

- A coupled electromagnetic-thermal-mass PINN was built for RF heating of oat seeds.
- Bayesian optimization tuned PINN hyperparameters.
- Temperature-moisture uniformity was optimized by Bayesian optimization.
- Improved heat-mass uniformity yielded more uniform microbial inactivation.
- Automatic differentiation uncovered mechanisms for improved uniformity.

**A heat-mass transfer coupled physics-informed neural network for optimizing radio  
frequency pasteurization uniformity of oat seeds**

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## Abstract:

Oat seeds are vulnerable to *Salmonella* contamination, making effective pasteurization technology essential for ensuring microbial food safety. Radio-frequency (RF) pasteurization is promising for foodborne pathogen control, but poor heating uniformity hinders its commercialization. Traditional optimization relies on time-consuming experiments or finite-element simulations, accurate but computationally expensive. Embedding microbial inactivation kinetics directly into multi-physics solvers further increases computational cost. According to reported correlations between thermal-moisture and pasteurization uniformity for low-moisture foods, this study established a physics-informed neural network (PINN)-based framework for RF pasteurization to optimize coupled electromagnetic-thermal-mass transfer performance. The PINN surrogate model enforced Maxwell's equations, the heat conduction equation, and Fick's moisture diffusion equation using multi-physics simulation datasets. Simulations and optimizations terminated at a volume-averaged moisture content of 8 % (w.b.), (safe-storage level). Two-stage Bayesian optimization tuned PINN hyperparameters and yielded optimal RF conditions (electrode gap: 149 mm, material height: 41 mm) at the pasteurization endpoint. The trained PINN predicted temperature, moisture, and electric-potential fields to compute simulation-based temperature (TUI) and moisture uniformity indices (MUI). Compared with non-optimized groups, the experimental heating uniformity index ( $\lambda_T$ ) was 22.14%-42.70% lower, while the experimental moisture uniformity index ( $\lambda_M$ ) improved by 26.81%-49.43%. Experimental validation of RF pasteurization against *Salmonella* Enteritidis PT 30 showed optimized parameters reduced the pasteurization

22 uniformity index (PUI,  $\lambda_P$ ) by 21.7 %, indicating improved heat-mass uniformity yields more  
23 uniform microbial inactivation. PINN automatic differentiation revealed that optimal  
24 parameters reduced coefficients of variation (CoV) in electric field, polarization, and  
25 thermal/moisture gradients. This study provides a computationally-efficient, physically  
26 interpretable approach for RF pasteurization optimization of low-moisture granular foods.

27 **Keywords:** Bayesian optimization; Hyperparameter adaptation; *Salmonella* Enteritidis PT 30;  
28 Heating uniformity;

## 1. Introduction

Oat seeds are an important low-moisture food commodity vulnerable to desiccation-tolerant *Salmonella* contamination (Lian et al., 2015; Jarvis et al., 2016). A 1998 multistate salmonellosis outbreak linked to toasted oats cereal (Centers for Disease Control and Prevention, 1998), alongside recent large-scale oat-product recalls (Food and Drug Administration, 2024), underlines the need for effective pasteurization before processing or consumption (Sánchez-Maldonado et al., 2018). Conventional hot-air and steam heating are often insufficient for low-moisture foods due to low heat-transfer efficiency; prolonged processing degrades flavor, color, and nutritional quality (Kim et al., 2023; Baker et al., 2025).

Radio frequency (RF) heating achieves volumetric heating using 13.56, 27.12, or 40.68 MHz electromagnetic waves (Jiao et al., 2018). Featuring deep penetration, rapid heating, and non-contact operation, it has been applied to disinfestation, pasteurization, drying, enzyme inactivation, and thawing (Shanmugam et al., 2025; Zhang et al., 2025; Liu et al., 2026; Song et al., 2026). Extensive studies have confirmed that RF pasteurization achieves reliable microbial inactivation with favorable quality retention across various low-moisture food matrices (Chen et al., 2019, 2020; Lian et al., 2026; Ou et al., 2026; Renzetti et al., 2026; Tang et al., 2026; Wu et al., 2026). However, non-uniform heating remains a commercial bottleneck. Material geometry, dielectric properties, and electrode configuration govern internal electromagnetic fields and frequently induce edge overheating, threatening product quality and safety (Tiwari et al., 2011; Tasci et al., 2024).

Various methods mitigate non-uniform RF heating, including dielectric-property modifying fillers, optimized electrode configurations, spouted-bed-assisted material movement, and tailored sample density arrangements (Jiang et al., 2024; Wang et al., 2024; Zheng et al., 2024; Altin et al., 2025; Bai et al., 2026). Trial-and-error approaches are time-consuming and offer limited mechanistic insight. Finite-element tools such as COMSOL Multiphysics simulate electromagnetic-thermal coupling for processing-parameter evaluation (Chen et al., 2015; Huang et al., 2015; Huang et al., 2018), yet high computational cost restricts global optimization. Most existing models also neglect mass transfer, which alters electromagnetic and temperature-field distributions. Machine-learning methods have accelerated RF-heating optimization (Gao et al., 2025b): Gao et al. (2025a) combined mechanistic modeling with gradient-boosted decision trees for canola-seed uniformity optimization, while Tao et al. (2026) used a literature-based machine learning approach to rank key parameters for RF heating uniformity in food-drying. Despite these advances, unconstrained purely data-driven models may predict physically invalid parameter combinations and yield unreliable outputs.

Physics-informed neural networks (PINNs), proposed by Raissi et al. (2019), embed governing partial differential equations as soft constraints in the loss function while using observational data to guide training. PINNs approximate high-dimensional nonlinear mappings while keeping predictions consistent with physical laws, making them suitable for forward simulation, parameter inversion, and optimization (Karniadakis et al., 2021). In electromagnetic-thermal coupling, PINNs can replace traditional solvers with maintained

accuracy and reduce computational cost. The performance, however, is sensitive to hyperparameters including network architecture, learning rate, loss weights, and sampling strategy, and optimal settings vary across problems (Wang et al., 2021; Wu et al., 2023). Manual tuning or grid search is inefficient and may not find the optimum. Bayesian optimization has therefore been applied to PINNs in various domains (Zhang et al., 2025; Roy Sarkar et al., 2026), improving accuracy and efficiency.

The objectives of this study were to: (1) develop an electromagnetic-thermal-mass transfer coupled PINN surrogate model for RF pasteurization of oat seeds, incorporating moisture transport based on Fick's second law and the influence of moisture content on dielectric properties; (2) optimize adaptive hyperparameter search of network architecture, learning rate, sampling strategy, and activation function using Bayesian method to achieve high-fidelity surrogate performance; (3) perform multi-objective parameter optimization that minimizes temperature and moisture uniformity indices strictly constrained at the practical pasteurization endpoint (volume-averaged moisture content of 8% w.b.), rather than arbitrary intermediate time points; (4) validate whether PINN-optimized uniformity improvement can correlate to real-case RF pasteurization of *Salmonella* Enteritidis PT 30 in oat seeds, and analyze the physical mechanisms underlying improved heating and moisture uniformity through automatic differentiation of the trained PINN.

## 2. Materials and methods

The optimization framework has six modules (Fig. 1): (i) COMSOL-based mechanistic modeling to generate training data, with simulations terminated when the volume-averaged moisture content reached 8% (w.b.); (ii) PINN surrogate model construction with physics-constrained loss; (iii) Bayesian optimization for hyperparameter tuning; (iv) multi-objective parameter optimization using the trained PINN, with temperature uniformity index (TUI) and moisture uniformity index (MUI) as evaluation criteria, both evaluated at the pasteurization endpoint (8% w.b.); (v) RF pasteurization experiments with *Salmonella* Enteritidis PT 30 in oat seeds to validate that PINN-optimized TUI and MUI improvements correspond to improved pasteurization uniformity (PUI); and (vi) physical mechanism analysis via automatic differentiation of the trained PINN to interpret uniformity improvements and parameter sensitivities.

### 2.1 Material preparation

Oat seeds (*Avena nuda* L.) were purchased from local farmers in Yangling, Shaanxi, China. Initial moisture content was  $10.3 \pm 0.6\%$  (w.b.) measured via oven drying. Following Yu et al. (2015), distilled water was sprayed onto seeds to adjust moisture to  $22.0 \pm 0.9\%$  (w.b.). Seeds were sealed in polyethylene bags and stored at  $4 \pm 1$  °C for 7 d, shaken three times daily to achieve homogeneous moisture distribution. After equilibration, bulk density ( $795 \text{ kg}\cdot\text{m}^{-3}$ ) was determined by the toluene displacement method (Razavi & Milani, 2006). Before RF experiments, seeds were held at  $20 \pm 0.5$  °C for 24 h. Oat material properties were measured following established protocols (Gao et al., 2025a). Dielectric properties were obtained using

an impedance analyzer (Agilent 4294A) across 20-110 °C and 10-35% (w.b.), with temperature-moisture correlations fitted by multiple linear regression ( $R^2 > 0.98$ ). Effective moisture diffusion coefficient, latent heat of vaporization, and GAB (Guggenheim-Anderson-de Boer) sorption-isotherm parameters were obtained from published literature. Detailed property values are listed in Table 1.

## *2.2 RF heating system*

A 6 kW, 27.12 MHz free-running oscillator RF system (SO6B, Strayfield International, UK) was used (Fig. 2a). It comprised a metal enclosure (1.2 m × 0.8 m × 0.6 m), generator, and parallel-plate electrodes. Oat seeds were held in a rectangular polypropylene container (260 mm × 175 mm × 100 mm) centered on the bottom electrode. Coupled RF power was adjusted via the electrode gap (90-170 mm). Bulk temperature was measured using a 6-channel fluorescent fiber-optic system (HQ-FTS-D120, Heqi Technology, Xi'an, China), with probes placed at the geometric center (Fig. 2a). Surface temperature was recorded by an infrared camera (A300, FLIR Systems, Billerica, MA, USA; accuracy  $\pm 2$  °C). Moisture content was measured gravimetrically at regular intervals.

## *2.3 COMSOL mechanistic model*

### *2.3.1 Geometric model*

The finite element model was developed in COMSOL Multiphysics V5.6 (COMSOL Co., Ltd., Shanghai, China). The geometry included the RF cavity, electrodes, and the oat seeds container (260 mm × 175 mm × 100 mm). The sample was at the center of the bottom electrode. Electrode gaps of 130, 140, 150, 160, and 170 mm and material heights of 25, 50, and 75 mm

were used. This parameter range was determined from preliminary experiments: excessively large electrode gaps result in impractically long experimental durations and prohibitive simulation computational cost, while small gaps lead to thermal runaway; the selected material heights correspond to low, medium, and high bed-loading levels referenced from existing relevant studies. Bulk density was  $795 \text{ kg}\cdot\text{m}^{-3}$ . Material properties are listed in Table 1.

**Table 1** Parameters and constants used in the COMSOL governing equations.

| Parameter                   | Symbol            | Value                                          | Unit                                                  | Reference                            |
|-----------------------------|-------------------|------------------------------------------------|-------------------------------------------------------|--------------------------------------|
| Vacuum permittivity         | $\varepsilon_0$   | $8.85 \times 10^{-12}$                         | $\text{F}\cdot\text{m}^{-1}$                          | (Mohret al., 2025)                   |
| Water vapor gas constant    | $R_v$             | 461.5                                          | $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$       | $R/M_w$                              |
| Bulk density                | $\rho$            | 795                                            | $\text{kg}\cdot\text{m}^{-3}$                         | Measured in this study               |
| Thermal conductivity        | $k$               | 0.14                                           | $\text{W}\cdot\text{m}^{-1}\cdot^\circ\text{C}^{-1}$  | Measured in this study               |
| Heat capacity               | $C_p$             | $2T+2418^{[\text{b}]}$                         | $\text{J}\cdot\text{kg}^{-1}\cdot^\circ\text{C}^{-1}$ | Measured in this study               |
| Dielectric constant         | $\varepsilon'$    | $(0.035T + 3.8) \times (1 + 0.02M)$            | -                                                     | Measured in this study               |
| Loss factor                 | $\varepsilon''$   | $(0.001T^2 + 0.08T + 0.35) \times (1 + 0.15M)$ | -                                                     | Measured in this study               |
| Latent heat of vaporization | $L_v$             | $2.26 \times 10^6$                             | $\text{J}\cdot\text{kg}^{-1}$                         | Standard value at $25^\circ\text{C}$ |
| Activation energy parameter | $E_a/R$           | 2500                                           | K                                                     | (Le et al., 2025)                    |
| Evaporation rate constant   | $k_{\text{evap}}$ | $1.2 \times 10^{-3}$                           | $\text{s}^{-1}$                                       | (Chen et al., 2022)                  |
| Dry matter density          | $\rho_d$          | $\rho \cdot (1+M)^{-1}$                        | $\text{kg}\cdot\text{m}^{-3}$                         | Calculated dynamically from $M$      |
| Monolayer moisture content  | $M_m$<br>(GAB)    | 0.08                                           | $\text{kg}\cdot\text{kg}^{-1}$                        | (Brett et al., 2009)                 |

|                                      |                       |                                                |                                                |                                                                            |
|--------------------------------------|-----------------------|------------------------------------------------|------------------------------------------------|----------------------------------------------------------------------------|
| GAB energy constant                  | $C$                   | 4.5                                            | -                                              | (Brett et al., 2009)                                                       |
| GAB heat constant                    | $K$                   | 0.85                                           | -                                              | (Brett et al., 2009)                                                       |
| Convective heat transfer coefficient | $h$                   | 35                                             | $\text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$ | (Altin et al., 2022)                                                       |
| Convective mass transfer coefficient | $k_m$                 | 0.03                                           | $\text{m}\cdot\text{s}^{-1}$                   | (Kaya et al., 2008;<br>Baptestini et al., 2017)                            |
| Saturation vapor pressure            | $p_{\text{sat,air}}$  | 15,752                                         | Pa                                             | (IAPWS-IF97)                                                               |
| Saturated water vapor density        | $\rho_{\text{v,sat}}$ | 0.1045                                         | $\text{kg}\cdot\text{m}^{-3}$                  | Calculated as $\rho = p_{\text{sat}}/(R_v\cdot T)$                         |
| Water vapor density in hot air       | $\rho_{\text{v,air}}$ | 0.0209                                         | $\text{kg}\cdot\text{m}^{-3}$                  | Calculated as $\rho_{\text{v,air}} = \text{RH} \times \rho_{\text{v,sat}}$ |
| Water vapor diffusivity in air       | $D_{\text{va}}$       | $2.5 \times 10^{-5}$                           | $\text{m}^2\cdot\text{s}^{-1}$                 | Used in Sherwood number calculation                                        |
| Saturation vapor pressure            | $p_{\text{sat}}$      | $610.78 \cdot \exp[17.27(T-273.15)/(T-35.85)]$ | Pa                                             | Antoine-type empirical equation                                            |
| Equilibrium moisture content         | $M_{\text{eq}}$       | GAB model                                      | $\text{kg}\cdot\text{kg}^{-1}$                 | Determined by GAB model                                                    |

$T$  = local temperature at each spatial position ( $^{\circ}\text{C}$ );  $M$  = dry-basis moisture content ( $\text{kg}\cdot\text{kg}^{-1}$ ). Both are field variables that appear in all temperature and moisture-dependent property correlations.

