

## Prediction of Thermal Conductivity Of Bentonite

*A minor project report submitted in partial fulfillment for the award of the degree of*

# Bachelor of Technology

*in*

# Civil Engineering

*By*

# Shivraj Gupta

**20101108047**

# Rahul Kumar

**20101108024**

# Ankit Kr. Singh

**20101108003**

# Sanu Kumar

**20101108016**

*Under the guidance of*

# Prof. Pawan Kishor Sah



**DEPARTMENT OF CIVIL ENGINEERING**  
**BHAGALPUR COLLEGE OF ENGINEERING**

**August, 2024**

## **ABSTRACT**

The abstract extracted from the project report is as follows:

"The first step involves gathering data on thermal conductivity from various sources in the existing literature. Once this data is collected, it will be meticulously analysed. The analysis aims to observe the impact of several factors on thermal conductivity. These factors include, but are not limited to, dry density, water content, and degree of saturation. The goal is to understand how these variables influence thermal conductivity as per the data collected from the literature.

In addition to the collection and analysis of thermal conductivity data, the data was also evaluated. This evaluation was carried out using various existing prediction models. These models helped in understanding the patterns and trends in the data, providing further insights into the effects of factors such as dry density, water content, and degree of saturation. This comprehensive approach ensures a thorough understanding of thermal conductivity based on the collected data."

The abstract provides an overview of the project's focus on thermal conductivity analysis and evaluation using data from existing literature sources.

## DECLARATION

I hereby declare that the work being presented in the **Bachelor of Technology Minor Project** “**Prediction of Thermal Conductivity Of Bentonite**”, in partial fulfillment of the requirements for the award of the Bachelor of Technology in Civil Engineering and submitted to the **Department of Civil Engineering of Bhagalpur College Of Engineering, Bhagalpur** is an authentic record of my own work carried under the supervision of our project guide **Pawan Kishor Sah**.

**Signature of Candidate:**

*Name: Shivraj Gupta  
Roll No. 20151*

**Signature of Candidate:**

*Name: Rahul Kumar  
Roll No. 20110*

**Signature of Candidate:**

*Name: Ankit Kumar Singh  
Roll No. 20104*

**Signature of Candidate:**

*Name: Sanu Kumar  
Roll No. 20116*

## **BONAFIDE CERTIFICATE**

Certified that this project report titled “**Prediction of Thermal**

**Conductivity Of Bentonite**” is the bonafide work of Shivraj Gupta (20101108047), Ankit Kumar Singh (20101108003), Rahul Kumar (20101108024) and Shanu Kumar (20101108016) who carried out the project under my supervision. Certified further, that to the best of my knowledge the work reported herein does not form part of any other project report or dissertation on the basis of which a degree or award was conferred on an earlier occasion or any other candidate.

**Signature of the Guide**

**Signature of the HOD**

**INTERNAL EXAMINER**

**EXTERNAL EXAMINER**

**DATE:**

## **ACKNOWLEDGEMENT**

We would like to express our deepest appreciation to all those who contributed to the success of this project. The outset, we express our sincere thanks to our project guide Mr. Pawan Kishor Sah (Assistant Professor), Civil Engineering, Bhagalpur College of Engineering, Bhagalpur, for their invaluable guidance, insightful feedback, and continuous encouragement. Your expertise and mentorship were instrumental in overcoming challenges and achieving our goal.

We are also grateful to Supporting Organizations or Departments for their support and resources, which were integral to the project's success. Your commitment to fostering a conducive environment for innovation and teamwork did not go unnoticed. Lastly, I want to thank everyone who played a part, big or small, in making this project a reality. Your collective efforts have made a lasting impact, and I am truly grateful for the privilege of working with such a dedicated and talented team.

<b>Shivraj Gupta</b>	<b>20151</b>
<b>Rahul Kumar</b>	<b>20110</b>
<b>Ankit Kumar Singh</b>	<b>20104</b>
<b>Sanu Kumar</b>	<b>20116</b>

## Table Of Contents

<b>TITLE</b>	<b>Page no.</b>
<b>Abstract</b>	<b>ii</b>
<b>Declaration</b>	<b>iii</b>
<b>Bonafide Certificate</b>	<b>iv</b>
<b>Acknowledgement</b>	<b>v</b>
<b>Table Of Contents</b>	<b>vi</b>
<b>1. INTRODUCTION</b>	<b>1</b>
<b>1.1 Objective</b>	<b>1</b>
<b>1.2 Necessity</b>	<b>2</b>
<b>1.3 Methodology</b>	<b>3</b>
<b>1.4 Model Development</b>	<b>6</b>
<b>1.5 Linear regression</b>	<b>7</b>
<b>1.6 Multiple Linear Regression</b>	<b>11</b>
<b>2. Literature Review</b>	<b>15</b>
<b>3. References</b>	<b>27</b>

# **1. INTRODUCTION**

As humanity, we are now facing big challenges. We need to rapidly reduce our CO<sub>2</sub> emissions - and create a more sustainable way of living. From this perspective, **nuclear energy** seems to be extremely interesting. Even though construction of the plants is costly both in terms of - CO<sub>2</sub> emissions and money, its operation is sustainable - with almost zero carbon footprint and with fuel being plentiful. However, there is a problem to solve - related to the nuclear waste produced by the power plants.

The amount of highly active waste created by the power plants - is not that large. Yet, it needs to be safely stored for a very long time. **All nuclear waste must be treated, stored and disposed. Thermal conductivity of compacted bentonite** is one of the most important properties in the design of high-level radioactive waste repositories where this material is proposed for use as a buffer. **Compacted bentonite is often considered as a possible buffer material for high-level radioactive waste disposal.** Its thermal conductivity is one of the key properties for the design of such disposal system.

## **1.1 Objective**

- The first step involves gathering data on thermal conductivity from various sources in the existing literature.
- Once this data is collected, it will be meticulously analysed.
- The analysis aims to observe the impact of several factors on thermal conductivity.
- These factors include, but are not limited to, dry density, water content, and degree of saturation.
- The goal is to understand how these variables influence thermal conductivity as per the data collected from the literature.
- In addition to the collection and analysis of thermal conductivity data, the data was also evaluated. This evaluation was carried out using various existing prediction models. These models helped in understanding the patterns and trends in the data, providing further insights into the effects of factors such as dry density, water content, and degree of saturation. This comprehensive approach ensures a thorough understanding of thermal conductivity based on the collected data.

- Based on the analysis a predictive model will be developed that will predict thermal conductivity by taking input values such as dry density , water content , quartz content, etc

## **1.2 Necessity**

Studying thermal conductivity from various research papers and comparing them is crucial for several reasons:

- **Understanding Material Properties:**

Thermal conductivity is a key property of materials, influencing how well they conduct or resist heat.

This understanding is vital in many fields, including engineering and material science.

- **Method Comparison:**

Different research papers may use different methods to measure thermal conductivity.

