Numerical Analysis of Small-Scale Heat Transfer in Diorite Rocks Validated with Experimental Data

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ABSTRACT

Thermo-active engineering projects such as deep geological repositories have prompted many experimental research ingestions involving the heating and subsequent testing of rocks and soils. Determining the heat development within test samples experimentally can be time consuming. This investigation aimed to create a numerical model that can simulate the heat development in a sample given the sample dimensions, thermal properties, and heat source. In this investigation small cylindrical samples of crystalline diorite rock and compacted bentonite were heated to 100 °C and the heat development within the samples were monitored. A model was then created in FLAC3D to simulate this heat development. The ability to predict temperature development within a test sample quickly by use of a numerical model will be useful for in scheduling test times and potentially limit the ambiguity in how long experimental trials will take.

RÉSUMÉ

Les projets d'ingénierie thermoactive, tels que les dépôts géologiques profonds, ont donné lieu à de nombreuses recherches expérimentales impliquant le chauffage et les tests subséquents des roches et des sols. Déterminer expérimentalement le développement de la chaleur dans les échantillons d'essai peut prendre beaucoup de temps. Cette étude vise à créer un modèle numérique capable de simuler le développement de chaleur dans un échantillon en fonction de ses dimensions, de ses propriétés thermiques et de sa source de chaleur. Dans cette étude, de petits échantillons cylindriques de roche diorite cristalline et de bentonite compactée ont été chauffés à 100 °C et le développement de la chaleur dans les échantillons a été surveillé. Un modèle a ensuite été créé dans FLAC3D pour simuler ce développement thermique. La capacité de prédire rapidement le développement de la température dans un échantillon d'essai à l'aide d'un modèle numérique sera utile pour planifier les temps d'essai et potentiellement limiter l'ambiguïté de la durée des essais expérimentaux.

1 INTRODUCTION

The effect of temperature on a rocks and soil's mechanical properties has become a focus of many geotechnical and geological engineering research. This is due to the increase in interest in projects such as geothermal energy exploitation, deep storage of natural gas, and deep geological repositories for the storage of spent nuclear fuel. This has led to a numerable amount of experimental research in which traditional testing such as unconfined compressive strength, and triaxial tests, has been adapted to be conducted at elevated temperatures.

For example, in 1982, Wai and Lo investigated the effect of temperature on the strength and deformation behaviour of rocks of Southern Ontario at temperatures ranging from 25 to 350 °C (Wai & Lo, 1982). Similar work was conducted by Chen, Ni, Shao, and Azzam in 2013, this research investigated the effect of temperature on the uniaxial compressive strength of granite in the range of 200 to 1000 °C (Chen, Azzam, & Ni, 2012). In both studies it was found that as the temperature of the rock increased, the peak stress and elastic modulus decreased. In 2015, Rodklang et. al investigated the effects of increasing temperature at various confining pressures on Tak granite (Rodklang, Khamrat, & Fuenkajorn, 2015). (Rodklang, Khamrat, & Fuenkajorn, 2015) determined that the granite rock samples strength decreased with increasing temperature, and increased with increasing confining pressure.

Research has also been conducted on the effect of temperature on the mechanical response of soils. In 1969, Laguros investigated the effect of temperature in the range of 2-40 °C on the engineering properties of various clay soils (Laguros, 1969). Laguros found that the unconfined compressive strength trended upwards with increasing temperature while other engineering properties, such as the liquid and plastic limit trended downwards with increasing temperature (Laguros, 1969). In 2016, Yavari et al investigated the effect of temperature on the shear strength of test sand, clay, and clay concrete interface. This investigation was conducted in the range of 5-40 °C to simulate thermoactive geostructures (Yavari, Tang, Pereira, & Hassen, 2016). It was found that the effect of temperature in this range on the shear strength of these interfaces was negligible.

