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Thermal Influence on Hydraulic Conductivity in Compacted Bentonite: Predictive Modeling Based on the Dry Density-Hydraulic Conductivity Relationship

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Hydraulic conductivity is a critical design parameter for buffers in high-level radioactive waste repositories. Most employed prediction models for hydraulic conductivity are limited to various types of bentonites, the main material of the buffer, and the associated temperature conditions. This study proposes the utilization of a novel integrated prediction model. The model is derived through theoretical and regression analyses and is applied to all types of compacted bentonites when the relationship between hydraulic conductivity and dry density for each compacted bentonite is known. The proposed model incorporates parameters such as permeability ratio, dynamic viscosity, and temperature coefficient to enable accurate prediction of hydraulic conductivity with temperature. Based on the results obtained, the values are in good agreement with the measured values for the selected bentonites, demonstrating the effectiveness of the proposed model. These results contribute to the analysis of the hydraulic behavior of the buffer with temperature during periods of high-level radioactive waste deposition.

Keywords: Hydraulic conductivity, Compacted bentonite, Buffer, Prediction model, Engineered barrier system

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1. Introduction

The buffer surrounding a canister containing spent fuels in a high-level radioactive waste (HLW) repository is affected by the decay heat from the canister; therefore, to design the buffer, the temperature of the buffer must be considered. Hydraulic conductivity is a design parameter of buffers for HLW repositories [1, 2]. The hydraulic conductivity of the buffer must be less than that of the ground, such as in the near-field rock, where an HLW repository is positioned to prevent the inflow of groundwater to the canister because nuclides leak from the canister and are transferred by the groundwater [1, 2]. Therefore, predicting the hydraulic conductivity of a buffer based on its conditions is important. The hydraulic conductivity of compacted bentonite, which is used as a buffer, is affected mostly by the dry density and temperature [3]. Therefore, many studies have been conducted to predict the hydraulic conductivity of compacted bentonite using these parameters [4-6]. However, it is difficult to apply a prediction model for hydraulic conductivity to various compacted bentonites because the hydraulic conductivity of compacted bentonite differs from that of bentonite [4-6]. There are various prediction models for hydraulic conductivity with different types of bentonite. Furthermore, various studies have shown that the hydraulic conductivity of compacted bentonite differs, even under the same conditions [3, 5].

In addition, the measured hydraulic conductivities did not coincide with the model values. Considering that the hydraulic conductivity of the buffer material should be lower than that of the near-field rock, ~10^{-12} $m \cdot s^{-1}$ [1], differences of the order of two or three times are not likely to have a significant impact when accounting for hydraulic conductivity variations. The determination coefficient of most prediction models for the normal hydraulic conductivity of compacted bentonite is significantly low to be considered as having no relationship or a weak relationship because the hydraulic conductivity of compacted bentonite is significantly low. Therefore, most prediction models for hydraulic conductivity use the logarithmic hydraulic conductivity to enhance the determination coefficient [4, 5]. However, logarithmic hydraulic conductivity is relatively counterintuitive compared to normal hydraulic conductivity.

Thus, an intuitive and integrated prediction model for hydraulic conductivity is necessary for effective research and development of HLW repository buffers. In this study, a prediction model for hydraulic conductivity according to temperature, which was applied to all types of compacted bentonite, was proposed to predict the reasonable hydraulic conductivity of compacted bentonite using the relationship between dry density and hydraulic conductivity based on theoretical and regression analyses.

2. Data Collection

Data from literature were used to develop and validate a prediction model for the hydraulic conductivity (K) of compacted bentonite. The data of hydraulic conductivities

Table 1. Basic properties of the samples

Sample	Specific gravity	Liquid limit (%)	Plastic limit (%)	Plasticity index	USCS	Montmorillonite (%)	Main exchanged cation	Reference
KJ-II	2.71	146.7	28.4	118.3	CH	61.9	Ca^{2+}	[12]
GMZ01	2.66	276	37	239	CH	75.4	Na^{+}	[13, 14]
MX-80	N/A	N/A	N/A	N/A	N/A	75	Na^{+}	[10]
KJ-I	2.74	244.5	46.1	198.4	CH	63.2	Ca^{2+}	[15]