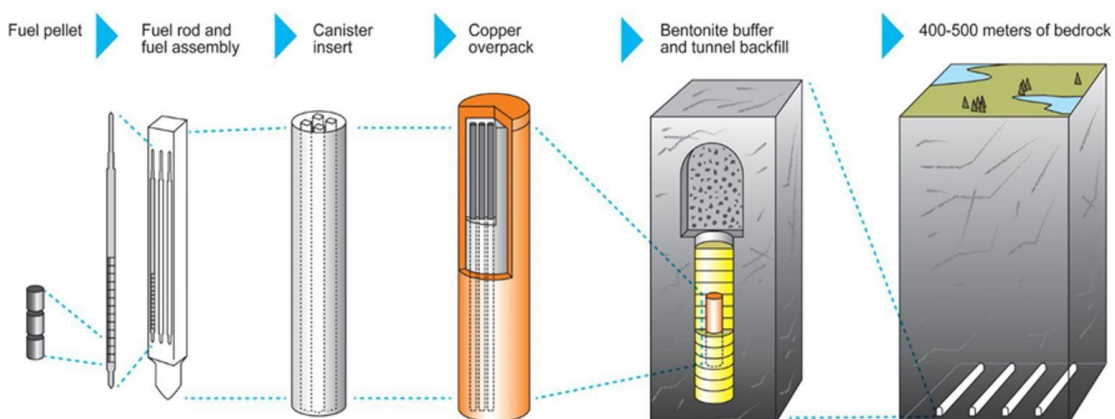
Comparing these methods can help identify the most accurate and efficient techniques.

- **Properties Assesment:**

Various factors such as dry density, water content, and degree of saturation can affect thermal conductivity. By comparing data from different papers, we can better understand these influences.

- **Application Selection:**

The study of thermal conductivity helps engineers select the appropriate material for specific applications. For example, in a heat exchanger, a good thermal conductor is ideal.





## fig 1.1 Bentonite as buffer material

In summary, studying and comparing thermal conductivity data from various research papers can lead to improved understanding, more accurate measurements, better prediction models, and more effective material selection.

### 1.3 Methodology

#### Data Collection Process:

- Begin by identifying and sourcing pre-existing research papers relevant to the study.
- From these papers, record data that has been collected under a variety of conditions.
- These conditions should include variations in dry densities, water content levels, and degrees of saturation.
- Ensure to note the specific conditions under which each data point was collected for future reference and analysis.
- This comprehensive data collection will provide a robust foundation for further study and understanding of the subject matter.

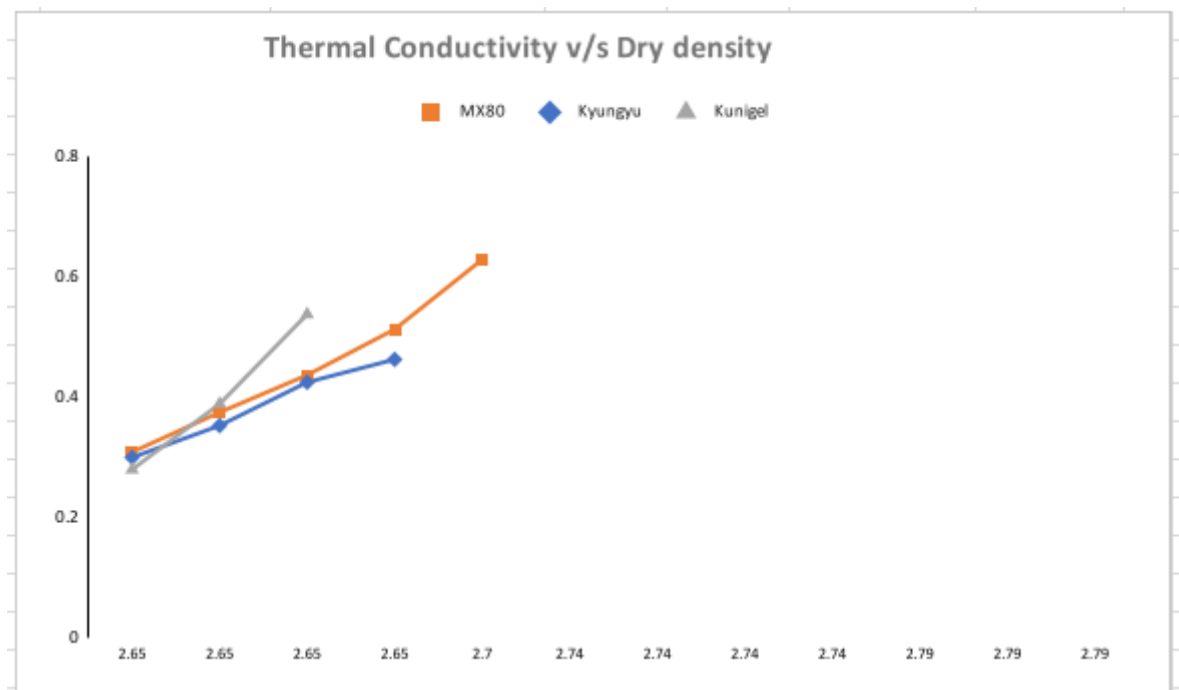
1	Author Name	Title of the paper	Quartz Cc	Particle siz	Specific (dry density	LL (%)	PL(%)	CEC(mec	Specific S	Porosity	Saturatio	Plasticity	Smectitie	(% K ( w/mK)	The water	temperatu	Bentonite Type
2	Zhao Zhang , Feng Zhan	Effect of air volu	17		2.79					0.409	100						
3	Zhao Zhang , Feng Zhan	Effect of air volu	17		2.79					0.3	95.03						
4	Zhao Zhang , Feng Zhan	Effect of air volu	17		2.79					0.4	95.98						
5	Zhao Zhang , Feng Zhan	Effect of air volu	17		2.79					0.5	96.89						
6	Zhao Zhang , Feng Zhan	Effect of air volu			2.79					0.3	0			0.539			
7	Zhao Zhang , Feng Zhan	Effect of air volu			2.79					0.4	0			0.39			
8	Zhao Zhang , Feng Zhan	Effect of air volu			2.79					0.5	0			0.281			
9	Zhao Zhang , Feng Zhan	Effect of air volu			2.79					0.3	0.09						
10	Zhao Zhang , Feng Zhan	Effect of air volu			2.79					0.4	0.18						
11	Zhao Zhang , Feng Zhan	Effect of air volu			2.79					0.5	0.17						
12	Anh-Minh TANG, Yu-Jun A	study on the ti	29-38		2.79	415	32		687				383				
13	Thermal Mechanical Be	Yu-Jun Cui, ANH-		64.5	2.79	474	27	73.2	687				447				
14	A Compilation and Evali	Won-Jin Cho, Jax			1.1									0.27	8	room temp	kunigel V1
15	A Compilation and Evali	Won-Jin Cho, Jax												0.26			
16	A Compilation and Evali	Won-Jin Cho, Jax												0.28			
17	A Compilation and Evali	Won-Jin Cho, Jax												0.24			
18	A Compilation and Evali	Won-Jin Cho, Jax												0.25			
19	A Compilation and Evali	Won-Jin Cho, Jax			1.2									0.3	8	room temp	kunigel V1
20	A Compilation and Evali	Won-Jin Cho, Jax			1.2									0.32			
21	A Compilation and Evali	Won-Jin Cho, Jax			1.2									0.33			
22	A Compilation and Evali	Won-Jin Cho, Jax			1.2									0.35			
23	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.28	0	room temp	kunigel V1
24	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.4	5		
25	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.48	8		
26	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.57	10		
27	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.63	13		
28	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.69	15		
29	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.39	8		
30	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.4	8		
31	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.41	8		
32	A Compilation and Evali	Won-Jin Cho, Jax			1.4									0.42	8		
33	A Compilation and Evali	Won-Jin Cho, Jax			1.5									0.53	8	room temp.	
34	A Compilation and Evali	Won-Jin Cho, Jax			1.5									0.54	8		
35	A Compilation and Evali	Won-Jin Cho, Jax			1.5									0.55	8		
36	A Compilation and Evali	Won-Jin Cho, Jax			1.6									0.42	0	room temp	kunigel V1
37	A Compilation and Evali	Won-Jin Cho, Jax			1.6									0.6	5		
38	A Compilation and Evali	Won-Jin Cho, Jax			1.6									0.69	6		
39	A Compilation and Evali	Won-Jin Cho, Jax			1.6									0.79	9		
40	A Compilation and Evali	Won-Jin Cho, Jax			1.6									0.96	12		

