

# Multiscale modeling for food drying: A Downscaling approach

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## ABSTRACT

Modeling cellular-level transport phenomena in plant-based food materials during drying remains a complex challenge. Intracellular water (ICW) plays a critical role in drying kinetics but is often overlooked in computational models. Multiscale modeling offers a potential approach to capture the effects of ICW; however, existing models frequently neglect ICW dynamics or predetermine its transport. This work aims to develop a multiscale downscaling model which can actively downscale a materials condition (dependent variables) to investigate the transport of ICW. Two different drying temperatures (47°C and 64°C) and the ICW transport at three different points of interest within the domain are investigated. The results were compared to experimental data and a control model. The downscaling model predicts drying at 47°C very well achieving mean relative errors (MREs) of 3.62% and 0.66% for the average moisture content and average temperature respectively. At 64°C, the model also predicts drying well achieving MREs of 8.38% and 0.90% for the average moisture content

23 and average temperature respectively. The ICW at each point of interest was calculated and its  
 24 trend through the cell wall revealed interesting findings.

25 **Keywords:** multiscale modeling, cell rupturing, food drying, downscaling

26 **NOMENCLATURE**

<b>Abbreviations</b>	
FW	Free water
ICW	Intracellular water
REV	Representative elementary volume
<b>Symbol</b>	
$a$	Constant
$C$	Macroscale instantaneous moisture concentration ( $\text{mol m}^{-3}$ )
$c$	Microscale concentration ( $\text{mol m}^{-3}$ )
$c_p$	Specific heat of apple tissue ( $\text{J kg}^{-1} \text{K}^{-1}$ )
$c_{p \text{ air}}$	Specific heat of air ( $\text{kJ kg}^{-1} \text{K}^{-1}$ )
$D$	Cellular diffusivity ( $\text{m}^2 \text{s}^{-1}$ )
$D_{H,eff}$	Upscaled effective moisture diffusivity ( $\text{m}^2 \text{s}^{-1}$ )
$D_{FW}$	Diffusivity of free water ( $\text{m}^2 \text{s}^{-1}$ )
$D_{ICW}$	Diffusivity of intracellular water ( $\text{m}^2 \text{s}^{-1}$ )
$h_{fg}$	Latent heat of evaporation ( $\text{J kg}^{-1}$ )
$h_m$	Mass transfer coefficient ( $\text{m s}^{-1}$ )
$h_T$	Heat transfer coefficient ( $\text{W m}^{-2} \text{K}^{-1}$ )
$k$	Thermal conductivity of apple tissue ( $\text{W m}^{-1} \text{K}^{-1}$ )
$k_c$	Gordon and Taylor constant
$L_c$	Characteristic length (m)

$M_{db}$	Moisture content dry basis (kg kg <sup>-1</sup> dry basis)
$M_{db}$	Dry basis moisture content (kg kg <sup>-1</sup> dry basis)
$\overline{M}_{db,num}$	Average predicted moisture content (kg kg <sup>-1</sup> dry basis)
$M_w$	Molar mass of water (kg mol <sup>-1</sup> )
$\mathbf{n}$	Unit vector normal to the boundary
$P_m$	Permeability of the cell wall (m s <sup>-1</sup> )
$p_{v\ air}$	Vapor air pressure of ambient air (Pa)
$p_{v\ eq}$	Equilibrium vapor pressure (Pa)
$p_{v\ sat}$	Saturated vapor pressure of water (Pa)
$q_c$	Mass flux (mol m <sup>-2</sup> s <sup>-1</sup> )
$R$	Universal gas constant (J mol <sup>-1</sup> K <sup>-1</sup> )
$t$	Time (s)
$T_{air}$	Drying air temperature (K)
$T_{cell}$	Temperature of the cell (K)
$T_g$	Glass transition temperature
$T_{g0}$	Initial glass transition temperature
$T_{gw}$	Glass transition temperature of water
$T$	Temperature (K)
$u_1$ and $u_2$	Corrective factors
$v$	Air velocity (m s <sup>-1</sup> )
$v_n$	Shrinkage velocity (m s <sup>-1</sup> )
$X$	Distance (m)
$WC_{ICW}$	Intracellular water content
$\beta$	Coefficients

$\psi$	Point of interest
$\rho$	Density of apple tissue ( $\text{kg m}^{-3}$ )
$\omega$	Area of the macroscale domain ( $\text{m}^2$ )

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## 28 **1. INTRODUCTION**

29 Plant-based food materials (PBFMs) have heterogeneous cellular structures comprising  
30 of three main cellular environments with each environment containing water of different  
31 characteristics: free water (FW) in intercellular spaces, intracellular water (ICW) in  
32 intracellular spaces and strongly bound water within the cell walls (Khan et al., 2018), Figure  
33 1. Drying PBFMs involves simultaneous heat and multiphase mass transfer which dynamically  
34 changes a material in terms of its properties, characteristics and final quality (Weligama  
35 Thuppahige et al., 2024). These changes originate within the heterogeneous cellular structure  
36 of the material and propagate across multiple length scales (cellular/microscale to  
37 tissue/macroscale). These changes are a direct result of the complex internal water migration  
38 during drying, specifically the transport of ICW is a major concern during drying due to its  
39 influence on materials cellular structure. However, the transport of ICW is complex as it  
40 depends on the spatial and temporal drying conditions in addition to the property changes the  
41 material is experiencing (Welsh et al., 2023). ICW can transport two main ways, apoplastic  
42 transport where ICW migrates from intracellular spaces to intercellular spaces after a cell  
43 membrane ruptures or through symplastic transport where ICW migrates from cell to cell via  
44 fine capillaries (Weligama Thuppahige et al., 2024). The use of computational mathematical  
45 models to understand and control the effects of migrating ICW is essential in designing optimal  
46 drying processes. However, ICW and its effects are rarely considered in mathematical models  
47 of food drying.

