Efficient design optimization of thermal battery using multi-fidelity surrogate modeling

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Abstract

Thermal battery (TB), a promising energy reserve system, has been widely studied due to its long-term storage capacity. However, due to exceptionally high computing costs of TB simulation models, research on the optimization of TB systems has received limited attention. To address these issues, an efficient TB design optimization methodology is developed to maximize the volumetric energy density of TB while satisfying target performances. In order to accurately and efficiently predict engineering performances of the TB system, a multi-fidelity (MF) surrogate method, which integrates high-fidelity (HF) and low-fidelity (LF) data, is applied. First, the detailed and effective heat transfer models of TB are used as respective sources of HF and LF data for a single working condition. Second, the MF surrogate model is generated for different working conditions utilizing a small number of HF data in the corresponding working condition and pre-obtained LF data from a different working condition. Third, a modified MF dataset selection indicator is proposed to maximize the use of MF surrogate models. The numerical results demonstrate that the proposed approaches greatly enhance the optimization efficiency by up to 60% while sacrificing little accuracy compared to the conventional one.
1. Introduction

Thermal battery (TB) is one of preserve batteries for preventing self-discharge using non-ion-conductive electrolyte (e.g., eutectic salts) in solid phase on shelf [Guidotti 1995; Butler et al. 2004; Guidotti and Masset 2006; Guidotti and Masset 2008]. When electric energy is required, pyrotechnic heat from heat pellets melts ion-conductive liquid electrolyte (EL) and discharge begins (i.e., activation process). Due to these characteristics, a TB system has a very high potential for application to equipment requiring long-term storage capacity, such as military equipment [Butler et al. 2004; Guidotti 2006; Park et al. 2021]. Due to the phase of EL being a discharge trigger, the temperature of EL must be maintained over its melting temperature (e.g., 443°C) despite the endothermic heat generation from chemical reaction and the heat loss to the surroundings [Haimovich et al. 2014; Jeong et al. 2019]. One of straightforward ways to maintain the temperature of EL above its melting temperature is adding or removing heat pellets that supply thermal energy or thermal insulators that minimize heat loss [Jeong et al. 2019]. However, heat pellets or thermal insulators are non-electro-active materials; hence, an excessive thermal design may reduce the electrical density of a battery system; that is, the volumetric energy density of TB system decreases inevitably. In addition, heat pellets that are overdesigned may produce thermal runaway by melting components or deteriorate temperature uniformity [Smith and Wang 2006; Jeong et al. 2019]. Therefore, for more efficient and safer use, the TB system should be designed with its thermal behavior and electric capacity from activation to the end of discharge.

Numerous research have attempted to predict the thermal behavior of TB systems [Schoeffert 2005; Freitas et al. 2008; Roberts et al. 2018; Cho et al. 2020; Luo et al. 2020; Im et al. 2021; Li et al. 2021; Voskuilen et al. 2021; Choi et al. 2022; Ran et al. 2022; Wang et al. 2022]. Research trends on TB systems can be classified into two categories: development of (1) high-fidelity (HF) and (2) low-fidelity (LF) models. In general, HF models are developed to more accurately predict the engineering performances of TB systems. As a result, the HF model naturally requires high computational cost. Specifically, a multi-physics model was proposed to account for thermal and electrochemical performances [Voskuilen et al. 2021]. Moreover, a three-dimensional (3-D) TB
simulation model was presented as opposed to a two-dimensional (2-D) model [Ran et al. 2022]. This 3-D simulation model has the advantage over 2-D simulation models in that it can calculate and achieve heat flow on the battery surface [Ran et al. 2022]. The LF model, on the other hand, aimed to reduce the computational cost of the HF model while slightly compromising its accuracy. Several thermal models have been developed by either considering only the activation time [Kang et al. 2016] or the working time after activation [Haimovich et al. 2009; Haimovich et al. 2014]. Recently, an effective TB model, which uses effective properties and heat sources, with high-power and large-capacity was proposed to reduce the computation time [Jeong et al. 2019]. When compared to the detailed TB model, the effective TB model achieved a temperature difference of less than 10°C while reducing simulation time to only 6% of the detailed TB model, resulting in an efficient LF simulation model [Jeong et al. 2019].

However, optimization of the TB system has received very little attention [Park et al. 2021]. This is mainly because there exist still limitations in performing the optimization process by selecting one of the currently developed thermal models based on their accuracy and efficiency. Due to the heavy computation required for a single analysis, it is hardly possible to perform optimization using the HF model. Even if optimization is performed, the computation time becomes impracticable again if TB models that account for more complex phenomena are developed. In contrast, the LF model enhances computational efficiency significantly when compared to the HF model, but its accuracy is rather low, making it difficult to use the LF model directly in the optimization process. Another issue is that TB systems used in military applications must be tailored to each mission’s requirements. In the worst-case scenario, optimization is prohibited since independent TB optimization results are required for multiple working conditions, not just one working condition. Therefore, a newly integrated optimization framework is required to efficiently optimize TB systems that are applicable in various situations.

To overcome these obstacles, it is vital to focus on research that improves computational efficiency by employing auxiliary information or prior knowledge. Multi-fidelity (MF) surrogate modeling is one of the representative methods using auxiliary information [Kennedy and O’Hagan 2000; Forrester et al. 2007; Shi et al. 2020; Guo et al. 2021; Zhang et al. 2021; Kaps et al. 2022; Lee et al. 2022]. The MF surrogate model, as opposed
to a single-fidelity (SF) surrogate model which uses only one fidelity data, integrates multiple fidelity data. HF data are typically more accurate but more time-consuming than LF data. The MF surrogate model is efficiently generated using a small amount of HF data and a large amount of LF data. Because the MF surrogate model integrates both types of data, it has the advantage of complementing the strengths and shortcomings of each type of fidelity data. In addition, the concept of transfer learning is well-known in the field of machine learning as an example of a way to exploit prior knowledge [Chakraborty 2021; Jung et al. 2022; Shin et al. 2023]. This method increases the efficiency of model generation by utilizing pre-trained prediction models in related domains when there are insufficient data in the area of interest.

In this paper, an efficient design optimization framework for a TB system under multiple working conditions is proposed. The main objective of the proposed method is to construct MF surrogate models using inexpensive or previously-obtained data as auxiliary information to reduce the computational cost. In addition, MF modeling is performed across various working conditions by using the concept of transfer learning. Next, optimization is performed based on these MF surrogate models to maximize the volumetric energy density of TB while meeting the target performance constraints. To maximize the effectiveness of the MF surrogate model, a strategy for effectively integrating HF and LF data is proposed here. We conclude by discussing the physical meaning of the optimization results and drawing insights from them.

