

Article

Sparse-Sensor Three-Dimensional Thermal-State Reconstruction for Black Tea Fermentation Using a CFD-Prior-Constrained Physics-Informed Neural Network

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Abstract

Internal temperature distributions in black tea fermentation regulate enzymatic oxidation, heat accumulation and fermentation uniformity, but continuous three-dimensional measurements remain difficult in practical processing. We developed a CFD-prior-constrained physics-informed neural network (PINN + CFD) to reconstruct the three-dimensional thermal state of a 1.35 m × 0.96 m × 0.08 m fermentation bed under sparse sensing. Nine sensors at $z = 0.04$ m were used for training, and six held-out depth-wise sensors at $z = 0.02$ m and $z = 0.06$ m were reserved for depth-wise validation. The model integrated measured temperatures, transient heat-transfer physics, convective boundary conditions and a CFD-derived volumetric soft spatial prior, which guided spatial extrapolation rather than serving as ground-truth temperature data. Although the multilayer perceptron achieved the lowest fitting error at the instrumented $z = 0.04$ m plane, PINN + CFD showed better depth-wise extrapolation, with RMSEs of 0.128, 0.129 and 0.296 °C across the three stages. However, its advantage was stage- and validation-target-dependent: the baseline PINN was slightly better in part of the dynamic-stage validation, and standalone CFD had the lowest surface infrared error in the constant-temperature stage, indicating that PINN + CFD mainly improved spatial extrapolation rather than uniformly minimizing all error metrics. The inferred apparent process-level heat-source index $Q_{\text{react}}(t)$ varied continuously, and its cumulative trajectory showed a descriptive association with cumulative polyphenol loss. These results indicate that PINN + CFD enables physically consistent thermal-state reconstruction within the tested sparsely instrumented black tea fermentation bed.

Keywords: black tea fermentation; physics-informed neural network; CFD prior; porous-medium heat transfer; infrared thermography; apparent process-level heat-source index



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1. Introduction

Black tea fermentation is a critical processing stage that determines the formation of color, aroma, taste and characteristic biochemical constituents. During fermentation, tea polyphenols, catechins and other endogenous compounds undergo oxidation, polymerization and transformation under the action of polyphenol oxidase and peroxidase, promoting the formation of quality-related compounds such as theaflavins and thearubigins and contributing to the typical “red liquor and red leaf” characteristics of black tea [1–4]. At the same time, enzymatic oxidation, material-state changes, environmental heat exchange and internal heat accumulation jointly drive the temperature evolution of the tea bed. Temperature not only affects the rate of enzymatic oxidation but also reflects heat

accumulation, boundary heat loss and batch uniformity during fermentation [5]. Therefore, obtaining the internal temperature distribution of the black tea fermentation bed is important for understanding the fermentation process, evaluating fermentation uniformity and optimizing temperature-control strategies.

Current monitoring studies on black tea fermentation have mainly focused on quality indicators and non-destructive sensing. Data-fusion systems, combining electrical properties with chemometrics, machine vision, hyperspectral imaging and transfer-learning models, have been used to evaluate fermentation quality, catechin changes and fermentation degree [6–10]. These studies demonstrate the value of intelligent sensing for online assessment in tea processing. However, their observations are mainly based on appearance, spectral responses or discrete chemical indicators, whereas the internal three-dimensional thermal state of the fermentation bed has received less attention. In practical production, internal temperature sensors can only be sparsely arranged because of sensor cost, disturbance to the loose tea bed and limited spatial accessibility. When a full temperature field is extrapolated from a limited number of measurements, conventional interpolation methods are simple to implement but lack heat-transfer and boundary-condition constraints, which may lead to physically inconsistent distributions in unmeasured regions.

Computational fluid dynamics (CFD) provides a mechanistic route for describing heat-transfer behavior during tea fermentation. Lian et al. simulated heat transfer and polyphenol oxidation during tea fermentation using CFD and revealed non-uniform thermal behavior within the fermentation bed [11]. At the engineering scale, bulk foods and biological materials are often treated as porous media, in which the solid matrix, pore gas and coupled heat and mass transfer are described using continuum parameters [12–15]. This treatment provides a basis for constructing a computable three-dimensional heat-transfer model for black tea fermentation beds. However, CFD predictions depend on effective thermophysical properties, boundary heat-transfer coefficients, porosity, permeability and internal heat-generation inputs, all of which are uncertain under real processing conditions. Studies on CFD verification, validation and uncertainty quantification also emphasize that numerical results should be regarded as computational evidence affected by model form, parameters and boundary conditions, rather than as unverified true temperature fields [16]. Thus, CFD is suitable for providing physically plausible spatial trends, but its systematic bias must be corrected using experimental data.

Physics-informed neural networks (PINNs) provide a framework for integrating sparse measurements with governing equations. Since the PINN framework was proposed by Raissi et al., it has been widely applied to forward and inverse problems governed by partial differential equations [17,18]. In heat-transfer research, PINNs have been used for heat conduction, convective heat transfer, source-driven thermal problems and forward or inverse heat-conduction analysis. Cai et al. demonstrated the applicability of PINNs to several heat-transfer problems [19]; Liu et al. reconstructed temperature fields in thermal-source systems using limited observations [20]; Koric and Abueidda applied physics-informed deep operators to heat-conduction equations with parameterized heat sources [21]; and He et al. used physics-informed deep learning for direct and inverse heat-conduction problems in materials [22]. For porous-media heat transfer, Xu et al. showed that PINNs can predict temperature fields, heat fluxes and effective thermal parameters [23]. In thermal-process modeling, PINNs have also been applied to temperature prediction, melt-pool flow estimation and thermal-parameter identification in additive manufacturing [24,25]. These studies indicate that PINNs can constrain the solution space using physical equations when measurements are sparse and can infer thermal states or heat-source terms that are difficult to measure directly.

Nevertheless, a baseline PINN does not automatically ensure reliable reconstruction in unmeasured regions. Previous studies have shown that imbalance among loss terms, gradient competition and biased training dynamics can cause convergence difficulties or overemphasis on local constraints [26–28]. When a baseline PINN is applied to black tea fermentation, these challenges are further compounded by practical modeling conditions: internal temperature measurements are limited, sensors are usually concentrated on representative planes or at a small number of depths, and boundary heat exchange, effective thermal properties and dynamic equivalent heat sources are all uncertain. Therefore, a PINN trained only with sparse temperature data and heat-transfer residuals may fit measured sensor locations but still lack sufficient constraints for spatial extrapolation. In contrast, CFD can generate a full three-dimensional temperature field based on heat-transfer mechanisms and provide a physically plausible spatial structure in unmeasured regions, although its absolute predictions may deviate from measurements because of uncertain properties, boundary conditions and heat-source settings.

Multi-fidelity physics-informed learning and data-assimilation studies provide methodological support for combining CFD with sparse measurements. He et al. showed that governing-equation residuals and sparse observations can jointly constrain unknown states and parameters in multiphysics data assimilation [29]. Previous multi-fidelity physics-informed learning studies have shown that lower-fidelity models, approximate physics or numerical information can be combined with limited high-fidelity data to improve prediction or inverse modeling in PDE-governed problems [30–32]. In the present study, the CFD-derived temperature field was introduced as a volumetric soft spatial prior during training, rather than as ground-truth temperature labels, to provide additional spatial constraints in unmeasured regions while retaining constraints from measured data and heat-transfer physics. This strategy is suitable for black tea fermentation temperature-field reconstruction: sparse sensors provide local experimental constraints, the governing equation constrains energy conservation, boundary conditions describe heat exchange between the tea bed and its environment, and the CFD prior supplements the three-dimensional spatial-distribution trend in unmeasured regions.

Based on this rationale, this study applies a CFD-prior-constrained physics-informed learning framework to three-dimensional thermal-state reconstruction in a black tea fermentation bed under sparse temperature sensing. The neural network directly predicts the temperature field, while its training loss incorporates measured temperature constraints, the transient heat-transfer residual with the time-dependent $Q_{\text{react}}(t)$ source term, convective boundary conditions and a CFD-derived volumetric soft spatial prior. The main contributions of this study are as follows: (1) a CFD-derived volumetric soft-prior strategy, grounded in established multi-fidelity physics-informed learning concepts, is adapted for sparse-sensor three-dimensional thermal-state reconstruction in black tea fermentation; (2) the reconstruction was assessed using the instrumented measurement plane, within-run leave-one-sensor-out spatial validation, six held-out depth-wise test points and held-out surface infrared thermography; and (3) an apparent process-level heat-source index $Q_{\text{react}}(t)$ is inferred from the macroscopic heat balance, and its association with tea-polyphenol changes is examined descriptively to characterize process-level thermal evolution. This work provides a physically interpretable modeling framework for low-cost three-dimensional thermal monitoring, fermentation-uniformity assessment and temperature-control optimization in black tea processing.

2. Materials and Methods

2.1. Experimental Setup and Sensor Layout

Fresh tea leaves were collected from Xianfeng County, Hubei Province, China ($29^{\circ}58' \text{ N}$, $109^{\circ}03' \text{ E}$; average altitude, 900 m). The fermentation experiment was conducted using an intelligent black tea fermentation system at Hubei Shuizhai Tea Co., Ltd. (Xianfeng, China). The tea cultivar was Lichuan black tea, and the processing strategy followed the principle of heavy rolling and light fermentation. The experimental material consisted of black tea leaves after withering and rolling. The leaves were uniformly spread in a fermentation tray and approximated as a cuboid tea bed with dimensions of $1.35 \text{ m} \times 0.96 \text{ m} \times 0.08 \text{ m}$. Before fermentation, the initial tea-bed temperature, ambient temperature, relative humidity, initial moisture content and quality were 21°C , 24°C , 96% RH, 55% and 10.472 kg, respectively. The experimental setup is shown in Figure 1.

