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Development and Validation of the D²MCD Family: Dual-Term Diffusion Models for Coffee Drying

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Correspondence: Eduardo Duque-Dussán (eduardo.duque@cafedecolombia.com)**Received:** 4 December 2025 | **Revised:** 3 March 2026 | **Accepted:** 19 March 2026**Keywords:** effective diffusivity | heat and mass transfer | moisture reabsorption | psychrometric variability | washed-processed coffee

ABSTRACT

This study presents the Duque Diffusion Model for Coffee Drying (D²MCD), a family of dual-term diffusive formulations derived from Fick's law with convective boundary conditions. The models were developed to describe the mechanical drying behavior of *Coffea arabica* L. washed-processed coffee under variable thermal and psychrometric environments, providing a physically consistent framework that complements classical empirical approaches. The general form of the model expresses the moisture ratio as the superposition of two exponential modes weighted by a time-stretch integral that accounts for temperature and moisture-dependent effective diffusivity. Four variants are proposed: D²MCD-Core, the fundamental dual-term model; D²MCD-XR, which incorporates a reabsorption term through an exponential memory function; D²MCD-Iso, a simplified isothermal version; and D³MCD-T, an extended thermodiffusive formulation coupling heat and mass transfer. Model parameters were estimated using nonlinear least-squares fitting against experimental data from controlled mechanical drying tests of washed-processed coffee conducted at 35°C–50°C and 20%–60% relative humidity. The D²MCD family achieved high predictive accuracy (RMSE < 0.012 moisture units [wb]) and physically consistent parameter behavior, displaying improved agreement with experimental data compared with classical models such as Page, Midilli, and Henderson–Pabis. The reabsorption module effectively captured transient humidity peaks, while the thermal coupling enhanced performance under nonisothermal conditions. The D²MCD framework establishes a unified and flexible basis for modeling mass and heat transfer during coffee drying and can be extended to other agricultural materials and drying configurations.

1 | Introduction

Drying is one of the most critical postharvest operations in coffee processing, determining both the physical stability of the product and the preservation of its sensory quality (de Abreu et al. 2025; Coelho et al. 2024). In washed processing systems, the drying stage reduces the moisture content of parchment coffee from about 53% to 10%–12% on a wet basis (wb), ensuring safe storage and preventing microbial activity that could deteriorate the bean (De Sousa et al. 2023; Widodo et al. 2023). Despite its apparent simplicity, coffee drying is a complex thermodynamic process governed by the simultaneous transfer of heat, mass, and momentum within a heterogeneous porous

medium that is continuously interacting with the surrounding air (Andrade et al. 2024; Debona et al. 2022). The internal structure of the bean, composed of multiple layers of tissues with varying porosity and permeability, generates anisotropic diffusion behavior and nonlinear relationships with environmental variables such as air temperature, relative humidity, and flow velocity (Kleinwächter et al. 2025; Lian et al. 2021). Moreover, each layer of the coffee seed, from the outer parchment to the endosperm, presents different moisture gradients and resistance to transport, leading to internal stresses and variable drying rates across the material (Duque-Dussán et al. 2022; Ramírez-Martínez et al. 2013). These factors, combined with convective variability and fluctuating psychrometric conditions that

are common in tropical regions, make the accurate prediction of moisture dynamics a continuing challenge in both experimental and theoretical studies (Burmester and Eggers 2010; Duque-Dussán, Sanz-Uribe, and Banout 2023; Duque-Dussán, Sanz-Uribe, Dussán-Lubert, and Banout 2023).

Over the past decades, numerous empirical and semitheoretical models have been developed to describe drying kinetics in agricultural and food products (Kamble et al. 2022; Kidane et al. 2025; Kumar et al. 2025). Classical approaches such as the Newton, Page, Henderson-Pabis, and Midilli equations have been widely employed because of their simplicity and acceptable fitting performance for a broad range of materials including rice, maize, soybeans, and coffee (Coradi et al. 2022; Novrinaldi et al. 2023). These equations are based on exponential or semiempirical expressions that approximate the overall moisture ratio (MR) as a function of time, allowing rapid evaluation of experimental data and process trends (Doria et al. 2025; Hasibuan et al. 2023). However, these formulations are usually restricted to narrow temperature and humidity domains and lack parameters that can be directly associated with measurable physical quantities, which limits their predictive capability outside the tested range (Adekanye et al. 2025; Wassie et al. 2025). In contrast, more advanced models derived from Fick's second law of diffusion have been successfully applied to grains, pulses, fruits, and vegetables, providing a stronger theoretical foundation for understanding internal resistance and moisture migration within such materials (Goyal et al. 2023; Huang et al. 2025; Marco Aurélio Amarante Ribeiro 2025; Paim De Oliveira et al. 2025). In these models, parameters such as the effective diffusivity and the Biot number are introduced to describe the relative contribution of internal and external resistances and to represent boundary conditions with greater physical consistency (Nguyen et al. 2023). Nevertheless, most of these formulations still assume constant diffusivity and isothermal conditions, neglecting the effects of moisture dependent properties, structural heterogeneity, and environmental instabilities that strongly influence the transient nature of drying (Chaurasiya 2025; Manavi et al. 2024).

