USE OF AN HEURISTIC METHOD AND PEST FOR CALIBRATION OF GEOTHERMAL MODELS

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ABSTRACT

This paper discusses inverse modeling coupled with an heuristic approach for calibration of geothermal reservoir models implemented with the TOUGH2 multi-phase flow simulator.

Given a pre-defined permeability distribution, the inverse modeling software suite PEST is utilized to automatically identify the values of the rock permeabilities that achieve the best fit between the model results and measured data. In order to gain further improvement in the model fit to the data, the permeability distribution is also refined in a heuristic manner by identifying the model domains that have the most effect in the model matching. This method is demonstrated using a model of a real geothermal field. The main calibration process involves the matching of the natural state temperatures taken from downhole well measurements. As a second stage, the production response of the field during the exploitation period, quantified by measurements of production enthalpies, is used to calibrate the model.

1. INTRODUCTION

By using a fully calibrated numerical model of heat and mass flowing underground in a geothermal reservoir, information on conditions and properties of the geothermal system can easily be obtained. This information is an important tool in deciding on a reservoir management strategy that will give rise to an optimum production scheme so that the production capacity of the field can be maximized without sacrificing the sustainability of the geothermal resource. Complex three dimensional reservoir models are commonly used to simulate complex geometry, structure, properties and spatial responses in the reservoir. A detailed three dimensional model of a field can provide an in-depth insight into the physical and chemical properties of the field as well as its transient responses.

Matching of the past behavior of the field with the model is an important first stage before it is used for forecasting. Then the model can be used for optimizing future production by comparing the predicted performance of the reservoir over its projected lifetime for various scenarios. As the model becomes more complex however, the difficulty of model calibration also increases substantially. Non-uniqueness of the reservoir description as a result of an increase in number of the parameters used may become an issue.

STAR (Pritchett, 1995), TOUGH2 (Pruess, 1991) and TETRAD (Vinsome and Shook, 1993) are among the commonly used reservoir simulators for modeling three dimensional, multi-phase, multi-component flows in geothermal reservoirs. There has been continual progress in both computational algorithms and hardware and many improvements have been made over the years to speed up geothermal model simulation. However, manual calibration of a geothermal model is still a slow process.

Tools for inverse modeling such as iTOUGH (Finsterle et al., 1997), UCODE (Poeter and Hill, 1999) and PEST (Doherty, 1994) are available for assisting with the selection of model parameters during calibration and for estimating the sensitivity of predictions of future production to the choice of model parameters. The goals in the use of these inverse modelling tools include (O'Sullivan, 2000):

- Automation of the time-consuming process of estimating reservoir properties.
- Minimizing the bias of the modeller in parameter selection.
- Providing correlation and uncertainty statistics for the parameters involved in the modeling process.

In a previous work, an automated calibration tool for TOUGH2 based on inverse modelling techniques was developed by Finsterle (1997) and implemented in the computer program iTOUGH2. The paper presents the result of calibration exercise of a geothermal model that uses the inverse modeling approach and a heuristic model structure refinement. Two software packages, TOUGH2 and PEST are used in a linked manner in this study.

- TOUGH2 (Pruess, 1991) is a numerical simulator for flows of multi-component and multi-phase fluids in porous medium commonly used in modeling of geothermal fields.
- PEST (Doherty, 1994) is a model-independent parameter estimation and uncertainty analysis software package developed by Watermark Numerical Computing. PEST is short for *P*arameter *EST*imation (Doherty, 2005).

The objective for the calibration of a geothermal model in this study is to identify the permeability values of the reservoir rocks defined in the model such that the mismatch between the model results and field data is minimized. The model is calibrated in two stages, first against the natural state data using the pre-exploitation temperature logs and secondly against the transient production response characterized by the well discharge enthalpy trend.

For some geothermal projects, transient pressure data may also be available but this was not the case for the model considered here. However the availability of an extra set of pressure data would not change the methodology described below.

2. MODELING OF GEOTHERMAL SYSTEMS

Predicting multiphase flow and mass transport processes in the subsurface by means of numerical simulation involves a number of steps, summarized below:

- Developing a conceptual model of the natural system.
- Assigning values to the input parameters and calibrating them with the available static and transient field data.
- Running the model in order to predict the future state of the system.
- Interpreting the results, assessing the uncertainty of the predictions and making decisions on field management.