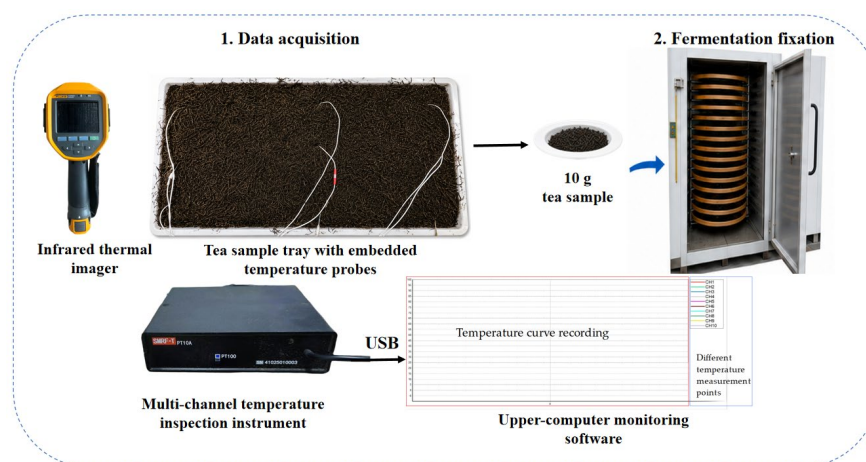


Figure 1. Experimental setup for black tea fermentation.

Nine temperature sensors were arranged in a 3×3 grid on the $z = 0.04 \text{ m}$ plane to monitor the internal temperature of the tea bed (Figure 2). T1, T4 and T5 represented the corner, edge and center of the tea bed, respectively. For held-out depth-wise test-point validation, six testing points were arranged at the same horizontal positions as T1, T4 and T5, with three points above the original measurement plane at $z = 0.06 \text{ m}$ and three points below it at $z = 0.02 \text{ m}$.

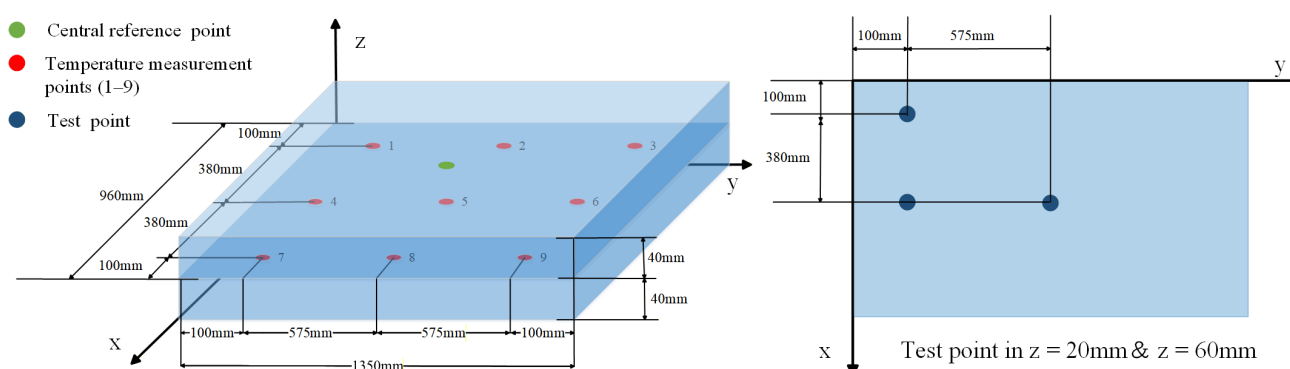


Figure 2. Sensor arrangement for black tea fermentation.

Temperature data were recorded every 30 s for 6 h using an SMRF-T multi-channel temperature recorder (Beijing Simairuice Technology Co., Ltd., Beijing, China) and transmitted to a host computer. The measurement accuracy of both the PT100 sensors and the SMRF-T recorder was $\pm 0.01\%$ of the measurement range.

To avoid information leakage, the six depth-wise validation points were excluded from model training, input/output normalization, CFD calibration, apparent heat-source estimation, hyperparameter selection and model selection, and were used only for final thickness-direction validation.

Surface temperature was measured using a FLUKE Ti32s thermal imager (Fluke Corporation, Everett, WA, USA). Radiometric .is2 files were used for temperature extraction. The camera was positioned approximately 0.50 m above the tea-bed surface for normal-incidence imaging, corresponding to a viewing angle of 0° relative to the surface normal, and the emissivity was set to 0.98. At each 30 min time point, three radiometric .is2 images were acquired and averaged to reduce imaging noise.

For surface-field validation, fixed pixel boundaries corresponding to the tea-bed region were used to define the pixel-to-physical coordinate mapping. The averaged infrared temperature matrix was linearly mapped to the physical tea-bed dimensions of 1.35 m × 0.96 m and then resampled onto the model surface grid. To assess local infrared–PT100 agreement, synchronous measurements were obtained at a surface calibration point located directly above the center of the tea bed. The infrared temperature at this calibration point was extracted from the averaged temperature matrix as the mean value within a 5 × 5-pixel ROI centered on the registered position of the calibration point, determined using the same coordinate mapping. The quantitative IR–PT100 agreement results and the key image-registration parameters are summarized in Supplementary Table S1.

Tea samples were collected every 30 min and immediately heated at 100 °C for 30 min using a tea baking machine (XS-6CHZ-9B, Fujian Anxi Xiangshan Machinery Co., Ltd., Quanzhou, China) to terminate enzymatic fermentation. After cooling, the tea's polyphenol content was determined according to GB/T 8313-2018.

2.2. Experimental Design

Based on previous studies on temperature-dependent quality formation and non-uniform heat transfer within tea beds [5,11], a three-stage temperature-control protocol was established to approximate typical temperature-variation patterns during practical black tea fermentation. The fermentation process comprised three sequential stages within the same continuous 6 h fermentation run under constant-humidity conditions. All training and validation data were obtained from this single run using one batch of rolled black tea leaves under the tested bed geometry and temperature-control protocol.

Linear-heating stage. Under constant-humidity conditions, the initial chamber temperature was 24 °C and the initial tea-bed temperature was 21 °C. The chamber temperature increased gradually from 24 °C to 28 °C during 0–7200 s. This stage was designed to examine the temperature-distribution response of the tea bed under a gradually increasing thermal boundary.

Constant-temperature stage. After the target fermentation temperature was reached, the chamber was maintained at 28 °C. This stage was used to observe the temperature-field response of the tea bed under a stable thermal boundary and to evaluate model prediction accuracy under quasi-steady heat-exchange conditions.

Dynamic-perturbation stage. To evaluate the applicability and robustness of the proposed model under dynamic conditions, a periodic thermal perturbation was applied to the fermentation chamber. Heating was automatically stopped when the chamber temperature reached 30 °C and restarted when it decreased to 28 °C. This control strategy produced an approximately triangular temperature fluctuation between 28 °C and 30 °C, simulating temperature oscillations caused by heater switching and non-ideal insulation in practical fermentation. This dynamic stage was used to test model accuracy and long-term stability under periodically varying thermal boundary conditions.

2.3. Equivalent Heat-Transfer Model of the Black Tea Fermentation Bed

The black tea fermentation bed was formed by the accumulation of rolled tea particles and contained both the solid tea matrix and pore air, giving it typical porous-medium characteristics. During fermentation, the temperature evolution of the bed was jointly affected by heat conduction through the tea solids, heat exchange with pore air, boundary heat loss and heat generation associated with fermentation reactions. Because the tea particles had irregular shapes and a complex pore structure, and because particle-scale heat transfer cannot be directly resolved under practical fermentation conditions, the tea bed was treated as a homogeneous porous medium at the engineering scale to describe the spatiotemporal evolution of the bulk temperature field [12–15].

For a general porous-medium heat-transfer problem with significant ventilation or pressure-driven airflow, the effective seepage velocity of pore air can be described by Darcy's law [11,33]:

$$\mathbf{u} = -\frac{K}{\mu} \nabla p \quad (1)$$

where $\mathbf{u}$ is the effective seepage velocity of pore air ($\text{m} \cdot \text{s}^{-1}$), K is the permeability of the tea (m^2), μ is the dynamic viscosity of air ($\text{Pa} \cdot \text{s}$) and p is the air pressure (Pa). Under such conditions, the energy equation should include the convective heat-transfer term induced by pore-airflow:

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \rho_f C_{p,f} \mathbf{u} \cdot \nabla T = \nabla \cdot (\mathbf{k}_{\text{eff}} \nabla T) + Q_{\text{react}}(t) \quad (2)$$

where ρ_f and $C_{p,f}$ are the density of air ($\text{kg} \cdot \text{m}^{-3}$) and the specific heat capacity of air ($\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$), respectively, and $Q_{\text{react}}(t)$ denotes the apparent process-level heat-source index, represented in the model as an equivalent volumetric source term during black tea fermentation ($\text{W} \cdot \text{m}^{-3}$). Its derivation and formal definition are provided in Section 2.5. This general form describes coupled heat and airflow transport under ventilation, pressure-gradient or forced-airflow conditions.