The following is a summary of the key contributions of this work:

- A framework for efficient optimization of a TB system is developed using the MF surrogate method.
- Under a single working condition, MF surrogate models are generated by integrating HF and LF data from detailed and effective TB models, respectively.
- MF surrogate modeling, which is relatively more accurate than the conventional method without additional cost, is proposed even if a sufficient amount of HF data cannot be obtained under multiple working conditions by setting previously-obtained data under different working conditions as LF data.
- A modified indicator for the selection of MF datasets is proposed to choose the LF output type that maximizes the performances of MF surrogate models from among various LF output types.
The remainder of the paper is organized as follows. Section 2 reviews conventional TB simulation models and MF surrogate method. Section 3 explains the proposed TB optimization framework. Section 4 demonstrates the superiority of the proposed method through numerical results and discusses physical meanings of optimal solutions. Finally, Section 5 summarizes the conclusion and future work.

2. Fundamentals of the proposed study

This section briefly provides fundamentals of the proposed study. Section 2.1 introduces the basic information of the TB system, which includes detailed and effective TB simulation models. Section 2.2 explains the concept of the MF surrogate modeling with a simple illustrative example.

2.1 Brief description of thermal model of a TB system

A TB system can generally be divided into three regions [i.e., upper & lower stacks and electro-active cells (EC)] enclosed by insulators $\alpha$, $\beta$, and $\gamma$ for thermal insulation, as shown in Figure 1(a) [Jeong et al. 2019; Cho et al. 2020; Im et al. 2021; Park et al. 2021]. Each region is composed of stacked elements: those are heat pellets $A_U$ & $A_L$ and insulators $B_U$ & $B_L$ in upper and lower stacks and heat pellet $A_C$, cathode, anode, EL and current collector in EC. Here, subscripts U, L, and C indicates the upper, lower, and center, respectively. There exist several forms of heat generation processes in the TB system. During activation process (i.e., melting of EL), pyrotechnic heat from heat pellets (exothermic) and latent heat from EL (endothermic) are involved. After activation process, Joule heating from cathode (exothermic) and chemical reaction heat from cathode and anode (endothermic) are countered. As done in Ref. [Jeong et al. 2019], Joule heating is applied only to the cathode, while chemical reaction heat is applied to both the cathode and anode. In addition, three working conditions of TB system are listed in Table 1, and Cases 1, 2, and 3 in Table 1 are the same as Cases 1, 3, and 3-1 in Ref. [Jeong et al. 2019], respectively. For convenience, elements working as heat source or heat sink (i.e., EC and heat pellets $A_U$ & $A_L$) are grouped as heat source elements. The detailed model of 54-stacked TB contains all the elements as well as heat sources in EC
separately. For transient thermal simulation, free convective \( (h = 10 \text{ W/m·K}) \) and radiative \( (\varepsilon = 0.11) \) heat losses are considered with ambient or initial temperature of 26.85°C (300 K) [Jeong et al. 2019]. More details (e.g., properties, dimensions, and compositions) of all elements and heat sources are provided in the previous work [Jeong et al. 2019].

<table>
<thead>
<tr>
<th>Table 1 Working conditions of the TB system</th>
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<tr>
<td>Case 1</td>
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<tr>
<td>( i_A ) (A/cm(^2))^*</td>
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<tr>
<td>( \partial U_o / \partial T ) (V/K)^*</td>
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</table>

* \( i_A \) represents current density and \( \partial U_o / \partial T \) denotes the change of open-circuit cell potential with respect to temperature, respectively [Jeong et al. 2019].

The effective TB model has been built by homogenizing properties and heat sources of EC, as shown in Figure 1(b) [Jeong et al. 2019]. Thermal conductivity, specific heat, and density are homogenized considering the anisotropic thermal resistance, mass, and volume, respectively. On the other hand, effective heat sources are obtained by volume average of the contribution of each element to heat sources. According to the activation time from the detailed TB model, effective heat sources before (pyrotechnic heat and latent heat) and after activation (Joule heating and chemical reaction heat) are applied to homogenized EC (HEC) [Jeong et al. 2019]. Initial and boundary conditions are identical to those of the detailed TB model.

The transient thermal behavior of TB is simulated using ANSYS® Fluent through text user interface with respect to design variables in MATLAB environment. In addition, Table 2 lists the computational costs of the detailed and effective TB models of the 54-stacked TB [Jeong et al. 2019]. In this study, the simulation cost of the detailed TB model is 8 times higher than that of the effective TB model.

<table>
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<th>Table 2 Information on two TB simulation models</th>
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<tr>
<td>Detailed TB model</td>
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<tr>
<td>Number of elements</td>
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<td>Simulation cost (min)</td>
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2.2 Review of MF surrogate modeling

Surrogate models such as response surface, Kriging, and neural network models are used to approximate performances of a real-world engineering system (e.g., thermal model of a TB system) [Kang et al. 2021; Kim et al. 2022; Yang et al. 2023]. If calculation time required to collect a sufficient amount of data for the corresponding system is burdensome, MF surrogate modeling can be a potential solution. The MF surrogate approach is to merge a small amount of accurate HF data with a relatively large amount of less accurate LF data [Kennedy and O'Hagan 2000; Forrester et al. 2007]. Therefore, the total computational cost for obtaining the output data is reduced while maintaining the accuracy of the surrogate model [Kennedy and O'Hagan 2000; Forrester et al. 2007].

Suppose that inputs of HF and LF samples are $S_{HF}$ and $S_{LF}$, respectively, and corresponding outputs are $Y_{S, HF}$ and $Y_{S, LF}$, respectively. Then, the LF surrogate model $\hat{y}_{LF}(x)$ or HF surrogate model $\hat{y}_{HF}(x)$ can be built using only LF data (i.e., $S_{LF}$ and $Y_{S,LF}$) or HF data (i.e., $S_{HF}$ and $Y_{S,HF}$), respectively. When both LF and HF data
are available, an MF surrogate modeling strategy has the potential to significantly improve overall process efficiency. In general, the MF surrogate model $\hat{y}_{MF}(\mathbf{x})$ can be expressed as

$$\hat{y}_{MF}(\mathbf{x}) = \rho \hat{y}_{LF}(\mathbf{x}) + \hat{\delta}(\mathbf{x})$$

(1)

where $\rho$ and $\hat{\delta}(\mathbf{x})$ are a constant scaling factor and discrepancy function between LF and HF models, respectively [Giselle et al. 2019]. In Eq. (1), $\hat{y}_{LF}(\mathbf{x})$ is the global trend part captured by LF data, and $\rho$ and $\hat{\delta}(\mathbf{x})$ serve to correct $\hat{y}_{LF}(\mathbf{x})$ by HF data.