The first conceptual modeling step involves sorting out the most significant physical properties of a geothermal reservoir based on diverse information and conflicting opinions (O'Sullivan et al., 2000). Once done, this conceptual model is converted into a mathematical model which numerically represents the actual system.

After generating the numerical model, important properties are then identified and values are assigned to the model. In order to produce an accurate model prediction, these model properties must be consistent with the real system. This is a problem with geothermal systems because the system properties on which the model is highly dependent are not directly measurable in the field. Despite the lack of a method for accurately identifying the reservoir parameters that affect the field response, there are state variables that can be easily measured in geothermal fields. Therefore, relevant system properties can be indirectly determined by calibrating the model to reproduce these measurable data. This calibration process involves adjustment of the model structure and parameters so as to best replicate the behavior of the system with the numerical model.

In geothermal modeling, the calibration process consists of two stages, namely, the natural state and production history calibration. The first stage of model calibration involves matching the natural state behavior of the system. The natural state temperature and pressure profiles in the wells are used to calibrate the location and magnitude of the deep inflows, and the permeability structure. The second stage of calibration involves matching the past production history. This is done by adjusting the model parameters such as permeability and porosity until there is good agreement between model results and measured values for pressure response and discharge enthalpy.

This entire calibration process is very tedious especially for large models with many unknown parameters. In the manual calibration of a geothermal model, a lot of trial-and-error changes have to be made to adjust parameters such as the permeabilities and porosities, the amount of heat and mass injected into reservoir base and productivity indices of the production wells.

2.1 Forward Modeling Technique

One of the commonly used tools for modeling of fluid and energy flow in a geothermal field is TOUGH2. It is a general-purpose program for the numerical simulation of multi-dimensional flow of heat and multiphase, multi-component fluid mixtures in porous and fractured media (Pruess, 1991). TOUGH2 solves mass and energy balance equations that describe general non-isothermal multiphase, multi-component fluid and heat flow in non-uniform anisotropic systems. The fundamental principles for multiphase flow simulation used in TOUGH2 are the laws of conservation of mass, energy and momentum. TOUGH2 uses a finite volume or integrated finite difference technique that requires the reservoir to be divided into several sub-volumes, commonly called blocks or elements.

2.2 Inverse Modeling Technique

Identifying the parameter values in the models in the present study is carried out using PEST. PEST is a collection of programs for parameter estimation, sensitivity analysis, and uncertainty propagation analysis. It is a model independent inverse modeling tool that can be easily integrated with a simulator like TOUGH2 for carrying out the forward calculation of non-isothermal multiphase flows in porous and fractured media such as those in geothermal models.

There are several advantages in using PEST rather than other available inverse modeling software. PEST is free, well documented, fully supported and the source code is publicly available. PEST, especially the parallel version, is multi-platform and can therefore work equally well on both Windows and Linux machines without the need of special configuration or software. Lastly, PEST being model-independent runs in a script-like manner working only on the input and output files. This feature enables users to use it without needing to modify the existing forward model simulation code. It can be adapted to any existing model simulator without needing to know the principles governing the model.

2.3 Non-linear Parameter Estimation Method in PEST

In the context of this work, the goodness of fit between the model results and field data is measured by a quantity known as the objective function, given by the equation below:

$$S(\Psi) = \sum_{i=1}^{n} [y_{oi} - f(x_i, \Psi)]^2 \qquad \text{(Eq. 1)}$$

Here, Ψ is the set of parameters that needs to be determined, y_{0i} is the field observation, $f(x_i,\Psi)$ is the model generated result, $y_{oi} - f(x_i, \Psi)$ is the residual or the difference between measured observation and model generated result and S is the objective function. The automated calibration process therefore involves searching for a set of model parameters that will give the lowest possible value of this objective function. In order to obtain the minimum of this function, we need to find the set of parameter Ψ which satisfies the equation:

$$\frac{\partial S(\Psi)}{\partial \Psi_j} = -2 * \sum_i \{[y_{0i} - f(x_i, \Psi)] * \frac{\partial f(x_i, \Psi)}{\partial \Psi_j}\} = 0 \qquad \text{(Eq. 2)}$$