DECOVALEX, an international research organization, has dedicated the past 20+ years to the understanding of coupled Thermo-hydro-mechanical-chemical (THMC) processes in porous media for applications to deep geological repositories (DECOVALEX, 2022). Much of this work has focused on the thermo-mechanical (TM) or thermo-hydro-mechanical (THM) coupled processes. For example, Task B in DECOVALEX 2011 conducted the Äspö Pillar Stability Experiment (ASPE) in which the spalling/yielding strength of a granitic rock mass as a time dependent coupled TM process in which maximum temperature was relatively low (<80 °C) (Kwon, Lee, Jeon, & Choi, 2013). The computer model and code were calibrated against large scale experimental investigations and was found to accurately estimate the temperature development and spalling strength (DECOVALEX, 2013)

While all this research has been conducted for a similar purpose, the methods used to heat the samples has varied. Some used heating chambers, while others have used heating coils or water-based systems. Due to this variability in technique, it may be difficult to predict the time to heat up samples for testing. Experimental investigations are inherently time consuming in comparison to numerical works, which can be conducted relatively fast. The ability to predict the heating time for samples would aid in scheduling test times and potentially limit some of the ambiguity in how long experimental trials will take.

This research investigation aimed to create a numerical tool using FLAC3D that could predict heating times for different samples. This was conducted for small cylindrical samples of compacted bentonite, as well as crystalline diorite rock cores. Results from the numerical model were compared to experimentally gathered data for heating times of the samples in question.

2 METHODOLOGY

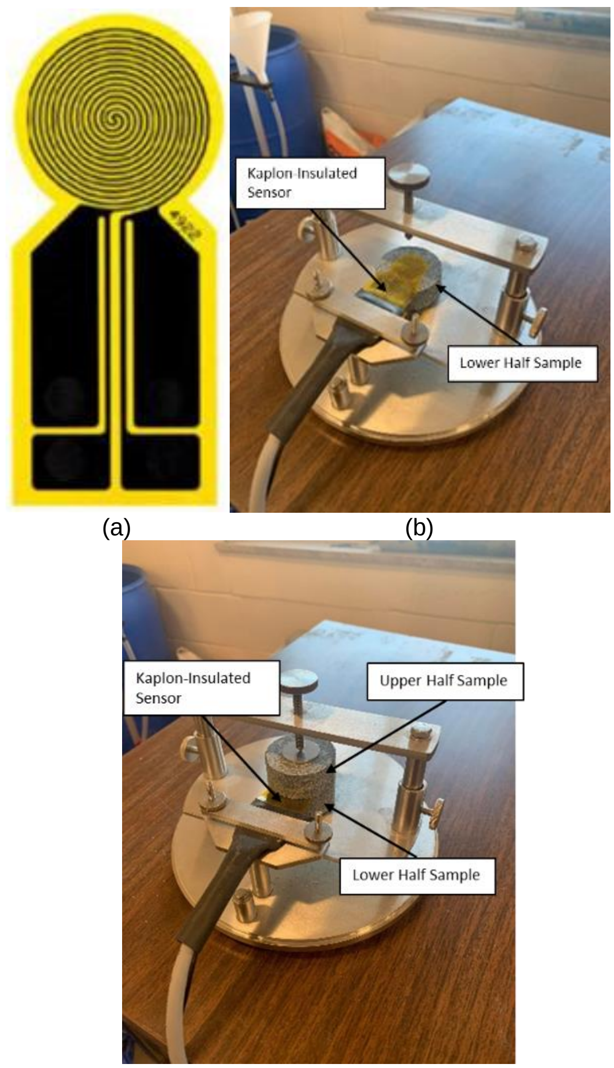
The adopted methodology in this study included experimental and numerical work. The experimental work included the measurement of temperature of heated samples under controlled conditions and the measurement of thermal properties of crystalline diorite and bentonite. The numerical work included the development of a numerical model to predict the temperature change with time. Details of both, experimental investigations, and numerical model development, will be explained in the proceeding sections.

2.1 Experimental program

2.1.1 Thermal Properties Measurements

The specific heat and thermal conductivity of the diorite rock cores were obtained using the Hot Disk Method, also known as the transient plane source (TPS) method (Mihiretie, et al., 2017). The Hot Disk device, shown in Figure 1, is capable of measuring the thermal properties of solids, powders and pastes with a minimum diameter of 40mm and thickness of 10mm, in the thermal conductivity range of 0.03 to 40 W/ (m·K) (Hot Disk M1, 2020). The samples were tested at saturated and dry conditions. The rock samples were submerged in water for 30 days to allow for saturation of the samples. Once 30 days had passed, the samples were surface dried with a towel and tested. The test is conducted by placing the Kapton – insulated sensor between two of the 20mm diorite disks to form a sandwich like structure. This is referred to as the double-sided method (Hot Disk M1, 2020). Figures depicting this can be seen in Figure 1 (b) and (c). After placing the Kapton sensor between the two samples, a small metal disk is placed on top of the upper sample and a small nominal force is applied to ensure contact between the samples throughout testing (Hot Disk M1, 2020).