### 2.3.2 Model assumptions

Assumptions: (1) uniform initial temperature and moisture; (2) constant porosity and bulk density; (3) negligible shrinkage or expansion; (4) equivalent continuum approach because oat seed particle diameter is much smaller than 1 cm (Huang et al., 2018). Under a fixed container

footprint, a higher bed increases total sample mass. This does not affect comparison because the optimization framework compares normalized spatial variability (TUI and MUI) at the same pasteurization endpoint (8% w.b.), not absolute heating rates or total energy.

### 2.3.3 Governing equations and boundary conditions

Neglecting magnetic field effects, the electric field distribution in the RF cavity is governed by the quasi-static form of Maxwell's equations (Marra et al., 2009). For a lossy dielectric material, the complex permittivity is  $\varepsilon = \varepsilon' - j\varepsilon''$ , and the electric potential satisfies (Birla et al., 2008):

$$-\nabla \cdot ((\sigma + j2\pi f \varepsilon_0 \varepsilon') \nabla V) = 0 \quad (1)$$

where  $\sigma$  is direct-current electrical conductivity ( $\text{S} \cdot \text{m}^{-1}$ ),  $j = (-1)^{0.5}$ ,  $f = 27.12$  MHz is the frequency (Hz),  $\varepsilon'$  is the dielectric constant,  $\varepsilon_0$  is the vacuum permittivity ( $8.85 \times 10^{-12} \text{ F} \cdot \text{m}^{-1}$ ),  $\varepsilon''$  is the dielectric loss factor, and  $V$  is the electric potential (V).

Heat conduction and the RF heat source were incorporated into the energy conservation equation (Marra et al., 2007):

$$\rho C_p \frac{\partial T}{\partial t} = \nabla(k \nabla T) + Q - L_v I_v \quad (2)$$

where  $\rho$  is the density ( $\text{kg} \cdot \text{m}^{-3}$ ),  $C_p$  is the specific heat capacity ( $\text{J} \cdot \text{kg}^{-1} \cdot ^\circ\text{C}^{-1}$ ),  $t$  is the process time (s),  $T$  is the temperature ( $^\circ\text{C}$ ),  $k$  is the thermal conductivity ( $\text{W} \cdot \text{m}^{-1} \cdot ^\circ\text{C}^{-1}$ ),  $L_v$  is the latent heat of vaporisation ( $\text{J} \cdot \text{kg}^{-1}$ ),  $I_v$  is the volumetric evaporation rate ( $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ ), and  $Q$  is the volumetric heat generation rate ( $\text{W} \cdot \text{m}^{-3}$ ) given by (Choi and Konrad, 1991):

$$Q = 2\pi f \varepsilon_0 \varepsilon'' |E|^2 \quad (3)$$

where  $E$  is the electric field intensity ( $V \cdot m^{-1}$ ) related to the voltage between two parallel electrodes:

$$E = -\nabla V \quad (4)$$

Moisture transport follows Fick's second law with an evaporation term (Khan et al., 2018):

$$\frac{\partial M}{\partial t} = \nabla(D_{\text{eff}}\nabla M) - \frac{I_v}{\rho_d} \quad (5)$$

Where  $M$  is the dry-basis moisture content ( $kg \cdot kg^{-1}$ ),  $D_{\text{eff}}$  is the effective moisture diffusivity ( $m^2 \cdot s^{-1}$ ),  $I_v$  is the evaporation rate ( $kg \cdot m^{-3} \cdot s^{-1}$ ), and  $\rho_d = \rho \cdot (1+M)^{-1}$  is the dry matter density ( $kg \cdot m^{-3}$ ).  $D_{\text{eff}}$  is the effective diffusivity ( $m^2 \cdot s^{-1}$ ):

$$D_{\text{eff}} = 2.5 \times 10^{-9} \exp(-2500/(T+273.15)) \quad (6)$$

where  $T$  is the temperature of the material at a given spatial position ( $^{\circ}C$ ).

The volumetric evaporation rate is expressed as (Zhang et al., 2021):

$$I_v = k_{\text{evap}} \rho_d (M - M_{\text{eq}}) \quad (7)$$

where  $k_{\text{evap}}$  is an evaporation constant, and  $M_{\text{eq}}$  is the equilibrium moisture content described by the GAB model (Timmermann et al., 2001).

$$M_{\text{eq}} = \frac{CKM_m a_w}{(1 - Ka_w)(1 - Ka_w + CKa_w)} \quad (8)$$

With  $M_m = 0.08 \text{ kg} \cdot \text{kg}^{-1}$ ,  $a_w = 0.938$ ,  $C = 4.5$ , and  $K = 0.85$  being the GAB parameters for oat seeds.

Before RF pasteurization, the samples were equilibrated to room temperature. The initial temperature was uniform ( $T_{\text{init}} = 20 \text{ }^{\circ}C$ ) and  $M_{\text{init}} = 0.282 \text{ kg} \cdot \text{kg}^{-1}$  dry basis (d.b.), corresponding to 22% (w.b.). The bottom electrode was grounded ( $V_{\text{bottom}} = 0$ ), and the cavity walls were

electrically insulated. The thermal boundary condition at air-exposed surfaces (Huang et al., 2018):

$$k \cdot \nabla T \cdot n|_{\text{boundary}} = h (T_{\text{air}} - T)|_{\text{boundary}} \quad (9)$$

where  $n$  is the surface normal vector,  $T_{\text{air}}$  is the air temperature (55 °C) inside the RF cavity, and  $h$  is the forced-convection heat transfer coefficient (35 W·m<sup>-2</sup>·K), whose value was adopted from Altin et al. (2022) for RF-cavity forced-convection conditions. The surface moisture flux is given by (Welty et al., 2008):

$$-D_{\text{eff}} \nabla M \cdot n|_{\text{boundary}} = k_m (\rho_{v,\text{surf}} - \rho_{v,\text{air}})|_{\text{boundary}} \quad (10)$$

where  $k_m$  is the convective mass transfer coefficient (m·s<sup>-1</sup>),  $\rho_{v,\text{surf}} = a_w \cdot p_{\text{sat}}(T_{\text{surf}}) / (R_v \cdot T_{\text{surf}})$  is the water vapor density at the material surface (kg·m<sup>-3</sup>),  $p_{\text{sat}}$  the saturation vapor pressure (Pa),  $R_v = 461.5 \text{ J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$  the gas constant for water vapor, and  $\rho_{v,\text{air}}$  the water vapor density in the 55 °C hot air.

Calibration against experimental heating rates was employed to determine the top electrode voltage, which is a standard and widely accepted procedure in numerical modeling of radio-frequency heating processes (Birla et al., 2008; Huang et al., 2018). In this work, a sinusoidal voltage of 5000 V at 27.12 MHz was applied to the top electrode. The resulting simulated heating rates matched well with the experimental measurements, and this voltage was fully consistent with the typical operating conditions of the 6 kW RF system.

#### 2.3.4 Simulation termination and time-stepping strategy

Simulation terminated when volume-averaged moisture content reached 8% (w.b.), corresponding to  $M_{\text{target}} = 0.087 \text{ kg} \cdot \text{kg}^{-1}$ . Total pasteurization time varied from ~36 min (75 mm

height, 130 mm gap) up to 358 min (25 mm height, 170 mm gap). Output sampling intervals were adjusted dynamically: (1) <60 min: every 5 min; (2) 60-120 min: every 10 min; (3) 120-240 min: every 20 min; (4) >240 min: every 30 min.

A free tetrahedral mesh with refinement near electrodes and the sample was adopted after mesh-independence verification, totaling about 1.8 million elements. Adaptive time stepping with a maximum step of 30 s ensured convergence. Relative tolerance was 0.001, maximum Newton iterations 25 for strong nonlinear coupling. MUMPS direct solver was used with relative tolerance 0.001. Each simulation took 35- 120 min on a Dell T3660 workstation (Intel i9- 13900K, 128 GB RAM). Parameter sweeps covered 5 electrode gaps and 3 material heights, giving 15 cases.

#### *2.3.5 Heat and mass transfer model validation*

RF pasteurization experiments were conducted at electrode gaps of 130, 150, and 170 mm, with a material thickness of 50 mm. Center temperature was measured with fiber optic sensors; surface temperature was recorded by an infrared camera at the pasteurization endpoint (8% w.b.). Average moisture was measured gravimetrically. Simulated and experimental time-temperature histories, surface temperature distributions, and moisture loss curves were compared. Agreement was quantified using root mean square error (RMSE) (Chai & Draxler, 2014):

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N [T_{exp}(i) - T_{sim}(i)]^2} \quad (11)$$

where  $T_{exp}$  and  $T_{sim}$  are the experimental and simulated temperatures ( $^{\circ}\text{C}$ ), respectively.

$N$  is the total number of points, and  $i$  is the data node number.

### 2.3.6 Data generation for neural network training

For each of 15 cases ( $5 \text{ gaps} \times 3 \text{ heights}$ ), electric potential  $V$ , temperature  $T$ , and moisture  $M$  were exported at dynamically determined time points, covering the entire pasteurization process (22% to 8% w.b.). These COMSOL simulations solved only coupled electromagnetic-heat-mass transfer without incorporating microbial inactivation kinetics, and microbial responses were evaluated exclusively by subsequent laboratory experiments. Latin hypercube sampling selected 2000 spatial points within the 3D oat domain at each time step (McKay et al., 1979). A fixed random seed ensured reproducibility. Coordinates and field values were saved in CSV format. The total number of output time steps accumulated across all 15 simulation cases was approximately 159, yielding a full dataset of around  $159 \times 2000 = 318\,000$  points. A leave-one-case-out cross-validation was applied: each of the 15 parameter cases served once as the independent test set, with the rest split 80%/20% for training and validation.

### 2.4 Construction of PINN model for RF pasteurization of oat seeds

As shown in Fig. 3, the electric potential  $V$ , temperature  $T$ , and moisture content  $M$  were approximated by the PINN surrogate model as continuous functions of spatial coordinates ( $x, y, z$ ), time  $\tau$ , and two process parameters: electrode gap  $d$  and material height  $h$ . The governing equations described in Section 2.3.3 were embedded as soft constraints in the loss function, and COMSOL simulation data were used to guide training. The total loss consisted of four

components: data loss, PDE residual loss, boundary condition loss, and initial condition loss, with weights dynamically adjusted by GradNorm. A fully connected feedforward network with  $L$  hidden layers and  $N$  neurons per layer was used; the input layer had seven nodes, and the output layer had three nodes. The hyperbolic tangent (tanh) was used as the activation function. Hyperparameters including  $L$ ,  $N$ , learning rate, number of collocation points, and activation function were optimized via Bayesian optimization. Collocation points were sampled using Latin hypercube sampling (LHS) and resampled every 500 epochs. Training used a two-stage strategy: Adam for 10,000 epochs followed by the limited-memory Broyden–Fletcher–Goldfarb–Shanno (L-BFGS) for up to 5,000 epochs. All derivatives in the PDE residuals were computed via automatic differentiation. Model performance was evaluated using  $R^2$ , MAE, and RMSE. Detailed formulations of the loss terms, PDE residuals, boundary conditions, initial condition loss, automatic differentiation, collocation sampling, Bayesian hyperparameter optimization, and training settings are provided in the Supplementary Material (Section S1).

## *2.5 Bayesian optimization of RF process parameters*

Tang et al. (2026) established a strong positive correlation between TUI, MUI, and PUI in low-moisture spices, suggesting that minimizing temperature gradients during RF heating would improve the uniformity of microbial inactivation. Therefore, TUI and MUI were chosen as the optimization criteria.

