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Evaluation of Thermal Properties for the Bentonil-WRK Bentonite

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The bentonite buffer material is a crucial component in an engineered barrier system used for the disposal of high-level radioactive waste. Because a large amount of heat from the disposal canister is released into the bentonite buffer material, the thermal conductivity of the bentonite buffer is a crucial parameter that determines the design temperature. At the Korea Atomic Energy Research Institute (KAERI), a new standard bentonite (Bentonil-WRK) has been used since 2022 because Gyeongju (KJ) bentonite is no longer produced. However, the currently available data are insufficient, making it essential to investigate both the basic and complex properties of Bentonil-WRK. Thus, this study evaluated its geotechnical and thermal properties and developed a thermal conductivity empirical model that considers its dry density, water content, and temperature variations from room temperature to 90°C. The coefficient of determination (R^2) for the model was found to be 0.986. The thermal conductivity values of Bentonil-WRK were 1–10% lower than those of KJ bentonite and 10–40% higher than those of MX-80 bentonites, which were attributable to mineral-composition differences. The thermal conductivity of Bentonil-WRK ranged between 0.504 and 1.149 W·(m^{-1}·K^{-1}), while the specific heat capacity varied from 0.826 to 1.138 (kJ·(kg^{-1}·K^{-1})).

Keywords: Bentonil-WRK bentonite, Thermal conductivity, Specific heat capacity, Regression analysis

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Table 1. Basic properties for KJ-II, Bentonil-WRK, and MX-80

	Specific gravity	Liquid limit (%)	Plastic limit (%)	Plasticity index (%)	USCS*	Swell index (ml/2 g)	Initial water content (%)	Specific surface area* ($m^2 \cdot g^{-1}$)	Grain-size distribution < 2 μm (%)
KJ-II	2.71	146.7	28.4	118.3	CH	6.5	11−12	61.5	48.4
Bentonil-WRK	2.548	97.1	42.4	54.7	MH	5	13−14	51.74	30
MX-80 [8, 11]	2.70	310	29	281	CH	48	10−17	569	81.9

*Note: Unified soil classification system (USCS): CH means high-plasticity clay, and MH means high-plasticity silt; Specific surface area was analyzed by the KAIST Analysis Center for Research Advancement.

1. Introduction

High-level radioactive wastes (HLWs) are inevitably produced by nuclear power plants, and they must be completely disposed in a deep geological site away from human life. Engineered barrier systems (EBSs) were suggested as a deep geological disposal system, comprising a disposal canister, buffer material, backfill material, etc. [1, 2]. The buffer material is placed between the disposal canister and rock-mass and has a crucial function in an EBS. Bentonite clay was selected as the most suitable buffer material [3-5] with specific functional criteria and technical design requirements defined for the buffer material [6]. In Korea, KJ bentonite (Ca-type) from the Gyeongju region has been studied for decades, and a new Ca-type bentonite, Bentonil-WRK, has been manufactured by Clariant Korea Corporation since 2022 as KJ bentonite is no longer produced in Korea. Since the Korea Atomic Energy Research Institute (KAERI) has selected Bentonil-WRK as a standard buffer material for research, investigating its various properties to evaluate its adaptability as a buffer material is necessary. Several indispensable thermal-hydraulic-mechanical (THM) properties are required in the bentonite buffer material to conduct safety analysis, and thermal conductivity is one of the most important parameters that determine the design temperature of the buffer material [1, 7-9].

Therefore, the objective of this study is to determine the thermal conductivity and specific heat capacity of Bentonil-WRK bentonite. These properties are utilized in numerical analyses for calculating buffer temperature. Accordingly, this paper measured the thermal conductivity of Bentonil-WRK considering various factors such as water content, dry density, and temperature variation, and specific heat capacity under certain dry density and water content values. Based on experimental results, this paper additionally suggested an empirical thermal conductivity model for the Bentonil-WRK bentonite, and thermal conductivity values of the Bentonil-WRK bentonite were compared with previous KJ and MX-80 (Na-type) bentonites.