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[Figure 1 can be placed here]

Whitaker (1977) theory forms the foundation for many modern mathematical models. The theory derives a mechanistic macroscale model using the concept of a representative elementary volume (REV) considering the microscale heat, mass and momentum conservation equations of each phase (solid, liquid water, water vapor and air). However, Whitaker theory fails to consider the material's heterogeneity and assumes no ICW exists, rather it assumes all water is located outside the solid matrix. **This often results in the Whitaker model performing better in the early stages of drying.** To overcome and compensate for this oversimplistic assumption, condition dependent properties are embedded within the computational models. Condition dependent properties (*i.e. diffusivity*) are properties which are accurate only when modeling the specific scenario/conditions in which the property was originally derived, for example properties which depend on a specific material, drying conditions (*i.e.* air temperature, air speed) and/or the dryer configuration. Additionally, the further the simulated conditions deviate from the original conditions in which the property was derived, the less accurate the property becomes. One approach which can aid in transitioning away from condition-dependent properties while considering ICW is multiscale modeling. Multiscale modeling considers a series of sub-models over multiple length scales, giving it the ability to incorporate large amount of physics for a reasonable computational cost (Welsh et al., 2018). There are two main types of multiscale models, one way coupled models and two-way coupled (concurrent) models (Welsh et al., 2018). A one way coupled multiscale model transfers information in one direction, either through upscaling or downscaling. In such models, properties are often computed considering the structure of the particular material and upscaled to inform a larger scale. Alternatively, dependent variables can be downscaled to analyze the behavior at a smaller scale. Concurrent or two way coupled models, on the other hand, allow bidirectional

73 information exchange. Here, data flows back and forth between scales, with each scale  
74 evolving simultaneously and influencing the other. This concurrent exchange includes  
75 upscaling, downscaling, and mutual information exchange throughout the simulation, enabling  
76 both scales to adjust based on the other's evolving state (Welsh et al., 2018). Multiscale  
77 modeling has gained recent attention in the field of food drying modeling with various  
78 multiscale **models** being developed based on various assumptions. Qiu et al. (2022) developed  
79 a pore scale multiscale model for impingement drying of a porous slab. The work demonstrated  
80 the strength of predicting the drying performance through their multiscale approach to transport  
81 properties rather than the traditional condition dependent approach. Tan et al. (2023) also  
82 developed a pore-scale model for the heat-moisture and stress-stain distributions for high-  
83 moisture porous media. However, these works failed to consider ICW as all water considered  
84 was located in the pores/capillaries rather than the solid material.

85 Over the years there has been a few cellular models and multiscale models which have  
86 considered ICW within the solid material. Fanta et al. (2013) developed a microscale model to  
87 better understand the underlying phenomena of pear dehydrating under isothermal conditions  
88 at 25 °C. The work considered water in each cellular environment, allowing the work to  
89 investigate the different pathways water can flow. The largest gradients in water content were  
90 observed across the cell walls and cell membranes. Rahman et al. (2018) also developed a  
91 micro-level transport model for drying apple parenchyma cells while considering ICW and  
92 conducting an in-depth sensitivity investigation. Prawiranto et al. (2018) constructed a cellular  
93 3D continuum model for the dehydration of apple. The study considered water in various  
94 cellular environments and modelled dehydration with a predetermined set of cellular  
95 changes/conditions (turgid, free shrinkage, lysis and plasmolysis). However, these works  
96 developed only cellular models rather than multiscale models, utilizing a single microscale  
97 domain to represent the transport occurring and often modelled predetermined

98 conditions/scenarios for deformation and/or relative humidity. During drying, significant  
99 spatial and temporal variations (in terms of moisture and temperature) develop within a product  
100 which cannot be fully understood/investigated with a singular microscale domain. These  
101 variations are especially evidence in the later stages of drying when the inner portion of the  
102 material can be fully wet/saturated, whereas the outer cells of the material can be fully dried  
103 and deformed. Recently, Welsh et al. (2021a) developed a multiscale model for predicting the  
104 diffusivity of apple through upscaling during convective drying. The work considered ICW  
105 coupled with predetermined temperature dependent domains. The authors later extended their  
106 multiscale approach to inversely calculate the temporal cellular diffusivity of ICW in apples  
107 (Welsh et al., 2021b) and to construct a generalized diffusivity tensor which is applicable to  
108 multiple materials and conditions (Welsh et al., 2023). However, again their work focused on  
109 multiscale models which upscaled properties by utilizing predetermined microscale domains  
110 and/or considered every possible microscale scenario rather than predicting the spatiotemporal  
111 conditions occurring throughout the material. To predict the spatiotemporal conditions the  
112 cellular structure is experiencing a multiscale model which is capable of downscaling is  
113 required.

114 This work aims to develop a multiscale model capable of downscaling the dependent variables  
115 to appropriately predict the spatiotemporal conditions a material's cellular structure  
116 experiences during drying. The work investigates two different drying temperatures (47°C and  
117 64°C) and focuses on the microscales at three different points of interest within the domain.  
118 Additionally, the trend of ICW and its flux through the cell wall is investigated. The  
119 downscaling approach also incorporated cellular shrinkage through the shrinkage velocity  
120 approach paired with X-ray Micro-Computed Tomography (X-ray  $\mu$ CT) data to future improve  
121 the generalizability of the multiscale model. The modeling results are also compared to  
122 experimental data and a single scale control model.