To intuitively demonstrate that the MF surrogate model can be superior to the HF surrogate model, a well-known 1-D illustrative example is utilized [Han and Görtz 2012]. Related HF analytical function and sampling location are $f_{HF}(x) = (6x - 2)^2 \sin(12x - 4)$ and $[0, 0.4, 0.6, 1.0]^T$, respectively; LF analytical function and sampling location are $f_{LF}(x) = 0.5f_{HF}(x) + 10(x - 0.5) - 5$ and $[0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0]^T$, respectively. As depicted in Figure 2, the MF surrogate model is more accurate than the HF surrogate model because the cheap LF data well catch up with the global trend of the HF system. In this study, the Kriging and hierarchical Kriging models are used as SF and MF surrogate models, respectively, and detailed descriptions can be founded in Ref. [Han and Görtz 2012].

![Figure 2](https://ssrn.com/abstract=4392562)

**Figure 2** Concept illustration of MF surrogate model using 1-D analytical function

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The nearest neighbor sampling (NNS), which ensures that HF sample set is a subset of the LF sample set, is widely used to build the MF surrogate model [Park et al. 2017]. The NNS generates the common samples between the HF and LF sample sets, and this characteristic has the advantage of allowing for the evaluation of the correlation between the LF and HF sample outputs. The NNS is divided into two steps: (1) HF and LF samples are independently generated by Latin hypercube sampling (LHS), and (2) the LF samples nearest to the HF samples are shifted to the HF samples to satisfy $S_{HF} \subset S_{LF}$. Figure 3 illustrates the design of experiment (DoE) process for a two-dimensional example with 10 HF and 40 LF samples to help understanding the NNS. As shown in Figure 3(a), 40 LF samples (both blue and green crosses) and 10 HF samples (red circles) are independently generated by LHS. Then, 10 LF samples (green crosses) closest to the HF samples are relocated to the matching HF samples. Finally, DoE is updated, as displayed in Figure 3(b).

![Figure 3](https://ssrn.com/abstract=4392562)

**Figure 3** Explanation of the NNS using 2-D illustrative example: (a) initial DoE and (b) updated DoE results

### 3. Efficient TB optimization framework using MF surrogate modeling

This section proposes an efficient TB optimization framework based on the MF surrogate method. Section 3.1 introduces the problem definition for TB system, which includes design variables, an objective function, and constraint functions, etc. Section 3.2 explains the concept of the proposed method. Section 3.3 presents how to select MF data for TB system to maximize the performances of the MF surrogate models. The performance
criterion used to evaluate surrogate models is explained in Section 3.4. Finally, the proposed overall optimization algorithm is illustrated in Section 3.5.

3.1 Problem definition for a TB system

Increasing the radius of EC is a simple way to increase the electrical capacity of a TB system because electrical energy is stored in EC. To increase the radius of EC while maintaining the radius of the enclosure, the width of the thermal insulator \(d_1\), the width of insulator \(\gamma\) in Figure 1(a) should be reduced. In this case, the thinner insulator may cause higher heat loss from EC to ambient and re-solidification of EL (i.e., end of discharge) before the desired working time (e.g., 600 s) [Jeong et al. 2019]. Therefore, \(d_1\), the volume of EC, and the working time (i.e., the moment when the re-solidification occurs) are adopted as a design variable, objective function, and constraint function, respectively. Furthermore, it is an important condition that the working time increases as the electrical capacity increases, and this is also included in the constraint function set. On the other hand, heat pellets and thermal insulators in upper and lower stacks also help increase the working time or retard re-solidification of EL. Especially, thicker heat pellets supply more thermal energy to the nearest EL that is vulnerable to re-solidification and, allowing for a longer working time with thicker heat pellets in the upper and lower stacks. However, it should be noted that excessive heat pellets in the upper and lower stack may cause overheating of EC near the upper and lower stacks or the non-uniform temperature distribution within EC or non-uniform electrical discharge. Thus, thicknesses of heat pellets and thermal insulators (i.e., \(d_2\) to \(d_5\) in Figure 1) are chosen as design variables. Overheating and temperature uniformity engineering performances are related constraints [Smith and Wang 2006; Jeong et al. 2019]. The thicknesses of insulators \(\alpha\) & \(\beta\) (i.e., \(L-2d_2-2d_3, L-2d_4-2d_5\)) are thus automatically modified to maintain the thickness of the upper and lower sides of EC.

Based on this information, the volume, which corresponds to electrical capacity, is maximized while satisfying the critical performance conditions. Hence, shape optimization for the TB system can be formulated as
find \( \mathbf{d} = [d_1, d_2, d_3, d_4, d_5]^T \)

minimize \( -V_{EC}(\mathbf{d}) \) mm³

subject to
- \( t_{\text{work}}(\mathbf{d}) \geq 600 \) s
- \( T_{\text{EL}}^{\text{overheating}}(\mathbf{d}) \leq 670^{\circ} \text{C} \)
- \( \Delta T_{\text{EL}}(\mathbf{d}) \leq 60^{\circ} \text{C} \)
- \( 0.90 \leq \eta(\mathbf{d}) \leq 1.10 \)
- \( d_i^{lb} \) mm \( \leq d_i \leq d_i^{ub} \) mm, \( i = 1 \sim 5 \)

\[ \Delta T_{\text{EL}}(\mathbf{d}) = T_{\text{EL}}^{\text{max}}(\mathbf{d}) - T_{\text{EL}}^{\text{min}}(\mathbf{d}) \]

\[ \eta(\mathbf{d}) = \frac{(V_{EC}(\mathbf{d}) - V_{EC}(\mathbf{d}^{\text{initial}}))/V_{EC}(\mathbf{d}^{\text{initial}})}{(t_{\text{work}}(\mathbf{d}) - 600)/600} \]

\[ \mathbf{d}^{\text{initial}} = [8.5, 1.8, 1.8, 1.8, 1.8]^T \]

\[ \mathbf{d}^{lb} = [1.0, 0.8, 0.8, 0.8, 0.8]^T \]

\[ \mathbf{d}^{ub} = [8.5, 2.8, 2.8, 2.8, 2.8]^T \]

where \( d_i \) is the \( i \)th shape design variable; \( V_{EC} \) is the volume of EC; \( t_{\text{work}} \) is the working time of a TB before re-solidification occurs; \( T_{\text{EL}}^{\text{overheating}} \) is the overheating temperature of EL; \( T_{\text{EL}}^{\text{max}} \) and \( T_{\text{EL}}^{\text{min}} \) are the maximum and minimum temperature of EL part at 600 s, respectively; \( \Delta T_{\text{EL}} \) is the difference between \( T_{\text{EL}}^{\text{max}} \) and \( T_{\text{EL}}^{\text{min}} \); \( \eta(\mathbf{d}) \) is the ratio of the increased volume of EC to working time which indicate whether \( t_{\text{work}} \) increases as the electrical capacity increases; \( \mathbf{d}^{\text{initial}} \) is the initial design vector; and \( \mathbf{d}^{lb} \) and \( \mathbf{d}^{ub} \) are the lower and upper bound vectors of \( \mathbf{d} \), respectively. The target values in Eq. (2) are conservatively set based on Ref. [Jeong et al. 2019], and the corresponding values can be changed as needed. In this work, surrogate-based optimization utilizing the infill-sampling method is applied to find the optimal solution of Eq. (2) [Forrester and Keane 2009; Han 2016].