The optimization objective was to minimize the TUI and MUI at the pasteurization endpoint, defined as the moment when the volume-averaged moisture content reached 8% (w.b.). This endpoint-based strategy ensured that the optimization criterion matched the

254 experimental validation protocol, where heating was terminated upon reaching the same  
 255 moisture level. The TUI was defined following Jiao et al. (2015):

$$\text{TUI} = \frac{\int_{V_{\text{vol}}} |T - T_{\text{avg}}| dV_{\text{vol}}}{(T_{\text{avg}} - T_{\text{initial}}) V_{\text{vol}}} \quad (12)$$

256 where  $T_{\text{avg}}$  is the average temperature of the material,  $T_{\text{init}} = 20$  °C, and  $V_{\text{vol}}$  is the material  
 257 volume. The moisture uniformity index was defined similarly:

$$\text{MUI} = \frac{\int_{V_{\text{vol}}} |M - M_{\text{avg}}| dV_{\text{vol}}}{|M_{\text{avg}} - M_{\text{initial}}| V_{\text{vol}}} \quad (13)$$

259 where  $M_{\text{avg}}$  is the average moisture content.

260 For a given  $(d, h)$ , the PINN found the time  $t_{\text{past}}(d, h)$  at which the volume-averaged dry-  
 261 basis moisture content reached  $M_{\text{target}} = 0.087 \text{ kg} \cdot \text{kg}^{-1}$ , corresponding to 8% (w.b.):

$$M_{\text{avg}}(d, h, t_{\text{past}}) = M_{\text{target}} \quad (14)$$

262 The TUI and MUI were then evaluated specifically at this time  $t_{\text{past}}$ :

$$\text{TUI}(d, h) = \text{TUI}(d, h, t_{\text{past}}(d, h)) \quad (15)$$

$$\text{MUI}(d, h) = \text{MUI}(d, h, t_{\text{past}}(d, h)) \quad (16)$$

263 The optimization was formulated to minimize a weighted sum of TUI and MUI subject to  
 264 constraints (Marler & Arora, 2004). Since TUI and MUI have different numerical ranges, both  
 265 indices were normalized using min-max scaling over the parameter space:

$$\text{TUI}_{\text{norm}} = \frac{\text{TUI} - \text{TUI}_{\text{min}}}{\text{TUI}_{\text{max}} - \text{TUI}_{\text{min}}} \quad (17)$$

$$\text{MUI}_{\text{norm}} = \frac{\text{MUI} - \text{MUI}_{\text{min}}}{\text{MUI}_{\text{max}} - \text{MUI}_{\text{min}}} \quad (18)$$

$$\min F(d, h) = w_T \cdot \text{TUI}_{\text{norm}}(d, h, t_{\text{past}}) + w_M \cdot \text{MUI}_{\text{norm}}(d, h, t_{\text{past}}) \quad (19)$$

With  $w_T = w_M = 0.5$ . The constraints were:  $130 \leq d \leq 170$  mm,  $25 \leq h \leq 75$  mm. Equal weights were applied, assuming equal importance of thermal and moisture uniformity; optimal  $(d, h)$  may shift with alternative weights. Full Pareto analysis can be explored in future work.

Bayesian optimization was again employed to solve this bi-objective optimization problem, using 50 initial points (Latin hypercube) and 100 iterations. At each iteration, the PINN evaluated  $t_{\text{past}}$  by a fast root-finding algorithm (secant method), then computed the corresponding TUI and MUI at that specific time. The combination that minimized  $F$  while satisfying all constraints was selected as the optimal processing parameters for experimental validation.

## *2.6 Experimental validation of RF pasteurization*

To validate the practical food-safety significance of the PINN-optimized parameters beyond temperature and moisture, the experimental validation was extended from thermal measurement to pathogen inactivation (Liu et al., 2018), following the "Temperature-Moisture-Pasteurization" uniformity framework proposed by Tang et al. (2026). *Salmonella* Enteritidis PT 30, one of the most frequently identified foodborne pathogens in low-moisture food matrices (Syamaladevi et al., 2016; Xu et al., 2019; Liu et al., 2025), was selected as the target microorganism for this study (Villa-Rojas et al., 2017).

### *2.6.1 Inoculum preparation and sample inoculation*

The full inoculum and sample-inoculation workflow (bacterial activation, suspension preparation, inoculation, equilibration) followed Tang et al. (2026). Briefly, 10  $\mu\text{L}$  frozen culture ( $-18^\circ\text{C}$ ) was transferred into 10 mL tryptic soy broth (TSB; Beijing Land Bridge,

Beijing, China) and incubated at 37 °C for 24 h. Cultures were streaked onto tryptic soy agar (TSA; Beijing Land Bridge, Beijing, China) for overnight incubation. A single colony was subcultured in TSB overnight; 100 µL was spread onto TSA and incubated. Cells were harvested by plate washing with 3 mL sterile 0.9 % saline and vortexed for 30 s. Oat samples (0.282 d.b.) were inoculated (1 mL suspension per 100 g) with a sterile spray bottle (10 mL, Langyue Trading Co., Ltd., Hengshui, China), followed by 10 min manual massaging for homogeneous inoculation. Inoculated samples were equilibrated at 25 °C for 48 h in a humidity-controlled chamber to achieve consistent thermal resistance of *Salmonella Enteritidis* PT 30 (Wei et al., 2018). All microbial experiments were performed with three independent biological replicates (separate inoculation batches), and each sample was plated in duplicate as technical replicates. All *Salmonella* Enteritidis PT 30 experiments were conducted in a certified biosafety Level 2 (BSL- 2) laboratory per institutional safety protocols.

#### 2.6.2 RF treatment groups and sampling strategy

Five parameter sets were designed: Groups 1-3 received full *Salmonella* pasteurization validation; Groups 4-5 (single-parameter perturbation) only underwent temperature-moisture measurement. All parameters were selected within the interior of the parameter domain without extreme boundary conditions. Treatments were terminated once the volume-averaged moisture content reached 8% (w.b.). As shown in Fig. 2b of Section 2.2, ten sampling locations (P<sub>1</sub>-P<sub>10</sub>) were defined, with P<sub>1</sub>-P<sub>5</sub> in the upper layer and P<sub>6</sub>-P<sub>10</sub> in the lower layer. P<sub>1</sub> and P<sub>6</sub> represented geometric cold spots of the two layers, whereas P<sub>2</sub>-P<sub>5</sub> and P<sub>7</sub>-P<sub>10</sub> corresponded to corner hot spots. All microbial experiments were performed in triplicate.

**Table 2** Parameter sets for experimental validation of RF pasteurization

| No. | Electrode gap (mm) | Material height (mm) | Note                             |
|-----|--------------------|----------------------|----------------------------------|
| 1   | 149                | 41                   | PINN-optimized                   |
| 2   | 140                | 48                   | Sub- optimized A                 |
| 3   | 158                | 34                   | Sub- optimized B                 |
| 4   | 149                | 52                   | Single- parameter perturbation A |
| 5   | 156                | 41                   | Single- parameter perturbation B |

### 2.6.3 Microbial enumeration and PUI

For each sampling location (P<sub>1</sub>-P<sub>10</sub>), 2 g of the treated sample was immediately transferred into a sterile Whirl-Pak bag (Dongguan Kaishi Electric Appliance Co., LTD, Dongguan, China) and cooled in an ice-water bath to terminate residual thermal inactivation. Then, 18 mL of sterile 0.9% saline solution was added, and the mixture was homogenized by manual rubbing for 3 min. Serial ten-fold dilutions were prepared, and 100 µL of each dilution was spread onto Tryptic Soy Agar (TSA; Beijing Land Bridge, Beijing, China) plates. The plates were incubated at 37 °C for 24-48 h, and characteristic colonies were counted. The initial *Salmonella* Enteritidis PT 30 population before RF treatment was determined using the same procedure from the equilibrated samples and was found to be  $8.10 \pm 0.03$  log CFU/g (n = 3). No significant difference in initial population was observed among the treatment groups (p > 0.05).

The experimental heating uniformity index ( $\lambda_T$ ) (Wang et al., 2005) and experimental moisture uniformity index ( $\lambda_M$ ) (Tang et al., 2026) were calculated as:

$$\lambda_T = \frac{\sqrt{\sigma_T^2 - \sigma_{Tinit}^2}}{\mu_T - \mu_{Tinit}} \quad (20)$$

$$\lambda_M = \frac{\sqrt{\sigma_M^2 - \sigma_{Minit}^2}}{|\mu_M - \mu_{Minit}|} \quad (21)$$

where  $\sigma_T$ ,  $\sigma_M$ ,  $\mu_T$ , and  $\mu_M$  are the standard deviation and mean after RF pasteurization, and  $\sigma_{Tinit}$ ,  $\sigma_{Minit}$ ,  $\mu_{Tinit}$ , and  $\mu_{Minit}$  are the initial values.

To quantitatively evaluate the uniformity of *Salmonella* Enteritidis PT 30 inactivation across the sample, the PUI ( $\lambda_P$ ) was adopted from Tang et al. (2026):

$$\lambda_P = \frac{\sqrt{\sigma_P^2 - \sigma_{Pinit}^2}}{\mu_P - \mu_{Pinit}} \quad (22)$$

where  $\sigma_P$  and  $\mu_P$  are the standard deviation and mean of the logarithmic microbial reductions (log CFU/g) of *Salmonella* Enteritidis PT 30 measured at the ten sampling locations (P<sub>1</sub>-P<sub>10</sub>) after treatment, respectively;  $\sigma_{Pinit}$  and  $\mu_{Pinit}$  are the initial standard deviation and mean before RF treatment. A smaller  $\lambda_P$  indicates a more spatially uniform pasteurization against *Salmonella* Enteritidis PT 30.

## 2.7 Physical mechanism analysis

Using the automatic differentiation capability of the trained physics-informed neural network, several physical quantities were computed and analyzed. The electric field intensity was obtained as  $E = |\nabla V|$ . The polarization intensity was obtained as  $P = \epsilon_0 (\epsilon' - 1) E$ . The temperature gradient  $\nabla T$  and moisture gradient  $\nabla M$  were also computed.

To quantify the spatial uniformity of these quantities, the coefficient of variation (CoV) was used. For a generic scalar field  $\phi$ , the CoV is defined as

$$\text{CoV}_\phi = \frac{\sigma_\phi}{\mu_\phi} \quad (23)$$

where,

$$\mu_\phi = \frac{1}{V_{vol}} \int_{V_{vol}} \phi dV_{vol} \quad (24)$$

$$\sigma_{\Phi} = \sqrt{\frac{1}{V_{vol}} \int_{V_{vol}} (\Phi - \mu_{\Phi})^2 dV_{vol}} \quad (25)$$

And  $V_{vol}$  is the material volume. For vector fields such as  $\nabla T$  and  $\nabla M$ , the magnitudes  $|\nabla T|$  and  $|\nabla M|$  were used in the CoV calculation. All CoV values were evaluated at the pasteurization endpoint  $t_{past}$ , at which the volume-averaged moisture content reached 8% (w.b.), using the PINN-predicted fields.

The sensitivities of the uniformity indices to the input parameters were obtained through partial derivatives, including  $(\partial TUI/\partial d)$ ,  $(\partial TUI/\partial h)$ ,  $(\partial MUI/\partial d)$ , and  $(\partial MUI/\partial h)$ .

## 2.8 Statistical analysis

One-way analysis of variance and Tukey's honestly significant difference post-hoc test were performed using RStudio with R version 4.4.1. Differences were considered significant at  $p < 0.05$ .

## 3. Result and discussions

### 3.1 Validation of heat and mass transfer model

The heat and mass transfer model was developed via COMSOL and validated against experimental measurements at electrode gaps of 130, 150, and 170 mm. Fig. 4a compares the simulated and experimental surface temperature distributions. The COMSOL-predicted distributions matched the infrared thermal images and correctly captured the characteristic "edge overheating and center underheating" pattern. Fig. 4b shows the comparison of simulated and experimental time-temperature histories at the geometric center. The simulated temperatures agreed well with the experimental data, with RMSE values of 3.966 °C, 3.554 °C,

and 2.939 °C for the three electrode gaps. Fig. 4c presents the moisture loss curves, which showed RMSE values of 1.181%, 1.291%, and 1.429% for the three validation cases. These results confirmed that the heat and mass transfer model accurately represented the physical RF heating process, providing reliable training data for the subsequent PINN model.

### 3.2 Bayesian optimization hyperparameter search results

As shown in Fig. 5, the validation loss decreased rapidly during the first 15 evaluations and then plateaued, with the Bayesian optimization process converging after 35 iterations of the 50 total evaluations. The optimal hyperparameter combination identified was:  $L = 6$  hidden layers,  $N = 128$  neurons per layer, initial learning rate  $\eta = 3.2 \times 10^{-4}$ , number of collocation points  $N_p = 1.5 \times 10^5$ , and activation function = tanh. The validation loss decreased from an initial value of 0.082 for the best random trial to 0.018 after Bayesian optimization, representing a 78% reduction, confirming the effectiveness of the adaptive hyperparameter search. This architecture balances representation capacity and overfitting risk for the current dataset scale.

### 3.3 PINN training and performance evaluation

The training loss curves in Fig.6 show stable convergence. The Adam optimizer reduced the total loss from 0.56 to 0.023 over 10,000 epochs, and L-BFGS further refined it to 0.014 after 3,200 additional epochs. The GradNorm mechanism balanced the four loss components with final weights of  $\lambda_{\text{data}} = 1.42$ ,  $\lambda_{\text{pde}} = 1.18$ ,  $\lambda_{\text{bc}} = 0.85$ , and  $\lambda_{\text{ic}} = 0.55$ , indicating that data fitting and physical constraints were optimized simultaneously without any single term dominating.

Fig. 7 presents parity plots of PINN predictions against heat and mass transfer model references for one representative test fold. Averaged across all 15 folds, the model achieved  $R^2 = 0.972$  for temperature,  $R^2 = 0.968$  for moisture, and  $R^2 = 0.978$  for electric potential, with corresponding MAE of 1.16 °C, 0.0125 kg·kg<sup>-1</sup>, and 27.5 V, respectively. Because the heat and mass transfer model training data are noise-free, the remaining prediction error mainly reflects the network's generalization error across unseen parameter combinations rather than measurement noise.