2. Test Setup

2.1 Basic Material Properties

In this study, basic geotechnical properties of the Bentonil-WRK bentonite, a Ca-type, were measured shown in Table 1. The specific gravity value of Bentonil-WRK was marginally smaller than previous bentonites and was classified as MH (highly plastic silt) based on the unified soil classification system [10]. The initial water content and swell index of the Bentonil-WRK bentonite were 13–14% and 5 ml/2 g. Especially, the swell index was 30% smaller than KJ-II bentonite. Fig. 1 shows the particle size distribution of the Bentonil-WRK bentonite. Table 2 shows the

Table 2. Quantitative XRD analysis (wt%) for mineral constituents [11]

Bentonite Type	KJ-II				Bentonil-WRK				MX-80
Sample No.	1	2	3	Avg.	1	2	3	Avg.	
Montmorillonite	63.4	61.7	60.5	61.9	68.8	70.7	72.6	70.7	78.2
Albite	19.4	22.8	20.4	20.9	16.8	13.2	13.3	14.4	10.3
Quartz	5.8	4.9	5.3	5.3	2.2	1.9	1.9	2.0	6.7
Cristobalite	4.0	4.5	3.7	4.1	12.2	14.3	12.2	12.9	3.6
Calcite	4.3	3.3	6.8	4.8					
Heulandite	3.0	2.7	3.3	3.0					

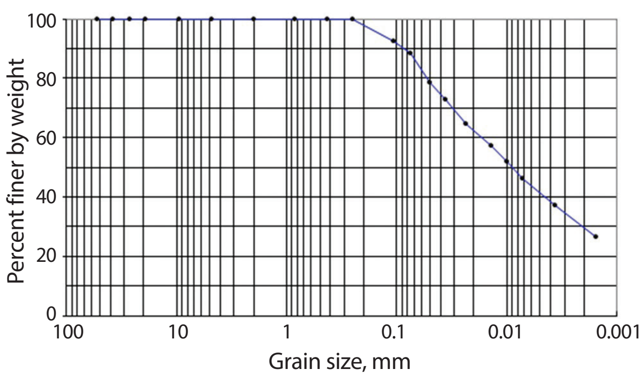
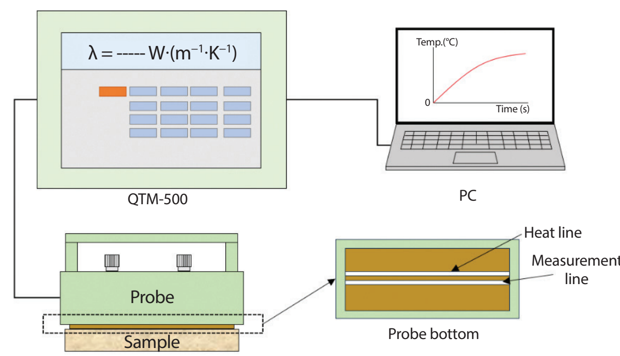
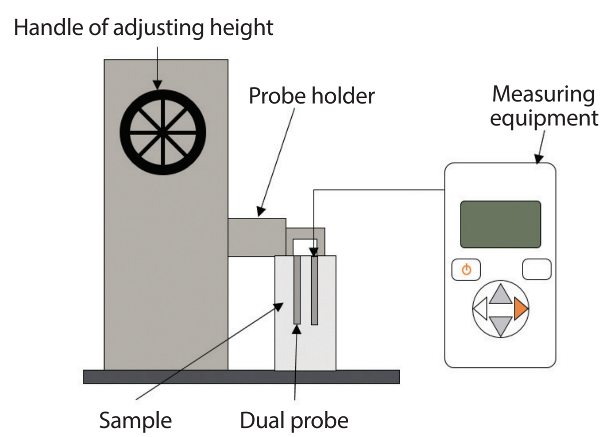


Fig. 1. Particle size distribution for the Bentonil-WRK bentonite.



(a) QTM-500



(b) KD2-pro dual probe

Fig. 2. Thermal property-measuring equipment.

mineral constituents for several previous bentonites including the Bentonil-WRK bentonite [11].

