with model and fall within one standard deviation and both are within less than 2°C of the model data. This shows the calibration Sydney Basin thermal model is approaching representative conditions with regards to temperature. The next step was to compare the thermal conductivity profiles of the model with measurements made on core samples in bore-holes Bulli 1, Woronora 1, Dural South 1 and Loder 1 (Figure 4).

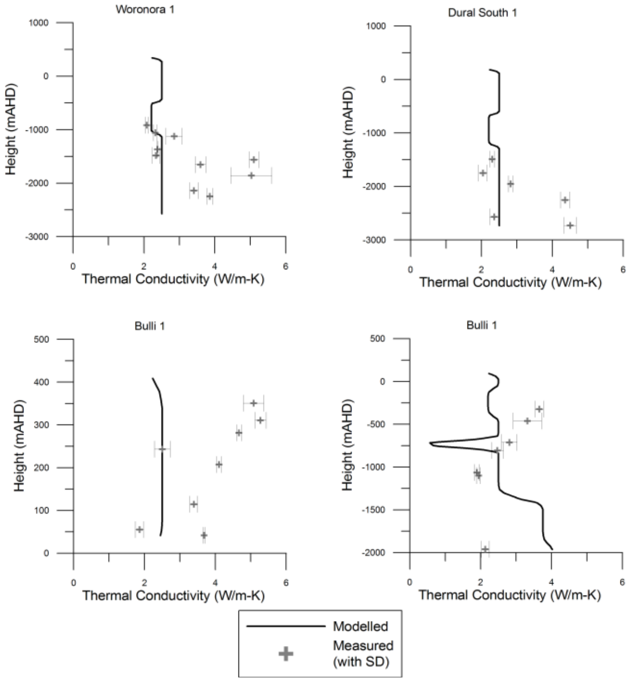

Figure 4. Comparison of model thermal conductivity (black line) and measured thermal conductivity of core samples (grey crosses) with measured standard deviation.

Figure 4 shows that matches of model assigned thermal conductivity to measured thermal conductivity are possibly ok in some lithologies but generally highlights the heterogeneity of the measured data over the model lithology. As detailed thermal conductivity measurements in the Sydney Basin are extremely limited this is an aspect of the model requiring further calibration.

Using the practical approach to create ensembles of best fit parameters and quantifying uncertainty an ensemble threshold of 0.1 was achieved with only 339 realisations on the objective (appraisal) function. For the Sydney Basin thermal model the largest sources of uncertainty, identified in the calibration process, were the parameters governing temperature dependent thermal conductivity, particularly in the basement and Permian Coal Measures (Figure 5) and the basal temperature condition and surface temperature (Figure 6). They have the least amount of constraining information but the strongest potential to impact the uncertainty of the model. The Lachlan basement exhibits strongest potential to generate uncertainty, from either its conductivity, heat production. The results show basement K_0 is close to the anticipated published values. The results of the optimal basal temperature suggest that at 12 km, 345°C with a standard deviation of 4.1°C represents the best 'regional' basal constraint, in that it produces the best fit with down-hole temperature measurements in the near surface. However the basal temperature may well change over the scale of a basin. Temperature dependent thermal conductivity for the Lachlan basement and Permian coal measures is difficult to optimize further without more constraints from observables. However these results show that even with the inherent uncertainties of insufficient heterogeneity the standard deviation is low. For the Lachlan basement K_0 is optimal at 3 W/m$^{-K,}$ which is comparable with published values, and K_{Crit} is optimal at 1.5 W/m^{-K}. The Permian coal measures have several down-hole temperature measurements which allow K_0 to be optimal at 1.2 W/m^{-K}.