The low total loss of 0.014, together with the balanced GradNorm weights, confirmed that the high data-fitting accuracy was achieved while maintaining consistency with the governing equations. Unlike purely data-driven models, the PINN predicts fields that satisfy Maxwell's equations, the heat conduction equation, and Fick's second law, which is essential for reliable parameter optimization.

### *3.4 Parameter optimization results*

The convergence of the Bayesian optimization for TUI and MUI minimization at the pasteurization endpoint (8% w.b.) is shown in Fig. 8, where the objective function decreased steadily and converged after 87 iterations. The optimal parameters were electrode gap = 149 mm and material height = 41 mm. At this optimum, TUI = 0.171, MUI = 0.112.

### *3.5 RF pasteurization validation results*

To validate the practical efficacy of the PINN-driven optimization, optimized and sub-optimized parameter sets were compared via RF pasteurization challenge studies with

*Salmonella* Enteritidis PT 30, with all treatments terminated at the 8 % (w.b.) pasteurization endpoint.

### 3.5.1 Temperature and microbial inactivation distributions

Under the sub-optimized conditions, a pronounced “periphery overheating-center underheating” pattern was observed, reflecting the edge effect of the parallel-plate RF electrode system. For Sub-optimized A (140 mm/48 mm), the upper-layer cold spot ( $P_1$ , center) reached  $82.5 \pm 1.1$  °C, while the upper-layer corner hot spots ( $P_3$ ) exceeded 109 °C. For Sub-optimized B (158 mm/34 mm), the upper-layer cold spot temperature was only  $63.9 \pm 0.9$  °C, and the upper-layer hot spots reached  $87.4 \pm 1.0$  °C. In contrast, under the PINN-optimized condition (149 mm/41 mm), the temperature gradient was substantially reduced: the cold spot reached  $71.4 \pm 1.2$  °C, and the upper-layer hot spots reached  $90.4 \pm 0.6$  °C. The maximum temperature difference among the ten locations decreased from 29.8 °C (Sub-optimized A) and 26.1 °C (Sub-optimized B) to 23.2 °C for the optimized condition. Temperature and moisture values at all ten sampling locations are summarized in Table 3.

**Table 3** Temperature (°C) and moisture content (w.b.) values at ten sampling locations ( $P_1$ - $P_{10}$ ), and  $\lambda_T$ ,  $\lambda_M$  for five RF treatment conditions.

| No.   | Parameter   | PINN-optimized     | Sub-optimized A    | Sub-optimized B    | Single-parameter perturbation A | Single-parameter perturbation B |
|-------|-------------|--------------------|--------------------|--------------------|---------------------------------|---------------------------------|
| $P_1$ | $T$<br>(°C) | $71.367 \pm 1.222$ | $82.533 \pm 1.113$ | $63.933 \pm 0.907$ | $67.067 \pm 0.961$              | $73.033 \pm 1.070$              |

|                 |              |                            |                            |                            |                            |                            |
|-----------------|--------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|
|                 | <i>M</i> (%) | 6.204 ± 0.182              | 5.566 ± 0.645              | 6.059 ± 0.201              | 5.174 ± 0.112              | 5.530 ± 0.482              |
| P <sub>2</sub>  | <i>T</i>     | 90.467 ± 0.929             | 108.633 ± 1.021            | 86.767 ± 1.026             | 93.533 ± 0.950             | 107.533 ± 1.350            |
|                 | <i>M</i>     | 6.009 ± 0.099              | 4.613 ± 0.743              | 5.816 ± 0.181              | 5.048 ± 0.274              | 5.136 ± 0.238              |
| P <sub>3</sub>  | <i>T</i>     | 90.367 ± 0.551             | 109.667 ± 1.102            | 87.400 ± 0.954             | 93.967 ± 1.060             | 109.050 ± 0.919            |
|                 | <i>M</i>     | 5.927 ± 0.190              | 4.272 ± 0.807              | 5.935 ± 0.161              | 5.070 ± 0.196              | 4.849 ± 0.240              |
| P <sub>4</sub>  | <i>T</i>     | 90.200 ± 0.889             | 108.267 ± 0.862            | 86.567 ± 0.961             | 93.033 ± 1.007             | 107.467 ± 1.124            |
|                 | <i>M</i>     | 5.814 ± 0.107              | 4.943 ± 0.153              | 5.569 ± 0.250              | 4.936 ± 0.021              | 5.412 ± 0.691              |
| P <sub>5</sub>  | <i>T</i>     | 90.633 ± 1.011             | 109.233 ± 0.950            | 87.267 ± 0.902             | 93.633 ± 0.971             | 108.133 ± 1.041            |
|                 | <i>M</i>     | 5.867 ± 0.131              | 4.685 ± 0.636              | 6.002 ± 0.297              | 5.011 ± 0.192              | 4.849 ± 0.136              |
| P <sub>6</sub>  | <i>T</i>     | 85.167 ± 1.119             | 85.800 ± 1.113             | 66.667 ± 0.961             | 69.567 ± 0.961             | 76.533 ± 0.971             |
|                 | <i>M</i>     | 9.722 ± 0.117              | 10.118 ± 0.074             | 10.924 ± 0.168             | 12.216 ± 0.177             | 11.998 ± 0.211             |
| P <sub>7</sub>  | <i>T</i>     | 94.567 ± 0.929             | 111.667 ± 1.026            | 89.2 ± 0.954               | 95.9 ± 1.113               | 110.7 ± 1.015              |
|                 | <i>M</i>     | 9.839 ± 0.047              | 9.994 ± 0.159              | 10.894 ± 0.137             | 12.117 ± 0.099             | 11.703 ± 0.366             |
| P <sub>8</sub>  | <i>T</i>     | 94.533 ± 0.551             | 112.333 ± 0.971            | 90.033 ± 1.070             | 96.433 ± 1.007             | 111.467 ± 0.814            |
|                 | <i>M</i>     | 9.760 ± 0.050              | 10.033 ± 0.333             | 10.773 ± 0.082             | 12.330 ± 0.026             | 11.482 ± 0.786             |
| P <sub>9</sub>  | <i>T</i>     | 94.233 ± 0.945             | 111.167 ± 0.862            | 89.033 ± 1.007             | 95.600 ± 0.917             | 110.167 ± 1.250            |
|                 | <i>M</i>     | 9.657 ± 0.085              | 9.965 ± 0.100              | 10.974 ± 0.122             | 12.209 ± 0.073             | 11.913 ± 0.062             |
| P <sub>10</sub> | <i>T</i>     | 94.633 ± 1.011             | 112.167 ± 1.002            | 89.733 ± 1.150             | 96.467 ± 1.150             | 111.067 ± 1.059            |
|                 | <i>M</i>     | 9.394 ± 0.855              | 10.544 ± 0.155             | 10.874 ± 0.156             | 12.367 ± 0.043             | 12.172 ± 0.507             |
| Mean ± SD       | <i>T</i>     | 89.62 ± 7.08               | 105.15 ± 11.18             | 83.66 ± 9.77               | 89.52 ± 11.26              | 102.46 ± 14.68             |
|                 | <i>M</i>     | 7.819 ± 1.880              | 7.473 ± 2.689              | 8.382 ± 2.515              | 8.648 ± 3.603              | 8.504 ± 3.385              |
|                 | $\lambda_T$  | 0.102 ± 0.003 <sup>a</sup> | 0.131 ± 0.002 <sup>b</sup> | 0.154 ± 0.002 <sup>c</sup> | 0.162 ± 0.002 <sup>d</sup> | 0.178 ± 0.002 <sup>e</sup> |
|                 | $\lambda_M$  | 0.445 ± 0.019 <sup>a</sup> | 0.628 ± 0.055 <sup>b</sup> | 0.608 ± 0.012 <sup>b</sup> | 0.880 ± 0.013 <sup>d</sup> | 0.822 ± 0.031 <sup>c</sup> |

416 Different lowercase letters in the same row indicate significant differences among treatment  
417 groups ( $p < 0.05$ ).

418 Corresponding *Salmonella Enteritidis* PT 30 inactivation results are presented in Table 4.

419 For all three conditions, the upper layer (P<sub>1</sub>-P<sub>5</sub>) exhibited lower reductions (2.54-2.91

420 log CFU/g) than the lower layer (P<sub>6</sub>-P<sub>10</sub>, 4.08-5.69 log CFU/g), indicating vertical

421 non-uniformity in microbial inactivation. The mean reductions were  $3.82 \pm 1.17$ ,  $3.91 \pm 1.31$ ,

422 and  $4.01 \pm 1.44$  log CFU/g for the optimized, Sub-optimized A, and Sub-optimized B

conditions, respectively. Although the optimized condition did not achieve the highest average reduction, it yielded the lowest  $\lambda_P = 0.274 \pm 0.004$ , which was significantly lower than those of Sub-optimized A ( $0.311 \pm 0.006$ ) and Sub-optimized B ( $0.350 \pm 0.004$ ) ( $p < 0.05$ ). A smaller  $\lambda_P$  indicates more uniform inactivation across the sample. The optimized condition reduced  $\lambda_P$  by 11.9 % and 21.7 % compared with Sub-optimized A and B, respectively.

**Table 4** Comparison of microbial reductions at ten locations ( $P_1$ - $P_{10}$ ) and PUI ( $\lambda_P$ ) under three different RF treatment conditions.

| No.                          | PINN-optimized      | Sub- optimized A    | Sub-optimized B     |
|------------------------------|---------------------|---------------------|---------------------|
| $P_1(\log \text{ CFU/g})$    | $2.86 \pm 0.17$     | $2.68 \pm 0.06$     | $2.57 \pm 0.16$     |
| $P_2(\log \text{ CFU/g})$    | $2.71 \pm 0.09$     | $2.71 \pm 0.04$     | $2.57 \pm 0.12$     |
| $P_3(\log \text{ CFU/g})$    | $2.80 \pm 0.12$     | $2.63 \pm 0.08$     | $2.54 \pm 0.11$     |
| $P_4(\log \text{ CFU/g})$    | $2.68 \pm 0.21$     | $2.69 \pm 0.16$     | $2.66 \pm 0.32$     |
| $P_5(\log \text{ CFU/g})$    | $2.91 \pm 0.04$     | $2.55 \pm 0.25$     | $2.67 \pm 0.05$     |
| $P_6(\log \text{ CFU/g})$    | $4.08 \pm 0.38$     | $5.43 \pm 0.19$     | $5.12 \pm 0.64$     |
| $P_7(\log \text{ CFU/g})$    | $4.44 \pm 0.51$     | $4.98 \pm 0.59$     | $5.33 \pm 0.28$     |
| $P_8(\log \text{ CFU/g})$    | $4.29 \pm 0.47$     | $4.80 \pm 0.46$     | $5.51 \pm 0.34$     |
| $P_9(\log \text{ CFU/g})$    | $5.69 \pm 0.06$     | $5.15 \pm 0.55$     | $5.61 \pm 0.21$     |
| $P_{10}(\log \text{ CFU/g})$ | $5.69 \pm 0.03$     | $5.44 \pm 0.37$     | $5.53 \pm 0.18$     |
| Mean $\pm$ SD<br>(log CFU/g) | $3.82 \pm 1.17$     | $3.91 \pm 1.31$     | $4.01 \pm 1.44$     |
| PUI ( $\lambda_P$ )          | $0.274 \pm 0.004^a$ | $0.311 \pm 0.006^b$ | $0.350 \pm 0.004^c$ |

Different lowercase letters in the same row indicate significant differences among treatment groups ( $p < 0.05$ ).

It should be noted that none of the three conditions reached the FDA- recommended 5- log reduction at all sampling locations. The lower reductions in the upper layer ( $P_1$ -  $P_5$ ) suggest that

the cold spots, particularly in the upper layer, received insufficient thermal treatment. However, the optimized condition minimized the spatial disparity in inactivation, which was critical for food safety because a uniform reduction ensured that no location fell below the required lethality. The average reduction alone can mask cold-spot insufficiency (Xu et al., 2020), as demonstrated by the sub-optimized conditions, where some locations reached  $>5$  log CFU/g while others remained below 3 log CFU/g. This study prioritized microbial inactivation uniformity over average lethality; the FDA-recommended 5 log CFU/g reduction across all sampling locations can be achieved in future work by extending processing time or increasing RF power.

### 3.5.2 Experimental temperature, moisture and pasteurization uniformity indices

The experimental  $\lambda_T$  followed the expected trend across all five conditions. As shown in Table 4,  $\lambda_T$  values were  $0.102 \pm 0.003$ ,  $0.131 \pm 0.002$ ,  $0.154 \pm 0.002$ ,  $0.162 \pm 0.002$ , and  $0.178 \pm 0.002$  for the optimized, Sub-optimized A, Sub-optimized B, single-parameter perturbation A, and single-parameter perturbation B conditions, respectively. The corresponding experimental  $\lambda_M$  values were  $0.445 \pm 0.019$ ,  $0.628 \pm 0.055$ ,  $0.608 \pm 0.012$ ,  $0.880 \pm 0.013$ , and  $0.822 \pm 0.031$ , respectively, following a similar spatial pattern. Across all non-optimized conditions, the optimized condition had  $\lambda_T$  values 22.14-42.70% lower and  $\lambda_M$  values 26.81–49.43% lower; both  $\lambda_T$  and  $\lambda_M$  were significantly lower for the optimized condition ( $p < 0.05$ ). The  $\lambda_p$  presented in Table 3 showed the same ranking of treatment effects, with the optimized condition achieving the most uniform microbial inactivation. The PINN-predicted MUI was 0.112 versus the experimental  $\lambda_M$  of 0.445. The magnitude gap arose because TUI and MUI

were full- field volume- integrated indices, while  $\lambda_T$ ,  $\lambda_M$ , and  $\lambda_P$  used only 10 discrete sampling points.

