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Thermal Multi-layer Perceptron Integrated Model for Grain Storage Temperature Forecasting

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Abstract: *The issue of grain loss and waste during the storage of grains has consistently represented a significant challenge to the security of stored grains. The prediction of grain temperature indicates the guidance of granary ventilation, with the objective of reducing the incidence of grain mold and deterioration due to excessive temperature. Current methods of grain temperature prediction mainly include thermal simulation and data-driven prediction. However, the former method has been found to have low accuracy due to an insufficient simulation of the environmental conditions within the grain storage, while the latter has been identified as lacking interpretability, especially for a large amount of historical grain temperature data. In light of the aforementioned limitations, this paper proposes a novel grain temperature prediction model that integrates thermal simulation and machine learning residual correction. The model employs a multi-layer perceptron (MLP) to refine the outputs of the JMAG thermal simulation of the grain storage. This approach not only preserves the interpretability of the thermal simulation but also improves the accuracy of grain temperature prediction.*

Keywords: *grain temperature prediction, thermal simulation, multi-layer perceptron, data driven forecasting*

1. Introduction

In recent years, economic growth and rising living standards have led to an increase in the availability and diversity of food in many countries; the issue of grain security remains a significant challenge and a matter of global concern. As indicated in the State of Grain Security and Nutrition in the World 2024 report, approximately 733 million individuals were affected by hunger in 2023, which means every one of 11 people in the world lacked access to sufficient food. Among the various issues pertaining to grain security, post-harvest losses of food have consistently been a matter of significant concern [1]. During the production and distribution of food, losses in quantity or quality may occur for a number of reasons. Such losses have a significant impact on the global food supply, particularly in regions experiencing grain insecurity and scarce resources. China, as the world's largest grain producer, recorded a total output of 695.41 million tons in 2023 [2]. Nevertheless, the annual post-harvest loss rate is as high as 15.69 percent, with an annual loss of approximately 35 billion kilograms, representing 8.1 percent of China's total grain output [3]. So, it is evident that the reduction of post-harvest grain losses represents a pivotal strategy for the assurance of global grain security.

Grain losses represent a significant proportion of overall losses incurred during the storage period, with a figure in excess of 20 percent being typical. The global annual loss of grain during storage is estimated at approximately 200 million tons [4], underscoring the critical importance of reducing grain losses during storage. A variety of factors may affect grain during the storage period, including temperature, humidity, light, pests and mold. Among these factors, grain is most sensitive to temperature. Fluctuations in temperature can result in the migration of internal moisture within the grain. An increase in temperature leads to the absorption of moisture by the grain, whereas a decrease in temperature causes the grain to lose moisture. An excess or deficiency of moisture may impact the quality and storage stability of grain. Besides, warm temperatures incur the proliferation of mold and pests. In the absence of human intervention and in the event of prolonged exposure to increasing temperatures, mold and pests multiply faster in grain piles, ultimately leading to a loss of grain quality and quantity. Furthermore, an increase in temperature results in an acceleration of the respiration of the grain and an increase in its metabolic rate. An increase in respiration rate leads to an accelerated deterioration and a decline in grain

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quality.

In light of the aforementioned background in grain storage safety, the real-time monitoring of grain temperature and the implementation of timely intervention measures when temperatures exceed upper limits represent effective strategies for the reduction of grain loss and waste. Currently, the monitoring of grain temperature in real-time is primarily dependent on the Internet of Things (IoT) and sensor technology [5]. The deployment of temperature sensors in the grain storage facility enables real-time acquisition of temperature data, which is then visualized through software or websites. Such a system helps grain managers remain updated on the temperature conditions of the grain pile, thereby facilitating the implementation of appropriate intervention before any issues arise.