In the present experiment, however, no defined air inlet or outlet was imposed on the tea bed, and the internal pressure gradient or pore-air velocity was not measured. Directly solving the Darcy velocity and pressure fields would therefore introduce additional unknown boundary conditions and parameter uncertainty. To avoid over-parameterization, the pressure field p and the Darcy velocity $\mathbf{u}$ were not explicitly solved. Instead, the effects of weak airflow, natural convection, tray contact heat transfer and boundary heat loss were represented through the effective properties $\mathbf{k}_{\text{eff}}$ and h . Based on this simplification, the governing equation used in both the CFD model and the PINN + CFD framework was expressed as a transient heat-transfer equation with the time-dependent $Q_{\text{react}}(t)$ source term [11–13,19,23]:

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} = \nabla \cdot (\mathbf{k}_{\text{eff}} \nabla T) + Q_{\text{react}}(t) \quad (3)$$

where T is the tea-bed temperature ($^{\circ}\text{C}$), $(\rho C_p)_{\text{eff}}$ is the effective volumetric heat capacity ($\text{J} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$), and $\mathbf{k}_{\text{eff}}$ is the effective thermal conductivity ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$). The initial condition was determined from the measured temperature at the beginning of fermentation:

$$T(x, y, z, 0) = T_0 \quad (4)$$

Here, T_0 denotes the measured initial tea-bed temperature ($^{\circ}\text{C}$). The tea-bed boundary was described by a Robin-type convective condition [19,33]:

$$-\mathbf{k}_{\text{eff}} \frac{\partial T}{\partial \mathbf{n}} = h [T - T_{\text{air}}(t)] \quad (5)$$

where n is the dimensionless outward unit normal vector, $T_{\text{air}}(t)$ is the ambient air temperature ($^{\circ}\text{C}$) and h is the effective convective heat-transfer coefficient ($\text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$). The top surface was the main heat-exchange interface directly exposed to air, whereas the side walls and bottom surface were affected by tray contact, air disturbance and weak heat exchange. A unified effective boundary heat-transfer coefficient was therefore used to describe the boundary heat exchange and to reduce the number of non-identifiable parameters associated with complex contact conditions.

Overall, the physical model represented the black tea fermentation bed as an equivalent porous medium and described its bulk temperature evolution using the effective-medium heat-transfer equation, an effective convective boundary condition and the time-dependent source term $Q_{\text{react}}(t)$ [11–15]. This formulation preserves the main porous-medium characteristics of the tea bed while avoiding an underdetermined airflow-pressure model under conditions without measured airflow or pressure boundaries. The model was therefore used as the common governing framework for constructing the CFD-derived temperature field and for imposing the physical constraints in the PINN + CFD model. The key effective thermophysical parameters used in the governing equation are listed in Table 1, and the complete porous-medium and air-property parameters are provided in Supplementary Table S2.

Table 1. Key effective thermal parameters used in the PINN + CFD model.

Parameter	Symbol	Value (Unit)	Source
Bulk density of tea layer	ρ_{bulk}	101.0 kg/m ³	$\rho_{\text{bulk}} = m_{\text{tea}}/V_{\text{bed}}$
Porosity	ε	0.85	[11,15]
Effective volumetric heat capacity	$(\rho C_p)_{\text{eff}}$	322,290.018 J/(m ³ · K)	[11]
Effective thermal conductivity	k_{eff}	0.0821 W/(m · K)	[11]
Convective heat-transfer coefficient	h	8.0 W/(m ² ·K)	Fixed engineering-empirical input

2.4. Construction of the CFD-Derived Volumetric Soft Spatial Prior

The CFD-derived temperature field was used as a volumetric soft spatial prior in regions not covered by internal sensors, rather than as ground-truth temperature data. Because CFD predictions depend on effective thermophysical properties, boundary conditions and heat-source settings, the CFD field was used to provide a physically plausible three-dimensional spatial trend for subsequent PINN reconstruction.

Using the equivalent heat-transfer model described in Section 2.3, CFD simulations were performed over the complete tea-bed domain defined in Section 2.1. The simulations were conducted in ANSYS Fluent 2022 R1 using a pressure-based transient solver framework. The tea bed was represented as a stationary solid-equivalent transient heat-conduction domain with effective thermophysical properties. Because internal airflow was not explicitly resolved, only the energy equation was solved, and no momentum equation, pressure field or turbulence model was included.

The transient energy equation was discretized using a finite-volume formulation on a structured hexahedral mesh. Conductive heat fluxes were discretized using a second-order central scheme, and the temporal derivative was treated using a second-order implicit scheme. A physical time step of 30 s was used, consistent with the experimental temperature-acquisition interval. Up to 30 iterations were performed at each time step, and a time step was considered converged when the scaled energy residual decreased below 1.0×10^{-8} . The computational domain was initialized using the measured tea-bed temperature at the beginning of fermentation. Detailed numerical settings are provided in Supplementary Table S3.

$T_{\text{air}}(t)$ was imposed as a time-dependent external boundary profile, with linear interpolation between successive 30 s measurements. A unified effective convective heat-transfer coefficient of h was applied to the external tea-bed surfaces. The $Q_{\text{react}}(t)$ sequence derived in Section 2.5 was implemented separately as a spatially uniform, time-dependent volumetric energy source in the solid-equivalent tea-bed domain using a compiled DEFINE_SOURCE UDF. The source value was evaluated according to the current solver time, with linear interpolation between successive data points. The CFD field was precomputed before PINN training and then kept fixed as the volumetric soft spatial prior. The held-out depth-wise sensors and infrared thermography data were excluded from CFD-prior construction, source-term inference, hyperparameter selection and model selection, and were used only for independent spatial-extrapolation evaluation.

Mesh independence was assessed using four structured hexahedral grids containing 4104, 27,216, 87,480 and 202,176 cells. The successive-grid RMSE between the 87,480- and 202,176-cell grids was 0.015–0.048 °C over the six output times, below the 0.10 °C acceptance criterion. Therefore, the 202,176-cell grid shown in Figure 3 was selected to generate the CFD-derived soft spatial prior. The mesh-convergence results are provided in Supplementary Figure S1 and Supplementary Table S4.

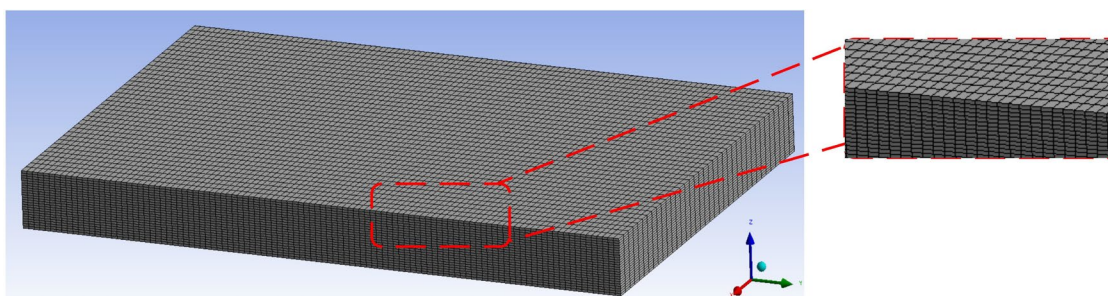


Figure 3. Structured hexahedral mesh of the CFD computational domain for the black tea fermentation bed and an enlarged local view.

To evaluate the robustness of the CFD prior to fixed effective parameters, one-at-a-time sensitivity analyses were performed for k_{eff} , h , porosity and $Q_{\text{react}}(t)$. The full perturbation ranges and corresponding CFD-prior and PINN + CFD results are provided in Supplementary Table S5.

2.5. Inference of the Apparent Process-Level Heat-Source Index

During black tea fermentation, changes in tea-bed temperature reflect both external heat exchange and internal process effects. Because biochemical heat release was not directly measured, a signed equivalent volumetric heat-source term, $Q_{\text{eff}}(t)$, was inferred from the nine training-plane sensors using a macroscopic heat balance. The mean bed temperature, $T_{\text{mean}}(t)$, was calculated as the arithmetic mean of the nine sensor readings. To reduce noise amplification during temporal differentiation, $T_{\text{mean}}(t)$ and $T_{\text{air}}(t)$ were smoothed using a third-order Savitzky–Golay filter with an 81-point window. The first-order derivative was then calculated using a numerical gradient, with centered finite differences at interior points and one-sided differences at the two endpoints:

$$\left. \frac{dT_{\text{mean}}}{dt} \right|_{t_i} \approx \frac{T_{\text{mean},i+1} - T_{\text{mean},i-1}}{t_{i+1} - t_{i-1}} \quad (6)$$

The signed equivalent heat-source term was calculated as

$$Q_{\text{eff}}(t) = (\rho C_p)_{\text{eff}} \frac{dT_{\text{mean}}}{dt} + \frac{hA}{V} [T_{\text{mean}}(t) - T_{\text{air}}(t)] \quad (7)$$

Here, A is the total external surface area used in the lumped heat-balance inversion (m^2) and $V = L_x L_y L_z$ is the tea-bed volume (m^3). The signed $Q_{\text{eff}}(t)$ was retained as an intermediate net heat-source quantity, allowing for possible net cooling, unresolved surface-specific boundary exchange and model discrepancy. The apparent process-level heat-source index $Q_{\text{react}}(t)$ was defined as the non-negative component of $Q_{\text{eff}}(t)$:

$$Q_{\text{react}}(t) = \max(Q_{\text{eff}}(t), 0) \quad (8)$$

$Q_{\text{react}}(t)$ is the apparent process-level source index reported in the results. This operation extracted the non-negative component of $Q_{\text{eff}}(t)$ without constraining the complete net energy balance to be non-negative. The resulting source profile was further processed and smoothed before being used as the dynamic source input in the CFD and PINN models. The smoothing and derivative-based source-estimation procedures follow established treatments of noise amplification and inverse heat-transfer problems [20,22,34–36].

To assess the sensitivity of the CFD prior and PINN + CFD reconstruction to $Q_{\text{react}}(t)$, the inferred source profile was scaled by 0.8, 0.9, 1.0, 1.1 and 1.2, while all other model parameters and training settings were kept unchanged.

2.6. Physics-Informed Neural Network and CFD-Prior-Constrained Training Framework

To reconstruct the continuous three-dimensional temperature field of the black tea fermentation bed under sparse sensing, a physics-informed neural network was constructed and the CFD-derived temperature field was introduced as a volumetric soft spatial prior during PINN training. The input variables were the normalized spatial coordinates, time and ambient air temperature, namely $(x, y, z, t, T_{\text{air}})$. The network output was the tea-bed temperature at the corresponding spatiotemporal location, denoted as $T_{\theta}(x, y, z, t)$. The overall model framework is shown in Figure 4.