[illegible]

## Sensitivity Analysis:

- Start by employing various statistical methods. These methods will help in identifying any existing trends and patterns within the collected thermal conductivity data.
- The aim is to understand the underlying structure of the data and how different variables interact with each other.
- Specifically, investigate the influence of factors such as dry density, water content, and degree of saturation on thermal conductivity.
- This involves analysing how changes in these factors impact thermal conductivity, thereby determining their sensitivity.
- The findings from this analysis can provide valuable insights into the relationships between these factors and thermal conductivity, and can guide future research and decision-making processes.

				MX80	
				(K v/s dry density)	
				Saturation = 0% dry density	K
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.65	0.31	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.65	0.376	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.65	0.438	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.65	0.514	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.7	0.63	
				Kyungyu	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.74	0.301	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.74	0.354	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.74	0.426	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.74	0.464	
				Kunigel	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.79	0.281	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.79	0.39	
Zhao Zhang , Feng Zhan	thermal conductivity of compacted bentonite materia	0	2.79	0.539	



## 1.4 Model Development

The primary goal is to predict the thermal conductivity of materials using various input properties, such as density, specific heat, temperature, and other relevant factors. The approach involves using both linear regression and multiple regression models. Linear regression assumes a single predictor variable, while multiple regression allows for multiple input properties to be considered simultaneously. This will help in understanding the combined effect of these properties on thermal conductivity.

**Linear Regression:** Begin by developing a simple linear regression model to predict thermal conductivity using one primary input property.

**Multiple Regression:** Extend the model to multiple regression by incorporating several input properties to improve prediction accuracy and capture the complex relationships between the properties and thermal conductivity.

**Evaluation:** Test the performance of both models using metrics such as R-squared, Mean Squared Error (MSE), and others. Compare the results to determine which model provides better predictive accuracy for the given dataset.

After validation, the model can be applied to predict thermal conductivity for new materials or under different conditions, offering valuable insights for material selection and engineering applications.

## **1.5 Linear Regression**

Linear regression is a fundamental statistical method used to model the relationship between a dependent variable and one or more independent variables. It is particularly useful in predicting outcomes and identifying the strength of the impact that independent variables have on the dependent variable.

- **Mathematical Formulation:** Present the general equation for a linear regression model:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \epsilon$$

where  $y$  is the dependent variable (thermal conductivity in your case),  $\beta_0$  is the intercept,  $\beta_1, \beta_2, \dots, \beta_n$  are the coefficients for each predictor variable  $x_1, x_2, \dots, x_n$ , and  $\epsilon$  is the error term.

### **Assumptions of Linear Regression**

- **Linearity:** Explain the assumption that the relationship between the independent and dependent variables is linear.
- **Independence:** Discuss the assumption that the residuals (errors) are independent.

### **Model and Data Selection:**

- **Data Sources:** We have reviewed from existing research papers, including the key variables we used to study thermal conductivity.
- **Data Preprocessing:** Include any data preprocessing steps, such as normalization or standardization of variables, handling missing data, or encoding categorical variables such as bulk density changes to dry density.
- **Training and Testing Data:** We have to split the data into training and testing sets to validate our model's performance. We kept 20 % of the data for testing and rest of the data are used to train the model.

```
#Import packages
import numpy as
np import
pandas as pd
from sklearn.model selection import
```

## Uploading Dataset

```
#load data
dataset = pd.read_csv('bentonite.csv')
X = dataset.iloc[:, :-
1].valuesy =
dataset.iloc[:, 3].values
```

```
↩ Bulk density Porosity Saturation Thermal conductivity
0      2.04      0.3      0.0      0.687
1      2.04      0.3      1.4      0.742
2      2.05      0.3      4.2      0.788
3      2.06      0.3      9.0      0.870
4      2.08      0.3     15.7      0.955
```