However, the impact of grain temperature on grain mold and deterioration is time-sensitive, meaning that if the temperature rises and is not handled properly in time, the quality of the grain will deteriorate rapidly. Real-time monitoring is, therefore, inevitable, and temperature prediction is also particularly important. By predicting the grain pile's temperature trend, managers can take necessary actions, such as ventilation, before the temperature reaches a dangerous threshold. This can prevent the quality of grain from deteriorating and thus reduce possible economic losses. Currently, scholars' predictions of grain temperature are based on two main approaches: thermal simulation based on numerical analysis [6] and data-driven prediction method [7]. The former method is founded upon the principles of physics, whereby a thermal simulation model is constructed to simulate the thermal changes that occur within the grain storage. The temperature changes within the grain storage are based on the laws of heat transfer theory, which is actually a more interpretive approach. However, the actual internal and external environment of the grain storage is very complex in a real granary, and thus, it is challenging to simulate the actual condition accurately for the whole granary. On the other hand, the data-driven prediction method uses a large amount of historical grain temperature data to train a statistical or machine learning model, and the trained machine learning model is used to predict grain temperature. This method has better accuracy than the former but requires more historical data to avoid model over-fitting, and it lacks interpretability compared to the thermal simulation.

In order to address the problems above, this paper proposes an integrated model of JMAG thermal simulation and Multilayer Perceptron (MLP), which employs MLP for residual correction based on predictions from thermal simulation, and exhibits a high accuracy rate and good interpretability.

2. Related Works

This section presents a more detailed review of previous research on two approaches to forecasting grain temperature: thermal simulation, numerical analysis, and data-driven prediction.

2.1. Thermal Simulations and Numerical Analysis Method

In the granary, the temperature changes observed at each sensor placed in the grain pile are subject to the laws of physics. As a porous medium, the temperature change in the grain pile is influenced by both external and internal transfer of heat. The process occurs through three main physical mechanisms: conduction, convection, and radiation. Among these, conduction is the primary mechanism for heat transfer. Mathematical models can be constructed using thermal modeling to simulate the temperature distribution of the grain pile under different storage conditions.

The fundamental principle underlying thermal modeling is the description of heat conduction processes. The conduction of heat in porous media is governed by Fourier's law, which states that the heat flux density is proportional to the temperature gradient. By establishing heat conduction equations, combining the material properties of the grain pile (such as thermal conductivity, density, specific heat capacity, etc.), and setting boundary and initial conditions, different storage environments can be simulated. These include different ventilation conditions, climatic conditions, as well as the structure of the granary [8] and the initial state of the grain pile [9]. This allows for a more realistic reflection of the temperature changes that occur during grain storage. Numerical analysis is a technique employed to solve thermal equations, such as finite element analysis (FEA) [10] or computational fluid dynamics (CFD) [11], which are typically applied to complex systems. By dividing continuous problems into a finite number of computational units, it is possible to make accurate predictions of parameters such as temperature and humidity.

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2.2. Data-driven Prediction Method

The complex and dynamic internal and external environments of grain storage make it difficult for physical models to simulate these conditions accurately. With advancements in computer science, data-driven prediction methods have emerged, focusing on learning patterns from grain temperature data without relying on physical laws. These methods typically involve inputting historical temperature data into statistical or machine-learning models to extract trends for prediction. The process begins by gathering comprehensive historical data, including temperature and environmental conditions, followed by feature engineering to identify key patterns such as temperature trends and periodic fluctuations. These features are then fed into models like regression, ensemble methods, or deep learning models, which are trained to capture relationships within the data. After training, the model's predictive accuracy is evaluated using validation data, with adjustments made as needed. Once optimized, the model can predict temperatures and analyze trends in real-time data.

In the field of machine learning, support vector machines (SVM), decision trees, and neural networks are frequently employed to predict grain temperature. Ni has optimized SVM through the application of intelligent algorithms in order to simulate the non-linear changes in grain temperature and other relevant indicators [12]. Guo et al. put forth a prediction model based on a synthesis of principal component analysis (PCA), Bayesian algorithms, and XGBoost to identify the optimal parameter combination and establish a grain temperature prediction model [13]. Wang et al. employed a particle swarm optimization technique to enhance a back propagation neural network, thereby developing a square bin grain temperature prediction model [14]. These methods offer a plethora of references and theoretical foundations for data-driven grain temperature prediction.

As a further development of machine learning, deep learning has also been employed to address the complexities inherent in grain temperature prediction [15]. Ge et al. developed an early warning model for grain situations by enhancing the Long Short-Term Memory (LSTM) model and evaluating its performance in comparison to the Recurrent Neural Network (RNN) model [16]. In a further development of the techniques already described, Qu et al. proposed a multi-output spatial-temporal model combining graph convolutional neural networks (GCN) and Transformer to predict grain temperature. GCN is employed to identify the spatial correlation and topological information inherent to the sensor network within the grain storage, while the Transformer is utilized to discern long-term and short-term temporal characteristics and to describe time dependence [17].