For this study, three sets of samples were tested. Each set of samples was measured 7 times at both 500 and 800MW. 10 minutes were allotted between the testing at 500 and 800MW to allow for a cooling time, in addition to this, 80 seconds were allotted between each of the 7 measurements at the respective wattage. In the hot disk method, one key assumption is that location of the sensor is within an infinite medium (Hot Disk M1, 2020).To ensure this assumption was valid the effective probing depth was compared to the thickness of the specimens. Finally, in an effort to maintain the water content of samples during testing and prevent evaporation, a plastic lid was placed over the device during testing. Once testing had been completed on the saturated samples, the samples were dried by being placed in an oven for 24 hours at a temperature of 100°C. Once drying had been completed the samples were placed in a sealed environment to return back to room temperature, the test methods for determining thermal properties were then repeated for dry conditions.



(c)

Figure 1: Kapton-insulated sensor b) half set up test c) "sandwiched" double sided

The thermal properties for bentonite samples were obtained from previous work conducted at the University of New Brunswick (Shafaei Bajestani & Nasir, 2021). (Shafaei Bajestani & Nasir, 2021) investigated the thermal properties of bentonite with dry densities of 1.4, 1.6, and 1.8 Mg/m^3, at saturations ranging from 0-100. The thermal properties were found using the same Hot Disk method described previously in which it was found that the thermal conductivity and specific heat of bentonite increased with increasing saturation and density (Shafaei Bajestani & Nasir, 2021).

2.1.2 Experimental investigation of heat development in samples

Experimental data of the heat development within the chamber and the sample was obtained via the setup shown in Figure *2*. The components of the setup were the Instron heating chamber, seen in Figure *3*, capable of heating samples up to a maximum temperature of 200 °C, a Dataq data acquisition system, two thermocouples, a steel base platen, and the test samples.

A steel base platen was used to cover the bottom opening of the heating chamber and a steel plate with a small hole drilled through it was used to cover the top opening of the chamber. This hole allowed for passage of the thermocouples into the chamber while allowing minimal heat to escape. A hole was drilled in the center of the sample and a thermocouple was placed within the center of the sample and secured with heat resistant silicone caulking. The second thermocouple was left to hang at the mid-height of the chamber. These thermocouples allowed for the monitoring of temperature development within the heating chamber and within the sample center.

To conduct the tests, the heating chamber door was shut, and the dial was set 100 °C. The temperature was monitored and recorded both within the oven and within the sample until both the oven and sample achieved the desired temperature. This was conducted for both a diorite sample and a bentonite sample separately. The diorite sample was 31.75mm in diameter and 63.5mm in length and can be seen in Figure *4*a. While the bentonite sample was 50mm in diameter and 100mm in length and can be seen in Figure *4*b.

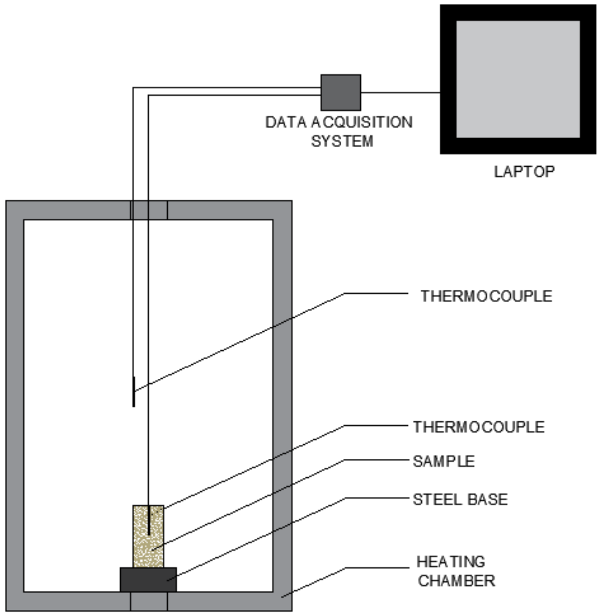
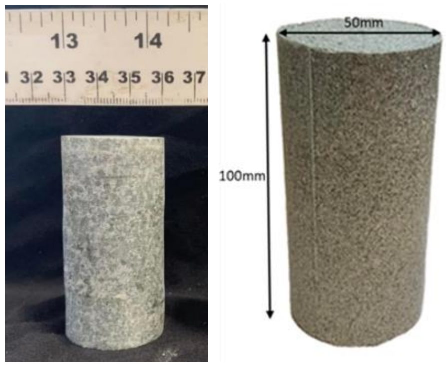