To intuitively understand Eq. (2), Figure 4 visualizes the key physical quantities of the TB system written in Eq. (2). Maximum, minimum temperatures and minimum liquid phase fraction are plotted when \( \mathbf{d} = [8.5, 1.8, 1.8, 1.8, 1.8]^T \) under Case 1 working condition. As shown in Figure 4, because the value of \( t_{\text{work}} \) (i.e., 616 s) exceeds 600 s, the corresponding constraint is satisfied, whereas the values of \( T_{\text{EL}}^{\text{overheating}} \) (i.e., 674°C), \( \Delta T_{\text{EL}/\text{work}} \) (i.e., 65°C), and \( \eta(\mathbf{d}) \) (i.e., 0) do not meet the desired requirements in Eq. (2). After applying the proposed
framework, all engineering performance conditions will be satisfied and the related quantitative results will be presented in Section 4.3.

Figure 4 Illustration of physical quantities of EL until $t = 1,000$ s in a logarithmic scale

3.2 Concept of the proposed optimization framework for a TB system

The main concept of the proposed optimization framework for the TB system is introduced in this section. The proposed method is developed based on the MF surrogate strategy. As shown in Figure 5, the proposed framework consists of two major stages: (1) MF surrogate modeling to replace the engineering performances of the TB system model under a single working condition and (2) extension of MF surrogate method to different working conditions.

The first stage is to build an MF surrogate model for Case 1 working condition. In this stage, HF and LF data are obtained from simulation results of detailed and effective TB models, respectively. Then, the optimal design point for Case 1 is efficiently obtained using MF-based optimization. In the second stage, the MF surrogate strategy is also used to find optimal design points for Cases 2 and 3 working conditions. In this process, the data generated from Case 1 working condition is treated as LF data meaning that the information gathered in Case 1
serves as prior knowledge. In Case 2, the MF surrogate model is constructed using a small number of HF data with the aid of these given data (i.e., LF data). In this way, the data from Case 1 can be fully utilized when building surrogate models for different working conditions. Similarly, in Case 3, MF models can be created by integrating the data from Cases 3 and 1. In other words, when creating a surrogate model for multiple working conditions, data from one case is utilized as pre-given LF data to maximize the efficiency of the entire surrogate modeling procedure.

![Figure 5 The proposed efficient TB system design framework](image_url)

### 3.3 The MF dataset utilization process for TB system

In general, the data mentioned in Section 3.2 cannot be used as LF data without any verification. For example, there may be various kinds of LF models, and the performance of the MF model may differ depending on which output is used in the selected LF model [Guo et al. 2018]. In addition, data collected under one working condition may not be related to data collected under different working conditions. In the worst-case scenario, the performance of the MF surrogate model may be rather poorer than that of the SF surrogate model using HF data only. Referring to reports of many previous studies, tendency such as high correlation between original HF and LF data should be good [Toal 2015; Giselle et al. 2019; Yong et al. 2019; Guo et al. 2021]. However, this method
still has drawbacks when the number of samples is small. Therefore, an indicator is required to determine whether or not to use MF data.

### 3.3.1 Difficulties of selecting MF datasets for TB systems

Several assumptions or techniques are generally incorporated into an HF system model in order to produce an LF system model. For instance, LF system models are generated by simplifying complex geometries of HF system models [Mundo et al. 2009; Yong et al. 2019; Ran et al. 2022], employing effective properties instead of original ones [Jeong et al. 2019; Liu et al. 2020], or reducing mesh size [Guo et al. 2021; Lee et al. 2022], etc. Due to these approaches, it is sometimes difficult to select an output response of the LF system model that corresponds to the HF system model. In this situation, there may be multiple candidate LF output responses corresponding to the HF output response. In particular, the performances of the MF surrogate models vary depending on which output responses are selected from the LF system model. Furthermore, if the LF data quality is poor, the performances of MF surrogate model may perform worse than those of the SF surrogate model, so it is not recommended to use the MF surrogate model in this case. Therefore, MF dataset selection is very important.

The physical quantities defined in the HF model may be impossible to define in the LF model. In the detailed TB model, the working time of a TB is defined when re-solidification occurs; that is when the minimum liquid fraction of EL becomes less than 1 after activation, as shown in Figure 6(a) [Jeong et al. 2019]. On the other hand, in the effective TB model, EC is homogenized and the phase change of EL is treated as heat sink [Jeong et al. 2019], and thus, the liquid fraction cannot be monitored. To obtain the working time from the same input design domain of detailed and effective TB models, we used the temperature as a parameter. Here, the melting temperature of EL (443°C) is adopted as a candidate criterion to decide the re-solidification and the end of discharge. In particular, since the EL disappears in the effective TB model, the melting temperature of the HEC (443°C) is used as shown in Figure 6(b). However, this is an uncertain information, and other temperatures, such as 470°C, may be more suitable. Therefore, when selecting the LF output responses in this study, it is necessary to determine from
a data point of view which type produces the MF surrogate model with better performances between physically inferred 443°C and randomly chosen 470°C. Furthermore, once either type of data is chosen, it is essential to assess whether the corresponding LF data is useful in creating the MF surrogate model.

**Figure 6** Process description of extracting $t_{\text{work}}$ from the (a) HF and (b) LF TB systems

### 3.3.2 Modified indicator for MF dataset selection

There were two representative temporary guidelines for MF dataset selection [Toal 2015; Guo et al. 2018; Giselle et al. 2019]. The first method (Method 1) is to use the normalized cross-validation error (NCVE) as the indicator [Guo et al. 2018], whereas the second method (Method 2) exploits the conventional Pearson correlation coefficient $r_c^2$ as the main measure [Toal 2015; Giselle et al. 2019] and their algorithms are as follows:

**Method 1:**

1. Create an SF surrogate model using HF data only and multiple MF surrogate models combining HF and LF data.
2. Calculate the NCVE values for each surrogate model and select the surrogate model with the lowest value as the best model.

**Method 2:**

1. Choose the LF type with the largest $|r_c^2|$ among various LF response types.
(2) If $|r_c^2|$ is greater than the predefined minimum threshold $r_{\text{min}}^2$, then select the corresponding MF surrogate model as the best model. Otherwise, choose the SF surrogate model as the best model.