PEST uses the Levenberg-Marquardt algorithm to solve the equation above and identify the parameter set Ψ. It can be written in the form:

$$\Delta\Psi = [J^T W J + \lambda_m I]^{-1} J^T W \Delta y \qquad \text{(Eq. 3)}$$

where J is the Jacobian matrix defined by

$$J_{ij} = \frac{\partial f(x_i, \Psi)}{\partial \Psi_j} \qquad \text{(Eq. 4)}$$

Thus J contains the rates of change in the model results with respect to the changes in the parameter values. W is the weight of the measured data, I is the identity matrix and λ_m is the Marquardt parameter. This method of nonlinear parameter estimation, upon which the PEST algorithm is based, is highly dependent on the evaluation of the gradients in the Jacobian matrix. These derivatives are calculated by PEST by taking the difference between two or three observations calculated on the basis of incrementally-varied parameter values. The derivative of each observation with respect to each parameter needs to be evaluated before the parameter identification step can be implemented and is therefore computationally expensive especially for models with many parameters.

2. PARAMETER ESTIMATION APPROACH

In modeling with TOUGH2, the reservoir system is divided into numerous elements or blocks. Hydrological and thermal properties are then assigned to each of the elements. For large models with a few thousand blocks, identifying the parameters for every block in the model is a very difficult task. Instead the model domain can be subdivided into a number of areas or volumes in which a certain physical property is assumed constant and is represented by a rock-type. Once this is done, PEST can then be used to estimate the best value of the permeability for each rock-type using the nonlinear parameter estimation method described above.

This process of defining the model structure is however highly dependent on the judgments of the modeler and is usually based on limited information. Therefore an optimal allocation of the rock-type is not guaranteed. As a consequence, even the best possible choice of rock-type parameters may still not give a satisfactory match between the model result and the measured data. Modifications to the rock-type structure as well as to the rock-type parameters may be required to further improve the model.

To overcome this problem, a heuristic model structure refinement was employed by systematically re-allocating the rock-types after each inverse model runs. This method requires the intensive use of the sensitivity result produced by PEST in order to identify the refinement that needs to be made. In this approach, the model calibration process is started with a simple permeability structure with as few rock-types as possible. Then PEST is used to identify the permeability values of the defined rock-types that will give the closest match between the model result and the measured data. During this calibration stage, the number of parameters varied in a PEST run is restricted partly because of the computation time, and mainly because if too many parameters or insignificant parameters are included, the minimization of the objective function may not make progress. As a general rule in this work, parameters whose sensitivity value are less than 10% of that for the most significant parameter are excluded in parameter estimation. Parameters whose values reach the modeler specified upper or lower bounds are also excluded. Choosing the parameters to exclude in the parameter estimation process is tricky because there is no way to know in advance if the model calibration will really benefit if a certain set of parameters is excluded from the optimization.

After each PEST optimization run, the resulting sensitivity file is reviewed to identify the most influential parameters. New rock-types are then created by subdividing the rock-types that have the most influence in the model. In this study the 5 most significant parameters are selected as the candidates for rock-type subdivision. This subdivision of rock-type is done iteratively after each PEST optimization cycle. The model domains occupied by these influential rock-types are then subdivided and more rock-types based on these five most influential rock types are created and assigned to the subdivided model domains. So for example a region containing one rock-type may be subdivided into two, or sometimes four, regions each with a new rock-type.

This subdivision of rock-type domains is done with consideration of the well locations and properties whenever possible. For example, areas in the model where wells are located (near the center) are separated from the areas where no wells are drilled. If a rock-type falls within these two areas and happens to belong to the group of five with the most influential parameters, a new rock-type with parameter values initially equal to this rock-type will be created. These two rock-types (the original rock-type and the new one) will then be assigned to each of the two regions (one an inner region including wells and the other an outer region) in the model previously occupied by a single rock-type. When the most influential rock-types fall in areas where no wells are present, the region is simply divided in half in either a north-south or east-west manner.

3. INVERSE MODELING CASE STUDY

The main objective for the calibration in this study is to identify the permeability values of the reservoir rock types defined in the model. This technique was applied in calibrating a working model of a geothermal field. The model was constructed using the MULGRAPH pre-processor (O'Sullivan and Bullivant, 1995) and run using the AUTOUGH2 simulator (a modified version of TOUGH2 developed at the University of Auckland, AUTOUGH2 notes, 2008). The model was set up with 17 rock-types distributed throughout the model based on detailed geological model of the field. As an initial guess, all the rock-types were assigned equal permeability values of 4 and 0.5 mD for the horizontal and vertical directions, respectively. The model was calibrated against the downhole temperature measured from the wells and the flowing enthalpy trend of the producing wells. The inverse runs for this model were carried out on a 32 processor Linux cluster at the University of Auckland.