### *3.5.3 Correlation validation of the temperature- moisture- pasteurization framework*

A Pearson correlation analysis (Schober et al., 2018) was performed on pooled experimental data from all three tested conditions ( $n = 9$ , combining triplicate runs) to verify the hypothesized link between thermal, moisture, and microbial uniformity. The  $\lambda_T$  showed a strong positive correlation with  $\lambda_M$  ( $r = 0.95$ ,  $p < 0.05$ ), confirming that more uniform heating corresponded to more uniform moisture redistribution across the sample. Furthermore, the  $\lambda_T$  showed an even stronger positive correlation with  $\lambda_P$  ( $r = 0.96$ ,  $p < 0.05$ ), aligning with the uniformity framework reported by Tang et al. (2026). The optimized condition, which had the lowest  $\lambda_T$ , also had the lowest  $\lambda_M$  and  $\lambda_P$ , confirming that PINN-predicted improvements in thermal uniformity translated into practical improvements in both moisture uniformity and pasteurization uniformity. These findings support the food-safety relevance of the PINN optimization framework, even though the average microbial reduction did not reach 5 log CFU/g under the tested conditions.

### *3.6 Analysis of electric field, temperature, and moisture distributions*

Fig. 9 presents PINN-predicted CoV for electric field, polarization, temperature gradient, and moisture gradient across the five conditions. The optimized condition (149 mm/41 mm) consistently exhibited the lowest CoV values across all four metrics, indicating the most uniform electromagnetic, thermal, and moisture fields. The sub-optimized and single-parameter perturbation groups showed notably higher CoV values. While the relative

ranking of the four metrics fluctuated slightly among the non-optimized groups, the overall trend strongly aligned with the  $\lambda_T$  and  $\lambda_M$  reported in Section 3.5. Specifically, the conditions with higher experimental  $\lambda_T$  and  $\lambda_M$  (Tables 3 and 4) also exhibited higher field CoVs in the PINN predictions.

This improvement in electromagnetic field uniformity produced more homogeneous temperature distributions. The maximum cold- to- hot- spot temperature difference was 23.2 °C under optimized conditions, notably lower than 29.8 °C (Sub-optimized A) and 26.1 °C (Sub-optimized B). Correspondingly, the optimized condition yielded the lowest PUI ( $0.274 \pm 0.004$ ), versus  $0.311 \pm 0.006$  for Sub-optimized A and  $0.350 \pm 0.004$  for Sub-optimized B (Table 4). These results confirmed that optimized parameters simultaneously improved electromagnetic, thermal, and moisture- field uniformity, ultimately producing more uniform microbial inactivation.

### 3.7 Sensitivity analysis

The spatial distributions of the first-order derivatives of TUI and MUI with respect to  $d$  and  $h$  are shown in Fig. 10. At the optimum (149 mm, 41 mm), all four derivatives were close to zero, confirming that this point was a local minimum. The sign reversal across the optimum indicated that any deviation from this point increased both TUI and MUI, thereby degrading uniformity. Furthermore, the magnitudes of the derivatives were consistently larger along the electrode-gap direction than those along the material-height direction. For instance, the maximum absolute values of  $\partial TUI/\partial d$  and  $\partial MUI/\partial d$  reached approximately  $0.010 \text{ mm}^{-1}$  and  $0.006 \text{ mm}^{-1}$ , respectively, whereas those of  $\partial TUI/\partial h$  and  $\partial MUI/\partial h$  were only about  $0.006 \text{ mm}^{-1}$

<sup>1</sup> and 0.004 mm<sup>-1</sup>, respectively. This indicates TUI is more sensitive to electrode gap than to material height near the optimum. Experimental  $\lambda_T$  also supported this observation. However,  $\lambda_M$  exhibited a different response, where perturbation in material height produced larger degradation in moisture uniformity. This discrepancy suggests moisture uniformity has complex coupled responses to geometry parameters. Therefore, the electrode gap should be prioritized for monitoring and control during industrial RF processing, while the optimum remains relatively robust to small variations in material height. Full sensitivity data are listed in Table S1 (Supplementary Material, uploaded with the manuscript).

### 3.8 Limitations and future perspectives

Since temperature and water activity-dependent D-values and z-values of *Salmonella* Enteritidis PT 30 in oat seeds under isothermal conditions were not determined in this study, and such data remain unavailable in the published literature to date. The PINN model developed in this work only solved coupled electromagnetic-heat-mass transfer multiphysics, without embedding microbial inactivation kinetics or thermal lethality (F-value) calculations within the simulation framework. All data for *Salmonella* Enteritidis PT 30 inactivation and PUI were obtained from separate post-hoc RF pasteurization experiments rather than direct numerical prediction. Although this strategy avoided extra computational overhead caused by additional microbial sub-models, the current model cannot independently predict microbial log-reduction without microbial experiments.

Another limitation is that, from a practical food safety perspective, none of the tested RF conditions achieved the FDA-recommended 5-log reduction of *Salmonella* Enteritidis PT 30

on average under the fixed 8 % (w.b.) moisture endpoint constraint. This study prioritized spatial uniformity of microbial inactivation over absolute lethality. Once these microbial inactivation kinetic parameters are experimentally characterized in future work, the kinetic parameters can be further integrated into the PINN workflow. With embedded microbial kinetics, the PINN will be capable of computing spatial microbial inactivation distributions and numerically predicting the PUI directly from simulated temperature and moisture fields. Multi-objective optimization can then simultaneously target TUI and MUI and microbial safety endpoints. Such improvement will reduce reliance on large-scale microbial inactivation trials and accelerate the development of RF pasteurization protocols for low-moisture granular food commodities. Additionally, future studies should further test the extrapolation performance of the PINN beyond the current parameter domain and explore model adaptability for larger industrial-scale RF systems.

#### **4. Conclusion**

The coupled electromagnetic-thermal-mass transfer model was validated against experimental temperature and moisture profiles during RF heating. Simulations terminated at 8 % (w.b.) volume-averaged moisture (oat safe-storage level), generating multi-physics datasets spanning 22 % to 8 % (w.b.) for PINN training. On held-out test sets from the cross-validation, the PINN attained  $R^2 > 0.96$  for all output fields (MAE: 27.5 V, 1.16 °C, 0.0125 kg·kg<sup>-1</sup>). Bayesian optimization identified optimal parameters (electrode gap 149 mm, material height 41 mm; TUI = 0.171, MUI = 0.112) at the end of pasteurization.

Experimental validation of RF pasteurization of *Salmonella* Enteritidis PT 30 obtained the lowest  $\lambda_P$  ( $0.274 \pm 0.004$ ) under optimized settings versus  $0.311 \pm 0.006$  and  $0.350 \pm 0.004$  for sub-optimized treatments, corresponding to 11.9 % and 21.7 %  $\lambda_P$  reduction and more uniform microbial inactivation. The strong correlation ( $r=0.96$ ) between  $\lambda_T$  and  $\lambda_P$  supported the “Temperature- Moisture- Pasteurization” framework. PINN automatic-differentiation analysis showed optimized parameters lowered CoV for electric- field intensity, polarization intensity, temperature- gradient magnitude, and moisture- gradient magnitude relative to Sub- optimized B (158 mm, 34 mm). Sensitivity analysis demonstrated that electrode gap dominated thermal- uniformity responses, whereas moisture uniformity depended on both electrode gap and material height; both parameters should be maintained near optimum for practical RF pasteurization.

This physically interpretable, computationally efficient framework enables fast parameter optimization under physical consistency, providing practical value for industrial-scale RF processing.

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**Fig. 1.** Flowchart of the PINN-based RF heating uniformity optimization framework.

**Fig. 2.** Schematic of the RF heating system and sample configuration. (a)

Experimental device; (b) Layered sampling positions in the oat seeds (Gao et al., 2025).

**Fig. 3.** Architecture and training scheme of the coupled electromagnetic-thermal-mass transfer PINN model.

**Fig. 4.** Validation of the coupled electromagnetic- thermal- mass- transfer model against experimental measurements at electrode gaps of 130, 150 and 170 mm. (a) Surface temperature distributions at the pasteurization endpoint (8% w.b. moisture); (b) Time-temperature histories at the geometric center of the sample; (c) Moisture loss during RF pasteurization.

**Fig. 5.** Convergence of Bayesian optimization for PINN hyperparameter tuning.

**Fig. 6.** Two-stage training loss curves of the coupled PINN model (Adam + L-BFGS).

**Fig. 7.** Parity plots of PINN predictions against references from the coupled electromagnetic- thermal- mass- transfer Multiphysics model on the test set. (a) Temperature; (b) Moisture; (c) Electric potential.

**Fig. 8.** Convergence of Bayesian optimization for RF process parameters. The y-axis shows the normalized composite objective function  $F$ . The annotation shows raw (non-normalized) TUI and MUI values at the optimum point ( $d = 149$  mm,  $h = 41$  mm).

**Fig. 9.** Coefficient of variation ( $CoV$ , dimensionless) of electric field intensity ( $CoV_E$ ), polarization intensity ( $CoV_P$ ), temperature gradient magnitude ( $CoV_{|\nabla T|}$ ), and

moisture gradient magnitude ( $CoV_{|V_M|}$ ) for five RF treatment conditions.

**Fig. 10.** First-order derivatives of TUI and MUI with respect to electrode gap ( $d$ ) and material height ( $h$ ): (a)  $\partial\text{TUI}/\partial d$ , (b)  $\partial\text{TUI}/\partial h$ , (c)  $\partial\text{MUI}/\partial d$ , and (d)  $\partial\text{MUI}/\partial h$ . The red dot marks the conditions:  $d = 149$  mm,  $h = 41$  mm.

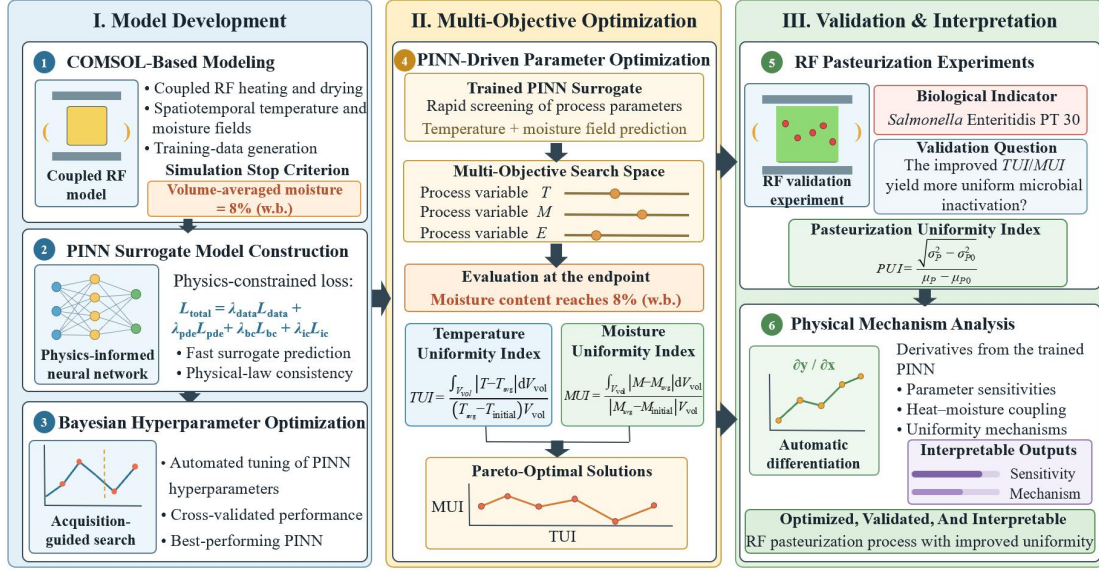


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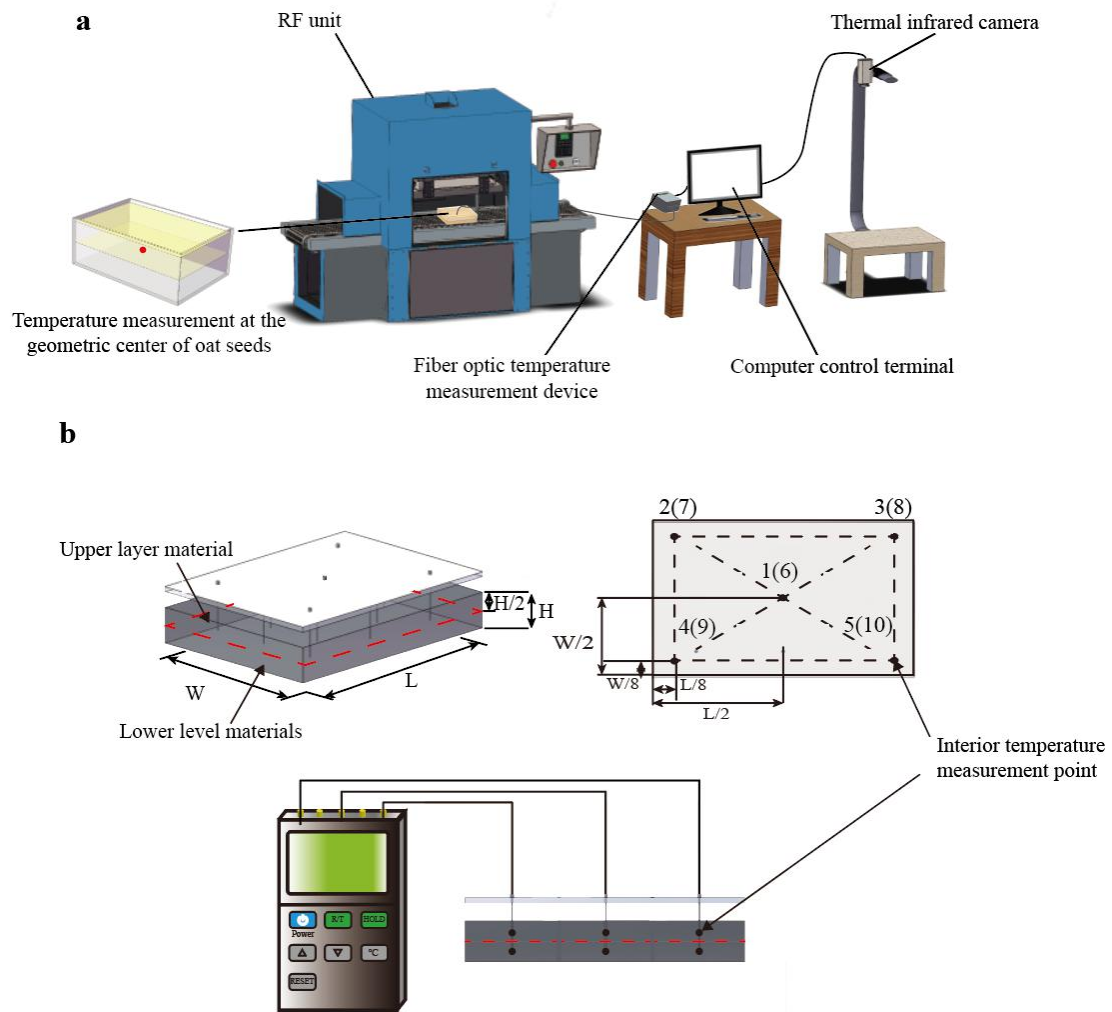