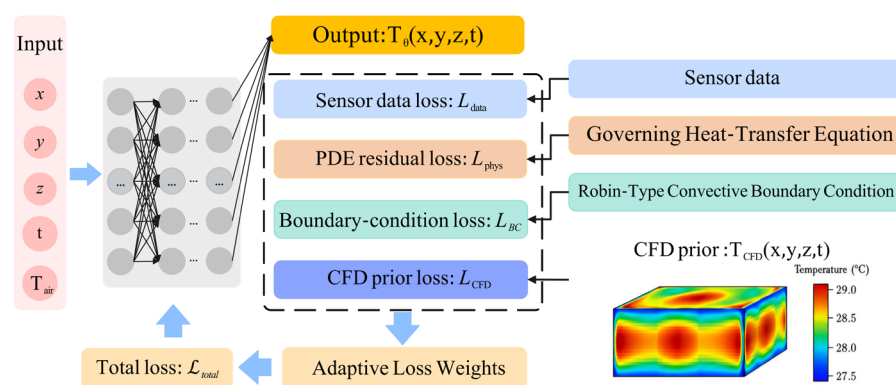


Figure 4. Framework of the CFD-prior-constrained physics-informed neural network.

All inputs were min–max normalized to $[-1, 1]$, and the output temperature was standardized using the mean and standard deviation calculated from the training data. The PINN was implemented in Python 3.6.5 with PyTorch 1.10.2 (CPU build) as a fully connected feed-forward network containing six hidden layers, 80 neurons per layer and tanh activation. Automatic differentiation in PyTorch was used to evaluate the derivatives in the heat-transfer and boundary residuals. The total loss combined the measured-temperature, physical-residual, convective-boundary and CFD-prior terms:

$$L = \lambda_d L_{\text{data}} + \lambda_p L_{\text{phys}} + \lambda_b L_{\text{BC}} + \lambda_c L_{\text{CFD}} \quad (9)$$

where λ_d , λ_p , λ_b and λ_c are the weights of the data loss, physical-residual loss, boundary loss and CFD-prior loss, respectively. Because the measured temperature samples at $t = 0$

were already included in L_{data} , the initial temperature was implicitly constrained through the data loss, and no separate initial-condition loss L_{IC} was introduced. The measured-data loss L_{data} was evaluated using the measured samples from the nine PT100 sensor locations:

$$L_{\text{data}} = \frac{1}{N_s} \sum_{i=1}^{N_s} [T_\theta(x_i, y_i, z_i, t_i) - T_{\text{meas},i}]^2 \quad (10)$$

The physical-residual loss L_{phys} , boundary loss L_{BC} and CFD-prior loss L_{CFD} were defined as follows [19,30–33]:

$$L_{\text{phys}} = \frac{1}{N_f} \sum_{i=1}^{N_f} \left[(\rho C_p)_{\text{eff}} \frac{\partial T_\theta}{\partial t} - \nabla \cdot (k_{\text{eff}} \nabla T_\theta) - Q_{\text{react}}(t) \right]^2 \quad (11)$$

$$L_{\text{BC}} = \frac{1}{N_b} \sum_{i=1}^{N_b} \left[-k_{\text{eff}} \frac{\partial T_\theta}{\partial n} - h(T_\theta - T_{\text{air}}) \right]^2 \quad (12)$$

$$L_{\text{CFD}} = \frac{1}{N_c} \sum_{i=1}^{N_c} [T_\theta(x_i, y_i, z_i, t_i) - T_{\text{CFD}}(x_i, y_i, z_i, t_i)]^2 \quad (13)$$

where $T_{\text{CFD}}(x_i, y_i, z_i, t_i)$ is the CFD-derived temperature prior ($^{\circ}\text{C}$) at a randomly sampled point (x_i, y_i, z_i, t_i) from the full three-dimensional CFD field; x_i , y_i and z_i are spatial coordinates (m); t_i is the sampling time (s); N_s , N_f , N_b and N_c denote the sample sizes used for the measured-data, physical-residual, boundary and CFD-prior losses, respectively; i is the sample index; $T_{\text{meas},i}$ is the measured temperature ($^{\circ}\text{C}$); and T_θ denotes the network-predicted temperature ($^{\circ}\text{C}$).

The baseline PINN and PINN + CFD used the same measured-temperature data, physical-residual formulation, boundary conditions, thermophysical parameters and $Q_{\text{react}}(t)$ sequence. Because the same $Q_{\text{react}}(t)$ sequence was also used to generate the CFD field, the CFD prior was data-informed rather than independent of the training measurements.

2.7. Adaptive Loss-Weighting Strategy

Because the data, physical-residual, boundary and CFD-prior losses may exhibit different numerical scales and convergence behaviors, fixed loss weights can lead to optimization imbalance in PINNs [26–28]. Therefore, a SoftAdapt-inspired, study-specific adaptive weighting rule was used to adjust the contribution of each loss term during training [37].

Before adaptive weighting, L_{phys} , L_{BC} and L_{CFD} were multiplied by 1.0×10^5 , 1.0×10^{-2} and 0.12, respectively, while L_{data} was left unchanged. These factors were numerical scaling coefficients rather than physical parameters. Let $L_i(k)$ denote the resulting value of the i -th loss term at training epoch k , where $i \in \{d, p, b, c\}$ represents the data, physical-residual, boundary and CFD-prior losses, respectively, and $m = 4$ is the total number of loss terms. The clipped loss-change ratio was calculated as:

$$r_i(k) = \text{clip} \left(\frac{L_i(k)}{L_i(k-1) + \varepsilon}, \frac{1}{\rho}, \rho \right) \quad (14)$$

Here, ε is a small positive constant, ρ is the clipping parameter, and $\text{clip}(\cdot)$ limits the ratio to the interval $[1/\rho, \rho]$. The adaptive weights were then obtained by exponential normalization:

$$\lambda_i(k) = \frac{\exp(r_i(k))}{\sum_{j=1}^m \exp(r_j(k))} \quad (15)$$

Here, j is the loss-term index in the normalization sum, and $\lambda_i(k)$ is the adaptive weight of the i -th loss term at epoch k . The four weights were initialized uniformly to 0.25,

and ρ was set to 4.0. The CFD-prior weight was capped at 0.95 to prevent the CFD prior from dominating the optimization in extreme cases.

The final CFD-prior-constrained PINN was initialized from the pretrained baseline PINN and then further trained after introducing the CFD-prior loss. The AdamW optimizer was used with an initial learning rate of 2.0×10^{-4} , a weight-decay coefficient of 1.0×10^{-6} and a total of 4200 training epochs. A stepwise learning-rate decay was applied in the later training stage, resulting in a final learning rate of 8.57×10^{-6} . Gradient clipping was applied with a maximum gradient norm of 1.0 to reduce local gradient fluctuations during multi-loss optimization.

The measured temperature dataset contained 720 sampling time points, with nine internal temperature sensors at each time point, resulting in 6480 measured temperature samples. In each epoch, up to 1024 measured samples were randomly selected to calculate the data loss, and 384 collocation points were randomly generated across the spatiotemporal domain to calculate the physical residual. In addition, 96 boundary points were generated in each epoch to calculate the convective boundary loss. The CFD-prior samples followed the volumetric sampling scheme in Equation (11) and were not limited to the instrumented $z = 0.04$ m plane. In each epoch, up to 2048 CFD-prior samples were randomly selected to calculate the CFD-prior loss.

To assess stochastic variability in the training procedure, the complete PINN + CFD workflow was repeated five times using different random seeds. The spatial training and validation partition, pretrained starting checkpoint, network architecture and training hyperparameters were kept unchanged across repetitions. The random seeds controlled the stochastic sampling procedures and optimization trajectory, including mini-batch, collocation-point, boundary-point and CFD-prior sampling.

2.8. Model Evaluation Metrics and Prediction

The trained models were evaluated under three representative fermentation stages: linear heating, constant-temperature fermentation and dynamic fermentation. Two-dimensional plane predictions were generated at $z = 0.04$ m for comparison with the interpolated sensor-based reference field. Three-dimensional temperature fields were predicted over the full tea-bed domain to analyze internal spatial temperature distributions. Surface temperature fields were predicted at $z = 0.08$ m and compared with infrared thermograms for held-out surface validation. Model performance was evaluated using the mean absolute error (MAE), root mean square error (RMSE) and maximum absolute error (MaxAE):

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^N (T_{\theta,i} - T_{\text{ref},i})^2} \quad (16)$$

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |T_{\theta,i} - T_{\text{ref},i}| \quad (17)$$

$$\text{MaxAE} = \max_i |T_{\theta,i} - T_{\text{ref},i}| \quad (18)$$

where N is the number of evaluation samples, $T_{\theta,i}$ is the model-predicted temperature ($^{\circ}\text{C}$) and $T_{\text{ref},i}$ is the corresponding reference temperature ($^{\circ}\text{C}$). These metrics were used to quantify prediction accuracy and, together with the physical-residual analysis, to assess the physical consistency of the reconstructed temperature field.

For the leave-one-sensor-out validation, model differences were assessed using paired fold-wise statistics because each held-out sensor yielded one RMSE value for each model. The same nine held-out-sensor folds were used for paired Wilcoxon signed-rank tests as a supplementary statistical analysis of the primary leave-one-sensor-out validation. This analysis was treated as an exploratory within-batch assessment rather than an independent validation experiment. Given the small number of folds and the fact that all folds originated

from a single fermentation batch with overlapping training data, the resulting p -values were interpreted as nominal, exploratory within-batch evidence.

3. Results

3.1. Training Convergence and Adaptive Loss-Weight Analysis

To evaluate the training stability of the CFD-prior-constrained PINN, the training losses and adaptive loss weights were first analyzed. The final model was trained jointly using L_{data} , L_{phys} , L_{BC} and L_{CFD} . As shown in Figure 5, the total loss decreased overall and reached a stable plateau in the later training stage. During the last 300 epochs, the mean total loss was 0.007986, with a range of 0.006128–0.011283, and no obvious divergence or large loss spikes were observed.