3.1 3D Reservoir Model Setup

The regular rectangular 3-dimensional grid shown below was used for the model. The computational mesh is composed of 26 layers, each layer having 754 elements except for the top 4 layers. The model consists of a total of 17,635 blocks with areas ranging from 90,000 m^2 (300 m x

300 m) near the wellbore to a maximum area 1,440,000 m^2 (1200 m x 1200 m) for some blocks at the edge of the model.

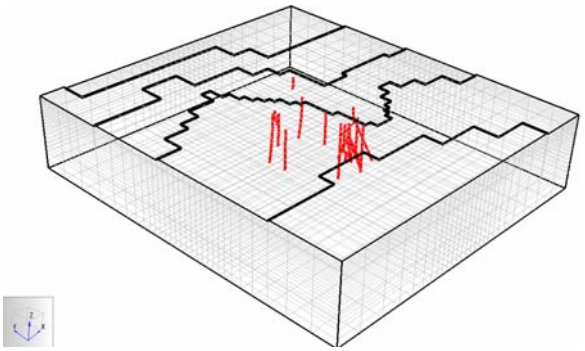

Figure 1: 3D computational mesh used in the model.

Small blocks are used around the center of the model where most of the wells are located while coarser blocks are used in the surrounding area to minimize the number of elements in the model. The entire model covers a total area of 243.3 km^2 (14.72 km x 16.52 km) which is large enough to minimize the artificial effects in the production and injection area due to the presence of the lateral boundary.

The elevation of the top-most layers of the model varies according to the location of the water table. This was estimated based on the measured water levels of the available wells and ranges from +590 mRSL to +300 mRSL. The base of the model is located at -3050 mRSL, ~900 m deeper than the maximum depth penetrated by the deepest well.

A closed, no flow, boundary condition where no energy and mass flows are allowed is used at the lateral boundaries. To impose atmospheric boundary conditions at the top of the model, the topmost blocks are connected to a thin element (0.00001 m thickness) with large volume (1E25 m^3) set at atmospheric conditions (T = 15 ^oC; P = 1.0E5 Pa). At the bottom, mass and energy are allowed to flow into the model to represent the conductive heating from the basement rock and upwelling of very hot fluid within the reservoir. This was achieved by adding a heat input throughout the blocks at the bottom of the model and injecting water with 1540 kJ/kg enthalpy (~330 ^oC) at the blocks in the conjectured upflow area. The heat flux applied ranges from 20 to 150 mW_t/m^2. A total of 77.9 kg/s of mass were injected at the bottom to represent the hot upflow in the reservoir.

For a complete model calibration process, the input of heat and mass at the base of the model could be adjusted but in the present study, they were held fixed.

3.2 Parameter Estimation Result

The inverse model starts with parameter estimation for the permeabilities of the 17 reservoir rock-types as defined in the TOUGH2 input file. Each of the rock-types contributes two parameters in the model, one for the horizontal and another for the vertical. Initially, permeability values of the reservoir rocks were assumed uniform using 4 mD for the horizontal permeability and 0.5 mD for the vertical permeability. Upper and lower bounds of 300 mD and 1 mD, respectively, were set for horizontal permeability while the vertical permeability was constrained to fall in the interval 0.1 to 5 mD.

In the first parameter estimation run, all the 34 parameters from the 17 rock-types were calibrated against the natural state temperature data. From the initial guess of parameter values, an objective function of 526,717 was calculated by PEST. It adjusts the parameters iteratively until convergence is achieved and the objective function is no longer decreasing. The result of this first optimization run showed a significant reduction in the objective function which reached a lowest value of 96,992. This corresponds to ~80% reduction in the objective function.

The sensitivity of the objective function to parameter variations was then used to identify the parameters that have the most influence and those with the least influence on the fit of model results to the data. This sensitivity information became the basis for implementing the selective parameter estimation (fixing the values of non-influential parameters) and the subdivision of model rock-types approach. It was observed that generally, rock-types that are assigned to a large area of the model and those near the wells appear to be the most influential ones. This observation further justifies the approach of iteratively subdividing the areas containing the most influential rock-types after each optimization run. After fixing the non-influential parameters and creating the new rock-types, a new optimization run using the parameter values obtained from the previous run as the initial guesses was then carried out to further reduce the objective function with the new set of parameters.