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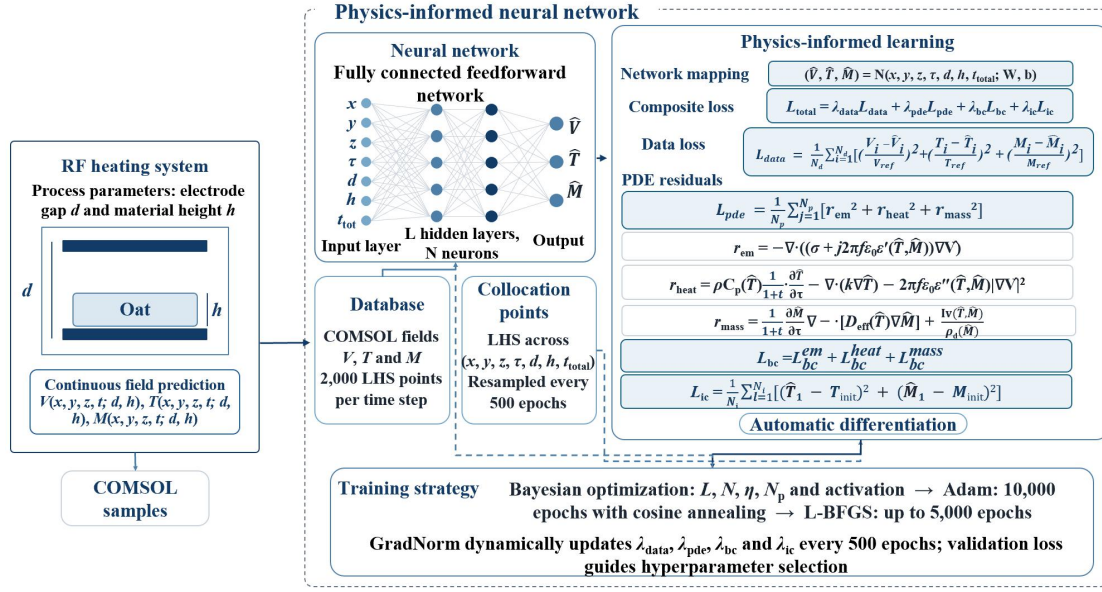


**Fig. 3.** Architecture and training scheme of the coupled electromagnetic-thermal-mass transfer PINN model.

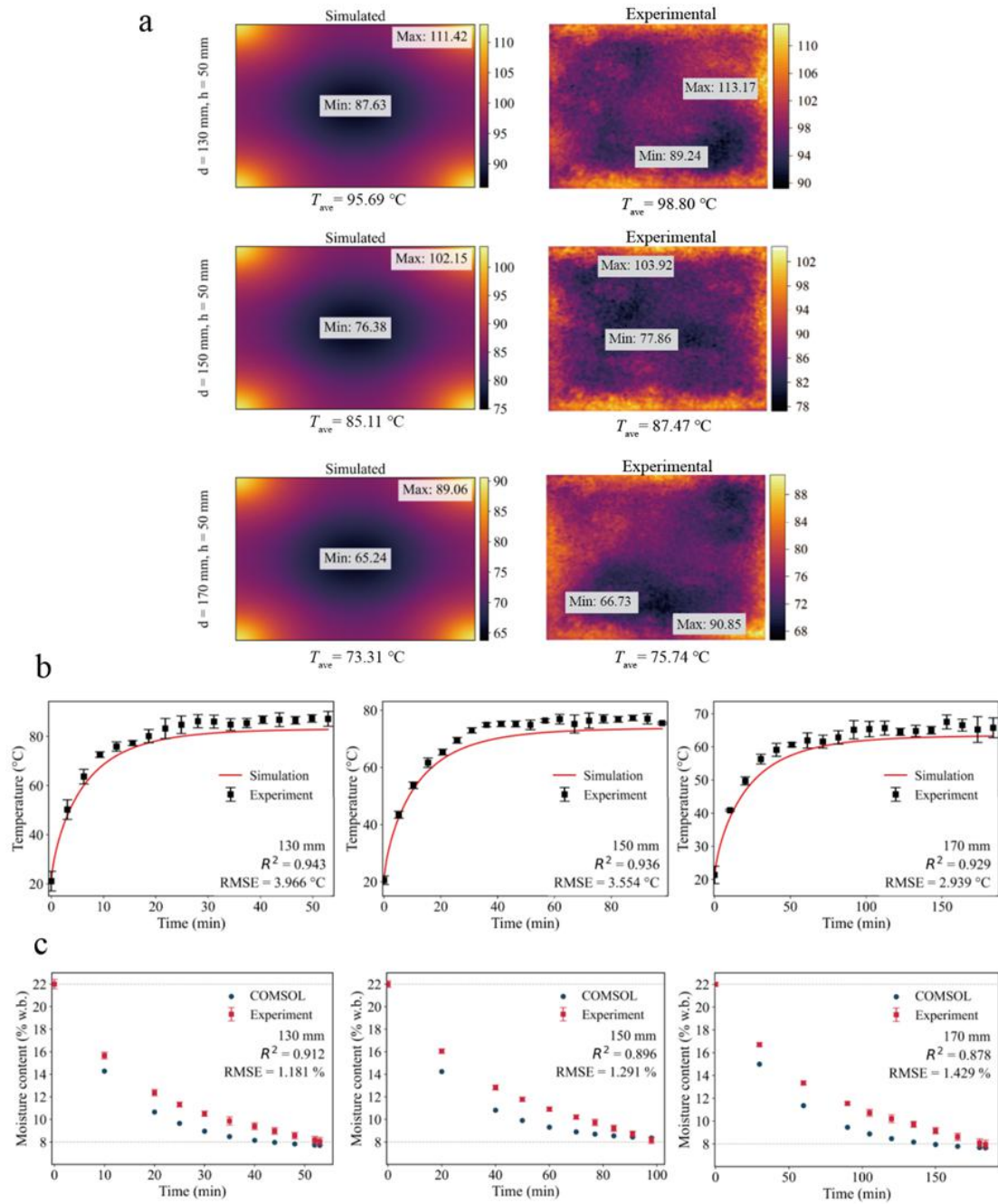


**Fig. 4.** Validation of the coupled electromagnetic- thermal- mass- transfer model against experimental measurements at electrode gaps of 130, 150 and 170 mm. (a) Surface temperature distributions at the pasteurization endpoint (8% w.b. moisture); (b) Time-temperature histories at the geometric center of the sample; (c) Moisture loss during RF pasteurization.

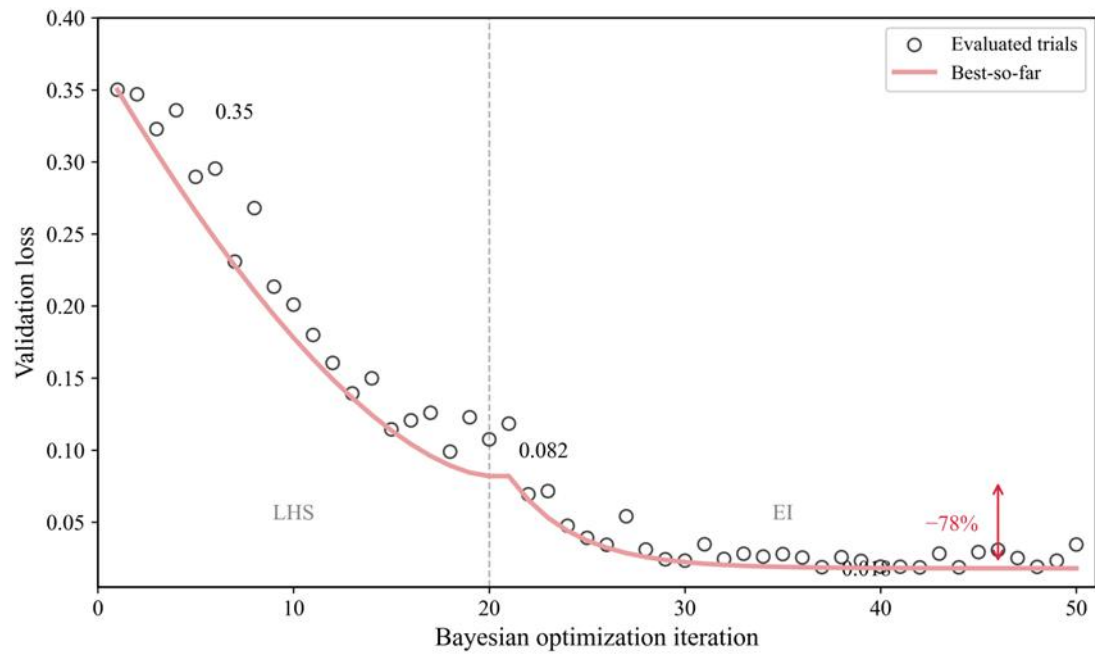


**Fig. 5.** Convergence of Bayesian optimization for PINN hyperparameter tuning.

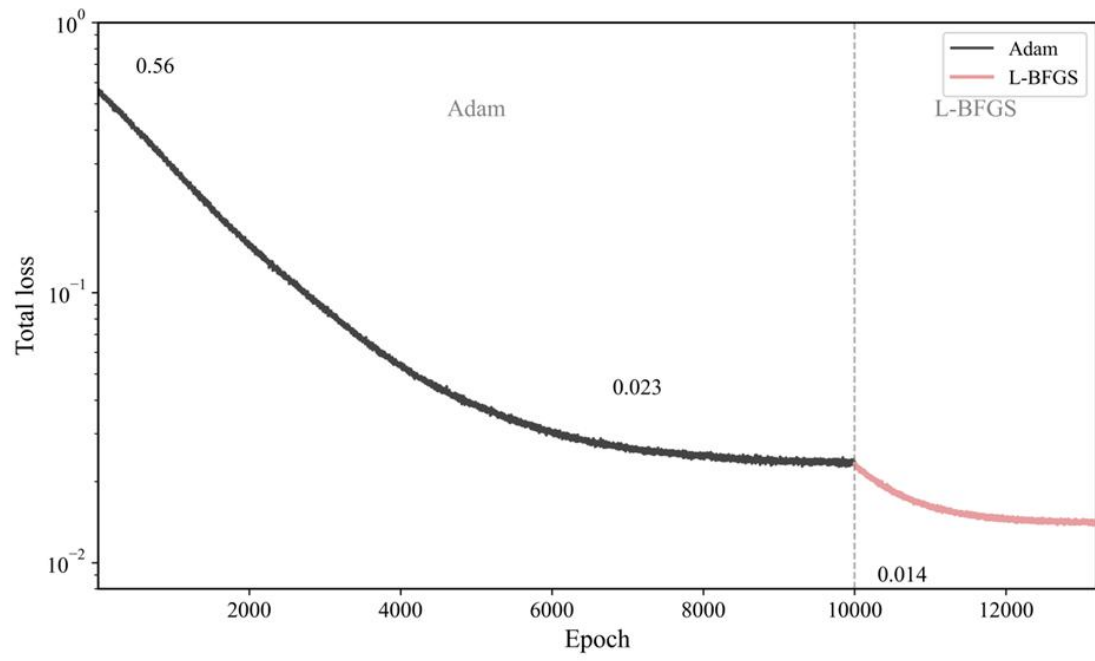


**Fig. 6.** Two-stage training loss curves of the coupled PINN model (Adam + L-BFGS)

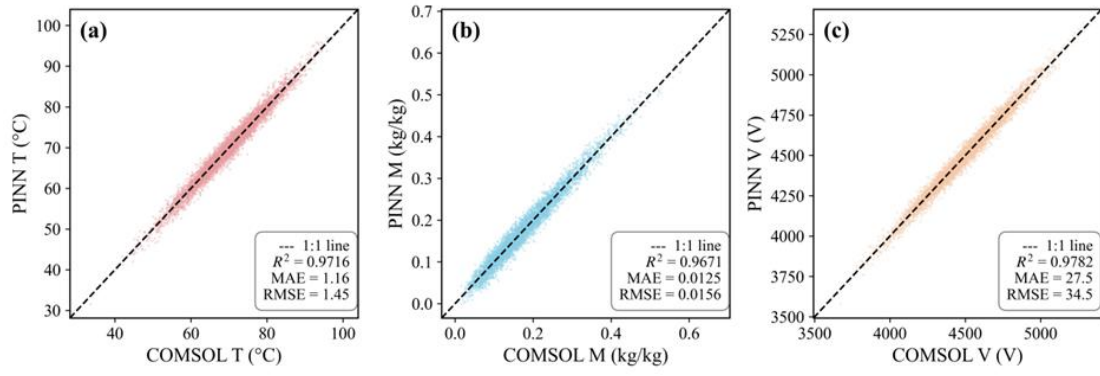


**Fig. 7.** Parity plots of PINN predictions against references from the coupled electromagnetic- thermal- mass- transfer Multiphysics model on the test set. (a) Temperature; (b) Moisture; (c) Electric potential.

