A STEM-Based Methodology for Designing and Validating a Cannabinoid Extraction Device: Integrating Drying Kinetics and Quality Function Deployment

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Section 1. Effect of geometrical parameters on D_{eff}

Taking into account the radius (R) and height (H) of the samples. The next mathematical model was developed

1.1 Cylinder mathematical model development and its comparison,

$$m(t) = (m_0 - m_e)e^{-kt} + m_e \qquad \text{(S1)}$$

Where: m(t) is the percentage of humidity at any time t; k is a drying constant (min^{-1});
t is a drying time; m_o is the initial humidity percentage at $t \to 0$; and m_e is the percentage of humidity when at $t \to \infty$; and from Eq.S1 we can construct the dehydration ratio $MR = \frac{m(t)-m_e}{m_0-m_e} = e^{-kt}$ and it is the left side of Fick's second law Eq.S2, which we can see below.

Due to the harvested FHB potentially exhibiting a cylinder morphology [22], the exact solution of the mathematical relationship between *MR* and Fick's second law is:

$$MR = \frac{m(t) - m_e}{m_0 - m_e} = e^{-kt} = \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} \frac{4}{\alpha_m^2} \frac{8}{(2n+1)^2\pi^2} e^{\left[-D_{eff}\left(\frac{\alpha_m^2}{R^2} + \frac{(2n+1)^2\pi^2}{H^2}\right)t\right]} \qquad \text{(S2)}$$

From Equation S1 (third and fourth terms), we derived Fick's second law diffusion model for moisture transport during the dehydration of a finite cylinder, where R is the radius (m), and H is the height (m). We also provide the standard analytical form for the moisture ratio and height, its application in estimating the D_{eff}, where D_{eff} is the effective diffusivity (m^2/min). When m=1 and n=0, through mathematical development, the $A_{10} = \frac{32}{\alpha_1^2\pi^2}$ is the Bessel function roots and $\alpha_1 \approx 2.4048$, we obtain:

$$e^{-kt} \approx A_{10} e^{\left[-D_{eff}\left(\frac{\alpha_1^2}{R^2} + \frac{\pi^2}{H^2}\right)t\right]} \qquad \text{(S3)}$$

$$ln[e^{-kt}] \approx ln\left\{A_{10}e^{\left[-D_{eff}\left(\frac{\alpha_1^2}{R^2}+\frac{\pi^2}{H^2}\right)t\right]}\right\} \quad \text{(S5)}$$

$$ln[e^{-kt}] \approx ln[A_{10}] + ln\left\{e^{\left[-D_{eff}\left(\frac{\alpha_1^2}{R^2}+\frac{\pi^2}{H^2}\right)t\right]}\right\} \quad \text{(S6)}$$

$$-kt \approx ln[A_{10}] - D_{eff}\left(\frac{\alpha_1^2}{R^2}+\frac{\pi^2}{H^2}\right)t \quad \text{(S7)}$$

$$k = D_{eff}\left(\frac{\alpha_1^2}{R^2}+\frac{\pi^2}{H^2}\right) \quad \text{(S8)}$$

$$D_{eff} = \frac{k}{\left(\frac{5.7831}{R^2}+\frac{\pi^2}{H^2}\right)} \quad \text{(S9)}$$

1.1.1. Calculation of m_e, k, and D_{eff}

The next steps were: (a) to obtain m_e from experimental data on the weight of the samples, we constructed more data by applying the mathematical model Eq.S1 by making time tend towards infinity; (b) All samples were modeled by applying Eq.S1 and substituting the constants m_0 and m_e as a function of time t; (c) calculate *MR* from Eq.S1 of the all experimental data profiles and to do a fitting of the profile; (d) Calculate *k* based on the exponential fitting applied Eq.S1 ; (e) calculate D_{eff} applied Eq.S9 for each sample.

1.1.2. Ratio calculation between D_{eff} Cylinder geometry and Slab geometry

Table S1. A ratio is calculated between the moisture diffusivity coefficients during the dehydration process of slab-shaped and cylindrical geometries, revealing a ratio with a constant trend. We hypothesize that several overlapping samples with slab geometries combine to form a cylindrical geometry, meaning they share the same physicochemical properties and are homogeneous due to originating from the same plant. Moisture refractive index (MR) is a dehydration moisture gradient, which allows us, using mathematical modeling and Fick's second law, to calculate the dehydration coefficient. The diffusivity coefficient (or diffusion coefficient) is a transport property that quantifies the ease with which particles (atoms or molecules) move through a medium. Its intrinsic physical properties depend primarily on the nature of the species involved and the environment.