Referring to literature survey, the proposed method is developed based on Methods 1 and 2. This approach computes $r_c^2$ by taking into account the correlation between original HF and LF data [Toal 2015; Giselle et al. 2019; Song et al. 2019]. However, if the number of HF samples is small, the accuracy of the correlation decreases. In other words, even though it is better to construct an MF surrogate model rather than an SF surrogate model with the current MF dataset, inaccurately estimated $r_c^2$ due to the lack of HF data may lead to a conclusion that it is not good to utilize the MF surrogate model. Furthermore, previous studies have reported that the performances of MF surrogate models are highly influenced by DoE results [Guo et al. 2018; Giselle et al. 2019]. To mitigate this issue, a modified indicator is proposed in this study for MF dataset selection. The proposed Pearson correlation coefficient $r_p^2$ is calculated considering correlation between original LF and predicted HF data from an MF surrogate model. Therefore, the proposed method can cope with the influence of the current DoE (e.g., the number and location of samples) and the failure of surrogate modeling (e.g., hyper-parameter optimization). Reflecting this idea, the proposed algorithm is as follows:

Proposed method:

(1) Select the LF type with the largest $|r_p^2|$ among several LF response types.

(2) If $|r_p^2|$ is greater than $r_{\text{min}}^2$, then select the corresponding MF surrogate model as the best model. Otherwise, select the surrogate model with the lowest NCVE value between the SF model and the selected MF model as the best model.

3.3.3 Illustrative example

In this section, the proposed method is explained using a one-dimensional illustrative example. Figure 7 well represents the necessity of the proposed measure, and corresponding numerical results are listed in Table 3.
The HF and LF functions used are the same as those presented in Section 2.2, and four cases are investigated. In all cases, the number and location of LF data are the same, but the number and location of HF data are all different, as shown in Figure 7. In particular, note that the number of HF samples used in Figures 7 (a), (b), (c), and (d) increases from 3 (Case A), 4 (Case B), and 5 (Case C) to 6 (Case D), respectively. As shown in Figure 7, in all cases, the MF surrogate model is almost identical with the true function whose correlation value $r_{\text{true}}^2$ is 0.74 as listed in Table 3. However, $r_c^2$ has a different value for each case. This is because $r_c^2$ is highly dependent on HF data. In Case A, even though the MF model was well built, $r_c^2$ is completely incorrectly predicted as $-0.06$. In addition, even Case D, which uses relatively large amounts of HF data, shows discrepancy in predicting the correlation. However, because it treats data predicted by the MF surrogate model as HF data, the proposed method accurately and robustly predicts the correlation $r_p^2$ for all cases if the MF surrogate model is well constructed. In conclusion, $r_p^2$ is independent not only of the number of HF data but also of DoE results, and this is why $r_p^2$ is utilized in this study instead of $r_c^2$. 
3.4 Performance criterion for surrogate model

The coefficient of determination $R^2$ (i.e., $R$-square) is adopted as the validation metric of the surrogate models. This criterion assesses the global accuracy of the surrogate models and it can be written as

$$R^2 = 1 - \frac{\sum_{j=1}^{N_{\text{test}}} (y_j - \hat{y}_j(x_j))^2}{\sum_{j=1}^{N_{\text{test}}} (y_j - \bar{y})^2}$$

(3)
where $N_{test}$ is the number of test samples; $y_j$ and $\hat{y}(x_j)$ represent the true and predicted output values of the $j^{th}$ test sample $x_j$, respectively; and $\bar{y}$ is the mean value of the true response values. The closer the value of $R^2$ is to 1, the more accurate the surrogate model of the corresponding output is, or vice versa [Song et al. 2019].

### 3.5 Overall optimization procedure

The overall algorithm of the proposed method is demonstrated in this section. The whole optimization procedure is illustrated in Figure 8 and it can be summarized as follows:

Step 1: Check if LF data is pre-given. If LF data is given, generate only HF samples using the LHS method, then obtain the output responses of corresponding samples through CFD simulations. Otherwise, perform the NNS method explained in Section 2.2, and then CFD simulations are conducted to obtain output responses of HF and LF samples.

Step 2: Construct multiple candidate MF surrogate models utilizing all HF and LF data as explained in Section 2.2 (e.g., Figure 2).

Step 3: Decide the best MF surrogate model among the candidate MF surrogate models created in Step 2 using the indicator proposed in Section 3.3.2.

Step 4: Find a predicted optimal HF design point using infill-sampling methods.

Step 5: Obtain the output responses at the HF sample point found in Step 4 through a real CFD simulation.

Step 6: Check all the constraints of a TB system given in Section 3.1. If the predicted optimal HF design point is satisfactory, then stop the overall procedure. Otherwise, update the DoE result and then repeat Steps 4 to 5 until the optimization results are satisfactory.
4. Results and discussion

Numerical results for evaluating the performances of the proposed algorithm and optimization are presented in this section. Sections 4.1 and 4.2 show the effect of the proposed MF dataset selection indicator and the performances of each surrogate model in terms of accuracy and efficiency, respectively. Optimization solutions and their physical meanings are presented in Section 4.3.

For fair comparison of the efficiency between surrogate models, the equivalent number of HF samples $N_{HFEqv}$ is used which is obtained as

\[ N_{HFEqv} \]
\[ N_{HF}^{equiv} = N_{HF} + \frac{N_{LF}}{\alpha} = N_{HF} + \frac{N_{LF}}{t_{HF}/t_{LF}} \]  

(4)

where \( N_{HF} \) and \( N_{LF} \) are the number of HF and LF samples, respectively; \( \alpha \) is a simulation cost ratio; \( t_{HF} \) and \( t_{LF} \) are the mean values of simulation time for HF and LF samples, respectively. In this study, \( t_{HF} \) and \( t_{LF} \) are 56 minutes and 7 minutes, respectively, as shown in Table 2, meaning that \( \alpha \) is 8. All surrogate models are built by modifying DACE Kriging MATLAB toolbox [Lophaven et al. 2002]. The CFD simulations of detailed and effective TB systems are conducted via ANSYS® Fluent. All tasks are implemented on a computer with an Intel® Core(TM) i9-10980XE CPU @ 3.00GHz with 128GB RAM. In this work, the value of the threshold parameter \( r_{min}^2 \) is set to 0.85 according to the previous studies [Toal 2015; Giselle et al. 2019; Yong et al. 2019; Guo et al. 2021].