As shown in Table 2, MX-80 has a montmorillonite content of 78wt%, while KJ-II has a montmorillonite content of approximately 62wt%. The Bentonil-WRK has a final montmorillonite content of 69–73wt%, and other minerals include 14wt% albite, 2wt% quartz, and 13wt% cristobalite. The average content of each mineral composition in both KJ-II and Bentonil-WRK adds up to 100%. However, for MX-80, the total is 98.8%, falling short by 1.2%. This discrepancy is attributed to the presence of trace mineral components in MX-80.

2.2 Measurement of Thermal Properties

This paper used QTM-500 (Kyoto Electronics) to measure thermal conductivity and a dual probe apparatus (KD2 Pro, Decagon device) to measure specific heat capacity for the Bentonil-WRK bentonite, as shown in Fig. 2. The QTM-500 is based on the transient hot-wire method [12], and the dual probe apparatus is based on the line source model [13]. The detailed explanation and measuring process of thermal conductivity and specific heat capacity have been reported previously [12, 13]. Prior to measuring thermal conductivity and specific heat capacity, the dried bentonite powders were mixed with deionized water using a three-dimensional mixer, and the mixed bentonite powders were compacted into a block measuring 5 cm in width, 10 cm in length, and 1 cm in height in a steel mold via a hydraulic press to a specific dimension and target density [12]. Bentonite blocks with varying water content ratios were produced by adjusting the amount of deionized water added to the bentonite powders. Then, the sample was placed in a constraint cell (Fig. 2(a)), ensuring stability in water content despite temperature increases. Consequently, both the initial dry density and initial water content remained constant during the thermal conductivity measurements.

3. Test Results

3.1 Thermal Conductivity

First, this paper measured the thermal conductivity of Bentonil-WRK considering dry density, water content, and temperature variation that were considered crucial factors influencing the thermal conductivity of bentonite buffer [1, 7, 8, 9, 12, 14]. The specimen was a rectangle of size 100×50×10 mm. It was hermetically sealed to prevent water evaporation under the high temperature condition. The dry density of the buffer must be higher than 1.6 g·cm^{-3} [15]. Accordingly, this paper used bentonite blocks with dry density (γ_d) of 1.61 g·cm^{-3} (± 1%). Fig. 3 shows the thermal conductivity variation according to water content under room temperature with a dry density of 1.61 g·cm^{-3}. The thermal conductivity was proportional to water content increase, which is consistent with previous research [1, 8, 9] and attributed to the thermal properties of water, air, and soil particles [16]. Fig. 4 shows thermal conductivity variation under the dried condition and room temperature based on the dry density of bentonite buffer materials. The larger the dry density, the higher the thermal conductivity of the bentonite buffer material [1, 12, 14] since thermal conductivity of the soil particle is significantly higher than that of air [16]. This paper also measured thermal conductivity from room temperature to 90°C under constant water content conditions. The repercussion of temperature increase on thermal conductivity was evident, similar to previous

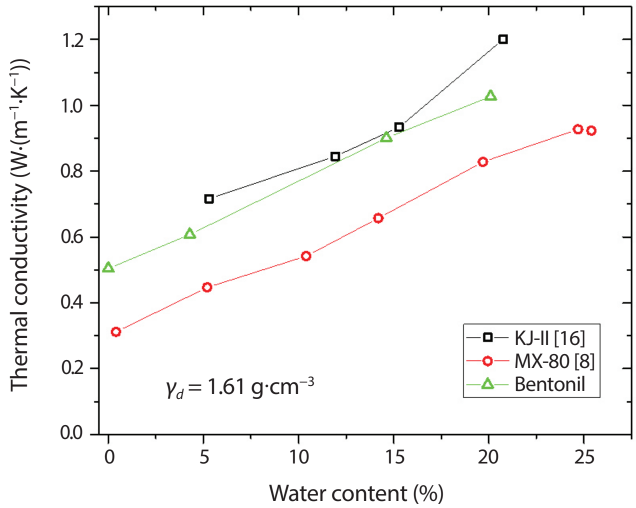


Fig. 3. Thermal conductivity variation according to water content.