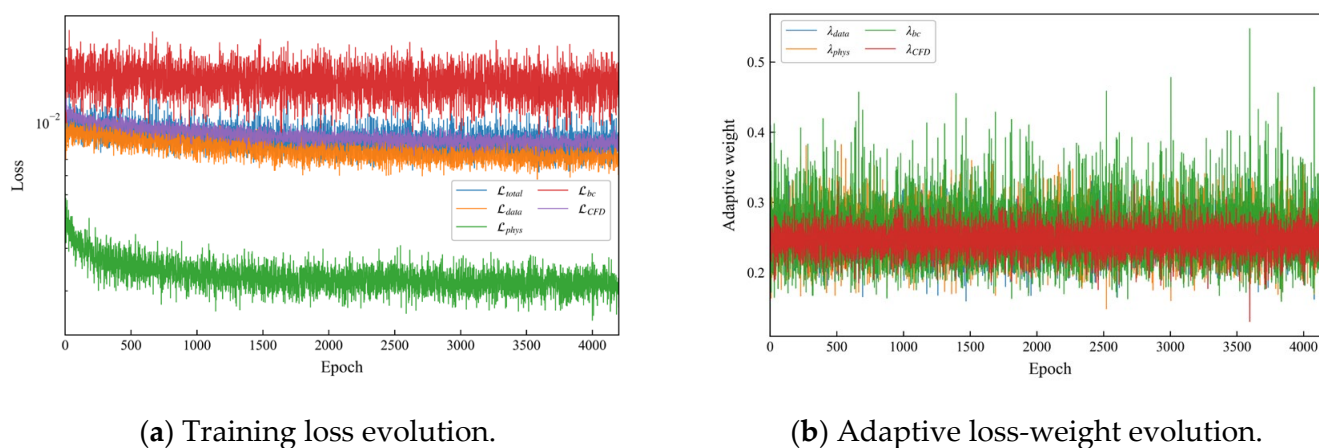


Figure 5. Training diagnostics of the CFD-prior-constrained PINN.

All loss components remained at relatively low levels during the later training stage, indicating that the model could fit the measured sensor temperatures while satisfying the equivalent heat-transfer equation and the convective boundary condition. The adaptive weights fluctuated naturally during late-stage training, with the CFD-prior weight ranging from 0.1671 to 0.2945. This result indicates that the CFD prior continuously contributed to model optimization but did not dominate the training process. Compared with a fixed-weight strategy, the adaptive weighting scheme helped reduce training instability caused by differences in magnitude and convergence rate among the loss terms.

Across the five random-seed repetitions, the MAE, RMSE and MaxAE were 0.416 ± 0.003 °C, 0.485 ± 0.003 °C and 1.553 ± 0.007 °C, respectively. These results indicate low stochastic variability under the fixed pretrained initialization, with the complete run-level results provided in Supplementary Table S6.

3.2. Predictive Accuracy and Within-Batch Spatial Validation

3.2.1. Stage-Dependent Fitting Performance at Instrumented Locations

Because the internal measured temperatures were mainly obtained from the nine sensors on the $z = 0.04$ m plane, model performance on this plane was first evaluated using prediction errors at the instrumented locations. This section compares the prediction accuracy of different models at the measured sensor locations and then further examines their ability to reconstruct the planar thermal state. To evaluate temperature prediction at the instrumented locations, the CFD-prior-constrained PINN (PINN + CFD) was compared with standalone CFD, a multilayer perceptron (MLP) and the baseline PINN. All models were evaluated using the same sensor data under the three representative fermentation stages, with MAE, RMSE and MaxAE used as the error metrics.

Table 2 reports the sensor-level prediction errors of MLP, CFD, PINN and PINN + CFD across the three fermentation stages. MLP achieved low errors at the instrumented locations, but it did not explicitly incorporate the heat-transfer equation, convective boundary condition or internal heat-source constraint. However, its low sensor-level error does not necessarily indicate reliable spatial extrapolation in unmeasured regions. The standalone CFD model showed relatively large errors in all three stages, indicating that the measured sensor temperatures could not be fully reproduced using only effective thermophysical parameters, boundary heat-transfer coefficients and the prescribed dynamic internal heat source. Thus, the CFD result is more suitable as a physical spatial prior for sensor-free regions than as a true temperature field.

Table 2. Sensor-level prediction errors under different fermentation stages.

Stage	Model Evaluation Metrics	MLP	CFD	PINN	PINN + CFD
Linear heating	MAE/°C	0.069	0.385	0.107	0.095
	RMSE/°C	0.089	0.475	0.129	0.119
	MaxAE/°C	0.294	1.095	0.531	0.406
Constant temperature	MAE/°C	0.053	0.337	0.084	0.084
	RMSE/°C	0.067	0.419	0.115	0.111
	MaxAE/°C	0.233	1.062	0.491	0.429
Dynamic perturbation	MAE/°C	0.041	0.447	0.103	0.105
	RMSE/°C	0.055	0.499	0.139	0.141
	MaxAE/°C	0.232	1.047	0.493	0.522

Compared with standalone CFD, both PINN and PINN + CFD substantially reduced sensor-level errors. PINN + CFD slightly improved the prediction accuracy relative to the baseline PINN during the linear-heating and constant-temperature stages, whereas its RMSE was slightly higher than that of the baseline PINN during the dynamic-perturbation stage. This suggests that the CFD prior can improve prediction stability under relatively stable boundary conditions but may introduce a small bias when the external thermal boundary fluctuates strongly. Therefore, in this study, the CFD-derived temperature field was introduced as a volumetric soft spatial prior during training rather than as a strongly supervised substitute for measured data.

3.2.2. Leave-One-Sensor-Out Spatial Validation

To further evaluate the within-batch spatial prediction ability of different models at unmeasured sensor locations, leave-one-sensor-out cross-validation was performed. For each held-out sensor, prediction errors were calculated over the full fermentation period to characterize spatial prediction performance during continuous fermentation. In each validation fold, the $Q_{\text{react}}(t)$ source term and CFD prior were reconstructed using only the remaining eight training sensors, and the data from the held-out sensor were not used. The complete temperature sequence of one sensor from 0 to 6 h was removed from the training set, the model was trained using the other eight sensors, and the full temperature trajectory of the excluded sensor was then predicted. This procedure was repeated for all nine sensors, yielding nine held-out sensor folds for within-batch spatial validation. All models used the same data partitioning, training epochs and evaluation metrics, thereby avoiding performance overestimation caused by temporally adjacent samples appearing simultaneously in the training and test sets. The same nine held-out-sensor folds were additionally used for paired fold-wise Wilcoxon signed-rank tests to assess the statistical significance of the observed RMSE differences. This analysis served as a supplementary

statistical assessment of the leave-one-sensor-out results, and detailed results are provided in Supplementary Table S7.

As shown in Table 3, MLP showed higher average MAE and RMSE in the leave-one-sensor-out validation than in the instrumented training-plane evaluation, indicating limited spatial extrapolation from sparse sensor data alone. The baseline PINN reduced the average RMSE by 7.4% relative to MLP and achieved lower RMSE in 8 of 9 held-out-sensor folds ($p = 0.045$). This represents a nominally significant paired decrease, but should be interpreted as exploratory within-batch evidence because the comparison was based on nine folds from a single fermentation batch.

Table 3. Leave-one-sensor-out spatial-validation performance.

Model	MAE/°C	RMSE/°C	RMSE SD/°C	MaxAE/°C
MLP	0.528	0.646	0.206	2.240
PINN	0.503	0.598	0.210	1.900
PINN + CFD fixed weights	0.476	0.572	0.179	1.833
PINN + CFD adaptive weights	0.501	0.594	0.187	1.733

The fixed-weight PINN + CFD model achieved the lowest average MAE and RMSE, reducing the average RMSE by approximately 11.4% relative to MLP. Its RMSE was lower than that of MLP in all nine held-out-sensor folds ($p = 0.004$), indicating a nominally significant paired decrease within this validation setting. Its lower RMSE standard deviation further indicated that the fixed-weight PINN + CFD framework achieved more consistent prediction errors than MLP across the held-out sensors.

The adaptive-weight PINN + CFD model had a slightly higher average RMSE than the fixed-weight model but achieved the lowest MaxAE. Compared with the baseline PINN, the adaptive-weight model reduced the average RMSE by 0.6% and achieved lower RMSE in all nine held-out-sensor folds ($p = 0.004$). Together with its lower MaxAE, this result indicates that adaptive weighting mainly reduced extreme errors at challenging spatial locations rather than consistently minimizing the mean error.

The fixed-weight PINN + CFD model achieved the lowest RMSE in all three stages, with values of 0.671, 0.467 and 0.486 °C, respectively. Thus, its lower spatial-prediction RMSE was maintained across the three tested fermentation stages, rather than arising only after aggregation over the full 6 h period, and detailed results are provided in Supplementary Table S8.

3.2.3. Qualitative Comparison of Planar Temperature-Field Trends

Based on the sensor-level error analysis, the planar temperature-field reconstructions of different models were further compared on the $z = 0.04$ m plane. Because the continuous true temperature field on this plane could not be measured directly, RBF interpolation of the measured sensor data was used only as a planar trend reference. This reference field represents a sparse-measurement-constrained two-dimensional temperature-distribution trend, not a ground-truth temperature field. It was used to assist comparison of how different models represented relative high-temperature regions, temperature-gradient directions and boundary-transition features.