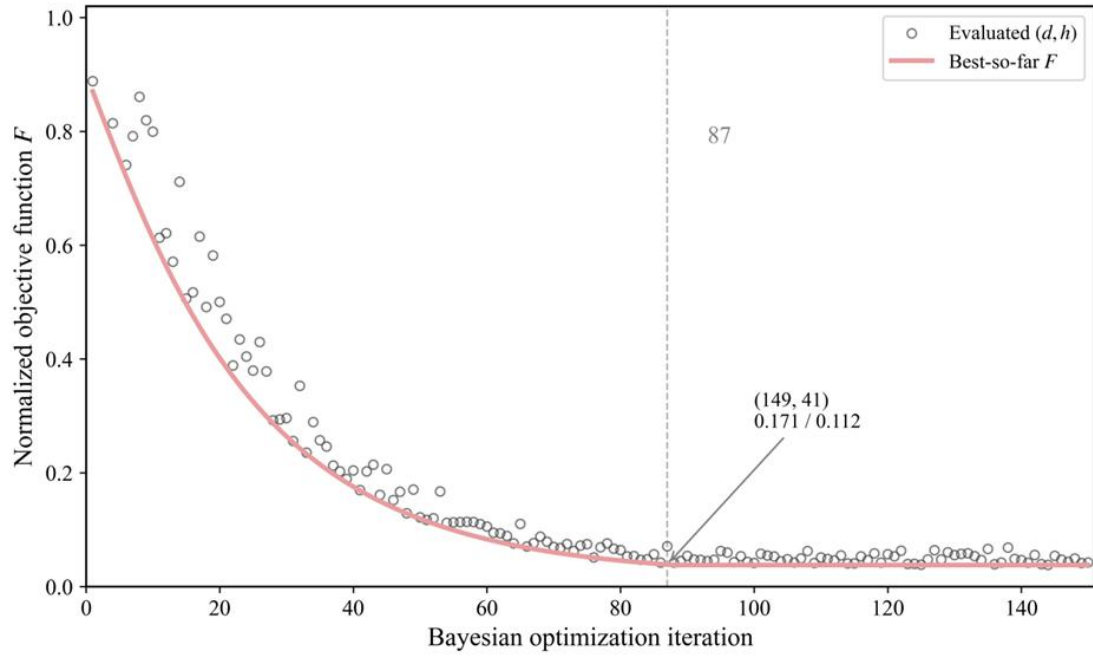


**Fig. 8.** Convergence of Bayesian optimization for RF process parameters. The y-axis shows the normalized composite objective function  $F$ . The annotation shows raw (non-normalized) TUI and MUI values at the optimum point ( $d = 149$  mm,  $h = 41$  mm).

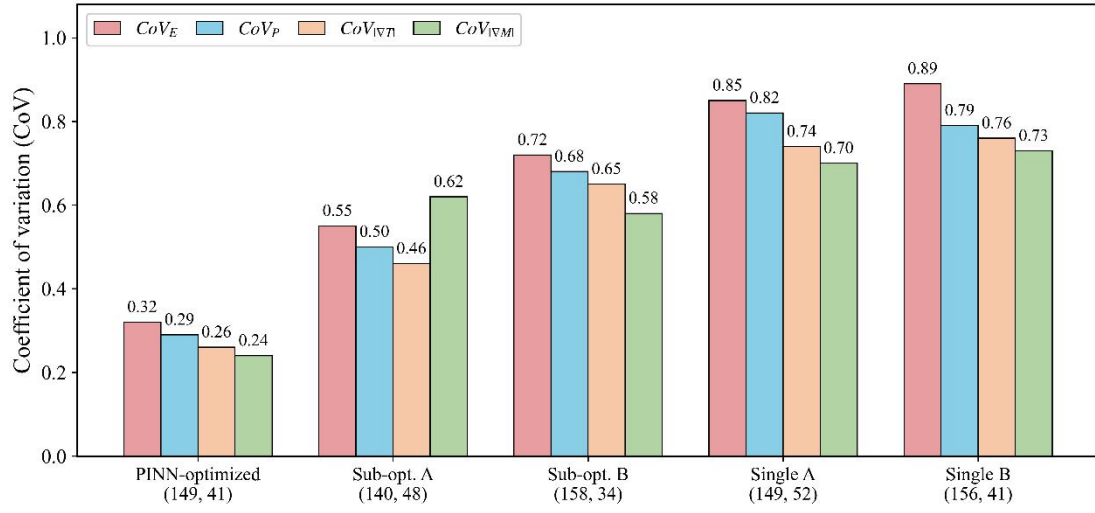


**Fig. 9.** Coefficient of variation ( $CoV$ , dimensionless) of electric field intensity ( $CoV_E$ ), polarization intensity ( $CoV_P$ ), temperature gradient magnitude ( $CoV_{|\nabla T|}$ ), and moisture gradient magnitude ( $CoV_{|\nabla M|}$ ) for five RF treatment conditions.

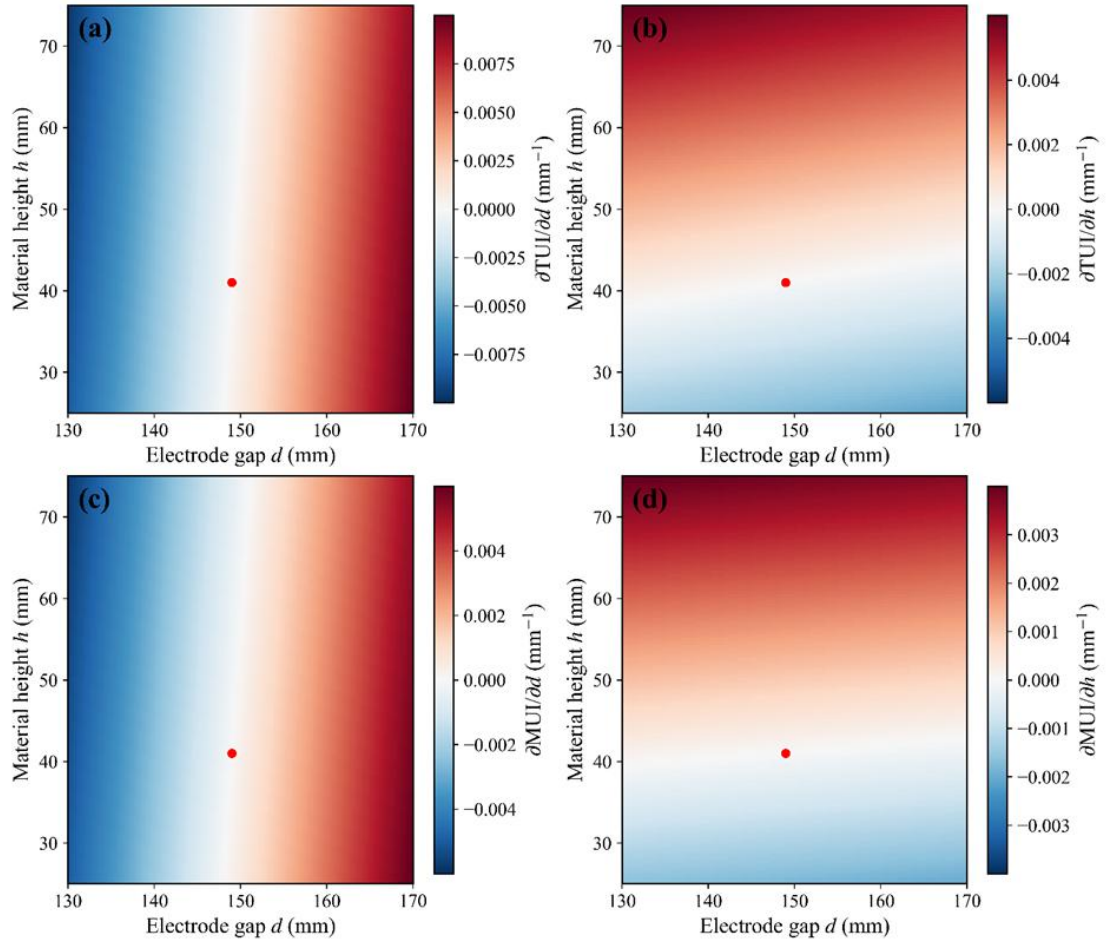


**Fig. 10.** First-order derivatives of TUI and MUI with respect to electrode gap ( $d$ ) and material height ( $h$ ): (a)  $\partial \text{TUI} / \partial d$ , (b)  $\partial \text{TUI} / \partial h$ , (c)  $\partial \text{MUI} / \partial d$ , and (d)  $\partial \text{MUI} / \partial h$ . The red dot marks the conditions:  $d=149$  mm,  $h=41$  mm.

## **Supplementary material:**

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## ***S1 Detailed formulation of the PINN model***

This supplementary material provides detailed formulations of the PINN model, including the physics-constrained loss function, PDE residuals, boundary conditions, initial condition loss, automatic differentiation, collocation sampling, Bayesian hyperparameter optimization, training strategy, and evaluation metrics.

### ***S1.1 Formulation for PINN modeling***

The RF heating process is governed by the PDEs in Section 2.3.3: electromagnetic equation (1), heat transfer equations (2) – (3), moisture diffusion equation (5), boundary conditions (9) - (10), and initial conditions ( $T_{\text{init}} = 20\text{ }^{\circ}\text{C}$ ,  $M_{\text{init}} = 0.282\text{ kg}\cdot\text{kg}^{-1}\text{ d.b.}$  at  $t = 0$ ). A PINN surrogate model approximates  $V = (x, y, z, \tau; d, h, t_{\text{total}})$ ,  $T = (x, y, z, \tau; d, h, t_{\text{total}})$ , and  $M = (x, y, z, \tau; d, h, t_{\text{total}})$  as continuous functions of spatial coordinates, time, and two process parameters: electrode gap  $d$  and material height  $h$ . Material density and placement were held constant.

A logarithmic time transformation  $\tau = \ln(1+t)$ , with  $t$  is in seconds, compresses the long-time scale while expanding the short-time scale, resolving both rapid initial heating and prolonged pasteurization. Total pasteurization time  $t_{\text{total}}$  for each parameter combination was included as an additional input feature.

### ***S1.2 Neural network architecture***

A fully connected feedforward network with  $L$  hidden layers and  $N$  neurons per layer was used. The input layer had seven nodes:  $(x, y, z, \tau, d, h, t_{\text{total}})$  after normalization to the interval  $[0,1]$ . The output layer contained three nodes:  $\hat{V}$ ,  $\hat{T}$ , and  $\hat{M}$ . The network function can be expressed as:

$$(\hat{V}, \hat{T}, \hat{M}) = N(x, y, z, \tau, d, h, t_{\text{total}}; \mathbf{W}, \mathbf{b}) \quad (\text{S1})$$

where  $N$  is the neural network mapping, and  $\mathbf{W}$  and  $\mathbf{b}$  are weights and biases. The hyperbolic tangent (tanh) was used as the default, but the activation function was also treated as a hyperparameter (Jagtap et al., 2020). The number of hidden layers  $L$  and neurons per layer  $N$  were hyperparameters determined by Bayesian optimization.  $t_{\text{total}}$  is the total pasteurization time for each  $(d, h)$  to reach 8% w.b., included to help the network learn widely varying time scales.

### *S1.3 Physics-constrained loss function*

The PINN was trained by minimizing a composite loss function that penalizes deviations from both the observed data and the physical laws (Karniadakis et al., 2021). The total loss  $L_{\text{total}}$  is a weighted sum of four components:

$$L_{\text{total}} = \lambda_{\text{data}} L_{\text{data}} + \lambda_{\text{pde}} L_{\text{pde}} + \lambda_{\text{bc}} L_{\text{bc}} + \lambda_{\text{ic}} L_{\text{ic}} \quad (\text{S2})$$

Where  $L_{\text{data}}$  is the data loss enforcing agreement with COMSOL data,  $L_{\text{pde}}$  is the PDE residual loss enforcing the governing equations,  $L_{\text{bc}}$  is the boundary condition loss,  $L_{\text{ic}}$  is the initial condition loss, and  $\lambda_{\text{data}}, \lambda_{\text{pde}}, \lambda_{\text{bc}}, \lambda_{\text{ic}}$  are loss weights that are dynamically adjusted during training using the GradNorm mechanism.