4.1 Effect of the proposed indicator for MF dataset selection

This section verifies the effectiveness of the proposed indicator for MF dataset selection. The goal of this numerical test is to show that the performances of MF surrogate models vary depending on the type of LF data used. The comparison results are listed in Tables 4, 5, and 6. MF15 (443°C) and MF15 (470°C) mean that HEC temperature is set to 443°C and 470°C, respectively, when obtaining the working time \( t_{work} \) of the LF model as mentioned earlier in Section 3.3.1. Therefore, one of the best surrogate models among HF15, MF15 (443°C), and MF15 (470°C) should be chosen for the performance related to the working time. For other performances (i.e., \( T_{overheating}^{el} \), \( T_{min}^{el} \), and \( T_{max}^{el} \)), the best surrogate model should be chosen between HF15 and MF15. Methods 1 and 2 in Section 3.3.2 are adopted for comparison.

In the case of \( t_{work} \), it can be seen from Table 4 that Method 1 selects HF15 with the lowest NCVE as the best model. Furthermore, Method 2 chooses HF15 with the lowest NCVE as the best model because \( r_c^2 \) values of both MF15 (443°C) and MF15 (470°C) are less than 0.85. However, the proposed method selects MF15 (443°C) as the best model because \( r_p^2 \) is greater than 0.85. As a result, in the case of \( t_{work} \), Method 1, Method 2, and the
proposed method choose HF15, HF15, and MF15 (443°C) as the best surrogate models, respectively. Table 5 summarizes the results of other performances.

Table 4 Comparison results of each surrogate model in Case 1

<table>
<thead>
<tr>
<th>Performance type</th>
<th>Model type</th>
<th>$N_{LF}$</th>
<th>$N_{HF}$</th>
<th>NCVE</th>
<th>$r_c^2$</th>
<th>$r_p^2$</th>
<th>$r_{true}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{work}$</td>
<td>HF15</td>
<td>-</td>
<td>15</td>
<td>0.089</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MF15</td>
<td>40</td>
<td>15</td>
<td>0.13</td>
<td>0.79  &lt;0.85</td>
<td>0.87  ≥0.85</td>
<td>0.91</td>
</tr>
<tr>
<td></td>
<td>MF15 (443°C)</td>
<td>40</td>
<td>15</td>
<td>0.19</td>
<td>0.57  &lt;0.85</td>
<td>0.75  &lt;0.85</td>
<td>0.88</td>
</tr>
<tr>
<td>$T_{overheating}^c$</td>
<td>HF15</td>
<td>-</td>
<td>15</td>
<td>0.12</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MF15</td>
<td>40</td>
<td>15</td>
<td>0.10</td>
<td>0.28  &lt;0.85</td>
<td>0.34  &lt;0.85</td>
<td>0.46</td>
</tr>
<tr>
<td>$T_{min}^c$</td>
<td>HF15</td>
<td>-</td>
<td>15</td>
<td>0.072</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MF15</td>
<td>40</td>
<td>15</td>
<td>0.079</td>
<td>0.85  ≥0.85</td>
<td>0.92  ≥0.85</td>
<td>0.93</td>
</tr>
<tr>
<td>$T_{max}^c$</td>
<td>HF15</td>
<td>-</td>
<td>15</td>
<td>0.27</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>MF15</td>
<td>40</td>
<td>15</td>
<td>0.18</td>
<td>0.94  ≥0.85</td>
<td>0.91  ≥0.85</td>
<td>0.97</td>
</tr>
</tbody>
</table>

* $r_c^2$ is calculated using 15 HF and 15 LF samples.
** $r_p^2$ is obtained from 40 virtual HF samples from MF surrogate model and 40 LF samples.
*** The correlation computed by 100 HF and 100 LF samples, which are 20 times the number of design variables (i.e., 5), is assumed to be $r_{true}^2$.
**** Case 1 is the working condition explained in Table 1.

Table 5 Selected surrogate models for each performance in Case 1

<table>
<thead>
<tr>
<th>Method</th>
<th>$t_{work}$</th>
<th>$T_{overheating}^c$</th>
<th>$T_{min}^c$</th>
<th>$T_{max}^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method 1</td>
<td>HF15</td>
<td>MF15</td>
<td>HF15</td>
<td>MF15</td>
</tr>
<tr>
<td>Method 2</td>
<td>HF15</td>
<td>MF15</td>
<td>HF15</td>
<td>MF15</td>
</tr>
<tr>
<td>Proposed method</td>
<td>MF15 (443°C)</td>
<td>MF15</td>
<td>MF15</td>
<td>MF15</td>
</tr>
</tbody>
</table>

Table 6 presents the performance results of the surrogate models selected in Table 5. $R^2$ values of $t_{work}$, $T_{overheating}^c$, $T_{min}^c$, and $T_{max}^c$ performances in HF15 are 0.38, 0.41, 0.51, and 0.69, respectively. Due to the effect of the MF method, results of all methods for each response are better than those of HF15. Next, when the performance results of the surrogate model selected by three selection methods are compared, the proposed method has the highest $R^2$ value of the surrogate model than other methods. In conclusion, the proposed $r_p^2$ is superior to other methods as an indicator of whether or not the MF surrogate model is used.
Table 6 Performance evaluation of each surrogate model according to the response selection of the LF model

<table>
<thead>
<tr>
<th>Method</th>
<th>$t_{\text{work}}$</th>
<th>$T_{\text{rel,overheating}}$</th>
<th>$T_{\text{rel,\min}}$</th>
<th>$T_{\text{rel,\max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method 1</td>
<td>0.38</td>
<td>0.87</td>
<td>0.51</td>
<td>0.92</td>
</tr>
<tr>
<td>Method 2</td>
<td>0.38</td>
<td>0.87</td>
<td>0.96</td>
<td>0.92</td>
</tr>
<tr>
<td>Proposed method</td>
<td>0.96</td>
<td>0.87</td>
<td>0.96</td>
<td>0.92</td>
</tr>
</tbody>
</table>

4.2 Performance evaluation results of the proposed surrogate models

The performances of the MF surrogate models are summarized in Tables 7 & 8 in terms of accuracy and efficiency. LF100 is built with 100 LF samples only, and HF50, HF20, and HF15 are generated with 50, 20, and 15 HF samples, respectively. MF15 (Proposed) is constructed integrating 15 HF and 40 LF samples. In addition, 15 HF samples used in both HF15 and MF15 (Proposed) models are identical to neglect the influence of the DoE results. The accuracy of each surrogate model is evaluated with $\bar{R}^2$, which is an average value of $R^2$. To evaluate $\bar{R}^2$, 100 HF samples generated through LHS are used as test samples. $\bar{R}^2$ of LF100 is $-0.75$ meaning that it is not suitable to construct a surrogate model using the effective TB model only in terms of accuracy. HF15 is not accurate either due to lack of HF samples. It can be seen from Table 7 that $\bar{R}^2$ of HF20 increases dramatically from 0.50 to 0.84 by using 5 more HF samples. However, MF15 (Proposed) shows much better accuracy ($\bar{R}^2$ of 0.93) which is comparable to HF50 ($\bar{R}^2$ of 0.98) with the same computational cost as that of HF20. Therefore, the numerical results show that proposed MF15 (Proposed) model for Case 1 minimize the computational cost while maintaining the acceptable level of accuracy of the surrogate models.