Figure 6 shows the reconstructed planar temperature fields at 3600, 10,800 and 18,000 s, corresponding to the three fermentation stages. During the linear-heating stage, the ambient temperature gradually increased and the internal temperature response of the tea bed was relatively mild. Both MLP and PINN approximated the RBF reference trend near the sensor locations, whereas the MLP distribution was mainly determined by data fitting. Compared with MLP, the PINN-based models produced smoother planar fields because

their predictions were constrained by the heat-transfer residual. In PINN + CFD, the additional CFD-derived volumetric soft spatial prior further guided the spatial trend in unmeasured regions.

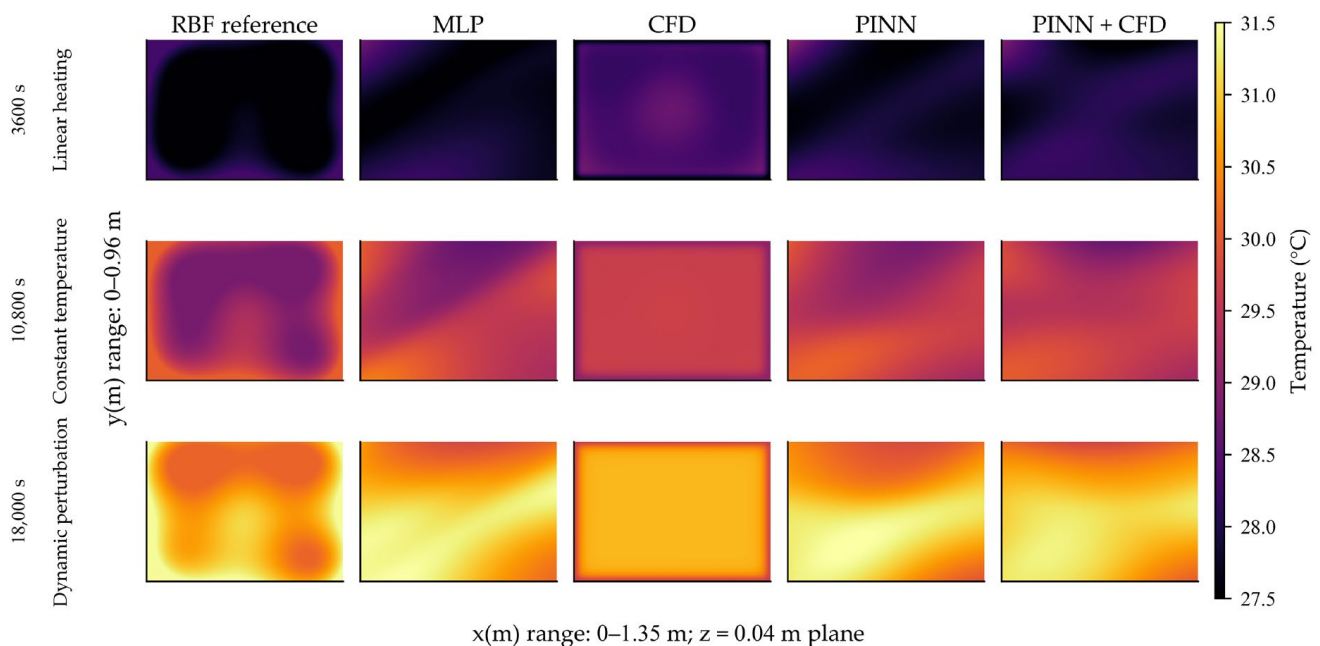


Figure 6. Two-dimensional temperature-field reconstruction on the instrumented plane.

During the constant-temperature stage, the internal temperature variation of the tea bed became relatively stable, and the balance between internal heat generation and boundary heat loss was more evident. In this stage, the RMSE of PINN + CFD was slightly lower than that of the baseline PINN. This result suggests that the CFD spatial prior provided a useful distributional constraint under relatively stable boundary conditions. In the reconstructed planar temperature field, PINN + CFD better preserved the overall temperature level and gradient direction, while reducing the absolute-temperature bias observed in standalone CFD.

During the dynamic-perturbation stage, the ambient temperature fluctuated because of heater switching, and the tea-bed temperature field showed stronger transient behavior. In this stage, the sensor-level error of PINN + CFD was slightly higher than that of the baseline PINN, indicating that the CFD prior may introduce a stage-dependent bias when the external thermal boundary changes rapidly. Nevertheless, the planar temperature trend reconstructed by PINN + CFD maintained good spatial continuity and showed no obvious local non-physical oscillations. This result supports the use of the CFD prior as a soft constraint in the dynamic stage, provided that measured data and physical residuals are retained to correct the prior while preserving a plausible spatial structure.

Overall, these planar comparisons indicate that sensor-level errors alone are insufficient for evaluating thermal-field reconstruction. Although MLP fitted the measured plane well and standalone CFD preserved a continuous spatial trend, the PINN-based models better maintained spatial continuity in unmeasured regions.

3.3. Ablation Analysis of L_{phys} , CFD Prior and Adaptive Weighting

The ablation analysis, as shown in Table 4, was used to clarify the separate roles of the physical residual, CFD prior and adaptive weighting. The comparison considered prediction accuracy, surface validation error and training stability, rather than only sensor-level fitting error.

Table 4. Ablation study of model components.

Model	L_{phys}	Q_{react}	CFD Prior	Adaptive Weights	$z = 0.04 \text{ m}$		Surface IR	
					MAE/ $^{\circ}\text{C}$	RMSE/ $^{\circ}\text{C}$	MAE/ $^{\circ}\text{C}$	RMSE/ $^{\circ}\text{C}$
MLP	No	No	No	No	0.054	0.072	2.177	2.270
CFD	CFD solver	Yes	No	No	0.389	0.465	1.383	1.394
PINN without Q_{react}	Yes	No	No	No	0.130	0.195	0.884	0.908
PINN	Yes	Yes	No	No	0.098	0.128	0.841	0.905
PINN + CFD fixed weights	Yes	Yes	Yes	No	0.093	0.127	0.733	0.834
PINN + CFD adaptive weights	Yes	Yes	Yes	Yes	0.092	0.124	0.713	0.812

First, L_{phys} constrained the network output to satisfy the transient heat-transfer equation with the $Q_{\text{react}}(t)$ source term. Its main contribution was not to further reduce fitting error at measured sensor locations, where MLP achieved the lowest errors in Table 2, but to suppress non-physical fluctuations and improve the interpretability of spatial extrapolation.

Second, the CFD-derived temperature field was introduced as a volumetric soft spatial prior through the CFD-prior loss L_{CFD} and supplied a three-dimensional spatial trend for regions without sensors. The standalone CFD model showed relatively large sensor-level errors, probably because of uncertainties in effective thermophysical properties, boundary heat-transfer coefficients and internal heat-source settings. When used as a volumetric soft spatial prior rather than as a final prediction, the CFD-derived temperature field helped regularize extrapolation in sensor-free regions while allowing measured data and heat-transfer residuals to correct CFD-related bias.

The one-at-a-time sensitivity analysis showed that porosity produced the largest variation in the standalone CFD prior, whereas the PINN + CFD reconstruction remained comparatively stable across perturbations of k_{eff} , h and porosity. Similarly, scaling $Q_{\text{react}}(t)$ produced a larger maximum RMSE change for the CFD prior than for PINN + CFD (37.7% versus 4.7%). These results indicate that the PINN + CFD reconstruction was less sensitive to uncertainty in the effective thermal properties and apparent heat-source amplitude than the standalone CFD prior. Complete results are provided in Supplementary Table S5.

Finally, adaptive weighting stabilized multi-loss training. The total loss reached a stable plateau, and the CFD-prior weight fluctuated within a moderate range, indicating that the CFD prior contributed to training without dominating optimization. Accordingly, the ablation analysis supports improved sparse-sensor extrapolation and training stability rather than universal error reduction across sensors, metrics or fermentation stages.

3.4. Three-Dimensional Thermal-State Reconstruction and Physical Consistency

Because the continuous internal three-dimensional temperature field was not directly measurable, the reconstructed maps were interpreted as physically constrained estimates rather than direct observations. Figure 7 displays the reconstructed three-dimensional thermal state at 3600, 10,800, and 18,000 s. These time points correspond to the linear-heating, constant-temperature, and dynamic-perturbation stages, respectively. They were selected for visualization only and do not define the spatiotemporal sampling of the CFD prior. Across the displayed times, the reconstructed field developed from weak gradients to more pronounced heat accumulation and inter-layer heterogeneity.

Table 5 shows small mean-temperature differences between CFD and PINN + CFD (-0.241 to 0.057 $^{\circ}\text{C}$), but larger spatial standard deviations and temperature ranges for PINN + CFD during the middle and later stages. The principal difference was therefore stronger reconstructed local heterogeneity rather than a shift in the overall temperature level. Together with the inter-layer patterns shown in Figure 7, these results indicate

temperature heterogeneity along the tea-bed thickness direction. A qualitatively similar thickness-direction heterogeneity was reported by Lian et al. [11], although the specific inter-layer temperature distributions are not directly comparable because the heat-transfer and boundary conditions differed between the two studies.

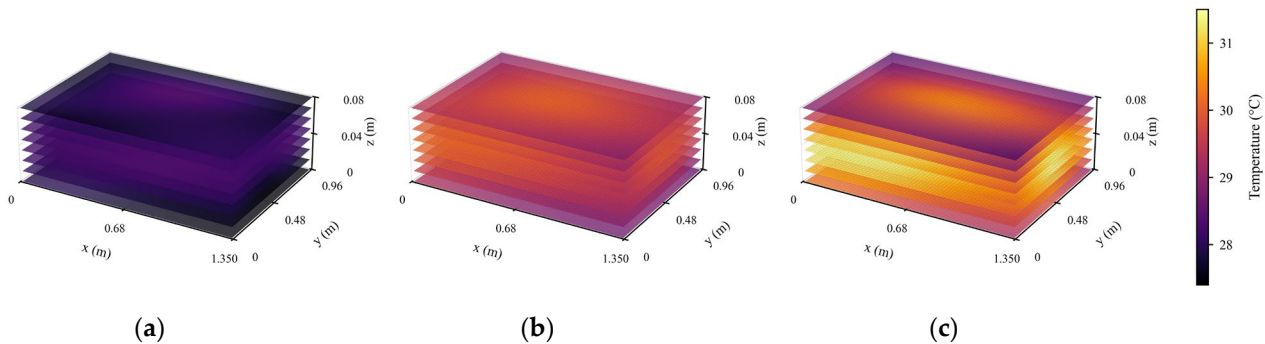


Figure 7. PINN + CFD-reconstructed three-dimensional thermal-state visualizations. (a) 3600 s, (b) 10,800 s, and (c) 18,000 s.