#### *S1.3.1 Data loss $L_{\text{data}}$*

To prevent the electric potential term from dominating due to its large magnitude, the three physical quantities were nondimensionalized:

$$L_{\text{data}} = \frac{1}{N_d} \sum_{i=1}^{N_d} \left[ \left( \frac{V_i - \hat{V}_i}{V_{\text{ref}}} \right)^2 + \left( \frac{T_i - \hat{T}_i}{T_{\text{ref}}} \right)^2 + \left( \frac{M_i - \hat{M}_i}{M_{\text{ref}}} \right)^2 \right] \quad (\text{S3})$$

Where  $N_d$  is the number of data points,  $V_i, T_i, M_i$  are the reference values from COMSOL simulations (electric potential in V, temperature in °C, dry-basis moisture

content in  $\text{kg} \cdot \text{kg}^{-1}$ ),  $\hat{V}_i$ ,  $\hat{T}_i$ ,  $\hat{M}_i$  are the corresponding PINN predictions at the same spatial coordinates, time, and process parameters, and  $V_{\text{ref}} = V_0 = 5000 \text{ V}$ ,  $T_{\text{ref}} = T_{\text{air}} - T_{\text{init}} = 35 \text{ }^\circ\text{C}$ ,  $M_{\text{ref}} = M_{\text{init}} - M_{\text{target}} = 0.195 \text{ kg} \cdot \text{kg}^{-1}$ .

### SI.3.2 PDE residual loss $L_{pde}$

With  $\tau = \ln(1+t)$ , derivatives with respect to  $t$  use the chain rule:  $\partial/\partial t = (1/(1+t)) \cdot \partial/\partial \tau$ . This term enforces the governing equations at collocation points  $(x_j, y_j, z_j, \tau_j, d_j, h_j, T_{\text{total},j})$  that are sampled independently of the training data. Three residual functions are defined based on Eqs. (1), (2), and (5):

Electromagnetic residual:

$$r_{\text{em}}(x, y, z, \tau, d, h, t_{\text{total}}) = -\nabla \cdot ((\sigma + j2\pi f \epsilon_0 \epsilon''(\hat{T}, \hat{M})) \nabla \hat{V}) \quad (\text{S4})$$

Where  $\hat{V}$  is the PINN-predicted electric potential (V).

Heat transfer residual:

$$r_{\text{heat}}(x, y, z, \tau, d, h, t_{\text{total}}) = \rho C_p(\hat{T}) \frac{1}{1+t} \cdot \frac{\partial \hat{T}}{\partial \tau} - \nabla \cdot (k \nabla \hat{T}) - 2\pi f \epsilon_0 \epsilon''(\hat{T}, \hat{M}) |\nabla \hat{V}|^2 + L_v I_v \quad (\text{S5})$$

Where  $\hat{T}$  is the PINN-predicted temperature ( $^\circ\text{C}$ ), and  $|\nabla \hat{V}|^2$  represents the squared magnitude of the electric field intensity ( $\text{V}^2 \cdot \text{m}^{-2}$ ).

Moisture transport residual:

$$r_{\text{mass}}(x, y, z, \tau, d, h, t_{\text{total}}) = \frac{1}{1+t} \frac{\partial \hat{M}}{\partial \tau} - \nabla \cdot (D_{\text{eff}}(\hat{T}) \nabla \hat{M}) + \frac{I_v(\hat{T}, \hat{M})}{\rho_d(\hat{M})} \quad (\text{S6})$$

Where  $I_v$  is the evaporation rate ( $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$ ), expressed as a differentiable function of  $\hat{T}$  and  $\hat{M}$  to enable automatic differentiation:

$$I_v = k_{\text{evap}} \cdot \rho_d \cdot (\hat{M} - M_{\text{eq}}) \quad (\text{S7})$$

the equilibrium moisture content ( $M_{\text{eq}}$ ) given by the GAB model:

$$M_{eq} = \frac{CKM_m a_w}{(1-Ka_w)(1-Ka_w+CKa_w)} \quad (S8)$$

All operations are implemented using Tensor Flow's differentiable operators.

The PDE loss was then defined as the mean squared value of these residuals over  $N_p$  collocation points:

$$L_{pde} = \frac{1}{N_p} \sum_{j=1}^{N_p} [r_{em}^2 + r_{heat}^2 + r_{mass}^2] \quad (S9)$$

Where  $N_p$  is the number of collocation points, and the derivatives are computed using automatic differentiation. The PDE residuals were non-dimensionalized using the same characteristic scales as the data loss to ensure balanced contributions from all loss terms.

### S1.3.3 Boundary condition loss $L_{bc}$

The boundary loss is decomposed into electromagnetic, thermal, and moisture parts:

$$L_{bc} = L_{bc}^{em} + L_{bc}^{heat} + L_{bc}^{mass} \quad (S10)$$

For the electromagnetic field, the bottom electrode is grounded ( $\widehat{V} = 0$ ) and the top electrode is set to  $\widehat{V} = V_0$  (5000 V). The cavity walls are electrically insulated, i.e.  $\nabla \widehat{V} \cdot n$ . The corresponding loss is:

$$L_{bc}^{em} = \frac{1}{N_{b,elec}} \sum_{k=1}^{N_{b,elec}} (\widehat{V}_k - V_{bc,k})^2 + \frac{1}{N_{b,ins}} \sum_{k=1}^{N_{b,ins}} (\nabla \widehat{V}_k \cdot n)^2 \quad (S11)$$

Where  $N_{b,elec}$  is the number of electrode boundary sampling points;  $N_{b,ins}$  is the number of insulated cavity-wall sampling points;  $\widehat{V}_k$  is the PINN-predicted electric potential (V);  $V_{bc,k}$  is the prescribed boundary potential, equal to 5000 V at the top electrode and 0 V at the bottom electrode;  $n$  is the outward unit normal vector;

and  $\nabla \hat{V}_k \cdot n$  is the normal derivative of the predicted potential, computed by automatic differentiation.

For the thermal boundary, the air-exposed surfaces follow a Robin condition:

$$k \nabla T \cdot n = h (T_{\text{air}} - T) \quad (\text{S12})$$

Therefore, the thermal boundary loss penalizes the flux residual:

$$L_{\text{bc}}^{\text{heat}} = \frac{1}{N_{\text{b,T}}} \sum_{k=1}^{N_{\text{b,T}}} \left[ k \nabla \hat{T}_k \cdot n - h (T_{\text{air}} - \hat{T}_k) \right]^2 \quad (\text{S13})$$

Where  $N_{\text{b,T}}$  is the number of thermal boundary sampling points on the air-exposed surfaces;  $k = 0.14 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$  is the thermal conductivity;  $\hat{T}_k$  is the PINN-predicted temperature ( $^{\circ}\text{C}$ );  $h = 35 \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$  is the convective heat transfer coefficient;  $T_{\text{air}} = 55 \text{ }^{\circ}\text{C}$  is the air temperature inside the RF cavity; and  $\nabla \hat{T}_k \cdot n$  is the normal temperature gradient computed by automatic differentiation.

For the moisture boundary, the diffusive flux equals the convective mass transfer:

$$- D_{\text{eff}} \nabla M \cdot n = k_m (\rho_{\text{v,surf}} - \rho_{\text{v,air}}) \quad (\text{S14})$$

The moisture boundary loss is therefore written as:

$$L_{\text{bc}}^{\text{mass}} = \frac{1}{N_{\text{b,M}}} \sum_{k=1}^{N_{\text{b,M}}} \left[ - D_{\text{eff}}(\hat{T}_k) \nabla \hat{M}_k \cdot n - k_m (\rho_{\text{v,surf}}(\hat{T}_k, \hat{M}_k) - \rho_{\text{v,air}}) \right]^2 \quad (\text{S15})$$

Where  $N_{\text{b,M}}$  is the number of moisture boundary sampling points on the air-exposed surfaces;  $D_{\text{eff}}(\hat{T}_k)$  is the effective moisture diffusivity;  $\hat{M}_k$  is the PINN-predicted dry-basis moisture content ( $\text{kg} \cdot \text{kg}^{-1}$ );  $k_m$  is the convective mass transfer coefficient;  $\rho_{\text{v,surf}}$  is the water vapor density at the material surface ( $\text{kg} \cdot \text{m}^{-3}$ );  $\rho_{\text{v,air}}$  is the water vapor density in the  $55 \text{ }^{\circ}\text{C}$  hot air; and  $n$  is the outward unit normal vector.

### S1.3.4 Initial condition loss $L_{ic}$

The initial condition loss enforced the initial temperature and moisture content at  $t = 0$ :

$$L_{ic} = \frac{1}{N_i} \sum_{l=1}^{N_i} [(\hat{T}_l - T_{\text{init}})^2 + (\hat{M}_l - M_{\text{init}})^2] \quad (\text{S16})$$

Where  $N_i$  is the number of initial sampling points,  $\hat{T}_l$  and  $\hat{M}_l$  are the PINN predictions at time  $t = 0$  for point  $l$ ,  $T_{\text{init}} = 20$  °C is the initial temperature (Section 2.1), and  $M_{\text{init}} = 0.282$  kg·kg<sup>-1</sup> (d.b.) is the initial moisture content.

### S1.4 Automatic differentiations for derivative computation

All derivatives in the PDE residuals are computed using TensorFlow's automatic differentiation, avoiding finite-difference approximations and yielding exact gradients at machine precision (Lu et al., 2021). Second-order derivatives are taken sequentially (Margossian, 2019).

### S1.5 Collocation point sampling strategy

Collocation points were generated using LHS across the continuous spatiotemporal-parametric space  $(x, y, z, \tau, d, h, t_{\text{total}})$ , independent of COMSOL data and used only for  $L_{\text{pde}}$ . LHS divides each input dimension into  $N_p$  equally probable intervals and randomly selects one point per interval (McKay et al., 1979). New collocation-point sets are generated periodically to avoid memorization of fixed point locations (Wu et al., 2023); in this work resampling is performed every 500 training epochs. Ranges:  $x \in [0, L_x]$ ,  $y \in [0, L_y]$ ,  $z \in [0, L_z]$ ,  $\tau \in [0, \ln(1+t_{\text{total, max}})]$  (where  $L_x, L_y, L_z$  are the dimensions of the oat container,  $t_{\text{total, max}} \approx 21,480$  s),  $d \in [130, 170]$  mm,  $h \in [25, 75]$  mm, and  $t_{\text{total}} \in [t_{\text{total, min}}, t_{\text{total, max}}]$  with values from 2,160 s to 21,480 s.

### *S1.6 Hyperparameter optimization via Bayesian optimization*

Bayesian optimization searched hyperparameters (Shahriari et al., 2016): hidden layers  $L \in [2, 8]$ , neurons per layer  $N \in [32, 256]$ , initial learning rate  $\eta \in [10^{-5}, 10^{-2}]$ , collocation points  $N_p \in [5 \times 10^4, 2 \times 10^5]$ , and activation function  $\in \{\tanh, \text{swish}, \text{gelu}\}$ . An initial set of 20 combinations was generated by LHS. Each was pre-trained for 2000 epochs, and validation loss was recorded. A Gaussian process surrogate modeled hyperparameters as inputs and validation loss as output. Expected Improvement selected the next set (Jones et al., 1998). The process ran for 50 evaluations (20 initial + 30 iterations). The combination with lowest validation loss was selected for full training.

### *S1.7 Training strategy and hardware*

The training dataset was generated from the COMSOL simulations described in Section 2.3. A total of 15 simulation cases were performed, covering five electrode gaps (130, 140, 150, 160 and 170 mm) and three material heights (25, 50 and 75 mm), with the material density fixed at  $795 \text{ kg}\cdot\text{m}^{-3}$  and the placement location fixed at the bottom electrode center. From each case, the electric potential, temperature, and moisture fields were extracted at dynamically determined time points as described in Section 2.3.4. To ensure a comprehensive and unbiased representation of the spatial field while maintaining computational efficiency, LHS was employed to select 2,000 spatial points within the three-dimensional oat domain at each time step, as described in Section 2.3.6. A leave-one-case-out cross-validation strategy was adopted: each of the 15 parameter cases served once as the independent test set, while the remaining 14 cases were split

80%/20% for training and validation within each fold. For enforcing PDE residuals, collocation points were generated using Latin hypercube sampling across the spatiotemporal domain and parameter space, with the number of collocation points  $N_p$  set to the value found by Bayesian optimization. To prevent over-fitting to specific points, collocation points were resampled every 500 training epochs. To prevent any single loss term from dominating the optimization, the gradient normalization method (GradNorm) was applied to dynamically adjust the loss weights  $\lambda_{\text{data}}$ ,  $\lambda_{\text{pde}}$ ,  $\lambda_{\text{bc}}$ , and  $\lambda_{\text{ic}}$  during training. Every 500 epochs, the gradient norm of each loss term with respect to the last layer's weights was computed. The weights were then updated via gradient descent to make all gradient norms converge to their average value. All loss weights were initialized to 1.0. A two-stage training strategy was adopted: The Adam optimizer was used for 10,000 epochs with a cosine annealing learning rate schedule, starting at the optimized learning rate, to achieve coarse convergence; subsequently, the L-BFGS optimizer (Nocedal, 1980) was used for up to 5,000 additional epochs (converged at 3,200 epochs in practice) for higher precision. All training was performed on an NVIDIA RTX 5090D v2 GPU (24 GB VRAM) using TensorFlow 2.10 with the DeepXDE library (Lu et al., 2021).

### *S1.8 Model evaluation metrics*

The predictive performance of the trained PINN was assessed using three standard metrics:

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2} \quad (\text{S17})$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |y_i - \hat{y}_i| \quad (S18)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2} \quad (S19)$$

Where  $y_i$  and  $\hat{y}_i$  represent the reference (COMSOL) and predicted values, respectively, and  $\bar{y}$  is the mean of the reference values.

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