## 123 **2. Model Development**

### 124 *2.1 Drying model*

125 A preliminary multiscale model was previously developed **considering** two spatial  
126 scales, a microscale and a macroscale (Welsh et al., 2021a), Figure 2. However, the previous  
127 model was only capable of upscaling information, specifically diffusivity, using **predetermined**  
128 conditions at the microscale. This study extends the preliminary model, allowing the model to  
129 downscale the required variables and evolve the microscale with time to investigate the  
130 different spatiotemporal conditions the cellular structure experiences throughout the entire  
131 material. Additionally, the ICW content required to calculate the diffusivity [Equation (16)], is  
132 **calculated** from the size of the intracellular space, outlined in 2.2.6, which is unique to this  
133 study. The modeling methods will present the multiscale governing equations, boundary  
134 conditions, properties, structure representation at each scale, computational approach, and  
135 temporal coupling. The modeling domains for both scales can be found in Figure 2.  
136 Additionally, the three points of interest, point 1 (P1), point 2 (P2) and point 3 (P3) are evenly  
137 distributed horizontally across the center of the macroscale [denoted by the red dots Figure 2  
138 (a)].

139 **[Figure 2 can be placed here]**

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### 141 *2.2 Structure Representation at each scale*

142 The macroscale can be considered as homogeneous following the common approach in  
143 literature, however, careful consideration needs to be taken when it comes to the microscale.  
144 Two common cellular structure definitions/classifications exist in the literature, (1)  
145 macroscopically connected and (2) disconnected inclusions, each effecting the model's  
146 assumptions and physics. Over the years, Perré (2019) has considered timber as connected

147 inclusions for their multiscale models, resulting in an additional “secondary flux” of the  
148 divergence of the microscopic flux being considered in the macroscale governing equations  
149 when completing the scaling (Perré, 2007, 2019). Karunasena et al. (2015) considered the food  
150 material as hexagon shaped cells evolving the porosity through removing some cells from the  
151 arrangement for their meshfree models. The resulting structure appears to be disconnected  
152 inclusions, though the work does not scale any results. Prawiranto et al. (2018) investigated the  
153 transport and cellular changes of a single cuboctahedron shaped apple cell during drying. The  
154 cell was located in the center of their 3D domain with voids (or pores) in all eight corners of  
155 the cube, however, only basic volume averaging was considered to interpolate the results to the  
156 macroscale. Fanta et al. (2014) and Rahman et al. (2018) considered an arrangement of multiple  
157 intracellular and intercellular spaces while modeling the transport within the cellular structure  
158 of PBFMs. The resulting structure is considered disconnected inclusions, though these works  
159 also considered cell walls within the domains. Additionally, these works only model the  
160 microscale transport phenomena and no scaling was conducted. In reality, fresh PBFMs  
161 generally contain disconnected inclusions (pores) and during drying the structure evolves and  
162 if cell rupturing occurs the inclusions will become connected. As a result, the model will  
163 consider the structure as connected inclusions, however, as the model is being applied to  
164 convective drying, internal convective flow can be neglected and the “secondary flux”  
165 representing the flow through the cell structure is not considered. Nevertheless, if the multiscale  
166 approach was applied to model other drying techniques (such as microwave drying) the  
167 secondary flux would need to be considered.

168         The size of the microscale is important due to its effect on computational cost and  
169 possible influence on the results. Additionally, the microscale must accurately represent the  
170 dynamic microstructure, specifically the domain must represent the two key characteristics  
171 which dynamically change during drying, namely the porosity and free/bound water.

172 Prawiranto et al. (2020) consider multiple domain sizes for dehydrating apple concluding  
173 0.5mm cubed to be sufficient to accurately represent the structure. Carr et al. (2013) developed  
174 a multiscale model for timber utilizing a microscale size of 50  $\mu\text{m}$  with two sub-domains, a  
175 cell and its cell wall. With this in mind, the microscale domain has a size of 250  $\mu\text{m}$  with an  
176 initial cell size of 215  $\mu\text{m}$  calculated from the obtained X-ray  $\mu\text{CT}$  images, visually displayed  
177 in Figure 2.

### 178 2.2.1 Macroscale conservation equations

179 In an axisymmetric coordinate system, the macroscale transport model was developed  
180 with the following assumptions: (1) internal convective flow and heat generation are negligible,  
181 (2) drying air properties remain constant, (3) heating is axisymmetric, (4) moisture evaporates  
182 solely from the surface, and (5) thermal equilibrium is maintained across all phases. The  
183 macroscale mass and energy conservation equations are derived using Fick's law of diffusion  
184 and Fourier's law of heat transfer. These equations determine the moisture concentration  $C$   
185 ( $\text{mol}/\text{m}^3$ ) and temperature  $T$  (K) as functions of position and time. The respective equations are  
186 as follows (Golestani et al., 2013).

$$187 \quad \frac{\partial C}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left[ -D_{H,eff} r \frac{\partial C}{\partial r} \right] + \frac{\partial}{\partial z} \left[ -D_{H,eff} \frac{\partial C}{\partial z} \right] = 0 , \quad (1)$$

$$188 \quad \rho c_p \frac{\partial T}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left[ -k r \frac{\partial T}{\partial r} \right] + \frac{\partial}{\partial z} \left[ -k \frac{\partial T}{\partial z} \right] = 0 , \quad (2)$$

189 where  $t$  is the time (s),  $\rho$  represents the density of the food tissue ( $\text{kg}/\text{m}^3$ ),  $c_p$  is the specific heat  
190 of the food tissue ( $\text{J}/(\text{kg}\cdot\text{K})$ ),  $k$  denotes the thermal conductivity of the food material ( $\text{W}/(\text{m}\cdot\text{K})$ )  
191 and  $D_{H,eff}$  is the upscaled effective moisture diffusivity ( $\text{m}^2/\text{s}$ ). The effective moisture diffusivity  
192 varies with temperature and  $WC_{ICW}$ , the ICW content (%).