## Splitting Data For Training(80%) And Testing(20%)

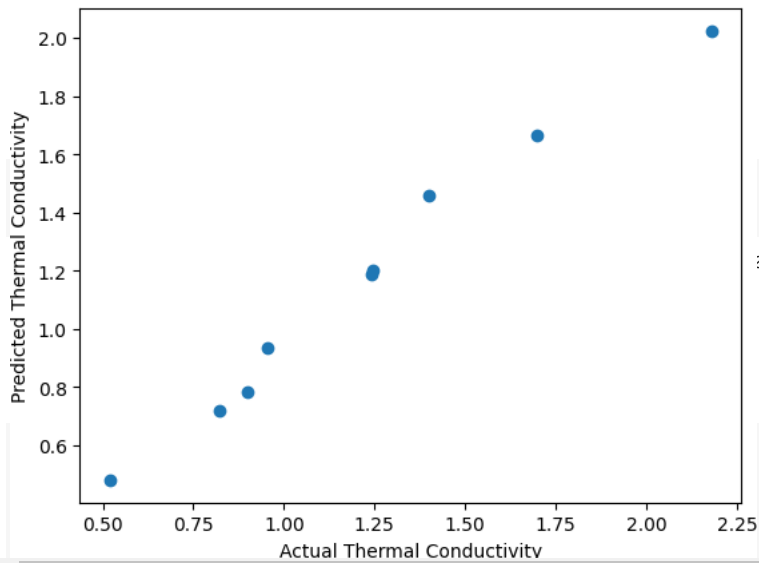
```
#split data
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 1/5, random_state
= 0)print("X_train :",X_train)
print("X_test
:",X_test)
print("y train
```

```
↩ X_train : [[ 2.18  0.42 99. ]
[ 2.02  0.4 61. ]
[ 2.49  0.3 56.3 ]
[ 2.06  0.54 98. ]
[ 2.05  0.3 4.2 ]
[ 1.71  0.63 2. ]
[ 2.43  0.3 38.6 ]
[ 2.35  0.3 10. ]
[ 1.84  0.39 2. ]
[ 2.36  0.3 15. ]
[ 2.03  0.54 90. ]
[ 2.12  0.3 0. ]
[ 2.4 0.3 96. ]
[ 2.11  0.3 25.6 ]
[ 2.38  0.3 21.4 ]
[ 1.88  0.46 3. ]
[ 2.32  0.3 0. ]
[ 2.03  0.46 97. ]
[ 2.3 0.3 86. ]
[ 1.64  0.46 2. ]
[ 2.04  0.3 1.4 ]
[ 1.8 0.4 6. ]
[ 2.28  0.3 54.5 ]
[ 2.2 0.46 98. ]
[ 2.17  0.39 99. ]
[ 2.17  0.3 45. ]
[ 2.05  0.39 62. ]
[ 2.2 0.47 30. ]
[ 2.56  0.3 82.3 ]
[ 2.46  0.3 48.6 ]
[ 2.17  0.3 17. ]
[ 1.67  0.54 3. ]
[ 1.92  0.56 3. ]
[ 2.06  0.3 9. ]
[ 2.04  0.3 0. ]]
X_test : [[ 2.08  0.4 75.6 ]
[ 2.36  0.47 91. ]
[ 1.85  0.4 18.7 ]
[ 2.08  0.3 15.7 ]
[ 2.2 0.3 27. ]
[ 1.78  0.4 0. ]
[ 1.87  0.4 24. ]
[ 2.2 0.3 29.2 ]
[ 2.05  0.5 98. ]]
y_train : [1.85 1.273 1.818 1.71 0.788 0.54 1.702 1.374 0.614 1.384 1.62 0.807
1.834 1.08 1.476 0.627 1.145 1.66 1.645 0.435 0.742 0.625 1.46 1.93
1.72 1.298 1.33 1.35 2.048 1.749 0.994 0.481 0.692 0.87 0.687]
y_test : [1.4 2.18 0.823 0.955 1.242 0.52 0.898 1.247 1.7 ]
```

## Fitting Data In Linear Regression Model

LinearRe

n()



0.93523462 1.18694108 0.48082812



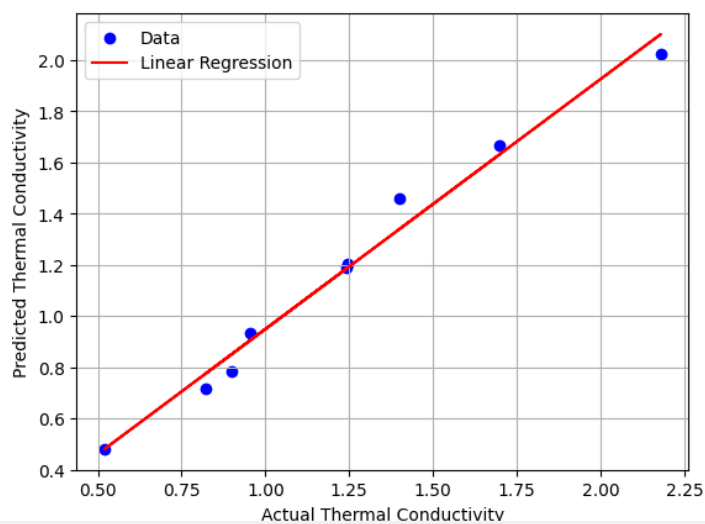
```
#regression
X = y_test.reshape(-1, 1) # reshape to a column
vector_y = pred_result.reshape(-1, 1)

# Create and fit the
model = LinearRegression()
model.fit(X, y)

# Predict values
y_pred = model.predict(X)

# Plotting
plt.scatter(X, y, color='blue', label='Data')
plt.plot(X, y_pred, color='red', label='Linear Regression')

plt.title('Actual Thermal Conductivity vs Predicted Thermal
Conductivity')plt.xlabel('Actual Thermal Conductivity')
plt.ylabel('Predicted Thermal
Conductivity')plt.legend()
plt.grid(True)
```



### Model Accuracy

```
# prompt: check accuracy of model

from sklearn.metrics import r2_score
r2_score_value = r2_score(y_test,
pred_result)print("r2
score:",r2_score_value*100)
#Since the target variable is continuous, you should use a regression metric to evaluate the model's
```

**r2 score: 96.9955605201356**



## **1.6 Multiple Linear Regression**

Multiple Linear Regression (MLR) is an extension of simple linear regression that models the relationship between one dependent variable and two or more independent variables.

The primary goal of MLR is to understand how changes in the independent variables are associated with changes in the dependent variable.

In the context of this study, Multiple Linear Regression is used to predict the thermal conductivity of compacted bentonite by considering several influencing factors simultaneously. This approach allows for a more nuanced understanding of how multiple variables interact to affect thermal conductivity.

The general form of the Multiple Linear Regression model is:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \epsilon$$

### **Assumptions of Multiple Linear Regression**

#### **Linearity**

MLR assumes that the relationship between each independent variable and the dependent variable is linear. It also assumes that the combined effect of the independent variables on the dependent variable is additive. This assumption can be assessed by plotting the residuals versus predicted values to check for any non-linear patterns.

### **Independence**

The residuals should be independent of each other. This assumption is particularly important when the data is collected over time or in sequences. Autocorrelation in residuals can be detected using the Durbin-Watson statistic.

### **No Multicollinearity**

Multicollinearity occurs when two or more independent variables in the model are highly correlated, making it difficult to distinguish their individual effects on the dependent variable.

Multicollinearity can inflate the variance of coefficient estimates and make the model unstable. It can be detected using Variance Inflation Factor (VIF) analysis, where a VIF value greater than 10 often indicates significant multicollinearity. E.g.-void ratio and porosity both can't be a factor together.

### **Model and Data Selection:**

- **Data Sources:** We have reviewed from existing research papers, including the key variables we used to study thermal conductivity.
- **Data Preprocessing:** Include any data preprocessing steps, such as normalization or standardization of variables, handling missing data, or encoding categorical variables such as bulk density changes to dry density.
- **Training and Testing Data:** We have to split the data into training and testing sets to validate our model's performance. We kept 20 % of the data for testing and rest of the data are used to train the model.