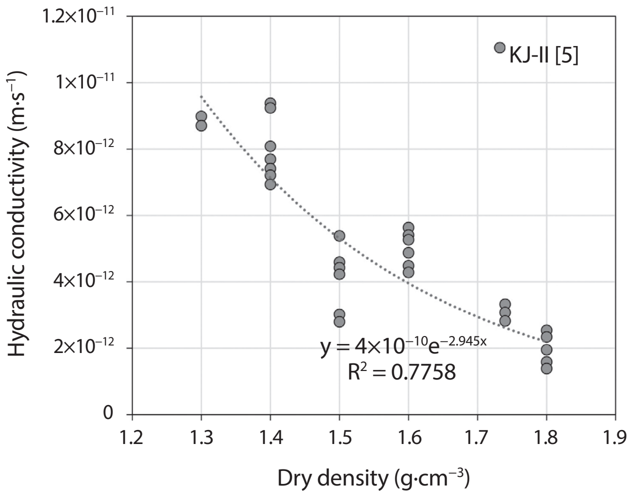


Fig. 1. Hydraulic conductivity with dry density for KJ-II.

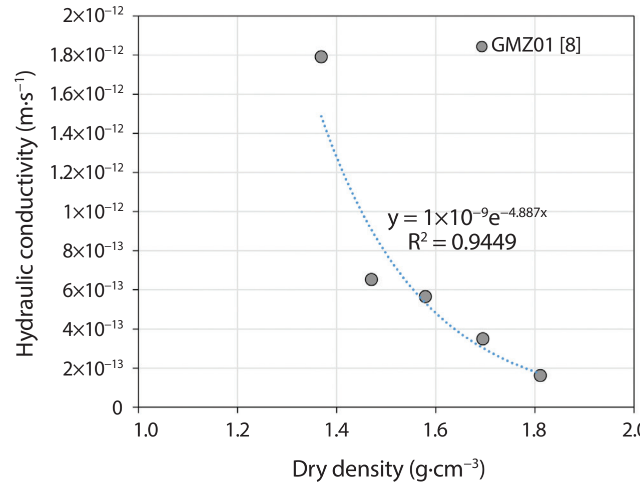


Fig. 2. Hydraulic conductivity with dry density for GMZ01.

with dry density (γ_d) and Celsius temperature (T) for KJ-II, GMZ01, MX-80, and KJ-I bentonites were collected by extracting data from the graphs and excerpting data from tables in the literature [5, 7-11]. The data for KJ-II and GMZ01 were used to derive the prediction model, whereas the data for MX-80 and KJ-I were used to validate the derived prediction model. The hydraulic conductivity was calculated using Darcy's law as follows:

$$K = \frac{Q \cdot L}{\Delta h \cdot A} \tag{1}$$

where Q is the injection flow rate, L is the sample thickness, Δh is the hydraulic head difference, and A is the cross-sectional area of the sample to the direction in which water flows. The basic properties of KJ-II, GMZ01, MX-80, and KJ-I are listed in Table 1 [10, 12-15].

3. Hydraulic Conductivity Relationships

KJ-II and GMZ01 have relationships between hydraulic conductivity and dry density as shown in Figs. 1 and 2, respectively. The increase in dry density implies a decrease in void ratio. Thus, the hydraulic conductivity of the sample decreases with an increase in dry density. Furthermore, in the case of bentonite, it expands upon contact with water, causing a reduction in pore volume. Therefore, as shown in Figs. 1 and 2, at approximately the same room temperature (~25°C), the hydraulic conductivities of KJ-II and GMZ01 exponentially decrease with increasing dry density.

4. Derivation of Hydraulic Conductivity Model

Hydraulic conductivity (K) has a relationship to permeability (k) as follows:

$$K = \frac{k \rho_w g}{\mu_w} \tag{2}$$

where ρ_w is the density of water, g is the acceleration due to gravity, and μ_w is the dynamic viscosity. To obtain the hydraulic conductivity according to the temperature in Eq. (2), the hydraulic conductivity can be derived using the hydraulic conductivity ratio according to the temperature (T) change from the initial temperature (T_o) as follows:

Table 2. Independent variable B for each dry density and temperature condition of KJ-II and GMZ01

Sample	A_2	γ_d	T	B
KJ-II [7]	2.945	1.3	30	0.0013253
	2.945	1.3	60	0.00082451
	2.945	1.3	90	0.00057227
	2.945	1.4	30	0.00057389
	2.945	1.4	60	0.00049712
	2.945	1.4	90	0.00038758
	2.945	1.5	30	0.00011922
	2.945	1.5	60	0.00016852
	2.945	1.5	90	0.00044238
	2.945	1.6	30	0.00014104
	2.945	1.6	60	0.0001323
	2.945	1.6	90	0.000093252
	2.945	1.74	30	0.000084471
	2.945	1.74	60	0.000076873
	2.945	1.74	90	0.000063568
GMZ01 [9]	4.887	1.7	20	0.0019213
	4.887	1.7	40	0.0020456
	4.887	1.7	50	0.0019728
	4.887	1.7	60	0.0019469

$$K(T) = K(T_o) \cdot \frac{k(T)}{k(T_o)} \cdot \frac{\mu_w(T_o)}{\mu_w(T)} \cdot \frac{\rho_w(T)}{\rho_w(T_o)} \tag{3}$$