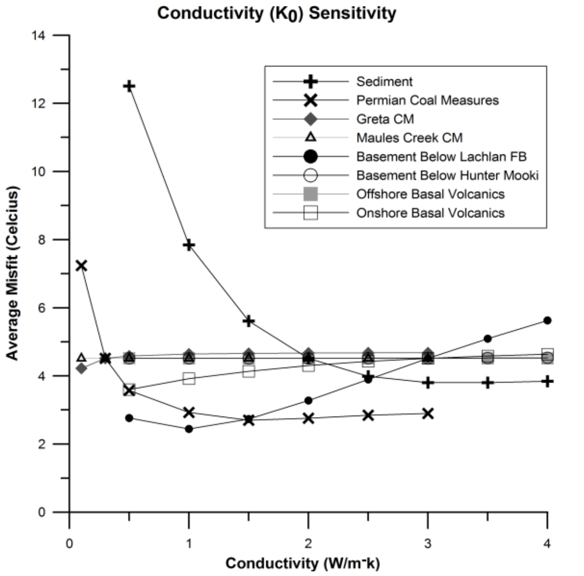

Figure 5. The difference in temperature, as an average across all observation points, between observed and model scenario when varying only the set of conductivity (K_0) parameters.

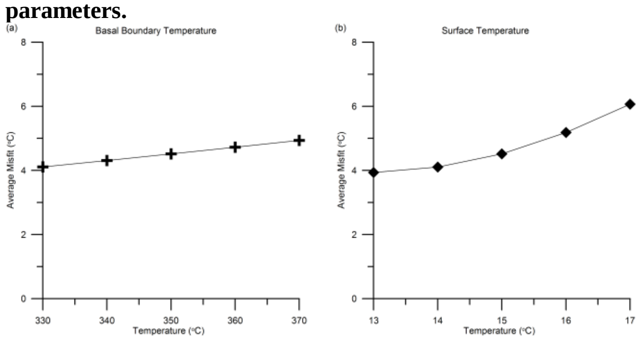

Figure 6. The difference in temperature, as an average across all observation points, between observed and model scenario when varying only (a) the basal boundary temperature and (b) the surface temperature.

The optimised model of the Sydney Basin estimates temperature at 5 km range from 150°C to 200°C with higher temperatures associated with areas of thick sediment and multiple coal measures. Uncertainty on the temperature estimates could be considered to be at least 5°C, based on the one standard deviation of the modelled average values and potentially as high as ± 40°C at 5km This is the difference between the maximum model temperature for the optimised model (220°C) and a model with no thermally insulating coal (170°C) (Danis *et al*. 2012) and incorporates a compounded error from the temperature sensor, climate correction and assumptions on thermal conductivity and basal boundary temperature.

CONCLUSIONS

Estimating subsurface temperature through thermal modelling contains many significant sources of uncertainty, especially when sparse datasets are involved. There is a critical need to identify, incorporate and constrain uncertainties in estimates of thermal structure and subsurface temperature. In the Sydney Basin the largest sources of uncertainty are the parameters governing temperature-dependent thermal conductivity, particularly in the basement and Permian coal measures; as well as the basal temperature condition, and unconstrained heterogeneities in the basement rocks.

Assessing the uncertainty and sensitivity of parameters during model calibration provides a degree of certainty and reliability to the results. Reliable observables are essential and the practical approach of developing ensembles constrained by these observables allows better understanding of the variance expected in the responses in subsurface temperature. The shallow and near surface temperature measurements from groundwater bores are suitable observables and their shear numbers have allowed for tight constraint on model parameters. Given an appropriate volume and spatial distribution, and consideration to their inherent uncertainties, shallow groundwater bores are a good substitute where deeper data is limited.

Whilst the Sydney Basin model may lack a degree of heterogeneity and/or the geometry is moderately incorrect to gain further certainty on the optimal parameters the results so far indicate it is fast approaching a state which best represents geological reality. Comparison of model results with measured temperature data from other boreholes not used in the calibration show good correlation. The lack of thermal conductivity values in the Australian thermal database is a fundamental knowledge gap with implications for many aspects of geodynamic research (i.e. plate tectonics, earthquakes) and resource exploration (i.e. geothermal, minerals, oil and gas). The comparison of model thermal conductivity values and measured core values clearly demonstrates this gap.

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