### 193 2.2.2 Boundary conditions

194 The macroscale boundary conditions for the mass flux and heat transfer at the exterior  
 195 surface was given by,

$$196 \quad \mathbf{n} \cdot [-D_{H,eff} \nabla C] = h_m \frac{(p_{v,eq} - p_{v,air})}{RT}, \quad (3)$$

$$197 \quad \mathbf{n} \cdot [-k \nabla T] = h_T (T - T_{air}) - h_m \frac{(p_{v,eq} - p_{v,air})}{RT} h_{fg} M_w, \quad (4)$$

198 where  $h_m$  is the mass transfer coefficient (m/s),  $h_T$  is the heat transfer coefficient (W/(m<sup>2</sup>·K)),  
 199  $p_{v,eq}$  is the equilibrium vapor pressure,  $p_{v,air}$  is the vapor air pressure of ambient air (Pa),  $\mathbf{n}$  is  
 200 the unit vector normal to the boundary,  $R$  is the universal gas constant (J/(mol·K)),  $T_{air}$  is the  
 201 drying air temperature (K),  $M_w$  molar mass of water (g/mol) and  $h_{fg}$  is the latent heat of  
 202 evaporation (J/kg). The equilibrium vapor pressure for apple can be determined from the  
 203 sorption isotherm. Thus, the equilibrium vapor pressure for apple ( $p_{v,eq}$ ) is (Ratti et al., 1989),

$$204 \quad p_{v,eq} = p_{v,sat}(T) \exp(-0.182 M_{db}^{-0.696} + 0.232 e^{-43.949 M_{db}} M_{db}^{0.0411} \ln[p_{v,sat}(T)]). \quad (5)$$

205 where  $M_{db}$  is the dry basis moisture content (kg/kg dry basis) (calculated through Equation A.1  
 206 in the supplementary material). The saturated vapor pressure is given by (Vega-Mercado et al.,  
 207 2001),

$$208 \quad p_{v,sat} = \exp \left[ \frac{-5800.2206}{T} + 1.3915 - 0.0486T + \right. \\ \left. 0.4176 \times 10^{-4} T^2 - 0.1445 \times 10^{-7} T^3 + 6.546 \ln(T) \right]. \quad (6)$$

209 The last boundary condition for the macroscale is the symmetric condition applied at  
 210  $r=0$  (Figure 2), defined as

$$211 \quad \mathbf{n} \cdot [-D_{H,eff} \nabla C] = 0, \quad (7)$$

$$212 \quad \mathbf{n} \cdot [-k \nabla T] = 0. \quad (8)$$

213 2.2.3 *Microscale mass conservation*

214 To develop the multiscale model, a microscale was defined at each point within the  
 215 macroscale to represent the heterogeneous structure of the food. This approach is valid when  
 216 the scale parameter approaches zero, causing the heterogeneities to vanish and resulting in a  
 217 homogeneous material (Pavliotis & Stuart, 2008; Welsh et al., 2021a). This assumption is  
 218 crucial for deriving a model through homogenization and is often referred to as the separation  
 219 of scales (Auriault et al., 2010; Carr & Turner, 2014). The microscale considered two sub-  
 220 domains, ICW denoted as  $\omega_{ICW}$  and intercellular water [free water (FW)] denote as  $\omega_{FW}$ , Figure  
 221 2 (b). The macroscale mass transport, Equation (1), is coupled to the microscale mass transport  
 222 equation defined as,

$$223 \quad \frac{\partial c}{\partial t} + \frac{\partial}{\partial x} \left( -D \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( -D \frac{\partial c}{\partial y} \right) = 0, \quad (9)$$

224 where  $c$  is the microscale concentration ( $\text{mol}/\text{m}^3$ ) and  $D$  is the cellular diffusivity ( $\text{m}^2/\text{s}$ )  
 225 equaling  $D_{ICW}$  if  $x,y \in \omega_{ICW}$  and  $D_{FW}$  if  $x,y \in \omega_{FW}$ .

226

227 2.2.4 *Microscale boundary conditions*

228 The coupling between the macroscale and microscale variables occurs at the boundary  
 229 of the microscale given by,

$$230 \quad c_{micro}(a, y) = c_{micro}(0, y) + a \frac{\partial C_{\psi}}{\partial r}, \quad 0 < y < b \quad (10)$$

$$231 \quad c_{micro}(x, b) = c_{micro}(x, 0) + b \frac{\partial C_{\psi}}{\partial z}, \quad 0 < x < a \quad (11)$$

232 where  $a$  and  $b$  are the size of the microscale domain and  $\psi$  is the point of interest. The fluxes  
 233 at the boundaries are also coupled through,

$$234 \quad \begin{aligned} q_c(0, y) \cdot \mathbf{n} &= q_c(a, y) \cdot \mathbf{n}, & 0 < y < b \\ q_c(x, 0) \cdot \mathbf{n} &= q_c(x, b) \cdot \mathbf{n}. & 0 < x < a \end{aligned} \quad (12)$$

235 The boundary condition for the cell wall is

$$236 \quad \mathbf{n} \cdot \left[ -D_{H,eff} \nabla C \right] = P_m (c - C), \quad (13)$$

237 where  $P_m$  is the permeability of the cell wall. The permeability of the cell wall does have some  
 238 uncertainty as the thickness of the cell wall changes during drying (Joardder et al., 2015) and  
 239 as such is investigated in a sensitivity investigation.

