Closed-Form Multi-Variable Correlation for Maximum Canister Surface Temperature in KBS-3V Repository Using Dimensionless Symbolic Regression

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Keywords : KBS-3V, Thermal dimensioning, Canister spacing, Symbolic regression, Dimensionless analysis

1. Introduction

Thermal performance is one of the dominant design constraints in deep geological repositories for spent nuclear fuel. In the KBS-3V disposal concept, decay heat from the canister induces transient heat conduction in the bentonite buffer and surrounding crystalline rock. The maximum temperature at the canister surface must not exceed the regulatory limit of 100 °C to preserve the long-term thermo-hydro-mechanical stability of the buffer.[1]

Existing design studies evaluate peak temperature primarily through numerical simulations while varying one parameter at a time, such as canister spacing or decay heat.[2] Although these parametric analyses provide valuable insight, they do not yield a closed-form multi-variable correlation directly applicable to engineering sizing problems.

The objective of this study is to derive a compact, closed-form correlation for the maximum canister surface temperature in KBS-3V repositories as a function of key design variables. A dimensionless formulation is adopted, and symbolic regression is employed to identify the optimal functional structure from a comprehensive dataset collected from SKB technical report.

2. Theoretical Background and Dimensionless Formulation

2.1 Governing heat conduction equation and thermal resistance formulation

Under saturated conditions, negligible advective transport, and insignificant radiative heat transfer in accordance with the assumptions adopted in the reference report, heat transfer in the buffer and rock is governed by the transient heat conduction equation in cylindrical coordinate system:

$$\rho c_p \frac{\partial T}{\partial t} = k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] + q'''$$

Assuming temperature-independent thermal properties(ρ, c_p, and k) in accordance with the reference report, the equation is linear in temperature. Consequently, temperature rise is proportional to the decay heat magnitude for identical geometric and boundary conditions.

Furthermore, since the normalized temporal profiles of Q(t) are nearly identical across cases-as can be quantitatively verified from the data-, the buffer region can be treated as quasi-steady at each instant, which justifies the use of the steady-state thermal resistance expression for R_{buffer}.

$$R_{buffer} = \frac{1}{2\pi L_{can} k_{buffer}} \ln\left(\frac{r_b}{r_c}\right)$$

2.2 Definition of dimensionless groups

To generalize the solution and reduce dimensional redundancy, Buckingham π theorem was applied. For the first-order model, the following variables were selected:

- Maximum canister surface temperature rise ΔT_{max} = $T_{max} - T_0$
- Decay heat at disposal per canister Q_{dep}
- Canister spacing along tunnel axis d
- Tunnel spacing s
- Rock thermal conductivity k_{rock}
- Buffer thermal conductivity k_{buffer}
- Canister radius r_c
- Outer radius of the buffer r_b
- Length of the canister L_{can}
- External boundary radius R_{ext}

The dimensionless maximum temperature rise is defined as:

$$\Theta_{max} \equiv \frac{\Delta T_{max}}{\Delta T_{ref}} \equiv \frac{2\pi L_{can} k_{buffer}(T_{max} - T_0)}{Q_{dep} \ln(r_b/r_c)}$$

Additional dimensionless groups are defined as:

$\Pi_d = d/r_b$,
$\Pi_s = s/r_b$,
$\Pi_k = k_{rock}/k_{buffer}$,
$\Pi_L = L_{can}/r_b$,
$\Pi_{ext} = R_{ext}/r_b$,
$\Pi_{geo} = r_c/r_b$,

Thus, the functional relationship becomes:

$$\Theta_{max} = F\left(\frac{k_{rock}}{k_{buffer}}, \frac{R_{ext}}{r_b}, \frac{d}{r_b}, \frac{s}{r_b}, \frac{L_{can}}{r_b}, \frac{r_c}{r_b}\right)$$

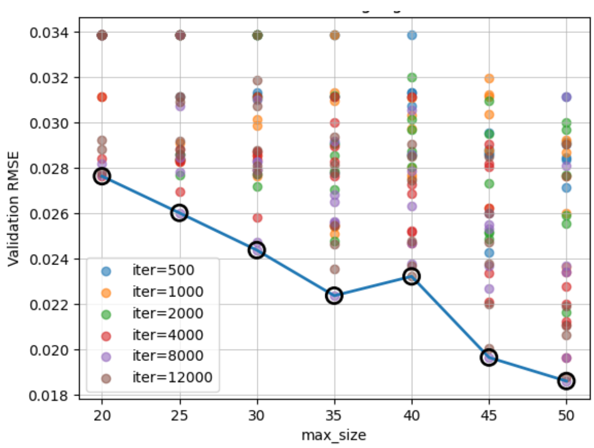
3. Data Collection and Methodology

Thermal analysis data were systematically digitized from publicly available repository design report, SKB TR-03-09. In this report, s, r_b, r_c, L_{can}, and R_{ext} are constants.[3] Thus, only Π_d and Π_k of dimensionless groups are used to express Θ_{max}. Extracted variables include peak temperature T_{max}, decay heat Q_{dep}, spacing d, and thermal conductivities k_{rock} and k_{buffer}. The final dataset consists of 432 data points.