In general, machine learning models demonstrate satisfactory predictive accuracy; however, it necessitates a substantial quantity of training data, is ill-suited to small data sets, and lacks sufficient interpretability.

3. Materials and Methodology

This section provides a detailed description of our model, including an introduction to the JMAG-based thermal simulation and software and the MLP model used for residual correction.

3.1. Grain Storage and Temperature Sensing System

In general, temperature sensing systems installed in a large flat-roofed granary are capable of monitoring multiple temperature measurement points in real-time. The system is typically comprised of many sensors and multiple temperature measurement cables. Each temperature measurement cable is equipped with a certain number (assumed to be k) of temperature sensors, which are arranged in the length and width directions of the grain storage and inserted vertically into the grain pile for the purpose of monitoring the temperature of the grain. Each temperature measurement cable in length (assumed to be L) direction of the grain storage is designated a region, from left to right, with the designation Region 1 to Region n. Similarly, the width (assumed to be W) of the grain storage is designated a point, from back to front, with the designation Point 1 to Point m. In the context of grain storage, the height (assumed to be H) of the storage is recorded as a layer per floor, from top to bottom, as Layer 1-Layer k. In this way, we can locate each temperature measurement point according to three-dimensional coordinates (n, m, k). The specific grain temperature monitoring system cross-sections are illustrated in Figures 1 and 2. Figure 1 depicts the front cross-section, which illustrates the sensor distribution in the length and height directions of the granary. Figure 2 presents the left-side cross-section, which shows the sensor distribution in the width and height directions.

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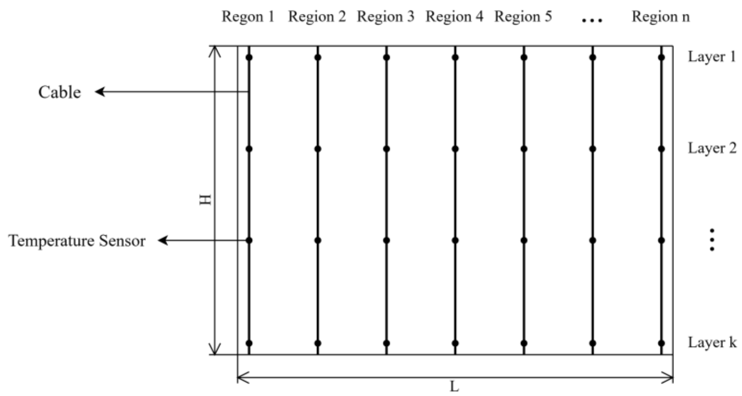

Figure 1: Front view of the sensor deployment in the granary.

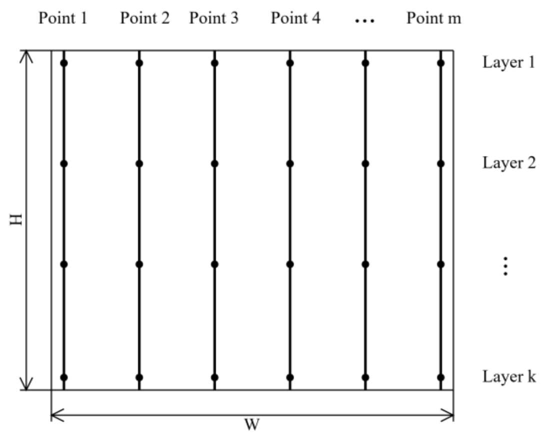

Figure 2: Left side view of the sensor deployment in the granary.

3.2. Temperature data collection and processing

Each sensor in the target grain storage is responsible for recording the temperature at its respective location and transmitting this data to the central control system via a dedicated cable. The control system collects and archives the temperature data from all measurement points on the server. A total of 168 measurement points were identified within a granary we monitored, resulting in the collection of 168 data points per day for three months between March 2023 and May 2023. Additionally, the temperature data for each day was also recorded. However, it should be noted that the data set inevitably experienced some degree of data loss.

The data uploaded after collection was processed preliminary, resulting in the calculation of the average, maximum, and minimum temperatures for each layer and the entire warehouse.