#### 240 2.2.5 Macroscale and microscale diffusivity

241 To complete the multiscale model the diffusivity for the macroscale and cellular  
 242 subdomains is required. The ICW diffusivity is (Welsh et al., 2021b),

$$243 \quad D_{ICW} = \exp \left[ -110.32 + 0.55536 T_{cell} + 0.095148 WC_{ICW} - 0.00090738 T_{cell}^2 - 0.0007235 WC_{ICW}^2 \right],$$

244 (14)

245 where  $T_{cell}$  is the cell temperature (K) and  $WC_{ICW}$  is the intracellular water content (mass %).  
 246 The diffusivity of FW is (Pace, 1962),

$$247 \quad D_{FW} = 2.26 \times 10^{-5} \left[ \frac{T}{273.15} \right]^{1.81}. \quad (15)$$

248 The model does not actively upscale the cellular properties to form the macroscale  
 249 diffusivity, rather the previously developed homogenized diffusivity is utilized (Welsh et al.,  
 250 2021a). The function for the macroscale diffusivity is (Welsh et al., 2023),

251  $D_{H,eff} = \exp\left[-106.6 + 0.5548T_{cell} + 0.029502WC_{ICW} - 0.00090648T_{cell}^2 - 0.00041019WC_{ICW}^2\right].$   
252 (16)

253 2.2.6 *Evolution of intracellular water- rupturing threshold*

254 The ICW diffusivity function [Equation (14)] incorporates all three transport modes  
255 (Welsh et al., 2023), **cell to cell, cell to pore and transport through cell rupturing**. Therefore,  
256 cell rupturing must be incorporated within the evolution of the ICW. Welsh et al. (2023)  
257 introduced a rupturing threshold, exploiting the macroscale equilibrium vapor pressure to  
258 determine if and when cell rupturing occurs within the material. **The model calculated the**  
259 **equilibrium vapor pressure at each point within the domain and once the average macroscale**  
260 **equilibrium vapor pressure of the domain reaches the threshold, cells will begin to rupture. The**  
261 **threshold was inversely calculated by evaluating the maximum average equilibrium vapor**  
262 **pressure when the domain was dried at 50°C, aligning with published experimental results**  
263 **(Halder et al., 2011; Khan et al., 2018)**. However, once the threshold was reached, Welsh et al.  
264 (2023) work utilized time dependent functions for ICW which require sophisticated microscale  
265 experimental techniques (such as nuclear magnetic resonance). This significantly limits the  
266 approaches applicability to other studies as these techniques are costly and not commonly  
267 available. As the current multiscale downscaling model includes an evolving microscale, the  
268 evolution of ICW can now be determined directly from the microscale. Therefore, when the  
269 cell is at its full size (215µm), the material is at its maximum ICW water content, 87.8% for  
270 apple (Khan et al., 2016). Once the cell rupturing threshold is reached the ICW is determined  
271 considering the change in cell size. The threshold of apple is considered as 7080 Pa for apple  
272 (Welsh et al., 2023).

273 2.2.7 *Intracellular deformation*

274 A shrinkage velocity approach was utilized to approximate the shrinkage of macroscale  
275 domain and the intracellular space given by (Tuly et al., 2023),

276 
$$\frac{\partial X}{\partial t} \cdot \mathbf{n} = v_n , \quad (17)$$

277 where  $v_n$  is the shrinkage velocity (m/s) and  $\partial X/\partial t$  is the change in distance over time. The  
278 shrinkage velocity for the macroscale domain was calculated by,

279 
$$v_n = a \cdot \frac{(T - T_g)}{(T_0 - T_{g0})} \quad (18)$$

280 where  $a$  is a constant inversely calculated from considering the average shrinkage velocity from  
281 the experimental data and the term  $(T - T_g)/(T_0 - T_{g0})$  represents the solid structure mobility factor.  
282 This factor characterizes the physical state transition (rubbery/glassy) while providing valuable  
283 insights into the correlation between the shrinkage kinetics and structural mobility (Tuly et al.,  
284 2025). The glass transition temperature ( $T_g$ ) can be calculated from the Gordon and Taylor  
285 equation given by (Joardder & Karim, 2019; Tuly et al., 2025),

286 
$$T_g = \frac{(1 - MC_{wb})T_{gs} + k_c MC_{wb} T_{gw}}{1 + MC_{wb}(k_c - 1)} \quad (19)$$

287 where  $T_g$  and  $T_{gs}$  are the glass transition temperature of binary mixture and dry matter at 47°C  
288 and 64°C respectively,  $T_{gw}$  is the glass transition temperature of water and  $k_c$  represents the  
289 Gordon and Taylor constant.

290 2.2.8 *Other input parameters*

291 The remaining input parameters are presented in Table 1.

292 **[Table 1 can be placed here]**

293 *2.2.9 Mass transfer coefficient*

294 The mass transfer coefficient is a parameter that varies with system conditions, heavily  
295 affected by the airflow pattern and the deformation undergone by the product (Defraeye &  
296 Radu, 2018). Khan et al. (2020) examined how spatial variations in heat and mass transfer  
297 coefficients impact drying behaviour, showing that neglecting airflow distribution can lead to  
298 substantial overestimations. To reduce the effect of this variability on the results, the mass  
299 transfer coefficient will instead be estimated using an inverse modeling approach. In the inverse  
300 problem approach, the mass transfer coefficient ( $h_m$ ) is treated as an unknown and is estimated  
301 by minimizing the discrepancy between simulated and experimental moisture drying curves.  
302 To achieve this, the Levenberg-Marquardt optimization algorithm was integrated with the finite  
303 element method, using the moisture data as the basis for the objective functions.

304 
$$OF(h_m) = \int \left[ \overline{M}_{db,exp}(t) - \overline{M}_{db,num}(t, h_m) \right]^2 dt, \quad (20)$$

305 where  $\overline{M}_{db,exp}$  is the average dry basis moisture content from the experimental investigation  
306 and  $\overline{M}_{db,num}$  is the average dry basis moisture content from the simulation.