Table 7 Performance evaluation of each surrogate model for Case 1

<table>
<thead>
<tr>
<th></th>
<th>$N_{\text{LF}}$</th>
<th>$N_{\text{HF}}$</th>
<th>$N_{\text{equiv,\HF}}$</th>
<th>$\bar{R}^2$</th>
<th>$\text{Obj}_N$</th>
<th>$\varepsilon_{\text{CV}}^\text{max}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LF100</td>
<td>100</td>
<td>-</td>
<td>12.5</td>
<td>-0.75</td>
<td>1.0100</td>
<td>102.2365</td>
</tr>
<tr>
<td>HF50</td>
<td>-</td>
<td>50</td>
<td>50</td>
<td>0.98</td>
<td>1.2191</td>
<td>0.6482</td>
</tr>
<tr>
<td>HF20</td>
<td>-</td>
<td>20</td>
<td>20</td>
<td>0.84</td>
<td>1.0377</td>
<td>72.7993</td>
</tr>
<tr>
<td>HF15</td>
<td>-</td>
<td>15</td>
<td>15</td>
<td>0.50</td>
<td>1.1867</td>
<td>93.7923</td>
</tr>
<tr>
<td>MF15 (Proposed)</td>
<td>40</td>
<td>15</td>
<td>20</td>
<td>0.93</td>
<td>1.1998</td>
<td>19.1067</td>
</tr>
</tbody>
</table>

* MF15 (Proposed) is built using the proposed method in Table 6.

The results for other working conditions (e.g., Cases 2 and 3) are presented in Table 8. As mentioned earlier in Section 3.2, the surrogate models for Case 1 in Table 7 can be LF data for Cases 2 and 3. In this study, HF I or
MF I in Table 8 is adopted as the LF model. In all cases, the MF surrogate models are constructed since $|r^2_n|$ is greater than $r_{\text{min}}^2$ (i.e., 0.85). Table 8 shows that both $R^2$ of MF II-1 and MF II-2 are much larger than that of HF II with the same computational cost. Since it is assumed that the surrogate model for Case 1 has already been built in the entire framework, there is no additional computational cost for other working conditions. Similar to Case 2, MF III-1 and MF III-2 with the based LF model yield better results than HF III.

<table>
<thead>
<tr>
<th>Based LF model</th>
<th>$N_{\text{HF}}$</th>
<th>$N_{\text{equiv}}$</th>
<th>$R^2$</th>
<th>$Obj_N$</th>
<th>$\bar{c}_{\text{CV}} \text{ max}$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF II</td>
<td>-</td>
<td>15</td>
<td>0.41</td>
<td>1.1714</td>
<td>77.8642</td>
</tr>
<tr>
<td>MF II-1</td>
<td>HF I</td>
<td>15</td>
<td>0.96</td>
<td>1.2257</td>
<td>9.8477</td>
</tr>
<tr>
<td>MF II-2</td>
<td>MF I</td>
<td>15</td>
<td>0.93</td>
<td>1.1884</td>
<td>22.7757</td>
</tr>
<tr>
<td>HF III</td>
<td>-</td>
<td>15</td>
<td>0.40</td>
<td>1.0891</td>
<td>3.9677</td>
</tr>
<tr>
<td>MF III-1</td>
<td>HF I</td>
<td>15</td>
<td>0.96</td>
<td>1.1908</td>
<td>12.5551</td>
</tr>
<tr>
<td>MF III-2</td>
<td>MF I</td>
<td>15</td>
<td>0.92</td>
<td>1.1372</td>
<td>6.7622</td>
</tr>
</tbody>
</table>

* HF I and MF I are HF50 and MF15 (Proposed) in Table 7, respectively.
** Since the LF data is assumed to be given, $N_{\text{HF}}$ and $N_{\text{equiv}}$ are the same.

From Table 7 & 8, it can be seen that MF surrogate models are successfully applied to the TB system. However, considering normalized objective function $Obj_N$ (i.e., $V_{EC}$) and maximum constraint violation $c_{\text{CV}} \text{ max}$, local accuracy of the predicted optimum needs to be improved. The refined numerical results to find the optimum are presented in the following sections.

### 4.3 Optimization results of a TB system

Surrogate-based optimization is performed for each case after surrogate models are constructed. Surrogate predictor focusing on exploitation is used as a criterion for adding samples as mentioned earlier in Section 3.1 [Forrester and Keane 2009; Han 2016]. The optimization results are summarized in Table 9. In each case, feasible solutions are obtained by adding 2, 6, and 2 samples, respectively. In addition, in all cases, the values of $Obj_N$ are increased from the initial value of 1 while satisfying all the constraint conditions.
Table 9 Optimization results of a TB system

<table>
<thead>
<tr>
<th></th>
<th>(d_1) (mm)</th>
<th>(d_2) (mm)</th>
<th>(d_3) (mm)</th>
<th>(d^*) (mm)</th>
<th>(d_4) (mm)</th>
<th>(d_5) (mm)</th>
<th>(\delta^*_2) (mm)</th>
<th>(N_{HF}^{Equiv})</th>
<th>(\text{Obj}_N)</th>
<th>(e_{CV}^{\text{max}}) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial design</td>
<td>8.5</td>
<td>1.8</td>
<td>1.8</td>
<td>13.0</td>
<td>1.8</td>
<td>1.8</td>
<td>13.0</td>
<td>-</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>MF I-2-opt</td>
<td>4.5</td>
<td>2.2</td>
<td>2.3</td>
<td>11.1</td>
<td>2.7</td>
<td>2.6</td>
<td>9.50</td>
<td>17</td>
<td>1.185</td>
<td>0.004</td>
</tr>
<tr>
<td>MF II-2-opt</td>
<td>4.4</td>
<td>2.5</td>
<td>2.5</td>
<td>10.2</td>
<td>2.4</td>
<td>2.6</td>
<td>10.3</td>
<td>21</td>
<td>1.193</td>
<td>0.000</td>
</tr>
<tr>
<td>MF III-2-opt</td>
<td>5.3</td>
<td>2.4</td>
<td>2.4</td>
<td>10.6</td>
<td>2.4</td>
<td>2.6</td>
<td>10.3</td>
<td>17</td>
<td>1.147</td>
<td>0.000</td>
</tr>
</tbody>
</table>

* \(\delta_1\) and \(\delta_2\) are \(L - 2d_2 - 2d_3\) and \(L - 2d_4 - 2d_5\) in Figure 1, respectively.