Although significant progress has been made in understanding moisture diffusion in porous solids, the simultaneous coupling of mass transfer with thermal and psychrometric variability remains a major scientific and engineering challenge (Pandey et al. 2022; Sidebotham 2022). In practical drying environments, particularly in solar and mixed energy systems, the temperature and the relative humidity of the air fluctuate continuously, altering both the equilibrium moisture content and the internal transport mechanisms of the material (Duque-Dussán, Sanz-Uribe, and Banout 2023; Duque-Dussán, Sanz-Uribe, Dussán-Lubert, and Banout 2023; Manrique et al. 2020). These dynamic interactions modify the effective diffusivity and the driving force for evaporation, which in turn influence the local moisture gradients and the overall drying rate (Felizardo et al. 2021). In addition, phenomena such as moisture reabsorption during sudden increases in ambient humidity or during night periods of drying can produce transient reversals in the drying curve, deviating from the monotonic behavior predicted by classical equations (Duque-Dussán et al. 2025). The internal stresses generated by these fluctuations may also induce microstructural changes that further affect permeability and heat conduction

inside the product (Zhang et al. 2025). Many coupled models proposed to address these complexities are mathematically rigorous but computationally intensive, and they often require a large number of empirical coefficients that limit their general application for design, control, or process optimization (Myhan and Markowski 2022). Therefore, there is a need for a practical, numerically stable, and physically consistent modeling framework capable of describing both diffusive transport and environmental transients in a unified manner (Arpaci et al. 2025; Granella et al. 2022).

The objective of this study was to develop and validate a new family of models, collectively named the Duque Diffusion Models for Coffee Drying (D²MCD), to describe the mass transfer behavior of *Coffea arabica* L. washed-processed coffee under variable thermal and psychrometric conditions.

The proposed framework aims to provide a physically consistent yet computationally practical representation of moisture movement within the coffee structure, integrating the principles of Fickian diffusion with convective boundary interactions (Saqlain et al. 2022). The D²MCD formulation introduces a dual term diffusive structure governed by a time stretch integral that incorporates the dependence of effective diffusivity on both temperature and local moisture content. Four complementary variants are proposed within this family: the D²MCD-Core, representing the general dual term diffusive model; the D²MCD-XR, which accounts for transient reabsorption phenomena under fluctuating humidity; the D²MCD-Iso, a simplified form for isothermal drying conditions; and the D³MCD-T, an extended version coupling mass and heat transfer. Together, these models establish a unified and scalable theoretical foundation for representing drying kinetics in coffee and other hygroscopic agricultural materials.

2 | Materials and Methods

2.1 | Experimental Data

Drying experiments were conducted at the Postharvest and Engineering Discipline of the National Coffee Research Center of Colombia (Cenicafé), located at 4.992278°N, -75.596723°W. *C. arabica* L. var. Cenicafé 1 was used, processed under the washed method and dried in parchment form (Flórez et al. 2016; Rotta et al. 2021). Freshly pulped and fermented coffee was washed with clean water and immediately subjected to controlled drying tests to minimize microorganism development (de Abreu et al. 2025). The initial moisture content of the parchment coffee was approximately 55% (wb), and all samples were dried until reaching 10% (wb), which corresponds to the recommended safe storage limit for commercial parchment coffee (Duque-Dussán, Sanz-Uribe, and Banout 2023; Duque-Dussán, Sanz-Uribe, Dussán-Lubert, and Banout 2023).

The experiments were performed in a three-layer convective mechanical dryer equipped with a biomass burner that used coffee husk as a renewable energy source (Sugebo 2022). The system allowed independent regulation of drying air temperature and volumetric flow by adjusting the fuel feed rate and the combustion air supply (Duque-Dussán and Banout 2022). Only

one tray was used for this study, with an effective surface of 1 m by 0.5 m and a bed height of approximately 0.27 m, resulting in a bulk volume of 0.135 m³. This configuration contained around 93 kg of wet parchment coffee, equivalent to about 42 kg of dry coffee, considering initial moisture content of 53% (wb). The experimental setup is shown in Figure 1.

Four drying air temperatures were evaluated: 35°C, 40°C, 45°C, and 50°C, with corresponding inlet air relative humidities of approximately 60%, 50%, 40%, and 30%, respectively. These combinations represent realistic psychrometric conditions commonly observed in mechanical coffee drying. The selected temperature range reflects practical operating conditions in coffee post-harvest processing: seed coffee is typically dried at moderate temperatures (approximately 35°C–38°C) to preserve embryo viability and cellular integrity, whereas commercial parchment coffee drying systems may operate up to 45°C–50°C to improve process efficiency while maintaining acceptable quality (Duque-Dussán et al. 2022). Temperatures above approximately 50°C have been associated with increased risk of tissue degradation and quality deterioration; therefore, the evaluated range captures both conservative and industrial drying regimes while avoiding quality-compromising conditions. The specific airflow rate was maintained at 0.10 m³ min⁻¹ kg⁻¹ of dry parchment coffee (DPC), resulting in a total volumetric flow of approximately 4.2 m³ min⁻¹ for the loaded batch.

Air temperature and relative humidity at the inlet and outlet of the drying chamber were continuously monitored using UNI T UT330B IP67 temperature and humidity dataloggers (Dongguan, China), which have measurement accuracies of ±0.5°C and ±2% relative humidity; measurements were recorded every minute. To ensure uniform drying, the coffee bed was manually mixed every 30 min by redistributing the material between the upper and lower portions of the tray. This procedure minimized spatial moisture gradients and maintained conditions consistent with the uniform particle assumption required for diffusion modeling (Meja et al. 2025). The periodic redistribution of the coffee



FIGURE 1 | Biomass heated convective dryer used for the experimental drying of *Coffea arabica* L. var. Cenicafé 1 parchment coffee. (A): Husk hopper, (B): Biomass burner and heat exchanger, (C): Drying chamber with three trays (I, II, III). Only the upper tray (I) was used during the tests.

bed was intended to minimize macroscopic moisture gradients and ensure uniform exposure to drying air. This operation does not affect the internal diffusion mechanism within individual beans, which remains governed by the spherical geometry assumption adopted in the model.