307 *2.3 Simulation Methodology*

308 The simulation procedure is outlined in Figure 3. The multiscale mathematical model  
309 was solved in LiveLink for MATLAB, a software package which combines COMSOL  
310 Multiphysics Simulations with MATLAB programming. Once the macroscale and microscale  
311 domains, governing equations, boundary conditions, properties and input parameters were  
312 defined, the model could be run from a MATLAB script file. To solve the multiscale model,  
313 the macroscale was first simulated for a single timestep, and the macroscale results were  
314 extracted. Then the required data was downscaled to the microscale and the microscale was  
315 simulated over its own timestep. Then, the extracted macroscale data was imported for the next

316 timestep, and the procedure is repeated until the drying is complete. Lastly, a sensitivity  
317 investigation was conducted.

318 **[Figure 3 can be placed here]**

319

### 320 *2.3.1 Macro-micro temporal coupling*

321 The temporal coupling is extremely important to consider in a multiscale model and  
322 various approaches for temporal coupling exist (Welsh et al., 2018). The current model utilizes  
323 a Multigrid/heterogeneous multiscale method (HMM) approach, as shown in Figure 4, where  
324 the microscale is not continuously simulated. Microscale simulation was conducted as  
325 different timesteps (Figure 3) and key data is downscaled at the exchange timesteps. The  
326 downscaling model has a macroscale timestep of 60 seconds, a micro timestep of 0.1 seconds  
327 and an exchange timestep of 600 seconds. Additionally, the macroscale is simulated for 21600  
328 seconds and 23400 seconds for drying at 47°C and 64°C respectively and the microscale is  
329 simulated for 5 seconds after each exchange step.

330 **[Figure 4 can be placed here]**

331

## 332 *2.4 Experimental Investigations*

333 Two separate experimental investigations were conducted, the macroscale drying  
334 experiments and X-ray  $\mu$ CT. The macroscale drying experiments were conducted to produce  
335 validation data to validate the output from the multiscale model whereas the X-ray  $\mu$ CT was  
336 conducted to investigate the evolution of the material's microstructure.

### 337 *2.4.1 Macroscale drying experiments*

338 Granny Smith apples at commercial maturity were purchased from a local supermarket  
339 and prepared following the standard sample preparation procedure (Asabe & Home). The

340 samples were washed and then cut into cylindrical shapes using a stainless-steel Cork Borer  
341 (JH-1225). Each sample consisted of the mesocarp (pulp) portion, initially measuring 30 mm  
342 in length and 18 mm in diameter. Convective drying was performed at two selected  
343 temperatures within the typical air temperature range for drying (40–80 °C): 47 °C and 64 °C,  
344 representing different levels of cellular deformation and ICW transport mechanisms. The dryer  
345 maintained an air velocity of 1 m/s and the airflow was perpendicular to the **sample along the**  
346 **x-y plane. A visual diagram of the dryer can be seen in Figure B.1 in the supplementary**  
347 **material.** Model validation was conducted using two data sets: average moisture content and  
348 average surface temperature of the samples. To measure moisture content, each sample was  
349 weighed individually at regular intervals. This occurred every 10 minutes during the first hour,  
350 then every 30 minutes until the drying process was completed. The samples were weighed  
351 using a digital balance with a 50 g capacity and  $\pm 0.001$  g accuracy, **with the measuring**  
352 **procedure being completed within 10 seconds (from removal to replacing the sample).** A FLIR-  
353 E6390 thermal imaging camera was used to record surface temperature. This experimental  
354 procedure was repeated three times. **The detailed drying experimental procedure and some of**  
355 **the results on the average macroscale moisture content and average surface temperature can be**  
356 **found in the authors' previous publication (Welsh et al., 2023).**

357

#### 358 2.4.2 X-ray $\mu$ CT Experiment

359 In order to extract the cellular deformation of dried apple cells, both the fresh and  
360 convective dried (both at 45 °C and 60 °C) cylindrical-shaped Granny Smith apple samples  
361 were scanned using an X-ray  $\mu$ CT scanner ( $\mu$ CT50, Scanco Medical, Switzerland). Apple  
362 samples were packed in foam and horizontally placed in scanning tubes with a diameter of  
363 34mm. The native resolution, electric potential, current and the power used for these scans  
364 were as  $10.3 \mu\text{m}^3$ , 55 kVp, 145  $\mu\text{A}$ , and 8 W, respectively with an average sample scanning

365 time of 1000 ms and an Aluminum filter (0.1 mm). The scans were carried out in triplicates.  
366 Once the scans were completed, the image stacks were exported as DIACOM files into Mimics  
367 (Version 24.0, Materialise NV, Belgium) for segmentation using semi-automated thresholding.  
368 The consistency of the segmentations was ensured by maintaining a constant threshold value.  
369 It should be noted due to the study requirements and equipment limitations the X-ray  $\mu$ CT  
370 experimentation was conducted on cylindrical samples with a height of 15 mm and a diameter  
371 of 8mm drying at an average temperature of 45°C and 60°C.

372

### 373 **3. Results**

374 The results are presented in six main sections, the cellular deformation, **the macroscale**  
375 **mass transfer coefficient**, the macroscale drying kinetics, the macroscale temperature  
376 evolution, the ICW results and a sensitivity investigation. Three points of interest within the  
377 macroscale domain, (P1, P2 and P3) were selected along the center of the domain to **analyze**  
378 the model and approach, visually shown in Figure 2. These points were selected as examples  
379 to demonstrate how the microscales vary spatially depending on their location in the  
380 macroscale. **Additionally, the points move in relation to the shrinkage occurring.** The multiscale  
381 downscaling model was compared to the experimental data and the single scale macroscale  
382 model without deformation as a control (Welsh et al., 2023). All properties and heat and mass  
383 transfer coefficients were the same for the control and downscaling model.