3.3. Thermal simulation based on JMAG

JMAG is primarily utilized for the analysis of electromagnetic devices [18]. However, its thermal simulation functionality can be applied to a range of fields, including the analysis of heat transfer in grain storage. The finite element method (FEM) allows JMAG to assist in the study of temperature distribution in grain storage, particularly with regard to heat conduction, heat transfer and temperature changes throughout the storage process. The aforementioned thermal simulation is of significant importance for the comprehension and optimization of the grain storage environment, thereby aiding the reduction of grain loss due to the presence of uneven temperatures.

Step 1. Create a geometric model. A geometric model of the grain silo must be constructed, including the layout of the shape and size of the granary. In order to ensure that the geometric model accurately reflects the physical structure of the granary, it is necessary to use the actual dimensions of the granary for modeling purposes.

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Step 2. Meshing. This is one of the key steps in the thermal simulation process, and it directly affects the accuracy of the simulation results and the efficiency of the calculation. When using the finite element method (FEM) to perform a thermal simulation of grain storage, meshing breaks down the entire grain storage model into many small, interconnected finite elements. Each finite element is calculated independently for temperature changes in the simulation.

Step 3. Set material properties. The material properties should be assigned to the various components of the model. For example, set the parameters for the thermal conductivity, specific heat capacity, and density of the grain pile.

Step 4. Define boundary conditions. Boundary conditions describe the manner in which the system exchanges heat with the external environment, thereby influencing the temperature distribution and changes within the grain pile. In accordance with the specific circumstances, the most prevalent boundary conditions encompass the reference temperature, the thermal conductivity of the granary wall, the conditions of the vents, the initial temperature, and natural convection. The reference temperature is typically specified as a function of time, allowing for the assessment of temperature changes in the external air environment surrounding the granary. The heat transfer coefficient of the granary wall can be employed to simulate the impact of the granary wall on the heat transfer dynamics of the grain pile. The temperature of the initial state of the grain pile is the temperature that is set prior to the commencement of the simulation. Owing to the constraints of the data acquisition process, there is no real-time humidity data or ventilation time available. Accordingly, to streamline the model, only the impact of external ambient temperature is taken into account, while ventilation conditions and natural convection are excluded.

Step 5. JMAG simulates the heat transfer process occurring within the grain storage, employing the Fourier heat conduction equation to facilitate the analysis of temperature changes occurring across different regions. In order to conduct a thermal transient state study, it is necessary to set the simulation step size and time interval. Furthermore, the actual temperature measurement points in the grain storage must be incorporated into the simulation model. This can be achieved by importing the three-dimensional coordinates of the 168 specific temperature measurement points into the Probes section of the study.

3.4. Multilayer perceptron

A multilayer perceptron (MLP) is a typical feed-forward neural network structure that is widely employed in fields such as classification, regression and pattern recognition [19]. An MLP comprises a minimum of three layers: an input layer, one or more hidden layers and an output layer. The neurons (nodes) in each layer are fully connected to the neurons in the next layer, with each connection characterized by a corresponding weight and bias. By propagating the input data layer by layer and performing nonlinear transformations, MLPs are capable of handling complex mapping relationships and are one of the most commonly used artificial neural networks (ANNs).

The input layer is responsible for receiving input data, with each input node corresponding to a specific feature of the data. The number of nodes in the input layer is equal to the dimensionality of the features of the data. The hidden layer comprises a number of neurons that process the linear combination of the input layer through the application of weights and biases. Each neuron in the hidden layer performs a weighted summation of the inputs from the upper layer and then applies a nonlinear activation function, namely the rectified linear unit (ReLU) function, thereby enhancing the network's expressive power. A significant attribute of the MLP is its capacity to discern high-level characteristics of the input data through the utilization of multiple hidden layers. The output layer is responsible for generating the final prediction result. The objective is to perform a regression task whereby a prediction result is generated using a linear activation function.