## 1.6.1 Source Code

```
Code Blame 39 lines (31 loc) · 1.4 KB Raw Copy Download Edit View
```

```
1 import streamlit as st
2 st.write('# Thermal Conductivity of Bentonite prediction')
3 # prompt: not use bentonite.csv use inout auto
4
5 import numpy as np
6 import pandas as pd
7 from sklearn.model_selection import train_test_split
8 from sklearn.linear_model import LinearRegression
9
10
11 #load data
12 dataset = pd.read_csv('bentonite.csv')
13 X = dataset.iloc[:, :-1].values
14 y = dataset.iloc[:, 3].values
15
16 # Split data into training and testing sets
17 X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)
18
19 # Train the model
20 model = LinearRegression()
21 model.fit(X_train, y_train)
22
23 # Function to take input and predict
24 def predict_thermal_conductivity_updated(bulk_density, porosity, saturation):
25     input_data = [bulk_density, porosity, saturation]
26     predicted_thermal_conductivity = model.predict([input_data])
27     return predicted_thermal_conductivity[0]
28
29
30 # Example usage
31 bulk_density = st.number_input('Bulk density') # g/cm^3
32 porosity = st.number_input('Porosity')# fraction
33 saturation = st.number_input('Saturation') # fraction
34 predicted_thermal_conductivity = predict_thermal_conductivity_updated(bulk_density, porosity, saturation)
35 print("Predicted Thermal Conductivity:", predicted_thermal_conductivity)
36 st.write('# Predicted Thermal Conductivity is ',predicted_thermal_conductivity)
37 st.write("---")
38
39 st.subheader("Under the guidance of Prof. Pawan Kishor Sah")
```

[Source Code link](https://github.com/iamrahul8/thermal-conductivity-prediction/blob/main/app.py)

<https://github.com/iamrahul8/thermal-conductivity-prediction/blob/main/app.py>

### Sample Output:

## Thermal Conductivity of Bentonite prediction

Bulk density

5.00

- +

Porosity

3.00

- +

Saturation

3.00

- +

## Predicted Thermal Conductivity is

**7.364769458392377**

Under the guidance of Prof. Pawan Kishor Sah

[App Link](https://thermal-conductivity-prediction-bentonite.streamlit.app/)

<https://thermal-conductivity-prediction-bentonite.streamlit.app/>

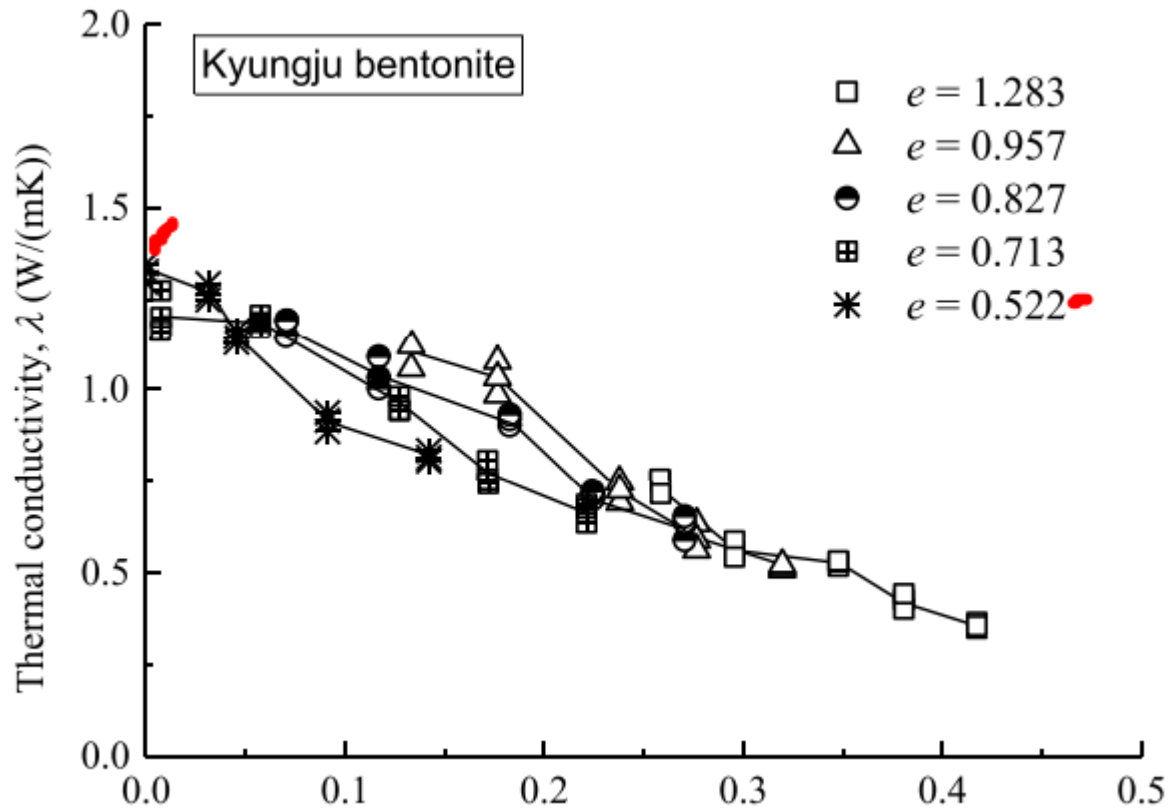


## **2. LITERATURE REVIEW**

### **2.1 Effect of air volume fraction on the thermal conductivity of compacted bentonite materials by Zhang et al. (2021)**

Due to their low permeability, good swelling property and high adsorption capacity, etc., compacted bentonite has been proposed as the candidate engineered buffer material in the deep geological repository for disposal of high-level radioactive waste (HLW) in many countries, e.g. MX-80 bentonite in Sweden (Johnsson and Sandén, 2013), Canada (Kim et al., 2012) and France (Wang et al., 2012; Molinero-Guerra et al., 2017), FEBEX bentonite in Spain (Villar and Lloret, 2004), Kunigel V1 bentonite in Japan (Sugita et al., 2003), GMZ bentonite in China (Zhang et al., 2016, 2019a; Zhang et al., 2018b, 2020), Kyungju bentonite in Korea (Cho et al., 2011; Lee et al., 2016). Once the disposal galleries are closed, the decay heat generated from the canister will transfer to the buffer materials and thus to the surrounding rock, ensuring the safety of the repository. Moreover, the generated temperature in the engineered barrier system must be lower than 100 °C (Svensk, 1983; Cho et al., 1999). Otherwise, mineralogical alteration will occur (e.g., illitization, silicification etc.) in the bentonite, leading to play a drastic role in the performance of bentonite buffer materials (e.g., swelling, mechanical, chemical performances etc.) (Lee et al., 2016). Thereby, in the assessment of repository performance, it is important to account for the thermal behaviour of compacted bentonite materials. It is well known that the thermal behaviour of compacted bentonite has been widely investigated in the laboratory (Borgesson et al., 1994; Tang et al., 2008; Xu et al., 2016; Chen et al., 2018; Yoon et al., 2018; Xu et al., 2019).