Figure 2: Diagram depicting arrangement of components used in experimental heat development monitoring


Figure 3: Setup for temperature development investigation



(a) (b)

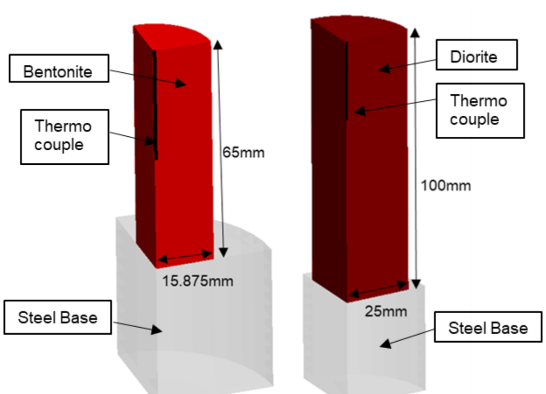
Figure 4: a) Diorite rock sample b) Bentonite clay sample

2.2 Numerical Program

2.2.1 Model Development and Validation

To develop a numerical model capable of simulating the heat development within the sample, FLAC3D (Itasca, 2021) was used. FLAC3D is described as a "a commercial software used for numerical analysis" (Itasca, 2021).

This model was developed to create a tool that can be used to approximate the time for a test sample to reach a desired temperature. This model was generated to resemble the bentonite and diorite test samples that were investigated experimentally for heat development within the Instron heating chamber. Due to symmetry, the modeled test samples represent a quarter of the experimental test samples. The radius and length of the modeled samples were the same as the test samples previously shown in Figure *4*. For the diorite, the dimensions of the model were 15.875mm in radius, and 63.5mm in height seen in Figure *5*a. The modeled bentonite sample had a radius of 25mm and a height of 100mm and can be seen in Figure *5*b. In addition to the samples, the steel base below the sample was included seen in grey in Figure *5*. The final addition to the model geometry was the thermocouple used to monitor the temperature, seen in black in Figure *5*.



(a) (b)

Figure 5: a) Modeled diorite sample b) Modeled bentonite sample

Each of these zones were assigned thermal properties to allow heat development to be predicted. The thermal properties for the diorite were obtained from the experimental investigation previously outlined using the Hot Disc device. The thermal properties for the dry bentonite were obtained from (Shafaei Bajestani & Nasir, 2021). Thermal properties for the steel base and thermocouple we obtained through literature (Lysesse & Rotta Loria, 2020), (Thermtest, 2021). A summary table of the density, specific heat and thermal conductivity for each of the materials in the models can be seen in Table *1*.

Table 1: Thermal properties of model materials

Group	Th. Conductivity (W/m·K)	Spec. Heat (kJ/m^{3}K)	Density (kg/m^3)
Steel Base	45	3120	7850
Dry Diorite Sample	2.800	1900	2950
Dry Bentonite Sample	0.479	1095	1600
Thermocouple	45	3120	7850

The final input needed for this model was the thermal initial and boundary conditions. This was obtained from the recorded temperature within the oven during the experimental investigation of heat development within the heating chamber previously outlined. The temperature within the oven from the 100 °C heating chamber tests can be seen in Table *2*. This temperature increase was applied to the external faces of the model simulate the conditions within the heating chamber. The temperature at 0 minutes represents the initial temperature condition of the oven and samples.

Table 2: Temperature development in oven from experimental heat development investigations

Time (minutes)	0	2	4	8	16+
Oven Temperature Dry Bentonite (°C)	21	56	74	88	100
Oven Temperature Dry diorite (°C)	24	63	80	95	100

The models were run for transient heat transfer until the modeled samples reached a homogeneous maximum temperature of ~100°C. The temperature development was tracked at the bottom of the thermocouple, at a location at the center of the sample roughly 31.6mm from the top surface. The temperature development in the modeled samples were then compared to the observed experimental temperature development within the samples from the heating chamber tests to validate the model.