In addition, it is found that the thicknesses of heat pellets and thermal insulators (i.e., insulator \(B_U\) & \(B_L\)) between heat pellets are increased. It seems that thicker heat pellets supply more thermal energy while thicker insulators work as bumper to prevent sudden increase of temperature near the heat pellets in the upper and lower stacks. Especially, the insulators and heat pellets in the lower stack tend to be thicker than those in the upper stack. This result is consistent with the previous work [Jeong et al. 2019] that reported the EL near the lower stack is more vulnerable to re-solidification. On the other hand, TB in Case 3 shows the smallest increment of EC volume (i.e., \(\text{Obj}_N\)) among all cases. This is because Case 3 has the highest endothermic heat generation and thus the heat loss should be minimized with thicker side insulator (i.e., insulator \(\gamma\)). It is also expected that the heat loss through side insulator becomes the highest compared to that through the upper and lower stacks after optimization because the thickness of insulator \(\gamma\) shows the largest deviation among the design variables.

For detailed analysis of the optimal results, thermal behavior of the TB system in Case 1 is investigated. Figure 9 shows transient thermal behavior of the optimal TB system. As shown in Figure 9 (a), the heat pellets in the upper and lower stacks show the highest temperature at completion of activation \((t = 3.36\ s)\). The generated thermal energy in the upper and lower stacks is then transferred to the inside of EC or outside of the case through thermal insulators. At the extended time \(t = 720\ s\), the temperature of EC becomes the highest among the elements due to heat diffusion from EC and the heat pellets in the upper and lower stacks to thermal insulators and case as well as heat loss to ambient. Moreover, it is found that the outer case near the side insulator shows higher temperature than that near the upper and lower stacks. This temperature distribution implies that the heat loss to
environment through the side insulator is greater than that through the upper and lower stacks. This result is consistent with the optimal values of $d_1$ which is the most sensitive to the working conditions among the design variables as listed in Table 9.

![Figure 9](image)

**Figure 9** Simulation results of optimal design for Case 1 working condition: (a) temperature contours at the completion of activation ($t = 3.36$ s) and the end of discharge ($t = 720$ s) and (b) physical quantities of EL until $t = 1,000$ s in a logarithmic scale

Figure 9(b) shows the maximum and minimum temperatures and minimum liquid phase fraction of EL. The minimum temperature of EL is higher than its melting temperature (443°C) from the completion of activation to 720 s. The working time of the optimal TB ($t_{\text{work}}^{(\text{opt})} = 720$ s) is extended by 20% compared to the target working time ($t_{\text{work}} = 600$ s). It is expected that the electrical capacity increased by 18.5% will be efficiently consumed during working time. In addition, the optimal TB shows improved temperature uniformity compared to the initial TB. As shown in Figure 9(b), the difference between the minimum and maximum temperatures of EL (i.e., temperature uniformity) becomes 45°C, which is well below the target temperature (50°C) and initial value (65°C). Furthermore, the maximum temperature of EL is lower than 670°C, which also satisfies the desired performance condition.
Finally, the volume of EC and the working time are examined. As listed in Table 10, working times of the optimized TB increase as the volumes of EC increase in all cases. It is obvious that higher increment of working time ensures effective usage of the TB systems. Moreover, TB in Case 3 could not achieve working time of 600 s due to its high endothermic heat generation from chemical reaction ($t_{\text{work}} = 574.02$ s) [Jeong et al. 2019]. However, in this study, working time longer than 600 s is achieved through the proposed efficient optimization framework. Therefore, the proposed efficient framework is successfully applied to the TB system. In the future, the presented framework will be applied to various engineering applications.

<table>
<thead>
<tr>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta V_{\text{EC}}(d^{\text{opt}})^{*} , (%)$</td>
<td>18.5</td>
<td>19.3</td>
</tr>
<tr>
<td>$\Delta t_{\text{work}}(d^{\text{opt}})^{*} , (%)$</td>
<td>20</td>
<td>18.0</td>
</tr>
<tr>
<td>$\eta(d^{\text{opt}})^{*}$</td>
<td>0.93</td>
<td>1.07</td>
</tr>
</tbody>
</table>

* $\Delta V_{\text{EC}}(d^{\text{opt}})$ and $\Delta t_{\text{work}}(d^{\text{opt}})$ are $(V_{\text{EC}}(d^{\text{opt}}) - V_{\text{EC}}(d^{\text{initial}}))/V_{\text{EC}}(d^{\text{initial}})$ and $(t_{\text{work}}(d^{\text{opt}}) - 600)/600$, respectively, where $d^{\text{opt}}$ is the optimal design vector.

5. Conclusion and future work

In this work, the MF surrogate modeling framework is proposed to improve the efficiency of optimization for TB system. Under a single working condition, the proposed method utilizes outputs of detailed and effective TB models as HF and LF data, respectively. Then, this information is utilized as LF data for different working conditions. In addition, a modified indicator for MF dataset selection is proposed to maximize the performances of MF surrogate models. The superiority of the proposed methods is verified step by step through numerical experiments. The first numerical results show that the proposed indicator for MF dataset selection outperforms conventional ones. This is because the proposed criterion can estimate a more accurate correlation between HF and LF data by coping with the influence of DoE (e.g., under the insufficient number of HF data) better than the existing ones. The second numerical results clearly show that the proposed MF surrogate models significantly improve the efficiency while maintaining the accuracy of the surrogate models. The superiority of the performance of the proposed MF surrogate model is validated by integrating the effective and detailed TB models under Case
1 working condition. For different working conditions (e.g., Case 2 and 3), the accuracies of the surrogate models are greatly improved without additional computational costs by utilizing the data from Case 1 as LF data. The final numerical results show that the optimal design for each working condition increases the electrical capacity by approximately 15~20% over the initial design while satisfying all target engineering performances.

In the future, experimental data as HF data will be integrated with LF data from simulation models in the proposed framework for more accurate MF surrogate modeling. In addition, the proposed algorithm will be applied to various thermal systems [Tang et al. 2019; Lee et al. 2020; Zhao et al. 2021; Demeke et al. 2022; Kalkan et al. 2022] as well as TB systems to enhance the scalability of the proposed method.

**CRediT author statement**

**Mingyu Lee:** Conceptualization, Methodology, Software, Investigation, Writing - original draft, Writing - review & editing. **Mun Goung Jeong:** Conceptualization, Methodology, Software, Investigation, Writing - original draft, Writing - review & editing. **Juyoung Lee:** Software, Writing. **Bong Jae Lee:** Conceptualization, Methodology, Writing - review & editing, Supervision. **Ikjin Lee:** Conceptualization, Methodology, Writing - review & editing, Supervision.

**Declaration of competing interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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