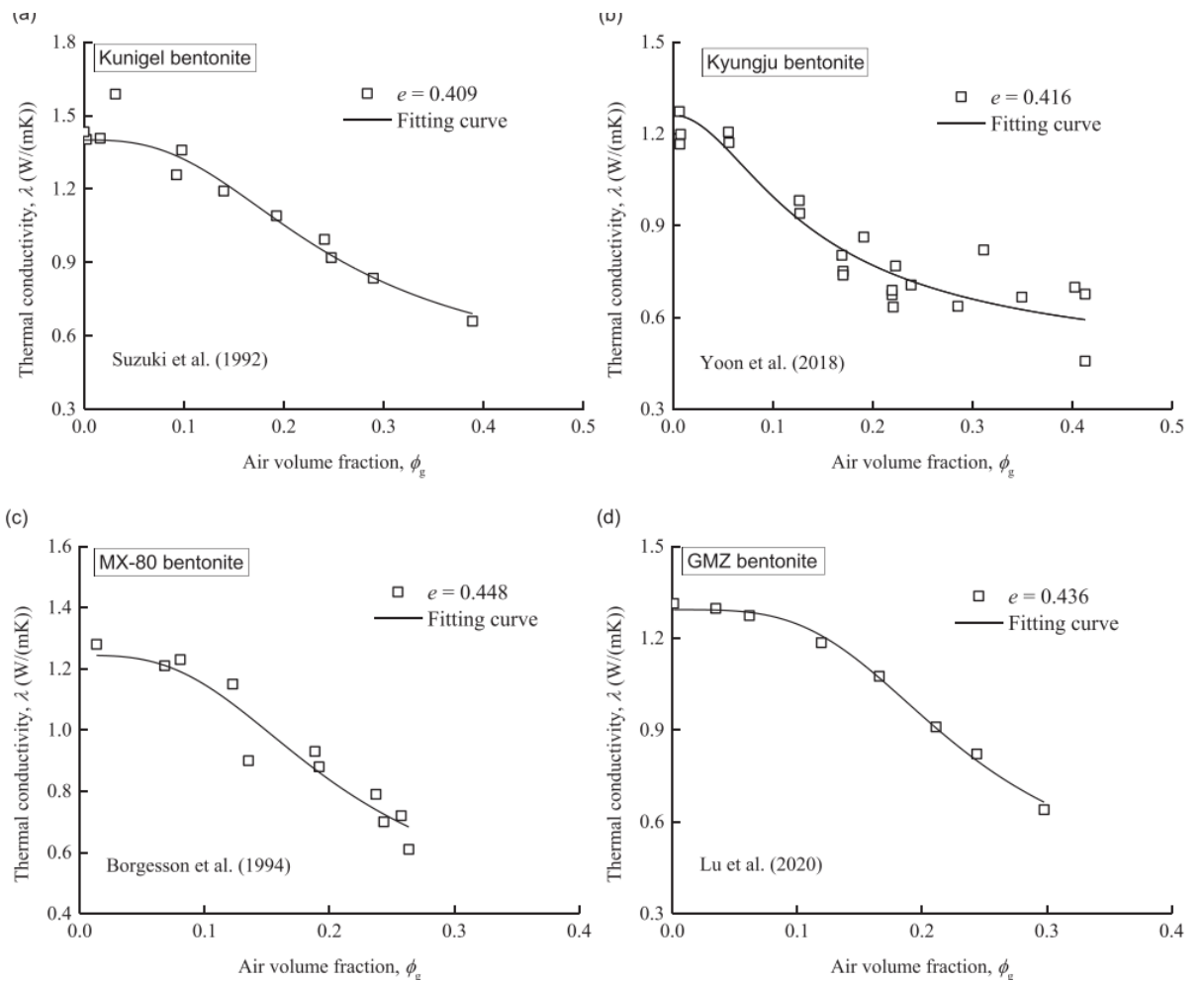
It was found that the thermal conductivity increased with the increase of water content (or degree of saturation) and dry density of soil, as well as the quartz fraction (Tien et al., 2010; Man et al., 2011; Saleh, 2012; Abootalebi and Siemens, 2018).



## CONCLUSION:

In this study, the effect of air volume fraction on the thermal conductivity of compacted bentonite materials was firstly analysed. Then a conceptual model and the corresponding mathematical formula were developed. Finally, this proposed method was verified from the existing results. The results and analyses made allow the following conclusions to be drawn.

The thermal behaviour of compacted bentonite materials can be roughly distinguished into three zones according to the air volume fraction. At low air volume fraction, the soil was nearly saturated, and the effect of air volume fraction was negligible. At medium air volume fraction, the channels for air were gradually increasing with the increase of air volume fraction, and in that case, the air volume fraction gradually became dominated parameter in controlling the soil thermal behavior. At high air volume fraction, the slight decrease of thermal conductivity with air volume fraction suggests that the channels for air were totally connected, and the air volume fraction had insignificant effect on the thermal conductivity.



A predictive model with consideration of air volume fraction was proposed, allowing the thermal conductivity for different kinds of compacted bentonite materials to be calculated. The good agreement between the predicted and measured thermal conductivities showed the performance of the proposed model, as well as the relevant mechanism identified in this study.



## **2.2 A study on the thermal conductivity of compacted bentonites by**

### **Tang et al. (2008)**

Compacted bentonite is often considered as a possible buffer material for high-level radioactive waste disposal. Its thermal conductivity is one of the key properties for the design of such disposal system (JNC, 2000). Several works have been done previously to study the thermal conductivity of compacted bentonites. Measured data can be found in the works of Villar (2000) on Febex bentonite, Ould-Lahoucine et al. (2002) on Kunigel bentonite, Madsen (1998) on MX80 bentonite, Coulon et al. (1987) on several smectite-based clays. These measurements show that the thermal conductivity of compacted bentonites depends on the dry density, the water content, and the mineralogical composition. These parameters, which are in general easily measurable, have been often used in order to predict the thermal conductivity of soil (Johansen, 1975; De Vries, 1963, Ould-Lahoucine et al., 2002; among others).

Clay	MX80 (Present work)	MX80 (Madsen, 1998)	Febex (Villar, 2000)	Kunigel (JNC, 2000)
Smectite (%)	92	76	92	46-49
Quartz (%)	3	15	2	29-38
w <sub>L</sub> (%)	520	-	102	415
w <sub>P</sub> (%)	42	-	53	32
I <sub>p</sub>	478	-	49	383
ρ <sub>s</sub> (Mg/m <sup>3</sup> )	2.76	2.76	2.70	2.79
S (m <sup>2</sup> /g)	-	562	725	687

**Table 1. Identification parameters.**

## CONCLUSION:

The thermal conductivity of compacted MX80 bentonite was measured using the heat method. The effect of the mineralogical composition was evident: the MX80 bentonite studied here contained a lower fraction of quartz than that studied by Madsen (1998) and had lower thermal conductivity. Water content, dry density, hysteresis, degree of saturation and volumetric fraction of constituents are also of influence. A good correlation between the volume fraction of air and thermal conductivity was observed. A linear correlation was proposed to predict the thermal conductivity of compacted bentonites.