Table S1. Relationship between D_{eff} Cylinder and D_{eff} Slab geometries

Sample	k (min^{-1})	Slab geometry D_{eff} (m^2min^{-1})	Cylinder geometry D_{eff} (m^2min^{-1})	D_{eff} Ratio (Slab/Cylinder)
S1	0.06999311	7.09175E-07	1.1179E-07	6.34379119
S2	0.05878736	2.38255E-06	3.75572E-07	6.34379119
S3	0.06967223	6.35332E-06	1.0015E-06	6.34379119
S4	0.05160196	1.30709E-05	1.8961E-06	6.89356937
SFP	0.0956193	1.55011E-07	3.85743E-08	4.01851884
SCP	0.12398211	1.13058E-05	2.24246E-06	5.04168497

Figure S1 shows D_{eff} values based on the SCP sample, varying the thickness or height. When L increases, D_{eff} increases too. That's why the milled samples were included for drying.

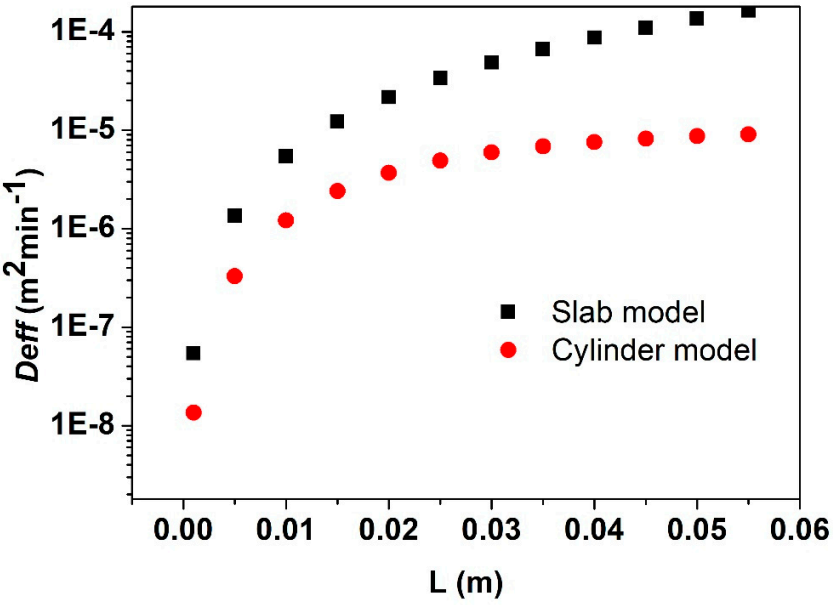


Figure S1. The relationship between the D_{eff} and the height or thickness (L or H) in the slab and cylinder geometry.

Figure S2 shows the D_{eff} values as a function of the Density; the trends are very similar to those found with slab geometry.

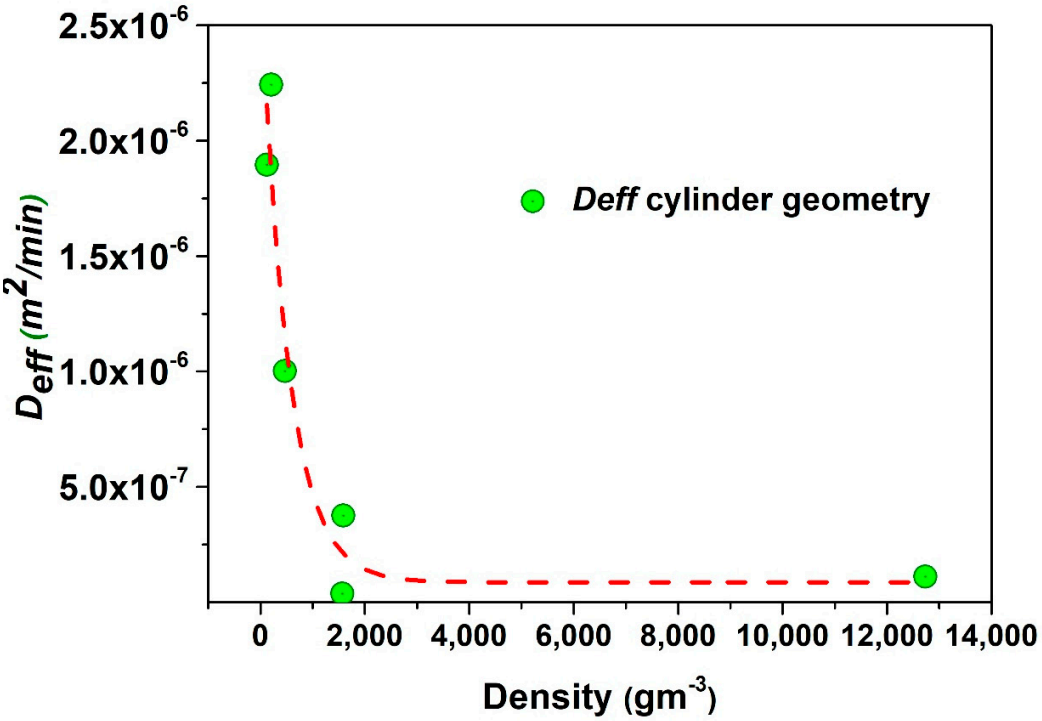


Figure S2. *Deff* values as a function of the Density of the six samples.