In Eq. (3), the water density term is negligible because the change in the density of water depending on the temperature is not sufficiently large to affect $K(T)$. Therefore, $K(T)$ can be expressed as follows:

$$K(T) = K(T_o) \cdot \frac{k(T)}{k(T_o)} \cdot \frac{\mu_w(T_o)}{\mu_w(T)} \tag{4}$$

$K(T_o)$ can be expressed as follows through the intercorrelation between dry density (γ_d) and hydraulic conductivity (K), as shown in Fig. 1:

$$K(T_o) = A_1\, exp(A_2\, \gamma_d) \tag{5}$$

where A_1 and A_2 are constants that vary depending on the relationship between K and γ_d. Based on the temperature coefficient (α_k), the permeability ratio ($k(T)/k(T_o)$) is derived as follows:

$$\frac{k(T)}{k(T_o)} = 1 + \alpha_k(T - T_o) \tag{6}$$

The dynamic viscosity of water with respect to temperature can be expressed as follows [16]:

$$\mu_w(T) = b_1 exp(-b_2 T) \tag{7}$$

where b_1 and b_2 are 5.091712×10^{-3} and 2.545425×10^{-2}, respectively [16]. Hence, $K(T)$ considering the dynamic viscosity ratio of water can be expressed as follows:

$$K(T) = A_1 exp(A_2 \gamma_d) \cdot (1 + \alpha_k(T - T_o)) \cdot \frac{\mu_w(T_o)}{b_1 \exp(-b_2 T)} \tag{8}$$

Eq. (8) can be summarized as follows:

$$K(T) = A_1 exp(A_2 \gamma_d) \cdot \frac{a_1 + a_2 T}{b_1 \exp(-b_2 T)} \tag{9}$$

where a_1 and a_2 are constants. $K(T)$ is represented by replacing "a_1+a_2T" with B as follows:

$$K(T) = A_1 exp(A_2 \gamma_d) \cdot \frac{B}{b_1 \exp(-b_2 T)} \tag{10}$$

The independent variable B is calculated for each dry density and temperature condition of KJ-II and GMZ01, as shown in Table 2. Since B varies with dry density and temperature, it is expressed as a function of known variables.

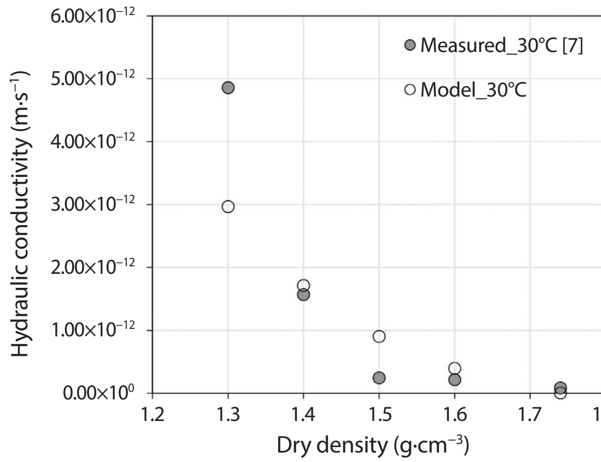
As A_1 has a significantly low value, almost 0 (~10^{-10}–10^{-9}), a function for the variable B with A_2, γ_d, and T as independent variables was derived through multiple regression analysis. The independence of the residuals was recognized to some extent because the Durbin–Watson value was 1.051. The determination coefficient (R^2) for function B was 0.943.

$$B = (-9.89 \times 10^{-4} A_2) + (-1.829 \times 10^{-3} \gamma_d) + (-2.028 \times 10^{-6} T) + 3.35 \times 10^{-4} \tag{11}$$