The fundamental principle is that the input data is passed through the layers and processed via the full connections between the neurons, resulting in the generation of the final output. The following procedure is to be followed:

Step 1. The forward propagation process is defined as follows: The nodes at each layer perform a linear transformation of the input data by applying weights and biases. This can be expressed as

$$z = W \cdot X + b \tag{1}$$

where W is the weight matrix, X is the input vector, b is the bias vector, and z is the result of the linear transformation. The result of the linear transformation is then non-linearly transformed by an activation function: ReLU (Rectified Linear Unit), the equation is as follows:

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$$f(x) = max(0, x) \tag{2}$$

The equation (2) indicates that the resulting output is zero when the input variable, designated as is less than or equal to zero. Conversely, when the input variable is greater than or equal to zero, the output is equal to the input value, i.e., x. The role of ReLU is to introduce non-linearity into the model, thereby enabling it to learn more complex patterns. Furthermore, it exhibits a faster convergence rate than traditional sigmoid or tanh activation functions and effectively alleviates the problem of gradient disappearance.

Step 2. Loss Function. The MLP employs a loss function to quantify the discrepancy between the model's predicted output and the actual, true value. In this paper, our model employs the mean square error (MSE) as the metric for quantifying the discrepancy between the model's prediction and the actual outcome.

Step 3. Backpropagation. The multilayer perceptron (MLP) employs the gradient descent algorithm to calculate the gradient of the loss function with respect to each weight through the backpropagation algorithm. The weights are updated in a sequential manner, progressing from the output layer to the input layer.

Step 4. Parameter Updating. The network parameters are adjusted using the Adam optimizer, which is an optimization method based on adaptive learning rate adjustment. Adam integrates the benefits of momentum-based gradient descent and RMS proportion, facilitating rapid convergence during training and enhancing the model's predictive precision.

3.5. Thermal Multilayer Perceptron Integrated Model

We now propose the TMPI model for grain storage temperature forecasting. Our integrated model firstly performs a thermal simulation based on the physical law of heat conduction to simulate the temperature distribution inside the grain pile. However, pure physical modeling may be biased in complex environments. Therefore, an MLP model is introduced for residual correction. The simulated temperature is compared with the actual monitored temperature, and the residual is calculated and used as training data for the MLP. The MLP corrects the simulation results by learning complex environmental factors not covered by the physical model.

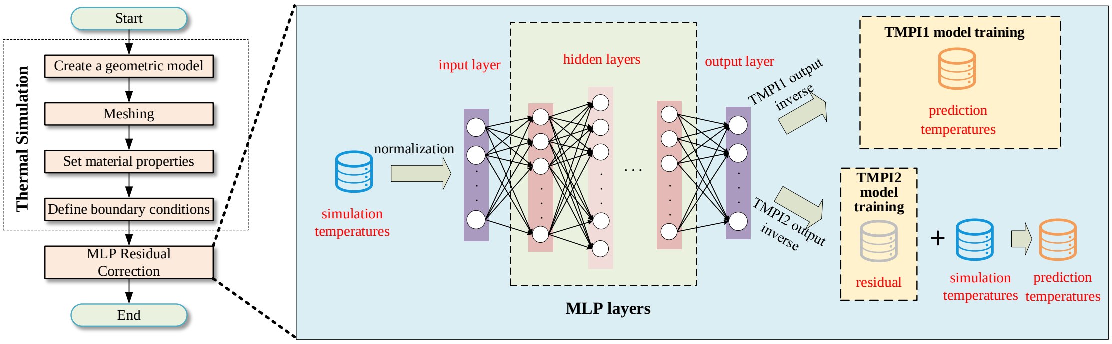

Figure 3: Flowchart of TMPI1 and TMPI2 models.

In this paper, we use two residual correction methods for comparison. The first correction method directly inputs the simulated value y_{sim} into the MLP, which produces the corrected predicted value $\hat{y}$. This can be expressed as

$$\hat{y} = MLP(y_{sim}) \tag{3}$$

aiming to adjust the simulated values of the 168 temperature measurement points to better match the true values, this method is named as TMPI1. In the second correction method named TMPI2, the simulated value y_{sim} is also used as the input to the MLP, but the output is the error value e (the difference between the true value y and the simulated value y_{sim}) calculated in equation (4).

$$e = y - y_{sim} \tag{4}$$

The corrected prediction is then obtained by adding the predicted error to the simulated value, i.e.,

$$\hat{y} = y_{sim} + MLP(y_{sim}) \tag{5}$$

The flowchart of TMPI1 and TMPI2 is shown in Figure 3.