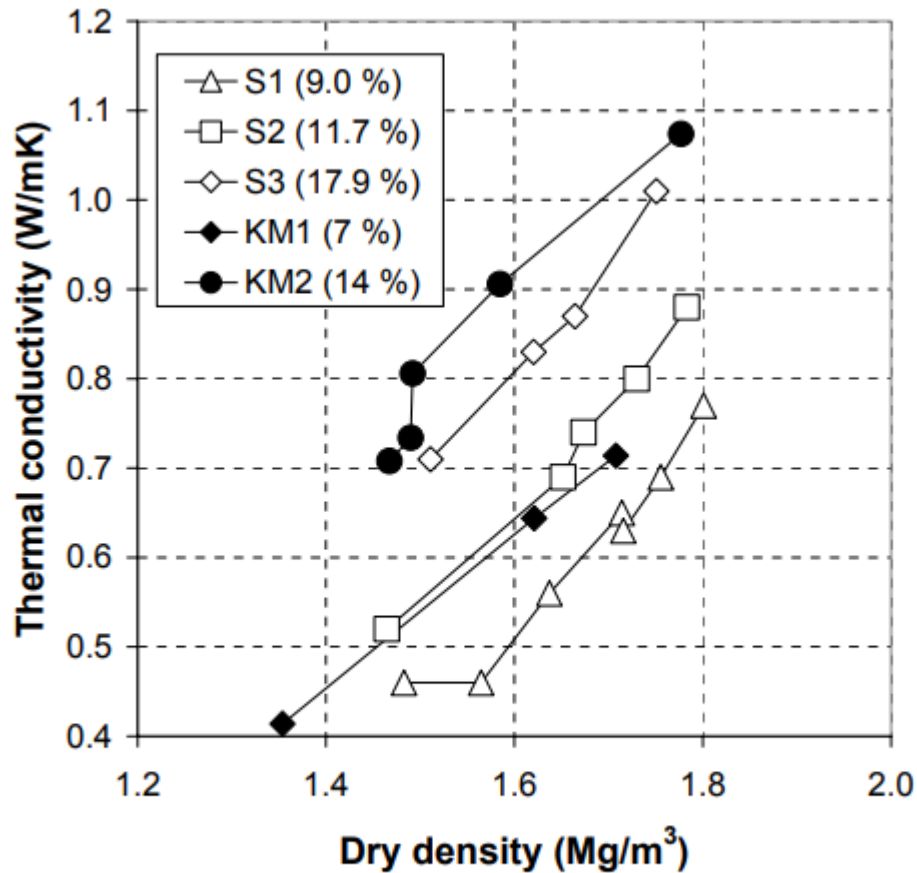
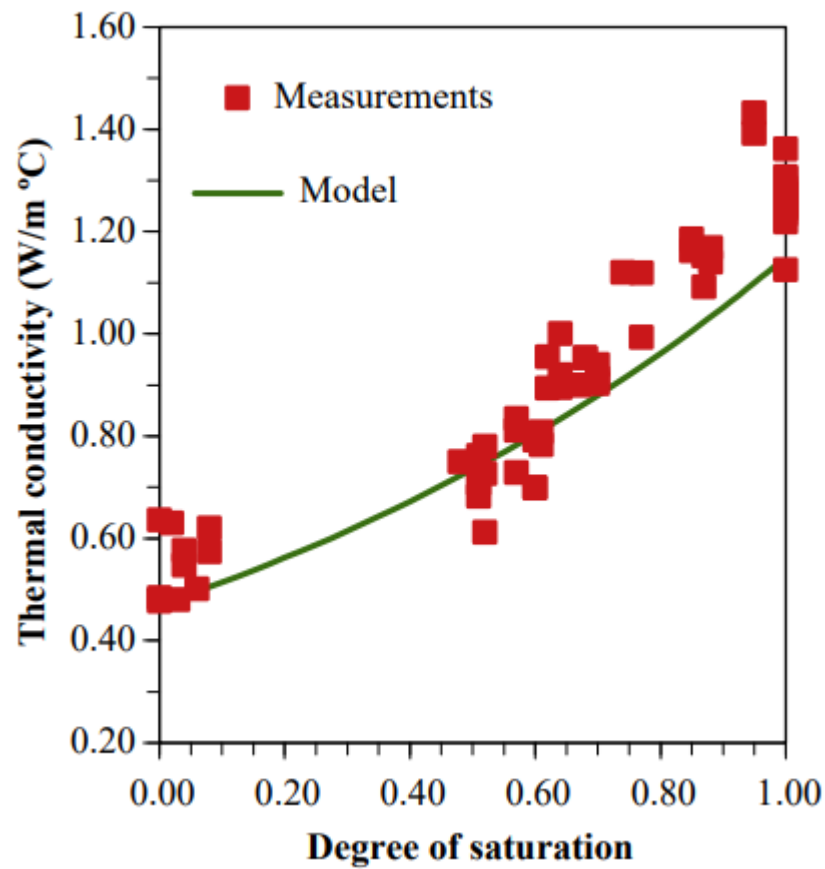


Figure 2. Thermal conductivity versus dry density.

### **2.3 Behavior of a bentonite barrier in the laboratory by Villar et al.**

**(2008)**

The conditions of the bentonite in an engineered barrier for high-level radioactive waste disposal were simulated in a series of tests performed in cylindrical cells (length 60 cm, diameter 7 cm). Inside the cells, six blocks of FEBEX bentonite compacted to dry density 1.65 g/cm<sup>3</sup> were piled up, giving rise to a total length similar to the thickness of the clay barrier in a repository according to the Spanish concept. The bottom surface of the material was heated at 100 °C and the top surface was injected with granitic water. The duration of the tests was 6, 12, 24 and 92 months. The temperatures inside the clay and the water intake were measured during the tests and, at the end, the cells were dismantled and the dry density, water content and hydro-mechanical properties were measured at different positions. The injection of water provokes, near the hydration surface, a decrease of the dry density due to the increase of the water content and the clay swelling, while heating gives rise to an increase of the dry density and a reduction of the water content in the hottest area.



At the end of all the tests there were important water content and dry density gradients along the bentonite column. The increase in water content caused by hydration is linked to a reduction in dry density as a consequence of swelling, whereas the decrease of water content caused by evaporation near the heater is linked to an increase of dry density as a consequence of shrinkage. The density and water content gradients will condition temporarily the hydro-mechanical properties of the bentonite that are dependent on both, as the permeability and the swelling capacity (Villar et al., 2005a, 2008).

## **2.4 Thermal Mechanical Behavior of Compacted GMZ Bentonite by Tang & Cui (2011)**

The preliminary long-term plan for the implementation of China's high-level radioactive waste repository (Wang et al., 2006) suggests that a high-level radioactive waste repository will be built in the middle of the 21st Century. In the Chinese concept of geological disposal, bentonite has been selected as the buffer/backfill material. The Gaomiaozi (GMZ) Na-bentonite taken from a large-scale deposit located in the North Chinese Inner Mongolia Autonomous Region (300 km northwest of Beijing) has been chosen for this purpose. After Wen (2006), preliminary research conducted on the swelling, mechanical, hydraulic, and thermal properties have shown that the GMZ bentonite is a good buffer/backfill material. Indeed, as reported by Wen (2006), it has relatively high thermal conductivity ( $K=1.51 \text{ W/mK}$  at a dry density of  $1.6 \text{ Mg/m}^3$  and a water content of 26.7%), quite low water permeability (at saturated state,  $k=1.94 \times 10^{-13} \text{ m/s}$  at a dry density of  $1.6 \text{ Mg/m}^3$  and a temperature of  $25^\circ\text{C}$ ), a relatively high unconfined compression strength ( $1.74 \text{ MPa}$  at a dry density of  $1.6 \text{ Mg/m}^3$  and a water content of 23.6%), and quite a high swelling pressure ( $3.17 \text{ MPa}$  at a dry density of  $1.6 \text{ Mg/m}^3$ ). Chen et al. (2006) completed the experimental investigation by determining the water retention curves of the GMZ bentonite and showed its high retention capacity.