Table 5. Three-dimensional temperature-field statistics of CFD and PINN + CFD.

Stage	CFD			PINN + CFD			Δ Mean/°C	Δ SD/°C	Δ Range/°C
	Mean/°C	SD/°C	Range/°C	Mean/°C	SD/°C	Range/°C			
3600 s	28.152	0.328	1.723	28.019	0.324	1.932	−0.133	−0.004	0.209
7200 s	28.917	0.254	1.116	28.775	0.371	1.977	−0.142	0.117	0.860
10,800 s	29.551	0.212	0.864	29.549	0.456	2.298	−0.002	0.243	1.434
14,400 s	29.951	0.407	1.554	30.008	0.568	2.845	0.057	0.161	1.291
18,000 s	30.580	0.438	1.785	30.399	0.714	3.423	−0.181	0.276	1.638
21,600 s	30.612	0.556	2.263	30.371	0.651	3.261	−0.241	0.096	0.998

3.5. Held-Out Depth-Wise Test-Point Validation

To assess thickness-direction extrapolation, the finalized models were evaluated against six held-out depth-wise test points defined in Section 2.1.

Table 6 compares the prediction errors of the four models at the untrained depths under the three fermentation stages. Although MLP achieved low errors on the instrumented $z = 0.04$ m plane (Section 3.2.1), it yielded the largest MAE, RMSE, and MaxAE at the depth-wise test points in all three stages. Standalone CFD generated a continuous three-dimensional field but remained less accurate than the PINN-based models, whereas the baseline PINN reduced the depth-wise errors relative to both MLP and CFD. PINN + CFD achieved the lowest MAE, RMSE, and MaxAE in every stage. Its RMSE values were 0.128, 0.129, and 0.296 °C during linear heating, constant-temperature fermentation, and dynamic perturbation, respectively. The corresponding MaxAE values were 0.263, 0.328, and 0.490 °C. The larger errors during dynamic perturbation showed that extrapolation was most difficult under a fluctuating thermal boundary.

These six held-out depth-wise test points provide point-wise descriptive evidence of local thickness-direction extrapolation within the limited spatial coverage of the test layout. Because they were fixed spatial test points from one continuous fermentation run, rather than independent cross-validation folds or replicated batches, they were not included in the nine-fold leave-one-sensor-out Wilcoxon analysis. Accordingly, the findings support local thickness-direction extrapolation at the tested locations. Height-stratified results in Supplementary Tables S9 and S10 showed that the pooled statistics were not dominated by either measurement height.

Table 6. Depth-wise reference-point validation errors under different fermentation stages.

Stage	Model Evaluation Metrics	MLP	CFD	PINN	PINN + CFD
Linear heating	MAE/°C	0.991	0.423	0.149	0.107
	RMSE/°C	1.515	0.525	0.187	0.128
	MaxAE/°C	4.239	1.503	0.516	0.263
Constant temperature	MAE/°C	0.409	0.309	0.162	0.111
	RMSE/°C	0.590	0.388	0.198	0.129
	MaxAE/°C	1.843	1.007	0.487	0.328
Dynamic perturbation	MAE/°C	0.622	0.437	0.293	0.262
	RMSE/°C	0.727	0.554	0.352	0.296
	MaxAE/°C	1.591	1.294	0.778	0.490

3.6. Held-Out Surface Infrared Thermography Validation

Infrared thermography was used as an independent surface-level validation source for model extrapolation at the upper surface of the tea bed ($z = 0.080$ m). The thermograms were not used for training MLP, CFD, PINN or PINN + CFD.

Figure 8 shows that the surface temperature field was spatially non-uniform at all three observed time points. At 18,000 s, boundary cooling was evident and the spatial heterogeneity became more pronounced. MLP exhibited an overall positive surface-temperature bias, whereas standalone CFD maintained spatial continuity but showed stage-dependent deviations from the infrared reference. PINN + CFD achieved the lowest surface prediction errors during linear heating and dynamic perturbation, whereas standalone CFD produced the lowest errors during constant-temperature fermentation.

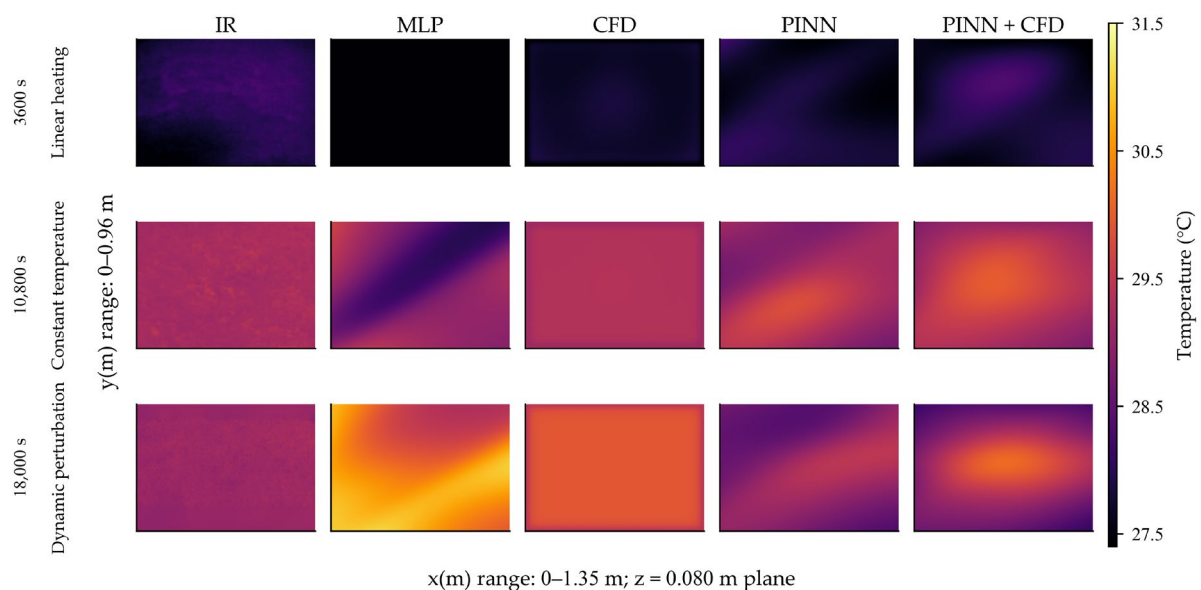
**Figure 8.** Comparison between infrared thermograms and surface temperature predictions from different models.

Table 7 shows a clear stage-dependent model ranking in surface-temperature validation against infrared thermography. MLP produced the largest MAE, RMSE, and MaxAE in all three stages, indicating limited surface extrapolation from the instrumented $z = 0.04$ m plane alone. Standalone CFD achieved the lowest values for all three metrics during constant-temperature fermentation, including an RMSE of 0.119 °C. This result suggests that the CFD formulation was more consistent with the measured surface thermal pattern under the relatively stable boundary condition. In contrast, PINN + CFD achieved the

lowest values for all three metrics during linear heating and dynamic perturbation, with RMSEs of 0.227 and 0.426 °C, respectively. Thus, no model was uniformly best across the tested thermal-boundary regimes, but PINN + CFD was more advantageous under the tested time-varying boundary conditions.

Table 7. Surface temperature validation errors against infrared thermography.

Stage	Model Evaluation Metrics	MLP	CFD	PINN	PINN + CFD
Linear heating	MAE/°C	2.360	0.292	0.352	0.191
	RMSE/°C	2.480	0.326	0.367	0.227
	MaxAE/°C	3.617	0.669	0.902	0.591
Constant-temperature	MAE/°C	0.548	0.104	0.254	0.283
	RMSE/°C	0.681	0.119	0.300	0.351
	MaxAE/°C	1.482	0.353	0.732	0.862
Dynamic-perturbation	MAE/°C	2.177	1.383	0.841	0.341
	RMSE/°C	2.270	1.394	0.905	0.426
	MaxAE/°C	3.511	1.819	1.432	1.091

3.7. Apparent Heat-Source Dynamics and Polyphenol Association

To evaluate consistency with the macroscopic energy balance, $Q_{\text{eff}}(t)$ was inferred from the temperature sequence and the equivalent heat-transfer model. $Q_{\text{react}}(t)$ was derived from $Q_{\text{eff}}(t)$ in Section 2.5.

Figure 9a shows that the inferred apparent process-level heat-source index $Q_{\text{react}}(t)$ varied throughout the continuous 6 h fermentation run. The stage-integrated $Q_{\text{react}}(t)$ values were 425.764, 314.237 and 365.353 ($\text{W}\cdot\text{h} / \text{m}^3$) during the linear-heating, constant-temperature and dynamic-perturbation stages, respectively (Table 8). This late-stage increase coincided with the stronger spatial heterogeneity described in Section 3.4.