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4. Experiment and Evaluation

4.1. Experiment setting

The target granary is situated in Jiangsu, China. It is a tall, flat-roofed granary with dimensions of 29.35 meters in length and 23.45 meters in width and a grain storage height of 6 meters (see Figure 4). A temperature measurement system has been installed within the granary to monitor several temperature measurement points within the grain pile in real time. The system comprises many temperature measurement cables. Seven temperature measurement cables are deployed horizontally within the granary at a spacing of 4.8 meters, while a further six are deployed vertically at a spacing of 4.5 meters. Each temperature measurement cable is integrated with four temperature sensors at a spacing of 1.8 meters, resulting in 168 embedded temperature measurement points within the grain pile. The aforementioned temperature measurement points collectively constitute a temperature measurement network, which ensures the monitoring of temperature changes across the entire grain pile.

Figure 4: Interior view of the targeted granary.

In the simulated experiments, the grain temperature was simulated in March, April and May, respectively, and the discrepancy between the simulation results y_{sim} and the actual measured values of y at 168 measurement points for each month was calculated.

4.2. Simulation setting

According to the simulation steps introduced in Section 3.3, the simulation parameters are designed as follows. A model of the granary with equal dimensions is created and meshed, with the mesh size set to 60 mm. In the material property settings, given that grain is a poor conductor of heat and its constant heat source density is very small with a thermal conductivity of only 0.13 ~ 0.16 $W/(m \cdot K)$ [20], it is possible to set the constant heat source density to 0.1. The conductivity is set to 0.159 $W/(m \cdot K)$, and the heat capacity is set to 1871 $J/(kg \cdot K)$ [21].

In defining the boundary conditions, the change in temperature over time in the collected data is used as the reference temperature. The heat transfer coefficient of the silo wall is defined as a constant value of 12 $W/(m^2 \cdot K)$. The initial temperature of the grain pile is established at the mean temperature recorded on the day preceding the simulation.

4.3. Evaluation

We simulated the temperatures of the grain storage temperature measurement points on some dates in March, April and May 2023, respectively, used the simulation data and the real data of March and April for the training of the MLP error correction, the data of May (5.1-5.17) was used for the test. Table 1 shows the average absolute errors of the test data in the simulation-only without MLP (denoted as “Thermal Simulation in table”), the direct input of the simulation results into the MLP correction (TMPI1 in table), and the prediction errors added back to the simulation values (TMPI2 in table), and the mean absolute error (MAE), which was calculated using the Equation (6)

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$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i| \tag{6}$$

where n is the number of samples, y_i is the i-th actual value, and $\hat{y}_i$ is the i-th predicted value.

Table 1: Comparison of MAEs for three models in 5.1-5.17.

Date	Thermal Simulation	TMPI1	TMPI2
5.1	3.590	0.612	1.527
5.2	3.580	0.782	0.919
5.3	3.787	0.829	0.891
5.4	3.879	0.800	0.942
5.5	3.805	0.763	1.069
5.6	3.820	0.787	1.196
5.7	3.832	0.825	1.354
5.8	3.892	0.863	1.427
5.9	3.478	1.278	1.728
5.10	3.991	0.914	1.227
5.11	4.151	0.930	0.994
5.12	4.264	0.947	1.017
5.13	4.530	0.932	0.953
5.14	4.905	0.936	0.987
5.15	5.044	0.954	1.010
5.16	4.962	0.967	1.062
5.17	4.905	0.998	1.057

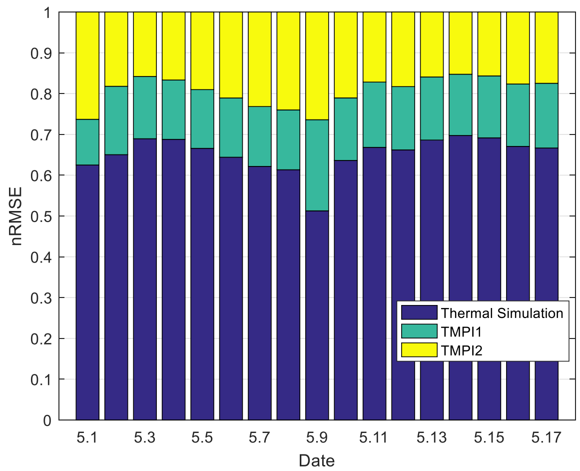

Figure 5: Comparison of the nRMSEs of the thermal simulation and the TMPI1 and TMPI2 models.