2.2.2 Model Application

With the model validated, the next goal was to further expand the capabilities of this model by investigating the effect of a wider range of thermal properties. Thermal conductivity and specific heat can greatly affect the temperature development within the sample. A lower thermal conductivity represents a material that transmits heat more poorly, therefore lengthening the time for heat development within a material (Connor, 2019). A greater specific heat capacity means the material requires more heat energy to raise in temperature, therefore, lengthening the time to reach the desired temperature within a material (Feidt, 2017),

Thermal properties of rock and soil are primarily controlled by the mineral composition of the porous media, however, another factor that can play a key role in the thermal properties of a porous materials is the porosity and subsequent saturation of that material (Nagaraju & Roy, 2014). Due to the variability in minerology, porosity, and saturation of rocks and soils, the thermal properties can range greatly. Thermal conductivity of rocks and soils usually fall within the range of 0.4-7.0 W/m·K (Labus & Labus, 2018) with the majority being within the range of 0.5-4.0 W/m·K (KodeSova, et al., 2013). The specific heat of soils and rocks regularly fall within the range of 1000-4000 kJ/m^{3}K (Feng, Gao, Zhu, Luo, & Zhang, 2013).

A series of model runs were completed with a range of thermal properties. The thermal conductivity ranged from 0.75-3.25 W/m·K and the specific heat ranged from 1000-4000 kJ/m^{3}K. A summary of the 24 combinations of thermal properties can be seen in Table *3*. These combinations were applied to a modeled 25mm radius, 100mm length sample.

Table 3: Combinations of thermal properties

Combination #	Th. Conductivity (W/m·K)	Spec. Heat (kJ/m^{3}K)
1, 2, 3, 4, 5, 6	0.75, 1.25, 1.75, 2.25, 2.75, 3.25	1000
7, 8, 9, 10, 11, 12	0.75, 1.25, 1.75, 2.25, 2.75, 3.25	2000
13, 14, 15, 16, 17, 18	0.75, 1.25, 1.75, 2.25, 2.75, 3.25	3000
19, 20, 21, 22, 23, 24	0.75, 1.25, 1.75, 2.25, 2.75, 3.25	4000

3 RESULTS AND DISCUSSIONS

3.1 Model validation

The temperature development of the modeled diorite sample was compared to the temperature development recorded during the experimental trial in which a diorite sample was heated to 100 °C within the heating chamber. The heat development within the sample in the numerical model was saved in multiple model states to show the temperature increase in temporal snapshots. In Figure 6 the temperature within the sample can be seen at 1 second, 60 seconds, 300 seconds, 900 seconds, and 1800 seconds.

While Figure 6 displays visual snapshots of the temperature development through time within the modeled sample, Figure 7 displays the comparison of continuous temperature development within the modeled and experimental diorite sample. In this figure it can be seen that in the experiential investigation, the Diorite sample took 1085 seconds to reach 100 °C, while in the numerical model, the sample took 928 seconds to reach 100 °C. This equates to a difference of 157 seconds.

When comparing these two temperature developments temporally, the difference to reach 100 degrees is ~16.9%. However, at a time of 928 seconds, the temperature of the sample in the experimental investigation is 97.5°C. Therefore, when analyzing the difference in these temperature developments through the perspective of temperature, the difference is much smaller at ~2.5%.

Figure *7* also shows the experimental and numerically modeled heat development in the bentonite sample. In this figure it can be seen that the sample took 3525 seconds to reach a temperature of 100 degrees in the experimental trial. While the numerical model took 3705 seconds. This equates to a difference of 180 seconds. When comparing these two temperature developments temporally, the percent difference to reach 100 degrees is ~4.9%

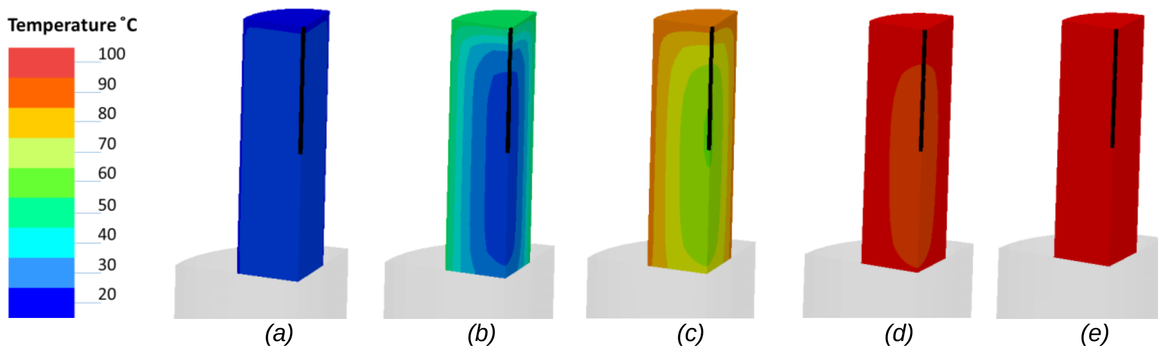


Figure 6: Temperature development in diorite sample at a) 1 second b) 60 seconds c) 300 seconds d) 900 seconds e) 1800 seconds