Figure 2 below shows the history of the objective function value calculated after each parameter optimization run. Twelve additional parameter estimation runs were carried out for the natural state model after the first optimization run. At the start before any PEST optimizations, the model results gave an objective function value of ~500,000. After each run, new rock-types were created as a result of the rock-type subdivision and additional non-influential parameters were fixed at their current values. After run #5, a sensitivity analysis of all the parameters, including those parameters whose values were fixed previously, was conducted to update the sensitivity ranking. The result of this sensitivity run showed that some of the parameters which were not very influential before became significant and thus needed to be included in the succeeding optimization run.

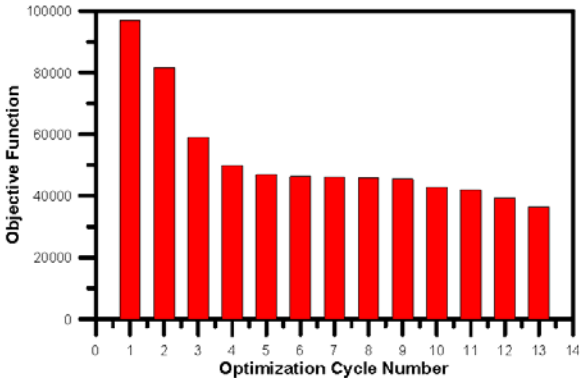

Figure 2: Objective function values during each optimization cycle of the steady state model.

Starting from optimization run #9, the automatic user intervention option was employed to allow PEST to search for additional parameters that could be fixed at their present

values to improve the model match with the data. In optimization run #13, some of parameter bounds were extended and that relaxation of the constraints allowed PEST to further improve the model. By the end of optimization #13, the total number of model parameters had increased from 34 (17 rock-types) to 114 (57 rock-types).

PEST run #	Number of rock-types	Parameters optimized	Final objective function	Remarks
0	---	---	526717	Initial guess
1	17	34	96922	
2	22	26	81781	
3	27	26	59111	
4	32	26	49909	
5	37	26	46800	
6	37	26	46235	New sensitivity data
7	39	30	46091	
8	45	26	45945	
9	45	26	45466	With automatic user intervention
10	51	26	42852	
11	51	102	41975	No automatic user intervention
12	51	102	39428	With automatic user intervention
13	57	26	36406	With automatic user intervention, bounds are widened

Table 1: Summary of optimization result for the natural state calibration.

After reaching an acceptable level of match to the observations with the natural state model, a simultaneous PEST optimization of both the natural state and production history was investigated. The purpose of this process was to try to improve the match between the enthalpy result from the production model and the measured enthalpy in the wells while at the same time maintaining the goodness of fit of the natural state data as much as possible. Parameter values obtained from the first natural state calibration stage were used as initial values for the second combined natural state/production history stage. In this second stage, the enthalpy data from the production wells were added into the calibration data set. Since the joint calibration involves two different types of data, temperatures and enthalpies, weights of the observation data were chosen so that the enthalpies have lower weights compared to the temperatures. Additionally, weights of the temperatures in wells that had good matches from the natural state calibration stage were increased so that the match would not be compromised when PEST tried to match the other data. The result of this run is summarized in Table 2.

PEST run #	Parameters optimized	Final objective function (total)	Enthalpy contribution to the objective function	Remarks
0	---	151839	91779	
1	26	118430	68603	Parameters chosen based on the sensitivity of the natural state model
2	114	151839	91579	All parameters are estimated
3	26	102440	43892	Parameters chosen based on sensitivity result of run #2
4	26	96834	39100	Parameters chosen based on sensitivity result of run #2 with respect to enthalpy only

Table 2: Summary of optimization run result for the combined natural state/production history calibration.

A large drop in the objective function (>90%) for the natural state model was achieved indicating that a significant improvement in the model match was obtained. The result of the calibration including the production history model however showed that PEST experienced difficulty in matching the model results to the measured production enthalpy of the individual production wells, especially those with two-phase enthalpies.