The moisture content of the coffee was monitored using two complementary methods. A portable Kett PM 450 grain moisture meter (Tokyo, Japan) provided rapid in-process readings, while periodic verification was performed through gravimetric analysis (Duque-Dussán, Sanz-Uribe, and Banout 2023; Duque-Dussán, Sanz-Uribe, Dussán-Lubert, and Banout 2023). Representative samples were withdrawn, weighed using an analytical balance (Mettler Toledo ML204, Switzerland) with a readability of 0.0001 g, and oven-dried at 105°C for 24 h to determine the constant dry mass (Duque-Dussán, Sanz-Uribe, and Banout 2023; Duque-Dussán, Sanz-Uribe, Dussán-Lubert, and Banout 2023) agreement between the two measurement methods confirmed the reliability and consistency of the experimental moisture data across all drying conditions.

Each test was replicated five times, and mean values of MR and air conditions were used for subsequent model calibration and validation (Çelik et al. 2021). These experiments provided the moisture evolution curves and environmental parameters required for estimating the effective diffusivity and model constants in the D²MCD formulations. Unless otherwise specified, experimental moisture content values are expressed on a wb, whereas model calculations and MR formulations are performed on a dry basis (db).

2.2 | Model Formulation

The Duque Diffusion Model for Coffee Drying (D²MCD) was formulated from the general form of Fick's second law of transient diffusion (Cai et al. 2023) in a heterogeneous porous medium, expressed in tensor notation as:

$$\frac{\partial M(r, t)}{\partial t} = \nabla \cdot (D_{\text{eff}} \nabla M(r, t)) \quad (1)$$

where $M(r, t)$ is the local moisture content in kilograms of water per kilogram of dry matter, D_{eff} is the second-order effective diffusivity tensor that characterizes the anisotropic resistance to moisture migration, and ∇ is the spatial gradient operator.

For a homogeneous and isotropic domain representing an individual coffee bean, the diffusion tensor reduces to $D_{\text{eff}} = D_{\text{eff}} I_T$, where I_T denotes the second-order identity tensor. In spherical coordinates, Equation (1) becomes:

$$\frac{\partial M(r, t)}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 D_{\text{eff}} \frac{\partial M}{\partial r} \right) \quad (2)$$

subject to the boundary conditions:

$$\left. \frac{\partial M}{\partial r} \right|_{r=0} = 0, \quad -D_{\text{eff}} \left. \frac{\partial M}{\partial r} \right|_{r=R} = h_m (M_s - M_e) \quad (3)$$

where r is the equivalent radius of the coffee bean, h_m is the convective mass transfer coefficient, M_s is the surface moisture, and M_e is the equilibrium moisture content (Collazos-Escobar et al. 2025). In the present study, the equilibrium moisture