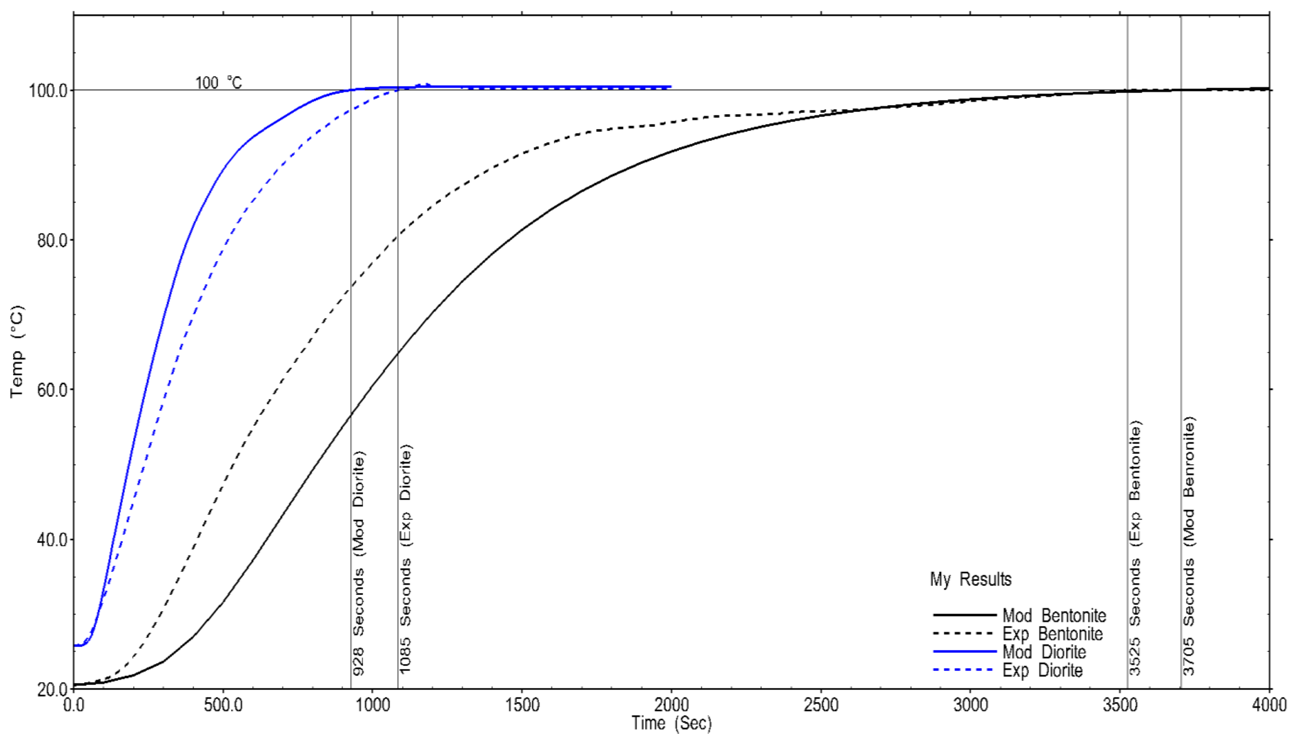


Figure 7: Experimental and numerically modeled heat development in diorite and bentonite samples

When comparing the heat development within the experimental observed and modeled samples, the difference in time to reach 100 °C for the diorite was ~157 seconds. In the bentonite samples, a 180 second difference in time to reach 100 °C was observed. This difference is not significant for use in scheduling experimental work, therefore, validating the model's accuracy.