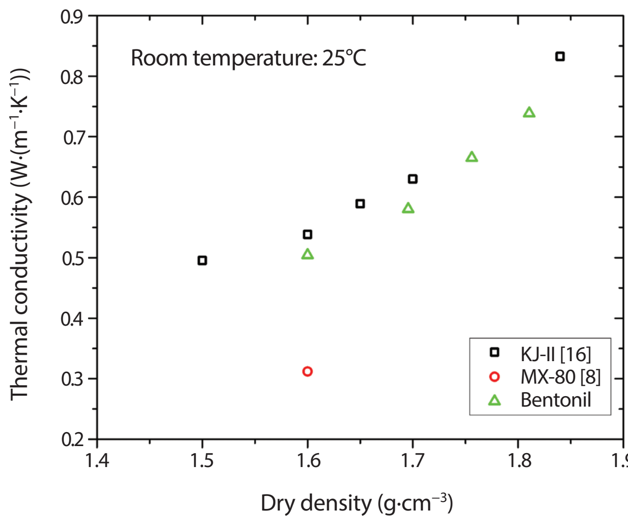


Fig. 4. Thermal conductivity variation according to dry density.

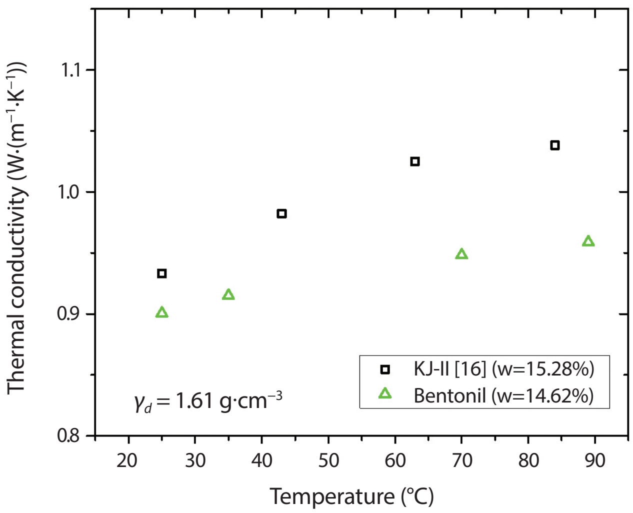


Fig. 5. Thermal conductivity variation according to temperature increase.

Table 3. Summary of thermal conductivity values

Bentonite	Dry density ($g \cdot cm^{-3}$)	Water content	Temperature (°C)	Thermal conductivity ($W \cdot (m^{-1} \cdot K^{-1})$)
MX-80 [8]	1.0–1.8	0.004–0.254	5–90	0.312–1.100
KJ-II [16]	1.314–1.836	0–0.234	25–87	0.388–1.536
Bentonil-WRK	1.519–1.811	0–0.210	25–90	0.504–1.149

researches [8, 16]. Thus, thermal conductivity due to water, air and soil particles increased with temperature [16, 17]. As the exact thermal conductivity values of MX-80 upon temperature increase were not available from previous research, the thermal conductivity values of KJ bentonite were compared with those of Bentonil-WRK bentonite.

The thermal conductivity of Bentonil-WRK bentonite was 1–10% lower than KJ bentonite, and 10–40% higher than MX-80 bentonite. Mineral composition has a high impact on the thermal conductivity of bentonite [1, 7, 18]. Thus, the thermal conductivity of montmorillonite is inferred to be the lowest among other minerals. That might be a major reason for the thermal conductivity of Bentonil-WRK bentonite being between that of KJ and MX-80 bentonites.

Table 4. Specific heat capacity values

Bentonite	Dry density ($g \cdot cm^{-3}$)	Water content	Specific heat capacity ($kJ \cdot (kg^{-1} \cdot K^{-1})$)
KJ-II	1.581/1.622	7.71/0	1.000/1.035
Bentonil-WRK	1.639/1.698	14.72/0	1.138/0.826

Table 3 summarizes the thermal conductivity variation for the different bentonites including Bentonil-WRK.

3.2 Specific Heat Capacity

This paper also measured the specific heat capacity of the Bentonil-WRK bentonite using a cylindrical KD-2 pro dual probe with a diameter and height of 30 and 60 mm, respectively. The initial water content and dry density were 14.72% and 1.639 $g \cdot cm^{-3}$. Table 4 represents the specific heat capacity values for the KJ and Bentonil-WRK bentonites. The specific heat capacity difference between the Bentonil-WRK and KJ bentonites was 10–20% because of variations in water content and dry density. However, no specific trend of specific heat capacity was evident. Hence, it was concluded that specific heat capacity was not strongly affected by water content and dry density. It could be perceived that numerous past studies used certain specific heat capacity, whereas thermal conductivity was often derived from a regression equation incorporating multiple independent variables, including saturation and dry density [1, 19, 20].