#### 384 *3.1 Cellular deformation*

385 X-ray  $\mu$ CT was utilized to extract the cellular deformation information of granny smith  
386 apple dried at 45°C and 60°C. **The quantitative values of the intracellular and pore space**  
387 **(surrounded by at least two or more cells) were extracted from the segmented scanned images**  
388 **using the in-built functions available in MIMICS software. Accordingly, 30 intracellular spaces**

389 and pore spaces were randomly selected across the top, middle and bottom slices of each  
390 scanned image. The boundaries of the selected intracellular and pore spaces were defined, and  
391  $L^{\perp}$ ; the minimal diameter orthogonal to the maximum length ( $L_{max}$ ) values have been  
392 extracted and performed in triplicates for higher accuracy. The mean average values for the  
393 extracted intracellular and pore sizes were statistically analyzed by performing one-way  
394 analysis of variance (ANOVA) at  $\alpha = 0.05$ , followed by the Turkey's test as the mean separation  
395 method using Minitab 18 (Minitab, version 18.1, Minitab LLC, Australia. Evaluating 30  
396 intracellular spaces resulted in average sizes of  $215.4 \pm 30 \mu\text{m}$  for fresh apple cells,  $128.15 \pm$   
397  $10 \mu\text{m}$  for dried apple cells using convective air at  $45^{\circ}\text{C}$  to a moisture content of  $0.8 \text{ kg/kg dry}$   
398  $\text{basis}$ , and  $119.10 \pm 10 \mu\text{m}$  for dried apple cells using convective air at  $60^{\circ}\text{C}$  to a moisture  
399  $\text{content of } 1.23 \text{ kg/kg dry basis}$ , (Figure 5). This resulted in condition dependent velocities of -  
400  $25 \times 10^{-9} \text{ m/s}$  and  $-30 \times 10^{-9} \text{ m/s}$  for drying at  $47^{\circ}\text{C}$  and apple dried  $64^{\circ}\text{C}$  respectively. It should  
401 be noted, the shrinkage velocity also had to consider the multiscale temporal coupling into its  
402 calculation due to the skipped portions of time.

403 **[Figure 5 can be placed here]**

### 404 3.2 Macroscale mass transfer coefficient

405 The downscaling model considered a deforming macroscale domain. Furthermore, the  
406 control model (Welsh et al., 2023) simulated drying without macroscale deformation. This  
407 resulted in unique mass transfer coefficients for each scenario, a mass transfer coefficient of  
408  $0.00699 \text{ m/s}$  when simulating drying with deformation compared to  $0.00381 \text{ m/s}$  for the control  
409 model (Welsh et al., 2023). The uncovered values were used for the remainder of the study.  
410 During drying, the mass transfer coefficient depends on the velocity field (spatially dependent)  
411 and macroscale deformation (temporal dependent) (Khan et al., 2020). When simulating drying  
412 without deformation like the control model, the mass transfer coefficient is significantly lower  
413 to compensate for the missing physics (deformation) and a non-spatially dependent mass

414 transfer coefficient. When drying is simulated with deformation, the mass transfer coefficient  
415 is much closer to the real scenario as the inverse study only has to compensate for the constant  
416 mass transfer coefficient.

417

### 418 3.3 Macroscale - Drying Kinetics

419 The downscaling model accurately predicted the moisture transport at 47°C achieving a mean  
420 relative error (MRE) of 3.62% when compared to the experimental results (Welsh et al., 2023),  
421 Figure 6. The control model (Welsh et al., 2023) achieved a similarly low MRE of 1.52%. The  
422 multiscale downscaling model slightly underpredict the experimental data in the middle stages  
423 of drying, 50-250 mins. In the later stage, the model slightly overpredicts the transport,  
424 demonstrating a trend opposite to that of the control. This is likely due to the inclusion of  
425 deformation in the downscaling model, whereas deformation was not considered in the control.

426 The downscaling model and control model resulted in almost identical diffusivities between  
427  $1.94 \times 10^{-10}$  and  $2.16 \times 10^{-10}$  m<sup>2</sup>/s for drying at 47°C, Figure 7. At 64°C the downscaling model  
428 predicted the moisture transport accurately achieving a MRE of 8.38% when compared to the  
429 experimental results, Figure 6. The control macroscale model achieved a similarly low MRE  
430 of 4.80%, predicting the experimental data slightly better. The multiscale downscaling model  
431 slightly underpredict the experimental data between 35-150 mins for drying at 64°C and then  
432 slightly overpredicted the experimental data in the later stages, following the same trend as  
433 predicting drying at 47°C. When drying at 64°C, the rupture threshold is reached, the ICW  
434 content in the domain changes quickly causing the diffusivity to abruptly change and the  
435 downscaling model estimated the ICW content from the change in cell size. This resulted in a  
436 diffusivity range of  $4 \times 10^{-10}$  –  $2.58 \times 10^{-10}$  m<sup>2</sup>/s which was slightly lower than the control model,  
437 Figure 7. The resulting diffusivities fell in the typically range of  $10^{-11}$  and  $10^{-9}$  m<sup>2</sup>/s for food  
438 material (Panagiotou et al., 2004; Saravacos & Maroulis, 2001).

439 The macroscale domain shrunk from an initial size of 30mm in height and of 18mm in  
440 diameter to a height of 25.1mm and a diameter of 13mm when drying at 47°C and a height of  
441 26.7mm and a diameter of 14.8mm when drying at 64°C. The macroscale shrinkage velocity  
442 was higher in the initial stages of drying and dramatically decreased in the later stage through  
443 considering the solid structure mobility factor, mimicking what occurs in the real world with  
444 the case hardening and the glass transition effect (Tuly et al., 2025). This results in varying  
445 shrinkage velocities of  $2.24 \times 10^{-7}$  to  $2.9 \times 10^{-8}$  for drying at 47°C and  $2.96 \times 10^{-7}$  to  $1.23 \times 10^{-8}$  for  
446 drying at 64°C. This nonlinear shrinkage can also be seen in Figure 9 and Figure 10. Drying at  
447 47°C resulted in more deformation due to the longer drying time, aligning with previously  
448 published results (Gulati & Datta, 2015; Tuly et al., 2025).