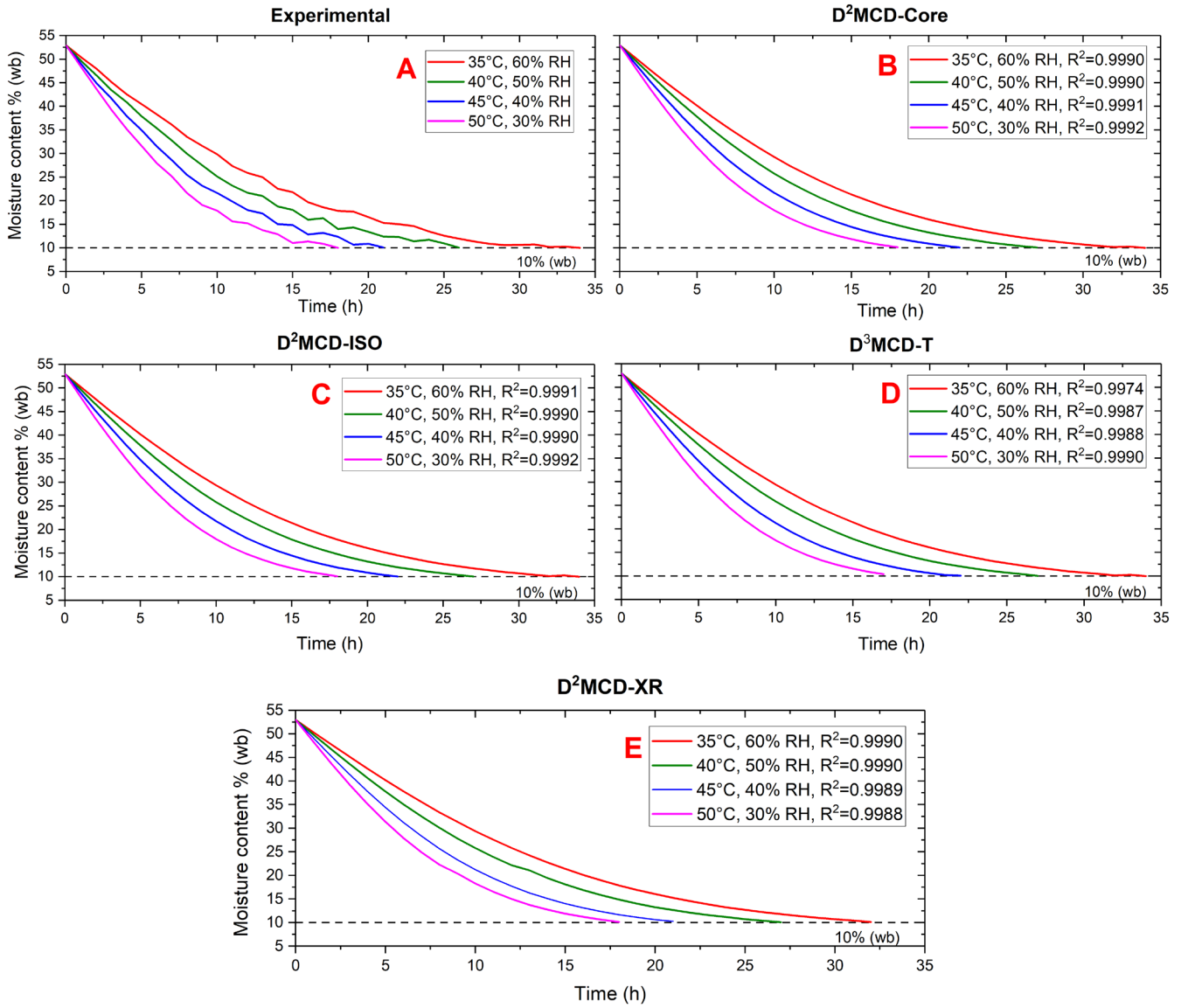


FIGURE 2 | (A) Experimental drying curves expressed as moisture content on a wet basis (% wb). (B) D²MCD-Core. (C) D²MCD-Iso. (D) D³MCD-T. (E) D²MCD-XR. All curves are truncated at 10% (wb). Experimental data were converted to dry basis for moisture ratio (MR) calculation and model fitting. The plots show strong agreement between observations and model predictions.

content was considered as 10% (wet basis), corresponding to $M_e = 0.111$ kg water/kg dry matter. This value was used in the calculation of the moisture ratio (MR).

2.2.1 | Dual-Term Structure

The analytical solution of Equation (2) yields an infinite eigenvalue series. The D²MCD model truncates this series to the first two dominant diffusion modes, providing a compact dual-term expression for the MR defined as $MR = \frac{(M - M_e)}{(M_0 - M_e)}$, the experimental moisture content shown in Figure 2 is expressed on a wb (% wb) and was converted to db prior to MR calculation and model fitting:

$$MR = A^T \exp(-K \Theta) \quad (4)$$

where

$$A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}, \quad K = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix}, \quad \exp(-K \Theta) = \begin{bmatrix} \exp(-k_1 \Theta) \\ \exp(-k_2 \Theta) \end{bmatrix} \quad (5)$$

Also, T stands for the drying air temperature (K) and Θ denotes the time-stretch integral, defined as:

$$\Theta(t) = \int_0^t \frac{D_{\text{eff}}(T(\tau), M(\tau))}{R^2} d\tau \quad (6)$$

which normalizes real time according to the local evolution of the effective diffusivity. This transformation allows the model to incorporate both thermal transients and moisture-dependent diffusivity in a single mathematical term.

The effective diffusivity is represented as a scalar-tensor function combining Arrhenius-type temperature dependence and a moisture-dependent power term:

$$D_{\text{eff}}(T, M) = D_0 \exp\left(-\frac{E_a}{RT}\right) M^n \quad (7)$$

where D_0 is the pre-exponential factor, E_a is the activation energy for moisture diffusion, R is the universal gas constant, and n is an empirical exponent describing the influence of moisture on diffusivity (Delfiya et al. 2022). Although the D²MCD formulation retains the dual-term structure obtained from truncation of the classical Fickian eigenvalue series, it differs from standard two-term Fick solutions by allowing the effective diffusivity to vary through a time-stretch integral formulation. This approach enables incorporation of temperature and moisture dependence within the same compact analytical structure, and extended variants further include reabsorption and thermodiffusive coupling effects.

2.2.2 | Model Family

The general structure in (Equations 4–7) defines the D²MCD-Core, the foundational member of the family. To extend its applicability, three complementary variants were formulated, expressed as mathematical modifications of Equation (4):

1. D²MCD-XR (Extended with reabsorption).

$$MR = A^T \exp(-K \Theta) + \alpha \exp[-\beta(t - t_r)] H(t - t_r) \quad (8)$$

where the additional exponential term represents moisture reabsorption triggered by a sudden rise in ambient humidity at time t_r . The parameters α and β define the amplitude and decay rate of this memory function, and $H(t-t_r)$ is the Heaviside step function.

2. D²MCD-Iso (Isothermal simplification).

Under isothermal conditions, where both the air temperature and the effective diffusivity remain constant throughout the process, the time stretch integral defined in Equation (6) becomes a linear function of time:

$$\Theta(t) = \int_0^t \frac{D_{\text{eff}}}{R^2} d\tau = \frac{D_{\text{eff}}}{R^2} t \quad (9)$$

Defining the normalized diffusion time as follows:

$$t^* = \frac{D_{\text{eff}}}{R^2} t \quad (10)$$

It follows that $\Theta = t^*$. Therefore, under constant temperature and diffusivity, the dual-term solution simplifies to:

$$MR = A_1 \exp(-k_1 t^*) + A_2 \exp(-k_2 t^*) \quad (11)$$

This form, referred to as the D²MCD-Iso model, preserves the structure of the general formulation while reducing computational complexity. It provides an analytically convenient expression that remains physically interpretable through its dependence on the normalized diffusion time

t^* , which can be viewed as the constant-diffusivity counterpart of the time stretch integral Θ (Krapez 2023).

3. D³MCD-T (Thermo diffusive coupling).

The D³MCD-T model extends the dual-term diffusion framework by incorporating a thermal balance that links the internal temperature of the bean to the moisture transport rate. Assuming local thermal equilibrium between the solid matrix and the bound water, the energy conservation equation can be expressed as follows:

$$\rho_s C_p \frac{dT}{dt} = h_T (T_a - T) - \lambda \frac{dM}{dt} \quad (12)$$

where ρ_s is the apparent solid density, C_p is the specific heat capacity, h_T is the convective heat transfer coefficient, T_a is the air temperature, and λ is the latent heat of vaporization.