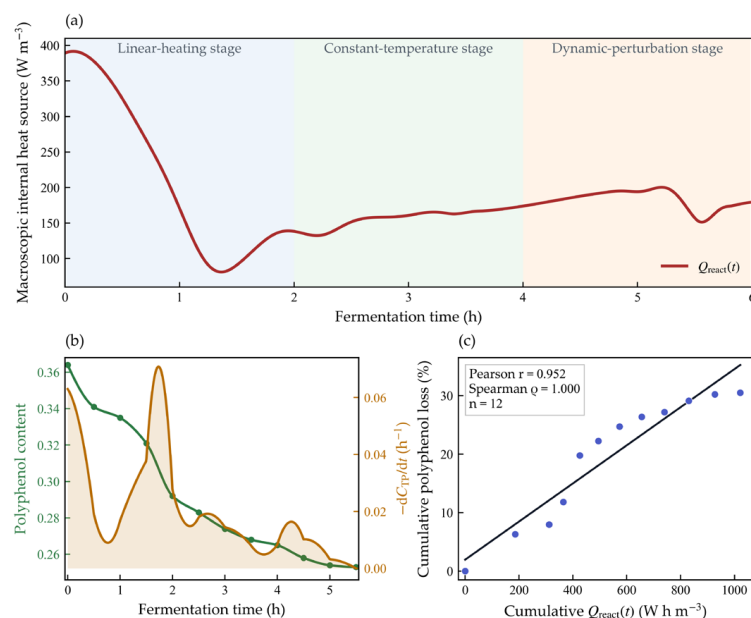


Figure 9. Apparent process-level heat-source dynamics and its association with polyphenol changes during black tea fermentation. (a) Continuous $Q_{\text{react}}(t)$ source profile during the linear-heating stage, constant-temperature stage and dynamic-perturbation stage. (b) Changes in polyphenol content and polyphenol decline rate during fermentation. (c) Relationship between cumulative $Q_{\text{react}}(t)$ and cumulative polyphenol loss.

Table 8. Stage-wise characteristics of $Q_{\text{react}}(t)$ and polyphenol loss.

Stage	Mean $Q_{\text{react}}(t)$ W/m ³	Peak $Q_{\text{react}}(t)$ W/m ³	Cumulative $Q_{\text{react}}(t)$ W · h/m ³	Polyphenol Loss /%
Linear heating	213.093	391.648	425.764	19.780
Constant temperature	157.114	173.114	314.237	7.418
Dynamic perturbation	182.651	200.400	365.353	3.297

The stage-dependent pattern was consistent with changes in the dominant thermal contributions across the fermentation run. External heating, initial-state adjustment, and internal heat accumulation jointly shaped the thermal response during linear heating. The lower constant-temperature value was consistent with a more stable balance between internal heat generation and boundary heat loss. During dynamic perturbation, boundary fluctuations, internal heat accumulation, and spatially non-uniform heat dissipation jointly influenced the thermal state. Because $Q_{\text{react}}(t)$ integrates both internal and boundary-related thermal contributions, it represents macroscopic thermal evolution rather than a directly measured biochemical heat-release rate.

Tea-polyphenol content decreased from 0.364 to 0.253, with stage-wise reductions of 19.780%, 7.418%, and 3.297% during linear heating, constant-temperature fermentation, and dynamic perturbation, respectively (Figure 9b; Table 8). Across all 12 sampling time points, instantaneous $Q_{\text{react}}(t)$ was not significantly associated with the instantaneous polyphenol-decline rate, whereas the cumulative quantities showed only a descriptive association (Figure 9c; Supplementary Table S11).

Accordingly, $Q_{\text{react}}(t)$ may serve as a process-level indicator of changes in the macroscopic thermal state of the tea bed, but it should not be interpreted as a direct biochemical marker. Replicated batch experiments, longer time-series analyses based on non-cumulative variables, and independently measured heat-release data are required to evaluate its mechanistic relevance and practical utility.

3.8. Limitations and Applicability Boundary

This study adapted a multi-fidelity physics-informed learning strategy to black tea fermentation by introducing a CFD-derived temperature field into a PINN as a volumetric soft spatial prior. This framework enabled three-dimensional thermal-state reconstruction of the tea bed under sparse sensing. However, to comprehensively assess its scientific boundaries and engineering applicability, the following limitations should be considered:

- (1) All model-development, parameter-calibration and validation data were obtained from one batch of Lichuan black tea during a single continuous 6 h fermentation run. Spatial validation was also limited to six fixed held-out depth-wise points and periodically acquired surface infrared thermograms. Although these measurements provided local spatial-validation evidence within the sampled regions, they do not establish the true temperature field throughout the entire tea-bed volume or demonstrate cross-batch generalization.
- (2) The linear-heating, constant-temperature and dynamic-perturbation periods were consecutive segments of the same fermentation run rather than independent experiments. Differences in stage-wise errors may therefore be confounded by fermentation time and concurrent changes in biochemical state, heat accumulation, moisture distribution and effective material properties. Independent replicated batches or stage-specific experimental designs are required to separate the effects of thermal-boundary conditions from the continuing fermentation process.

- (3) The tea bed was treated as an effective porous medium for estimating its bulk thermo-physical properties, whereas the final CFD calculation represented it as a stationary solid-equivalent heat-conduction domain without explicitly resolving Darcy airflow or the pressure field. The use of constant effective properties and a unified convective heat-transfer coefficient does not account for possible variations associated with cultivar, moisture content, packing density and airflow conditions. Under a $\pm 20\%$ global perturbation of h , the PINN + CFD RMSE changed by only -0.6% to $+0.9\%$, indicating limited sensitivity to the tested global perturbation. However, this result does not validate the spatial distribution of local boundary heat loss or account for unresolved airflow effects.
- (4) The high correlation between cumulative $Q_{\text{react}}(t)$ and cumulative polyphenol loss was calculated from only 12 monotonically cumulative observations. The reported Pearson and Spearman coefficients may therefore largely reflect a shared temporal trend rather than a direct biological relationship. This association should be treated as descriptive evidence rather than as evidence of biochemical causality. The absence of a significant association between instantaneous $Q_{\text{react}}(t)$ and the instantaneous polyphenol-decline rate further limits its biological interpretation.
- (5) The CFD prior was data-informed because the measurement-derived $Q_{\text{react}}(t)$ sequence inferred from the training-plane sensors was also used to generate the CFD field. Excluding the held-out depth-wise test points and infrared thermograms prevented their direct leakage into evaluation but did not eliminate this coupling. Such coupling arises because spatially resolved boundary heat exchange and internal heat generation are only partially observable in engineering thermal processes, making a measurement-informed effective source term necessary to render the reconstruction problem identifiable. Nevertheless, this coupling limits the interpretation of the present results to the integrated data-informed modeling framework. Its reproducibility and external validity across batches remain to be established through independent batch experiments and independently characterized heat-source and boundary inputs.

Future work should include independent batches, multiple cultivars and bed geometries, denser multi-depth measurements, spatially resolved boundary characterization, and independently measured moisture, airflow and heat-source inputs. Longer time series analyzed using non-cumulative, detrended or lagged variables are also required before the framework can be extended to industrial monitoring or closed-loop control.

4. Conclusions and Outlook

Black tea fermentation is a spatially heterogeneous and dynamically evolving multi-stage process, yet the continuous internal three-dimensional temperature field is difficult to measure under practical processing conditions, leaving only sparse spatial observations. This study therefore applied a CFD-prior-constrained PINN to reconstruct the three-dimensional thermal state of the tea bed during a continuous 6 h run. The framework was evaluated using within-run leave-one-sensor-out spatial validation, six held-out depth-wise test points and stage-wise surface validation based on the available infrared thermograms.

The results showed that MLP achieved the lowest error at the trained $z = 0.04$ m plane, whereas PINN + CFD showed more consistent spatial extrapolation performance across leave-one-sensor-out validation, held-out depth-wise test-point validation and most surface infrared thermography scenarios, although it did not dominate every metric in every stage. In particular, PINN + CFD achieved RMSE values of 0.128, 0.129 and 0.296 °C in the held-out depth-wise test-point validation during the linear-heating, constant-temperature and dynamic-perturbation stages, respectively. The reconstructed thermal field captured heat accumulation, boundary heat loss and spatial heterogeneity within the tea bed. The inferred

apparent process-level heat-source index $Q_{\text{react}}(t)$ showed stage-dependent macroscopic thermal evolution, but its association with polyphenol loss remained descriptive rather than causal.

Within the tested bed configuration, the reconstructed thermal state could help identify regions of heat accumulation and boundary cooling that are not resolved by sparse point sensors, thereby informing sensor placement and fermentation-uniformity assessment. However, the present evidence was derived from a single continuous fermentation run and does not establish full-volume validation, cross-batch generalizability or closed-loop control performance. Future work should therefore evaluate the framework across independent batches and bed configurations using independently characterized thermal inputs before its generalizability and process-control relevance can be established.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/fermentation12080345/s1>, Table S1: Paired infrared and PT100 measurements, quantitative agreement, and key image-registration settings at the tea-bed central surface reference point; Table S2: Thermophysical and boundary parameters used in the CFD model and PINN physical constraints [11,15,38–40]; Table S3: CFD solver settings, discretization schemes, and convergence criteria used to generate the CFD-derived volumetric soft spatial prior; Figure S1: Mesh-independence analysis of the CFD model for the black tea fermentation bed; Table S4: numerical settings and mesh-independence results for the CFD-derived temperature prior; Table S5: One-at-a-time sensitivity sweep of k_{eff} , h , porosity, and $Q_{\text{react}}(t)$ amplitude for the CFD prior and PINN + CFD reconstruction; Table S6: Five-seed repeatability of the PINN + CFD reconstruction on the primary spatial-validation field; Table S7: Paired fold-wise statistical comparison of RMSE values in leave-one-sensor-out validation; Table S8: Stage-wise leave-one-sensor-out spatial-validation performance; Table S9: Error statistics for held-out depth-wise test points at $z = 0.02$ m; Table S10: Error statistics for held-out depth-wise test points at $z = 0.06$ m; and Table S11: Correlation analysis between the apparent process-level heat-source index $Q_{\text{react}}(t)$ and tea polyphenol indicators.

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