**Table 1. Mineral composition of some bentonites**

Mineral	Kunigel V1 <sup>a</sup>	FoCa <sup>b</sup>	MX80 <sup>c</sup>	FEBEX <sup>d</sup>	GMZ <sup>e</sup>
Montmorillonite (%)	46–49	80% (interstratified smectite/ kaolinite)	79	92 ± 3	75.4
Plagioclase (%)	—	—	9.2	2 ± 1	—
Pyrite (%)	0.5–0.7	—	0.–	0.02 ± 0.01	—
Calcite (%)	2.1–2.6	1.4	0.8	Traces	0.5
Dolomite (%)	2.0–2.8	—	—	0.60 ± 0.13	—
Gypsum (%)	—	0.4	—	0.14 ± 0.01	—
Halite (%)	—	—	—	0.13 ± 0.02	—
Analcite (%)	3.0–3.5	—	—	—	—
Mica (%)	—	—	< 1	—	—
Feldspar (%)	2.7–5.5	—	2.0	Traces	4.3
Cristobalite (%)	—	—	—	2 ± 1	7.3
Kaolinite (%)	—	4	—	—	0.8
Quartz (%)	29–38	6	2.8	2 ± 1	11.7
Field organic	0.31–0.34	—	0.1	0.35 ± 0.05	—

<sup>a</sup>JNC (2000); <sup>b</sup>Guillot et al. (2002); <sup>c</sup>Montes-H. et al.(2003); <sup>d</sup>ENRESA (2000); <sup>e</sup>Wen (2006).

**Table 2. Physical properties of some bentonites**

Parameter	Kunigel-V1 <sup>a</sup>	FoCa <sup>b</sup>	MX80 <sup>c</sup>	FEBEX <sup>d</sup>	GMZ <sup>e</sup>
Particle < 2 $\mu\text{m}$ (%)	64.5	—	60	68	60
CEC (meq/100 g)	73.2	54	82.3	102 <sup>j</sup>	77.30
Base cations Exchange	Na–Ca	Ca	Na	Ca–Mg	Na–Ca
$w_L$ (%)	474	112	519	102	313
$w_P$ (%)	27	50	35	53	38
$I_P$	447	62	484	49	275
$\rho_s$ (Mg/m <sup>3</sup> )	2.79	2.67	2.76	2.70	2.66
$S$ (m <sup>2</sup> /g)	687	300	522	725	570

<sup>a</sup>Komine (2004); <sup>b</sup>Marcial et al. (2002); <sup>c</sup>Tang and Cui (2005); <sup>d</sup>ENRESA (2000); <sup>e</sup>Wen (2006).

## CONCLUSION:

- i) The montmorillonite content of GMZ bentonite is lower than that of MX80 bentonite and FEBEX bentonite but it is higher than that of Kunigel-V1 bentonite. That explains the large values of its cations exchange capacity (CEC) and specific surface area  $S$ . In general, good correlations can be established between the montmorillonite content and the CEC values or the specific surface area  $S$  (Table 2). Nevertheless, no direct correlation can be made between the montmorillonite content and the basic geo-technical properties; other factors, such as the nature of base exchangeable cations, also appear to have a significant influence.
  
- ii) The same observation has been made in terms of swelling potential. In general, the higher the montmorillonite content, the higher the swelling potential. However, a Ca-based bentonite generally shows lower swelling potential than a Na-based bentonite. For GMZ bentonite it was observed that wetting (suction decreased from 110 to 9 MPa) induced a swelling volumetric strain of 30%. That is lower than MX80 (50%) and higher than that of other bentonites (less than 20%).
  
- iii) The quartz content of GMZ bentonite is relatively high (11.7%) just behind KunigelV1 bentonite (29-38%). This could explain their relatively large values of thermal conductivity. Note that compared to the values for other bentonites, the difference is too small to allow for a relevant correlation to be drawn between their thermal conductivity and the quartz content.

iv) The coefficient of thermal expansion of the compacted GMZ bentonite is  $2.10 \cdot 10^{-4} \text{ } ^\circ\text{C}^{-1}$ , that is similar to the values obtained for the compacted MX80 bentonite (Tang et al.,

2008a) and the compacted FEBEX bentonite (Romero et al., 2005). As the compacted MX80 bentonite, the GMZ bentonite also showed a thermal expansion upon heating at high suctions (39 and 110 MPa) and a thermal contraction at lower suction (9 MPa). v)

The effect of suction and temperature on  $\kappa$  and  $\lambda(s)$  of GMZ bentonite is similar to MX80:  $\kappa$  and  $\lambda(s)$  increase with decreasing suction but are independent of the temperature changes. Compared to other bentonites, GMZ bentonite has the highest values of  $\lambda(s)$ : 0.12-0.16 at  $s=9\text{-}110 \text{ MPa}$ .

vi) The effect of temperature on the yield stress  $p_0$  of the GMZ bentonite has been found to be insignificant. A similar observation was made for MX80 bentonite by Tang et al. (2008a). In contrast, a significant suction effect was identified. As is also the case for MX80 bentonite and FEBEX bentonite, the yield stress  $p_0$  of the GMZ bentonite decreased significantly, at a rate similar to that of FEBEX bentonite but lower than that of MX80 bentonite.



### **3. References**

- I. Behavior of a bentonite barrier in the laboratory: Experimental results up to 8 years and numerical simulation by M.V. Villar, M. Sánchez, A. Gens (2008).
- II. Effects of ammonium ion and bentonite content on permeability of bentonite-clay mixture by Wen-Jing Sun et al. (2021).
- III. Thermal Mechanical Behavior of Compacted GMZ Bentonite by tang & cui (2011).
- IV. A study on the thermal conductivity of compacted bentonites by Tang et al. (2008).
- V. Effect of air volume fraction on the thermal conductivity of compacted bentonite materials by Zhang et al. (2021).
- VI. Effects of mineralogy on thermo-hydro-mechanical parameters of MX80 bentonite by A. M. Tang, Y. J. Cui
- VII. Controlling suction by vapour equilibrium technique at different temperatures, application to the determination of the water retention properties of MX80 clay by Anh-Minh Tang and Yu-Jun Cui
- VIII. Thermal Conductivity of Korean Compacted Bentonite Buffer Materials for a Nuclear Waste Repository by Seok Yoon, WanHyoung Cho, Changsoo Lee and Geon-Young Kim.
- IX. Gas transport in granular compacted bentonite: coupled hydro mechanical interactions and microstructural features by Laura Gonzalez-Blanco, Enrique Romero and Paul Marschall.
- X. <https://sci-hub.se/> for research paper collection.
- XI. <https://scholar.google.com/> for research paper collection.