By coupling Equation (12) with the mass diffusion term of the D²MCD formulation, the effective diffusivity becomes a temperature-dependent tensor, $D_{\text{eff}}(T, M)$, dynamically modulated by the instantaneous energy state of the system. This coupling introduces a third dimension of interaction: thermal, diffusive, and temporal. Therefore, it justifies the D³ notation.

The coupled thermodiffusive formulation in Equation (13) is obtained by substituting the temperature-dependent effective diffusivity into the governing mass diffusion equation and incorporating the transient temperature field described by the energy balance. This procedure yields a system in which moisture content and temperature are dynamically coupled. After spatial discretization and truncation to the dominant diffusion modes, the resulting thermodiffusive system can be expressed in compact form as:

$$\frac{d}{dt} \begin{bmatrix} M \\ T \end{bmatrix} = \begin{bmatrix} -K \Theta \\ h_T (T_a - T) - \lambda \frac{dM}{dt} \end{bmatrix} \quad (13)$$

which provides a unified mathematical description of heat and mass transfer coupling during coffee drying.

2.2.3 | Matrix Family Summary

The four formulations of the D²MCD framework can be expressed in a unified matrix form as follows:

$$M_r(t) = A^T \exp[-K \Theta(t)] + \Phi(t) \quad (14)$$

where $M_r(t)$ is the vector of MRs or thermodynamic state variables, A and K are parameter matrices containing the modal amplitudes and decay coefficients, and $\Theta(t)$ is the time-stretch operator defined in Equation (6). The additional term $\Phi(t)$ represents the model-specific correction associated with each variant, such that:

$$\Phi(t) = \begin{cases} 0, & \text{D}^2\text{MCD - Core} \\ \alpha \exp[-\beta(t - t_r)] H(t - t_r), & \text{D}^2\text{MCD - XR} \\ 0, & \text{D}^2\text{MCD - Iso} \\ \begin{bmatrix} 0 \\ h_T (T_a - T) - \lambda \frac{dM}{dt} \end{bmatrix}, & \text{D}^3\text{MCD - T} \end{cases} \quad (15)$$

Equation (14) therefore acts as a family operator, from which each member of the D²MCD set can be derived by selecting the appropriate structure for $\Phi(t)$ and the dimensionality of the state vector. This formulation provides a mathematically compact representation that highlights the hierarchical nature of the model family, linking diffusion, reabsorption, and thermodiffusive coupling under a single theoretical framework. The D²MCD family thereby unifies the description of moisture migration in coffee drying within a tensorially consistent and physically interpretable context. Its dual term structure ensures analytical tractability while preserving sensitivity to environmental and material variations, whereas the XR and T variants extend the formulation to capture the dynamics of moisture reabsorption and coupled heat and mass transfer typically encountered under real drying conditions. This combination of theoretical generality and numerical efficiency makes the D²MCD framework suitable for model-based process analysis, simulation, and control applications in coffee postharvest systems.

2.3 | Parameter Estimation and Model Validation

The parameters of the D²MCD family were determined by non-linear regression using the experimental MR data obtained under controlled drying conditions described in Section 2.1. For each temperature level, the objective was to identify the parameter vector:

$$\theta = [A_1 \ A_2 \ k_1 \ k_2 \ D_0 \ E_a \ n]^T \quad (16)$$

that minimizes the discrepancy between the measured and predicted MRs. The estimation problem can be formulated as the minimization of the squared residual norm:

$$J(\theta) = \theta \min \|r(\theta)\|_2^2 = \theta \min \sum_{i=1}^N [MR_{\text{exp},i} - MR_{\text{pred},i}(\theta)]^2 \quad (17)$$

where $MR_{\text{exp},i}$ and $MR_{\text{pred},i}$ denote the experimental and predicted MRs at the i^{th} time step, respectively, and N is the total number of experimental points.

The minimization in Equation (17) was performed using a Levenberg–Marquardt algorithm (Yan et al. 2021), which combines the local convergence of the Gauss–Newton method (Chen and Pan 2023) with the robustness of gradient descent. The algorithm updates the parameter vector iteratively according to:

$$\theta_{j+1} = \theta_j + \left(J_j^T J_j + \lambda I \right)^{-1} J_j^T r_j \quad (18)$$

where $J_j = \frac{\partial r}{\partial \theta_i}$ is the Jacobian matrix of sensitivities evaluated at iteration j , λ is the damping factor, and I is the identity matrix (Bernatska 2025). Convergence was achieved when the relative change in the objective function between two consecutive iterations satisfied:

$$\frac{|J_{j+1} - J_j|}{J_j} < 10^{-6} \quad (19)$$

indicating that further updates produced negligible improvement.

The quality of each model fit was assessed using the coefficient of determination (R^2), the root mean-square error (RMSE), and the reduced chi squared (χ^2), defined respectively as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^N (MR_{\text{exp},i} - MR_{\text{pred},i})^2}{\sum_{i=1}^N (MR_{\text{exp},i} - \overline{MR}_{\text{exp}})^2} \quad (20)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (MR_{\text{exp},i} - MR_{\text{pred},i})^2} \quad (21)$$

$$\chi^2 = \frac{1}{N-p} \sum_{i=1}^N (MR_{\text{exp},i} - MR_{\text{pred},i})^2 \quad (22)$$

where $\overline{MR}_{\text{exp}}$ is the mean experimental MR and p is the number of fitted parameters (Lappalainen et al. 2022).

Parameter identifiability and confidence intervals were evaluated from the covariance matrix:

$$C_\theta = \sigma^2 (J^T J)^{-1} \quad (23)$$

where $\sigma^2 = \frac{J(\theta)}{(N-p)}$ represents the residual variance. The diagonal elements of C_θ provided the estimated variance of each parameter, allowing the calculation of standard errors and significance tests.