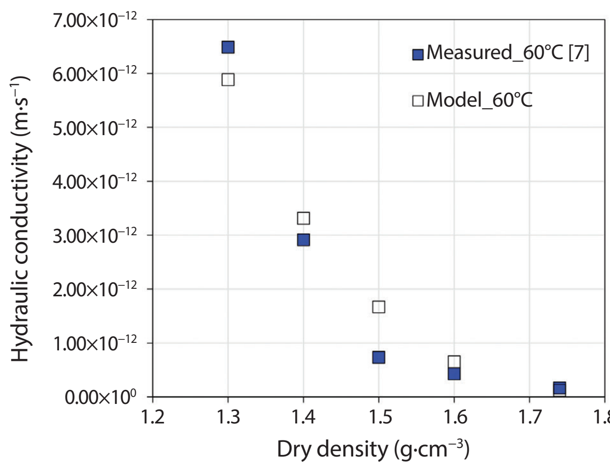
Finally, the prediction model of $K(T)$ is as follows:

$$K(T) = A_1\, exp(A_2 \gamma d) \cdot \frac{(-9.89 \times 10^{-4} A_2) + (-1.829 \times 10^{-3} \gamma_d) + (-2.028 \times 10^{-6} T) + 3.35 \times 10^{-4}}{b_1 exp(-b_2 T)} \tag{12}$$

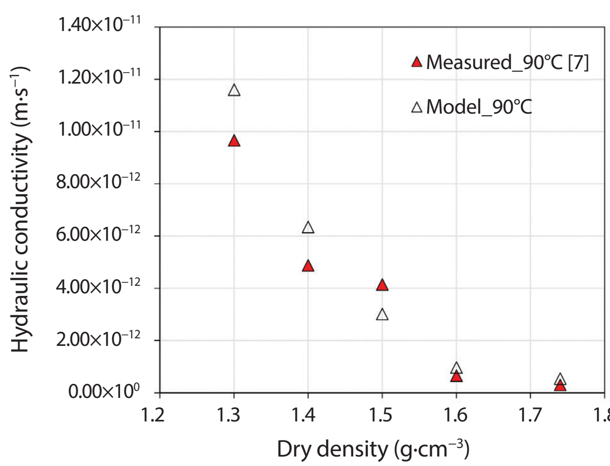
This model exhibited a strong relationship with the



(a) At 30℃



(b) At 60℃



(c) At 90℃

Fig. 3. Comparison of predicted and measured hydraulic conductivities according to temperature and dry density for KJ-II.

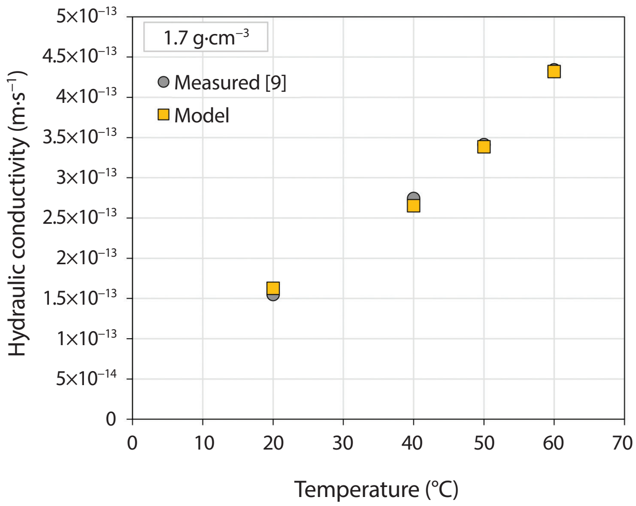


Fig. 4. Comparison of predicted and measured hydraulic conductivities according to temperature for GMZ01 at a dry density of 1.7 g·cm^{-3}.

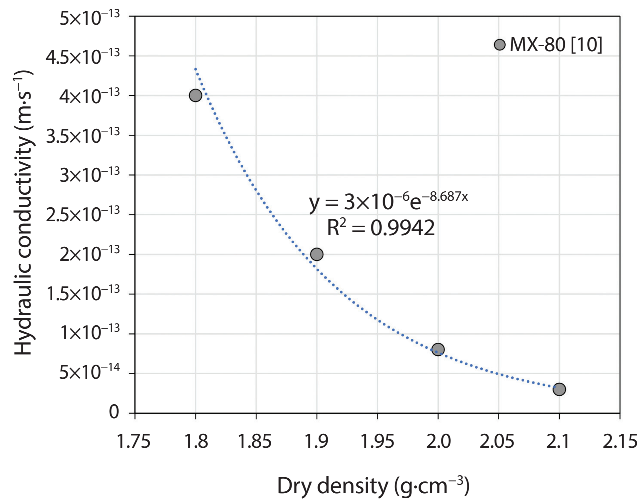


Fig. 5. Hydraulic conductivity with dry density for MX-80.

measured hydraulic conductivities of KJ-II and GMZ01, as shown in Figs. 3 and 4, respectively. Fig. 3 shows that the prediction values for KJ-II based on temperature at a dry density above 1.7 g·cm^{-3} align very well with the measured values, similar to the results for GMZ01 in Fig. 4.