Data were randomly divided into training (70%), validation (15%), and test (15%) sets. Symbolic regression was performed using a genetic programming framework to search over functional forms composed of algebraic operations. Hyperparameter sweeps were conducted for population size(population_size), iteration number(iter), and maximum expression complexity(max_size).

Model performance was evaluated using RMSE and R^2 metrics.

4. Results



[Fig.1] Pareto frontier between max_size and RMSE

[Fig.1] shows the Pareto frontier between model complexity (max_size) and validation RMSE. The frontier represents non-dominated solutions that achieve the best performance for a given level of complexity.

Validation RMSE decreases as model complexity increases. The optimal performance on the Pareto frontier is obtained at (iter, population, max_size, seed) = (8000, 800, 50, 1), achieving:

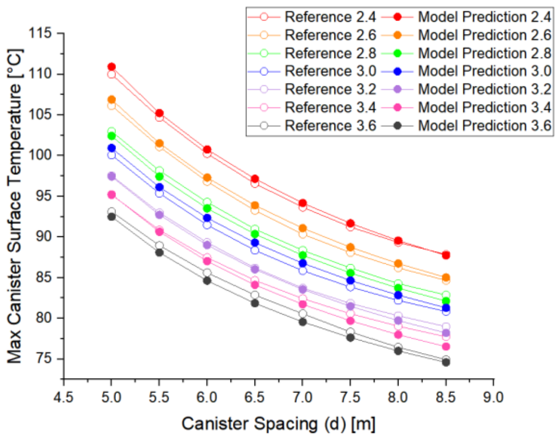
Validation RMSE = 0.0186
Validation R^2 = 0.9957

Accordingly, the optimal correlation equation was derived from this configuration:

$$\Theta_{max} = \Pi_k^{1/4}\left(-1.826 + \frac{0.0007}{2.774 - \Pi_k} + \frac{13.037 - \frac{0.005}{\Pi_k - 2.393} - \frac{0.007}{\Pi_k - 3.106} + \frac{0.005}{(\Pi_k - 3.254)(\Pi_k - 2.587)}}{\Pi_k(\Pi_d - 1.514)}\right) + 3.837$$

$$\left(\Pi_d = \frac{d}{r_b}, \quad \Pi_k = \frac{k_{rock}}{k_{buffer}}\right)$$

The proposed dimensionless correlation exhibits a structured form that captures the combined effects of thermal conductivity contrast and canister spacing on heat transfer behavior. The overall form $\Theta_{max} = \Pi_k^{1/4} F(\Pi_k, \Pi_d) + C$ indicates that the influence of the thermal conductivity ratio Π_k is sublinear, reflecting the multi-layer conduction through the canister–buffer–rock system rather than a single-medium response. The dominant term of the form $1/[\Pi_k(\Pi_d - \Pi_{d,crit})]$ reveals that thermal interaction between adjacent canisters governs the temperature rise, with $\Pi_{d,crit}$ ~1.51 representing an empirical critical spacing near which thermal interference increases rapidly. Additional rational-function terms in Π_k act as nonlinear corrections accounting for multi-scale heat transfer, including the transition from cylindrical conduction near canister to three-dimensional heat spreading in rock. The constant term C ~3.84 corresponds to the asymptotic temperature rise of an isolated canister, representing the baseline self-heating effect in the absence of thermal interaction.



[Fig.2] Comparison between Reference data and Model Prediction

As shown in [Fig.2], the proposed correlation shows excellent agreement with the reference data, accurately reproducing both the overall trend and magnitude of the maximum temperature across all conditions. The temperature variation with canister spacing is well captured, including the nonlinear behavior at small spacing, with only minor deviations observed throughout the range.

5. Conclusions

This study establishes a closed-form design correlation for the dimensionless maximum temperature in the KBS-3V repository concept using symbolic regression. Through systematic hyperparameter exploration, and analysis based on model performance and reproducibility of the data, the optimal model was identified at (8000, 800, 50, 1), providing the best predictive accuracy.

The proposed equation converts numerical thermal analysis results into a directly usable engineering design tool. It reflects nonlinear interactions among key dimensionless parameters without assuming a predefined functional form.

Overall, this work demonstrates that data-driven symbolic regression can yield physically interpretable, high-accuracy, and implementation-ready design equations for deep geological repository thermal assessment.

REFERENCES

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