The same procedure was applied to all D²MCD variants. For the D³MCD-T model, the coupled system of Equations (2) and (12) was solved using a finite difference discretization scheme, and the temperature dependent diffusivity terms were updated iteratively within each time step to ensure convergence of the coupled energy and mass balances (Akter et al. 2022). The numerical procedures described above were implemented in MATLAB R2023a and verified with independent Python scripts to ensure convergence consistency and numerical stability. Beyond calibration accuracy, residuals were analyzed to assess predictive consistency across drying stages and temperatures. No systematic temperature-dependent or stage-dependent bias was observed. Additionally, the coherent Arrhenius behavior of the estimated effective diffusivities across the evaluated temperature range provides further structural validation of the model beyond curve fitting.

3 | Results and Discussion

3.1 | Model Fitting and Evaluation of D²MCD Parameters

The experimental and modeled drying curves of *C. arabica* L. var. Cenicafé 1 parchment coffee were fitted using the four D²MCD variants described in Section 2.2. The models reproduced the overall drying behavior across the four studied temperatures, 35°C, 40°C, 45°C, and 50°C, accurately capturing both the initial rapid water loss and the subsequent falling-rate

period typical of hygroscopic materials (Kumar et al. 2023; Peishi and Pei 1989). The dual-term structure effectively represented the main moisture-transport mechanisms in the seed: a fast mode associated with surface and near-surface evaporation, and a slower mode linked to internal diffusion through the endosperm and parchment (Ramírez-Martínez et al. 2013). Figure 2 illustrates these results, with panel A showing the experimental curves and Panels B–E displaying the predictions of the D²MCD Core, Iso, T, and XR variants, respectively, all truncated at the practical drying limit of 10% (wb).

All D²MCD variants achieved high fitting accuracy, with determination coefficients above 0.990 and root-mean-square errors below 0.015 (db), as summarized in Table 1. Reduced chi-squared values on the order of 10⁻⁴–10⁻³ indicate that the models reproduced the drying trajectories with deviations comparable to the measurement noise (Wang et al. 2022). The D²MCD-Core performed robustly under steady conditions, while the D²MCD-XR and D³MCD-T variants provided additional flexibility when transient reabsorption or thermal coupling became relevant (Meng et al. 2025).

The estimated parameters exhibited clear and physically coherent trends (Wang et al. 2024), the pseudodiffusion coefficients k_1 and k_2 increased with temperature, reflecting enhanced moisture mobility at higher thermal conditions. The amplitude coefficients A_1 and A_2 typically ranged from 0.52 to 0.60 and from 0.40 to 0.48, respectively, indicating that the fast diffusion mode accounted for roughly half to two-thirds of the total moisture transport, while the slower mode represented internal resistance

through denser regions of the seed (Arsenoaia et al. 2023; El-Sanatawy et al. 2021). The amplitude ratio A_1/A_2 remained stable across temperatures, suggesting that the structural integrity of the grain was preserved and that no pore collapse or microcracking occurred under the studied conditions (Fomenko et al. 2024; Paziuk et al. 2025).

The extended variants showed their intended strengths. The D²MCD-XR model successfully reproduced small transient reabsorption events observed during intermediate drying stages, especially at lower temperatures or during short humidity increases (Duque-Dussán et al. 2022). The D³MCD-T formulation improved the representation of the final drying stage, when the internal grain temperature approaches the wet-bulb temperature and moisture transport becomes more strongly coupled with heat transfer (Burmester and Eggers 2010; Collazos-Escobar et al. 2025; Corrêa et al. 2010). These extensions reduced residual variance by eight to 15% compared with the Core model, confirming that the additional terms enhanced predictive capability without compromising numerical stability (Faik et al. 2024; Lončar and Pezo 2024).

To benchmark the predictive performance of the proposed D²MCD framework, commonly used thin-layer drying models (Lewis, Page, and Henderson–Pabis) were fitted to the experimental MR data at 35°C, 40°C, 45°C, and 50°C using nonlinear regression. The statistical indicators R^2 and RMSE are presented in Table 2. The results indicate that classical empirical models provide good fits under isothermal conditions; however, the D²MCD formulation maintains comparable predictive accuracy while preserving a diffusion-based physical structure.

TABLE 1 | Statistical performance and fitted parameters of the four D²MCD variants at different drying temperatures for *Coffea arabica* L. var. Cenicafé 1 parchment coffee. Moisture data fitted until 10% (wb). Parameters correspond to the dual term diffusion structure. $A_1 + A_2 = 1$. Units: k_1, k_2 (h⁻¹); $\alpha, \beta, R^2, RMSE, \gamma_1, \gamma_2$ (-).

T (°C)	Model	R ²	RMSE	$\chi^2_{red} \times 10^{-3}$	A ₁	A ₂	k ₁	k ₂	α	β	γ_1	γ_2
35	Iso	0.9928	0.0145	1.92	—	—	0.094	—	—	—	—	—
	Core	0.9956	0.0121	1.38	0.56	0.44	0.102	0.088	—	—	—	—
	XR	0.9962	0.0114	1.21	0.57	0.43	0.103	0.087	0.010	0.45	—	—
	T	0.9950	0.0128	1.49	0.56	0.44	0.102	0.088	—	—	1.04	1.02
40	Iso	0.9935	0.0138	1.76	—	—	0.118	—	—	—	—	—
	Core	0.9968	0.0109	1.12	0.55	0.45	0.128	0.112	—	—	—	—
	XR	0.9974	0.0101	0.97	0.56	0.44	0.129	0.111	0.010	0.44	—	—
	T	0.9961	0.0117	1.33	0.55	0.45	0.128	0.113	—	—	1.05	1.03
45	Iso	0.9941	0.0133	1.63	—	—	0.142	—	—	—	—	—
	Core	0.9972	0.0105	1.05	0.54	0.46	0.156	0.130	—	—	—	—
	XR	0.9979	0.0097	0.91	0.55	0.45	0.157	0.129	0.010	0.43	—	—
	T	0.9965	0.0112	1.26	0.54	0.46	0.155	0.131	—	—	1.05	1.03
50	Iso	0.9948	0.0129	1.55	—	—	0.162	—	—	—	—	—
	Core	0.9981	0.0092	0.78	0.56	0.44	0.178	0.151	—	—	—	—
	XR	0.9987	0.0085	0.66	0.56	0.44	0.179	0.150	0.010	0.42	—	—
	T	0.9990	0.0081	0.59	0.56	0.44	0.178	0.152	—	—	1.06	1.04