A comparison of the measured data and model result during the steady state calibration is presented in the scatter plot and histogram of the residuals in Figure 3. The scatter plot shows a relatively narrow distribution of points around the measured temperature = simulated temperature line (red line) indicating a close match between the model result and measured data. The production history calibration however did not go as well as the calibration of the natural state model. The result of production history matching against flowing enthalpy is summarized in Figure 4. The scatter plot shows a wide distribution of points around the measured enthalpy = simulated enthalpy line. It can also be seen that a larger density of points appear below this line indicating that the model generally produced lower enthalpy values than the measured data.

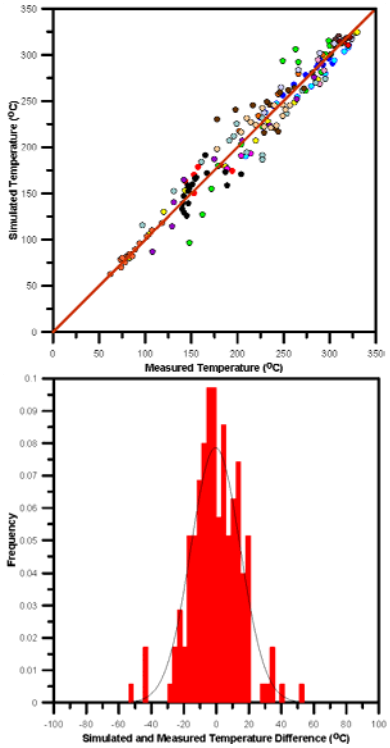

Figure 3: Comparison of the model result versus measured temperature data for the natural state calibration of model A.

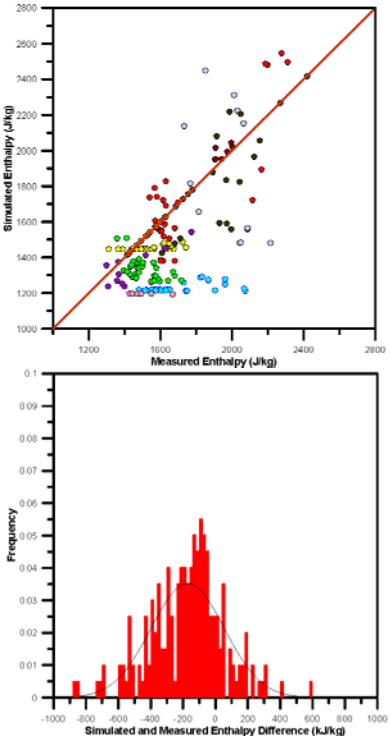

Figure 4: Comparison of the model result versus measured enthalpy data for the production history calibration of model A.

4. CONCLUSIONS AND FURTHER WORKS

The main objective of this study was to demonstrate the use of the PEST software package for automated calibration of geothermal models and the heuristic approach of model structure refinement. Calibration of models of geothermal systems is a challenging problem in geothermal reservoir engineering. The process is necessary since most, if not all, parameters on which the model response depends are not directly measurable and can only be inferred from the system response measured in the field. Good calibration of the model is required so that reliable long term predictions can be made despite the lack of direct information about the reservoir parameters.

For the model used in this study, the matches to the natural state temperature obtained after calibration were generally good. Difficulties in enthalpy matching were encountered with the model. Most of simulated enthalpies are lower than the measured ones and more boiling needs to be induced in the reservoir. This mismatch in enthalpy could be attributed to the nonlinear dependence of the enthalpy to the changes in the permeability values.

Overall, PEST proved to be a very powerful tool for automated calibration of models of geothermal systems but some difficulties were encountered. The difficulties include the following:

- Selecting the appropriate weights for the measured data.
- Deciding on the number of parameters to be used in the parameter estimation.
- Deciding which approach to use in order to get the lowest objective function possible.
- Forward model specific problem such as models not reaching the desired end time due to unrealistic parameters used by PEST.
- Long run times due to the large number of forward runs required for the calculation of the Jacobian matrix.
- Limitations in the precision of the model output thus limiting PEST's ability to accurately calculate the Jacobian matrix.
- Difficulties with getting PEST to match enthalpy data.

The functionality of PEST however extends beyond what was investigated in this work and further experimentation with other PEST options may help to identify how to best use this tool for geothermal modeling.

The combination of PEST and the heuristic approach for rock-type refinement still requires considerable manual intervention. Our long term aim is to automate the whole process.

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