3.2 Model application

A series of runs were conducted on the 25mm radius, 100mm length modeled quarter sample to create a series of scenarios that could be used for future research. The curves can be seen in Figure *8* (a to d). These scenarios represent different combinations of specific heat capacity and thermal conductivity. The heating time to temperatures of 20-100 °C can be estimated by using these curves by selecting the thermal conductivity and specific heat that are representative of the material in question and following the appropriate scenario to the temperature of interest. For example, if a 50mm diameter sample of Granite with a thermal conductivity of ~2.75 W/m·K and a Specific heat capacity of 2000kJ/m^{3}K, then the teal curve in Figure *8*, b can be used to approximate the 100 °C heating them to be roughly 1700 seconds.

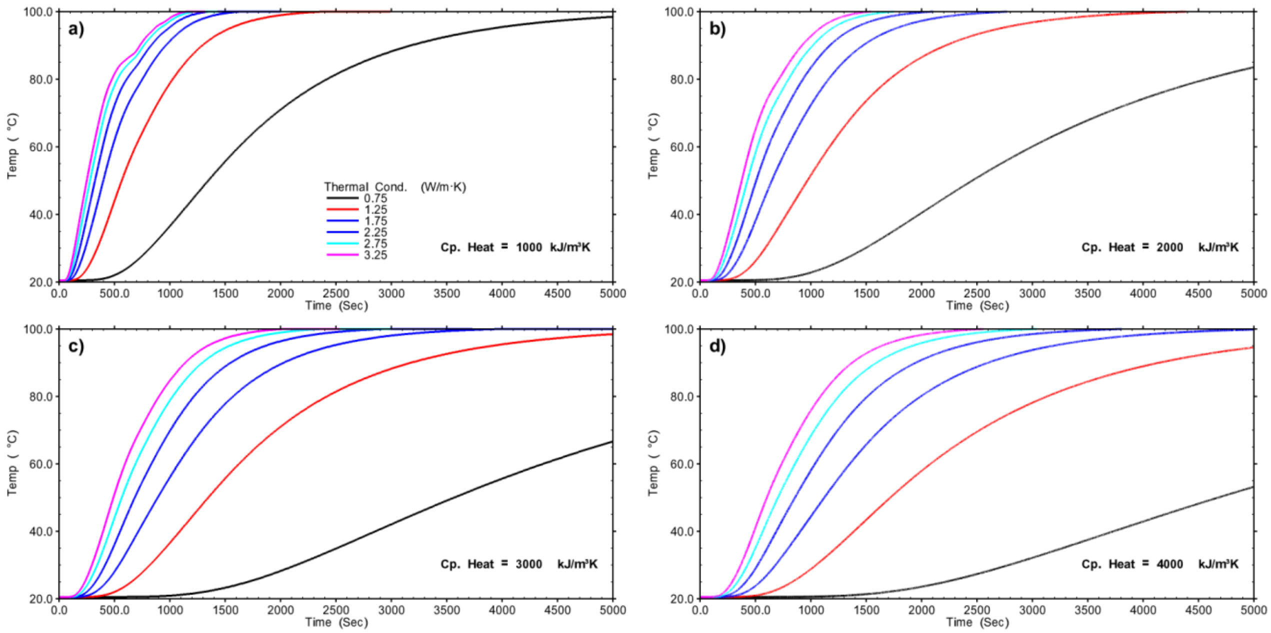


Figure 8: Temperature development application for 25mm radius samples with variable thermal properties

4 GENERAL CONCLUSIONS AND RECOMMENDATIONS

The model created using FLAC3D was validated to be accurate by comparing the modeled heat development within the modeled sample to experimentally collected data for both a 25 mm radius sample of bentonite, and a 15.875 mm radius diorite sample. In both cases the modeled samples reached 100 °C within 180 seconds of the experimentally determined time.

With the model validated a series of application trials were ran with variable thermal properties in which the thermal conductivity ranged from 0.75-3.25 W/m·K and the specific heat ranged from 1000-4000 kJ/m^{3}K. With this data, curves were created that can be used by future researchers to estimate heating times in the range of 25-100 °C for 25 mm radius, 100mm length samples of rocks or soils.

When using these curves, we need to assume that the heating conditions applied to the sample are similar to those used in this model. If heating conditions are within similar ranges, and thermal properties for the sample are accurate, these curves can be used as a tool for estimating heating times for research that involves heating samples.

Using the original code, more accurate temperature development estimations can be determined as the model had been created such that all parameters can be easily adjusted including the sample dimensions, heating conditions, and thermal properties.

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