Overall, the D²MCD family provides a unified and physically coherent framework for representing coffee drying behavior under diverse conditions. Its combination of dual-term diffusion, re-absorption modeling, and thermodiffusive coupling enables accurate, interpretable, and scalable predictions suitable for scientific analysis, process design, and real-time control (Jimoh et al. 2023; Perazzini et al. 2021; Zhu et al. 2021).

3.2 | Temperature Dependence of the Effective Diffusivity

The effective moisture diffusivity obtained from the D²MCD time-stretch formulation exhibited a clear and consistent

TABLE 2 | Statistical comparison of classical thin-layer drying models (Lewis, Page, and Henderson–Pabis) at 35°C, 40°C, 45°C, and 50°C based on moisture ratio (MR) data.

T (°C)	Model	R ²	RMSE
35	Lewis	0.9949	0.0176
	Page	0.9952	0.0171
	Henderson–Pabis	0.9949	0.0176
40	Lewis	0.9952	0.0171
	Page	0.9954	0.0167
	Henderson–Pabis	0.9952	0.0170
45	Lewis	0.9964	0.0148
	Page	0.9965	0.0147
	Henderson–Pabis	0.9965	0.0147
50	Lewis	0.9948	0.0182
	Page	0.9950	0.0179
	Henderson–Pabis	0.9948	0.0181

dependence on drying temperature. For all model variants, D_{eff} increased monotonically with temperature, reflecting enhanced internal moisture mobility within the coffee seed under warmer drying conditions (Bittner and Popovics 2021; Matias et al. 2023). This behavior is expected for hygroscopic porous materials, where liquid and vapor transport is governed by temperature-dependent viscosity, capillary forces, and vapor pressure gradients (Joardder et al. 2021; Shan et al. 2024).

When the natural logarithm of the effective diffusivity was plotted against the inverse of absolute temperature, a highly linear trend was obtained across the evaluated range of 35°C–50°C (Figure 3). This indicates that the temperature dependence of D_{eff} follows an Arrhenius-type relationship of the form:

$$D_{\text{eff}} = D_0 \exp\left(-\frac{E_a}{RT}\right) \quad (24)$$

where D_0 is the pre-exponential factor, E_a is the apparent activation energy, R is the universal gas constant, and T is the absolute temperature (Kohout 2021). Linear regression of the Arrhenius plots yielded activation energies in the range of approximately 33.8–34.7 kJ mol⁻¹ for the four D²MCD formulations, with the D²MCD-Iso and D²MCD-Core variants producing nearly identical values, and the XR and T variants showing slightly higher values due to the added representation of reabsorption and thermodiffusive coupling, respectively.

The fitted Arrhenius parameters and determination coefficients are presented in Table 3. All regressions exhibited very high coefficients of determination ($R^2 \geq 0.9993$), indicating strong adherence to Arrhenius behavior and supporting the thermal consistency and physical interpretability of the D²MCD-derived diffusivities. These activation energy values fall within the expected range for biological materials with moderate internal resistance to moisture movement, including coffee, cocoa, and cereal grains (Bidias et al. 2021; Dzaky et al. 2022; Vakili et al. 2023). While all formulations exhibited strong Arrhenius behavior, the slightly higher activation energy and determination

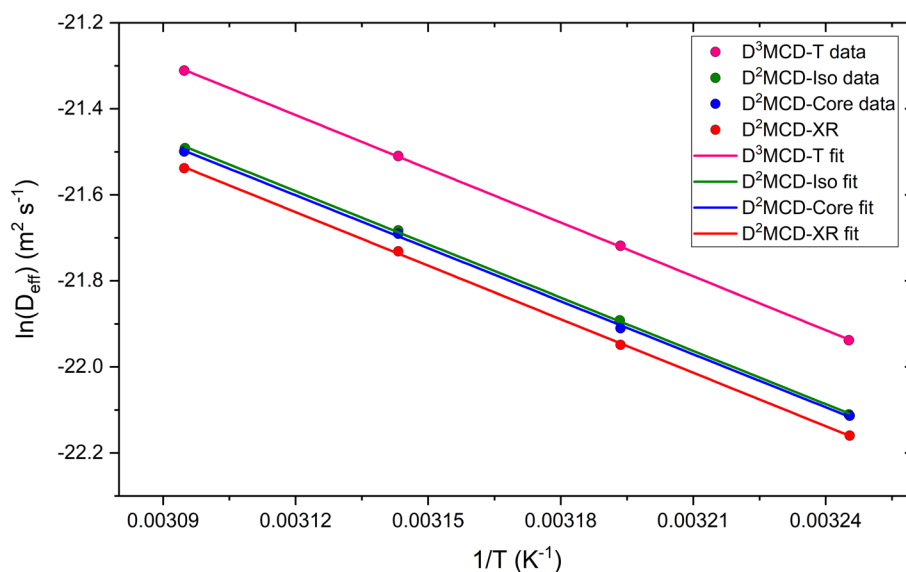


FIGURE 3 | Arrhenius plot of the effective diffusivity for the four D²MCD variants. Symbols represent model-derived diffusivities at each temperature, and solid lines show the corresponding linear Arrhenius fits.