5. Validation of the Prediction Model

A prediction model for hydraulic conductivity was applied to MX-80 and KJ-I to validate the prediction model. The MX-80 and KJ-I data from previous literature were not used to derive the prediction model for the hydraulic conductivity. The relationships between hydraulic conductivity and dry density for MX-80 and KJ-I are shown in Figs. 5 and 6, respectively. For both MX-80 and KJ-I, the predicted hydraulic conductivity exhibited a strong relationship with the measured hydraulic conductivity (Fig. 7). The prediction model for both MX-80 and KJ-I was evaluated using the root mean squared error (RMSE) among the evaluation indices as follows:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{n}} \tag{13}$$

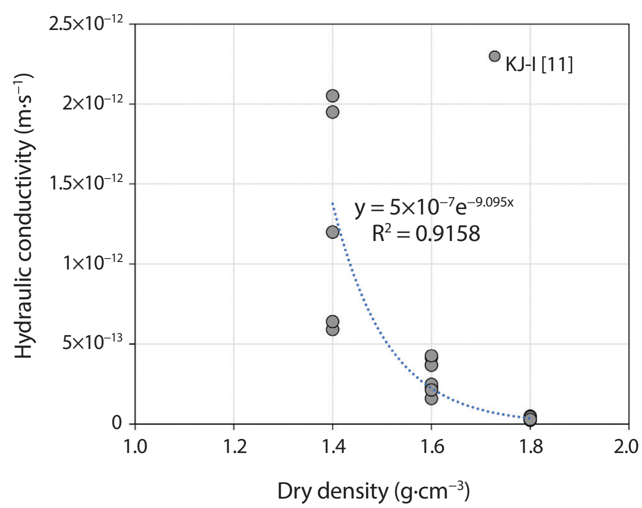
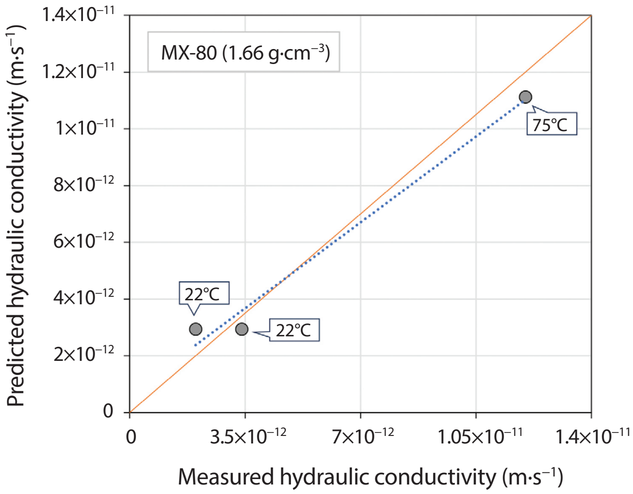
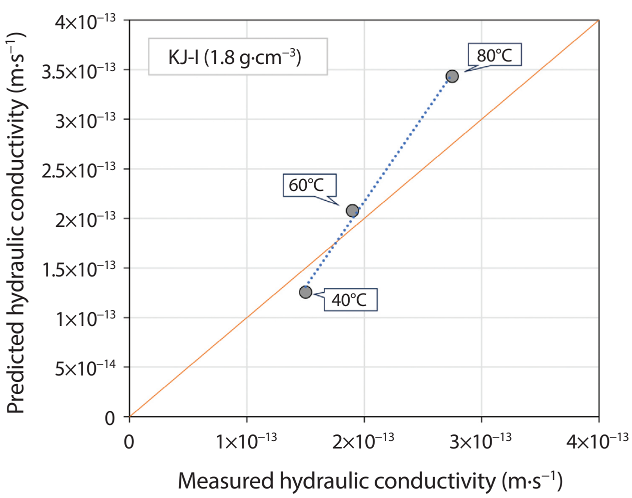


Fig. 6. Hydraulic conductivity with dry density for KJ-I.