4. Regression Analysis

As thermal conductivity can be used as the input parameter in the safety analysis of the EBS, this paper suggested the thermal conductivity prediction model of Bentonil-WRK bentonite buffer using three independent variables based on multiple regression analysis. Table 5 summarizes the statistical quantities for three independent variables

Table 5. Statistical quantities for several variables

	N	Minimum	Maximum	Average	Skewness	Kurtosis
Water content	64	0	0.210	0.091	0.055	−1.350
Dry density ($g\cdot cm^{-3}$)		1.519	1.811	1.665	−0.054	−0.865
Temperature (°C)		25	90	54.484	0.201	−1.462
Thermal conductivity ($W\cdot(m^{-1}\cdot K^{-1})$)		0.504	1.149	0.844	−0.108	−1.223

Table 6. Multiple regression analysis results

	B	Standard error	t	P-value	VIF
Constant	−1.694	0.065	−25.937	< 0.01	
X_1 (water content)	2.811	0.053	65.102	< 0.01	1.265
X_2 (dry density)	1.338	0.038	35.218	< 0.01	1.236
X_3 (temperature)	0.001	0.000	8.929	< 0.01	1.034
R^2	0.986				
${}_{adj}R^2$	0.986				

B: non-standardized coefficient, *t*: *B*/standard error, VIF: variance inflation factor

(water content, dry density, and temperature) and one dependent variable (thermal conductivity) used in the multiple regression analysis. Thermal conductivity can be predicted as Eq. (1), and Table 6 represents the multiple regression analysis. To use a regression analysis model, several assumptions must be satisfied, such as *T*-tests, ANOVA, and residual analysis [16, 21]. When selecting independent variables, ensuring their mutual independence is crucial. This is because if the independent variables are interrelated, they may exert overlapping influences on the dependent variable. In this analysis, the independence of the independent variables was confirmed by examining the variance inflation factors (VIFs) for each variable, all of which were below 10 [21]. The water content, dry density, and temperature showed high correlation with thermal conductivity, as demonstrated in Table 6. Hence, the three independent variables can be used to predict thermal conductivity.

Furthermore, Eq. (1) was pertinent to follow every regression analysis assumption with high R^2 value.

$$\lambda = -1.694 + 2.811\omega + 1.338\rho_d + 0.001T \tag{1}$$

where λ is thermal conductivity ($W\cdot(m^{-1}\cdot K^{-1})$), ω is water content, ρ_d means dry density ($g\cdot cm^{-3}$), and T is temperature (°C). In Eq. (1), of the three independent variables, the sample's water content exerts the most significant influence on thermal conductivity, as indicated by its B value. The dry density of the sample follows in terms of influence.

5. Conclusions

This study measured the thermal conductivity and specific heat capacity of the Bentonil-WRK bentonite that is selected as a new reference buffer material in KAERI. The suggestions and new findings in this study are summarized as follows:

• The thermal conductivity of Bentonil-WRK, considering its dry density, water content, and temperature, was identified for the first time.

- The thermal conductivity of Bentonil-WRK bentonite was 1–10% lower than KJ bentonite and 10–40% higher than MX-80 bentonites.
- Their mineral compositions are assumed to have a major impact on thermal conductivity.
- Furthermore, the thermal conductivity prediction model for the Bentonil-WRK bentonite with 64 datasets is suggested.
- Additionally, it has been shown that the specific heat of Bentonil-WRK bentonite differs by 10–20% from that of KJ bentonite.

Hence, Bentonil-WRK can be applied as a buffer material based on basic, mineralogical, and thermal properties although thermal conductivity was marginally lower than KJ bentonite. However, its hydraulic-mechanical properties must be investigated to evaluate safety performance as a further study in the future.

Conflict of Interest

No potential conflict of interest relevant to this article was reported.

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