As above, Figure 5 shows the normalized root mean square error (nRMSE) of the three models, which is another metric used to compare prediction errors relative to some characteristic of the data, and calculated as in Equation (7).

$$Normalized\ RMSE = \frac{RMSE}{\max(y) - \min(y)} \tag{7}$$

In the equation above, the formula for RMSE is as follows:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)} \tag{8}$$

where $\max(y) - \min(y)$ is the maximum minus the minimum of the true data, other parameters are the same as in MAE equation.

From Table 1 and Figure 5 we can find that both MAE and RMSE after MLP correction of the simulation results are much higher than the predictions from the simulation only, and of the two ways of using MLP for error correction, the direct correction model is better than the prediction errors added back to the simulation values model.

For further analysis, we compare the proposed TMPI model with a simple thermal simulation and the

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representative machine learning method LSTM in terms of prediction performance at specific temperature measurement points. Figures 6 and 7 show the predicted temperature of the temperature measurement points (1, 6, 4) and (5, 2, 4) for the three models, as well as the actual temperature value of this point.

It is evident from the figures that there is a significant residual between the thermal simulation results and the observed values, which can be substantially reduced after MLP correction. In most cases, our TMPI1 model demonstrates a superior correction effect compared to the TMPI2 model. However, at certain points, such as point (1, 6, 4) in Figure 7, the TMPI2 model exhibits relatively higher accuracy after the first day. For the LSTM model, the small amount of data limits its ability to accurately predict the grain temperature trend. This comparison further highlights the advantages of the TMPI models when data availability is limited.

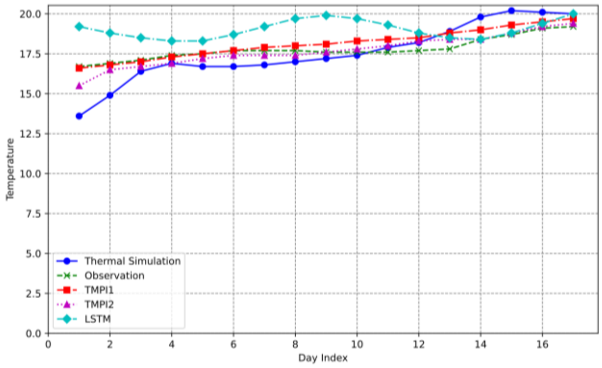

Figure 6: Comparison of Observation, Thermal Simulation, TMPI1, TMPI2 and LSTM models of point (1, 6, 4).

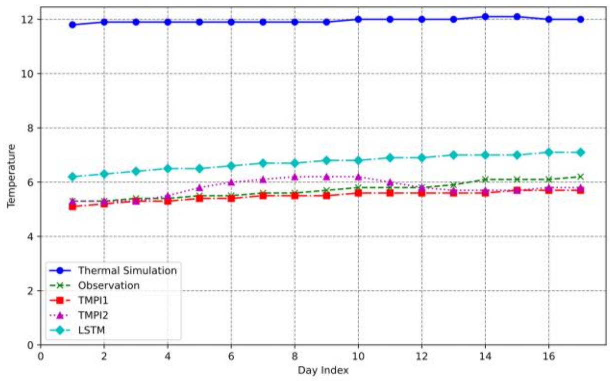

Figure 7: Comparison of Observation, Thermal Simulation, TMPI1, TMPI2 and LSTM models of point (5, 2, 4).

5. Conclusion

This paper proposes a temperature prediction model based on physics thermal simulation and machine learning MLP residual correction, which is capable of more accurate grain temperature prediction without the necessity for extensive data training. The underlying model is based on thermal simulation, thus enabling model interpretation.

However, MLP may not be the optimal model for correcting simulation residuals, and it also exhibits inaccuracies when correcting the temperature. The residual correction model can be optimized in future research to achieve higher prediction accuracy. Furthermore, our predictions are all based on existing temperature measurement points. Thermal simulation can simulate the temperature of any point in the grain storage, which may not be the coordinate point where the sensor is located. However, we do not have the actual temperature of these non-sensor points as a reference for residual correction. Our future work is to propose a grain storage temperature prediction model that can accurately predict the temperature of any location in the grain storage.

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