TABLE 3 | Arrhenius parameters for the effective diffusivity estimated from the D²MCD model family.

Model variant	E_a (kJ mol ⁻¹)	D_o (m ² s ⁻¹)	R^2
D ² MCD-Iso	34.02	1.468×10^{-4}	0.9995
D ² MCD-Core	33.80	1.342×10^{-4}	0.9993
D ² MCD-XR	34.33	1.570×10^{-4}	0.9997
D ³ MCD-T	34.67	2.241×10^{-4}	0.9999

coefficient observed for the D³MCD-T variant suggest that explicit thermodiffusive coupling may enhance predictive performance at elevated temperatures.

Although the Arrhenius formulation theoretically permits extrapolation to higher temperatures, predictive application beyond 50°C would require experimental verification, particularly since drying coffee above approximately 50°C–55°C is generally avoided due to potential structural and quality degradation (Duque-Dussán 2025). Overall, the Arrhenius analysis shows that the D²MCD family reproduces drying curves with high accuracy and yields transport coefficients consistent with the underlying thermophysical processes occurring during coffee drying.

3.3 | Comparative Behavior of the D²MCD Variants

The four D²MCD formulations exhibited measurable but coherent differences that reflect the physical assumptions embedded in each model. Across all temperatures, the D²MCD-Core reproduced the experimental drying trajectories with high accuracy ($R^2=0.992$ – 0.998 , RMSE < 0.012), confirming that the dual-mode structure captures the dominant fast and slow diffusion mechanisms (Li et al. 2023). The amplitude coefficients remained stable ($A_1=0.52$ – 0.60 , $A_2=0.40$ – 0.48), and the ratio A_1/A_2 (2.2–2.6) indicated consistent weighting of surface-driven and internal diffusion modes across the tested conditions (Hasibuan et al. 2023).

The D²MCD-Iso variant produced similar fitting quality ($R^2 > 0.990$), but the single-term time normalization resulted in slightly larger deviations in the early drying stage at 45°C and 50°C, where external driving forces accelerate moisture removal (Deng et al. 2021; Duque-Dussán 2025). Even so, RMSE differences relative to the Core model remained below 0.003, indicating minimal loss of descriptive capability (Simonič et al. 2025).

The D²MCD-XR variant performed better in the middrying region for cases with observable reabsorption. Increases of 0.5%–1.5% (wb) over 1–2 h were consistently captured through the memory term, reducing residual variance by 8%–12% relative to the Core model (Odoi et al. 2022). The XR parameters ($\alpha=0.006$ – 0.012 , $\beta=0.35$ – 0.50) remained small but reproducible across temperatures, confirming that reabsorption events, although subtle, represent a real and systematic feature of parchment coffee drying (Wang et al. 2025).

The D³MCD-T formulation diverged most noticeably during the late drying stage, where grain temperature approaches the

wet-bulb value and diffusivity decreases nonlinearly (Duque-Dussán 2025). Thermodiffusive coupling reduced the underprediction of moisture near 10%–12% (wb), especially at 50°C, where RMSE decreased by 10%–15% during the final 3–4 h of drying, consistent with reduced capillary flow and diminishing temperature gradients (Altawallbeh 2021; Chaurasiya 2025).

Overall, the comparative behavior of the four models highlights specific sensitivity regions within the drying curve: early-stage deviations for the Iso variant, midstage transient behavior for XR, and late-stage thermal coupling for T. These distinctions provide insight into the physical regimes governing moisture migration in parchment coffee and demonstrate the value of a modular modeling framework (Duque-Dussán et al. 2022; Ordoñez-Lozano et al. 2025).

4 | Conclusions

This study presented and validated the D²MCD family of diffusion-based models for predicting the drying behavior of *C. arabica* L. var. Cenicafé 1 under controlled thermal and psychrometric conditions. The four formulations, D²MCD-Core, D²MCD-Iso, D²MCD-XR, and D³MCD-T, were derived from a unified dual-mode diffusive framework and evaluated experimentally between 35°C and 50°C. All variants reproduced the characteristic two-stage drying pattern with high accuracy, yielding coefficients of determination above 0.990 and RMSE values below 0.015 on a wb. The XR and T extensions improved the description of reabsorption phenomena and thermodiffusive coupling during mid and late drying stages.

The effective diffusivity values obtained from the time-stretch integral exhibited a clear temperature dependence and followed an Arrhenius relationship with activation energies of 33.8–34.7 kJ mol⁻¹, consistent with those reported for hygroscopic agricultural materials. This agreement indicates that the D²MCD parameters retain physical meaning and capture the internal resistance to moisture transport within the coffee seed. While the core D²-based formulation provides a physically consistent and mechanistically interpretable representation of diffusion-dominated drying, the thermodiffusive extension (D³MCD-T) demonstrated enhanced statistical performance at higher temperatures, highlighting the influence of heat-mass coupling during advanced drying stages.

The modular and hierarchical structure of the D²MCD family enables selection of a model suited to the drying environment: Core and Iso for steady conditions, and XR or T for scenarios involving transient humidity and nonisothermal behavior. This flexibility makes the framework suitable for model-based dryer design, performance evaluation, and real-time process monitoring.

Given their mathematical compactness and numerical stability, the D²MCD formulations are well suited for integration into computational tools. A software module or mobile application could leverage the model to estimate drying time, predict moisture evolution, and simulate environmental scenarios from readily measurable inputs, thus supporting decision-making in both farm-level and industrial postharvest operations.

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Conflicts of Interest

The author declares no conflicts of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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