where n is the number of measured values, Y is the measured, and $\hat{Y}$ is the predicted values, respectively. The RMSE was significantly small when considering the measured hydraulic conductivity for each dry density, which was 7.9 × 10^{-13} m·s^{-1} and 4.3 × 10^{-14} m·s^{-1} for MX-80 and KJ-I, respectively. In addition, the prediction model newly proposed by this research showed the highest overall accuracy compared with other prediction models [3, 5] for the hydraulic conductivity of compacted bentonite

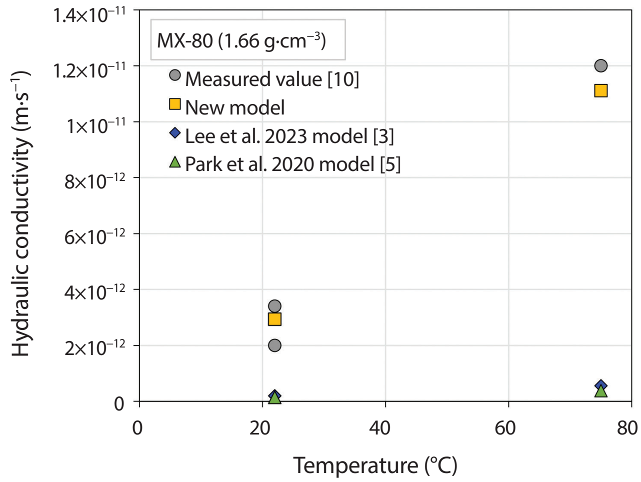


(a) For MX-80

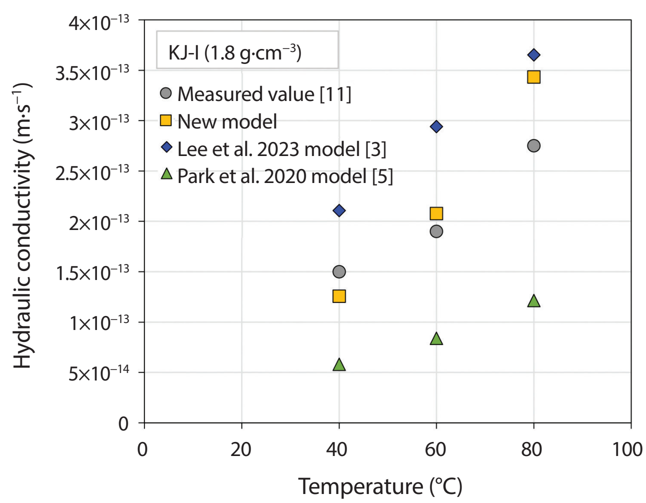


(b) For KJ-I

Fig. 7. Validation of the prediction model by comparison of the predicted hydraulic conductivity to the measured hydraulic conductivity with temperature for MX-80 and KJ-I.



(a) For MX-80 with dry density of 1.66 g·cm^{-3}



(b) For KJ-I with dry density of 1.8 g·cm^{-3}

Fig. 8. Comparison of the prediction model with other prediction models with temperature for MX-80 and KJ-I.

with temperature (Fig. 8). In the case of other models, the difference between the predicted and measured values for MX-80 was larger than that for KJ-I, unlike the discrepancy for the MX-80 and KJ-I samples exhibited by the newly proposed model in this study. The above existing models have a limitation in that they cannot be applied to compacted bentonite of the KJ type. However, it was confirmed that the new model predicted the hydraulic conductivity of compacted bentonite with high accuracy, even though the bentonite types were different.

6. Conclusions

In this study, an integrated prediction model for hydraulic conductivity based on the relationship between hydraulic conductivity and dry density, which can be applied to all types of compacted bentonite, was presented.

1) A new model for predicting the hydraulic conductivity of compacted bentonite with respect to temperature was derived using theoretical and regression analyses.
2) The new model predicts that the hydraulic conductivity of compacted bentonite depends on the temperature when the relationship between dry density and hydraulic conductivity is known.
3) The new model for the hydraulic conductivity of compacted bentonite with temperature predicts the hydraulic conductivity with higher accuracy than existing prediction models.
4) Through the relationship between dry density and hydraulic conductivity, it is possible to predict hydraulic conductivity according to temperature, thereby reducing the time and cost required to measure hydraulic conductivity according to temperature.

Therefore, it is believed that the results of this study will be useful for modeling the hydraulic characteristics according to temperature in an HLW repository, enhancing the predictive capability for a more precise assessment of hydraulic conductivity variations at real disposal sites, irrespective of the bentonite type.

Conflict of Interest

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

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