449 [Figure 6 can be placed here]

450 [Figure 7 can be placed here]

451

#### 452 3.4 Macroscale – Temperature evolution

453 The downscaling model accurately predicted the average sample temperature for drying  
454 at both 47°C and 64°C, with MREs of 0.66% and 0.90% respectively, Figure 8. Similarly, the  
455 control model achieved MREs of 0.46% and 0.89% respectively when compared to the  
456 experimental results, Figure 8. The downscaling model predicted the temperature evolution  
457 much more consistently when drying at 47°C than at 64°C. Although having a low MRE, the  
458 downscaling model predicted an unusual trend for drying 64°C, underpredicting and  
459 overpredicting the temperature throughout the drying time. The only notable difference  
460 between the downscaling model and the control model at both drying temperatures is the  
461 inclusion of moisture-dependent density in the downscaling model and macroscale  
462 deformation. Additionally, no properties within the heat transfer are in terms of ICW, rather

463 just macroscale moisture. Both the multiscale downscaling model and the control model  
464 significantly overpredicted the experimental data in the early stages of drying. It should be  
465 noted, the experimental data is of a sample under convective drying with perpendicular airflow  
466 on the x-y plane due to the location of the inlet and outlet within the dryer (shown in Figure  
467 B.1 in the supplementary material). Due to the perpendicular airflow, a large ‘dead zone’  
468 existed behind the trailing edge of the sample during drying and thus, the heat transfer  
469 coefficient heavily effected in this region of the sample, demonstrate by Khan et al. (2020).  
470 Furthermore, in real life the heat and mass transfer coefficient also evolves as the sample  
471 shrinks corresponding to the change in its characteristic length (Welsh et al., 2021a). As a result,  
472 the temporally and spatially constant heat transfer coefficient contributed heavily to the initial  
473 overprediction.

474 **[Figure 8 can be placed here]**

475

### 476 3.5 *Intracellular water transport*

477 The spatial moisture profile at macroscale and the three locations of interest can be seen  
478 in Figure 9 and Figure 10 for drying at 47°C and 64°C respectively. Within this figure the  
479 dashed circle denotes the original cell size and the dashed rectangle denotes the original size  
480 of the macroscale domain. It should be noted, the moisture profile shown in Figure 9 and  
481 Figure 10 are at the exchange steps. As expected, each point of interest has its own temporal  
482 moisture profile corresponding to the macroscale conditions occurring at that particular point.  
483 This is unlike the existing microscale models in literature which utilize a single domain to  
484 characterize the sample transport (Rahman et al., 2018). As the moisture profile develops  
485 within the sample, the intracellular space at the outside point (P3), dries first. As expected, in  
486 the later stages, the intracellular space at P3 is almost entirely dry whereas the intracellular

487 space at P1 only starts to dry. This trend observed in both drying temperatures. Additionally,  
488 due to the temporal coupling and the size of the exchange time step utilized, there can be a  
489 delay in the moisture transfer between the end of the microscale and the initialization of the  
490 microscale. The microscale is only simulated for 5 seconds after an exchange step and the data  
491 exchange only occurs every 600 seconds (10 mins). This creates a time skip of 595 seconds.  
492 Evidence of this delay can be seen in the microscale at P3 at 100 minutes in Figure 9.

493 **[Figure 9 can be placed here]**

494 **[Figure 10 can be placed here]**

495

496 The average moisture content of the intracellular spaces at each point of interest can be  
497 found in Figure 11 (a). Throughout drying, the flux through the cell wall at P3 (point closest to  
498 the exterior wall) is significantly larger than the flux at P2 and P1, especially in the middle  
499 portion of drying. This trend is consistent for both drying temperatures. **Furthermore, a  
500 comparison between the predicted ICW content and the predicted macroscale moisture content  
501 at each point interest can be seen in Figure 11 (b). The downscaling model preserves the  
502 average across the microscale domain at each point of interest, causing the ICW content to  
503 slightly lag behind the macroscale due to the intracellular space acting as an additional barrier  
504 or storage domain. The flux through the cell wall can be seen in Figure 12, where (a) shows  
505 the flux through the cell wall when the downscaling model does not consider macroscale  
506 deformation and (b) shows the downscaling model when macroscale deformation is  
507 considered. Both scenarios result in very different flux evolutions. When macroscale  
508 deformation is not considered the flux through the cell walls at each point exhibit peaks at  
509 different stages of drying and as expected drying at higher temperatures resulted in additional  
510 flux through the cell wall. P3 near the outside wall peaks first at 110 mins for drying at 64°C  
511 with a magnitude of  $-4.33 \times 10^{-7}$  mol/m<sup>2</sup>s. For drying at 47°C, P3's peak occurs later at 170**

512 mins. Furthermore, the evolution of the macroscale and microscale moisture content  
513 distribution for simulating the downscaling model without deformation can be found in the  
514 Supplementary material (Appendix C). When macroscale deformation is considered, the cells  
515 and thus points of interest move as the domain shrinks. The points of interest move in  
516 proportion to the change in domain size (the points of interest are always assumed to be equally  
517 spaced along the sample). This assumption affects the resulting flux the cell wall experiences  
518 and result in the flux at each point of interest increasing over time, following a similar trend of  
519 the moisture content evolution, Figure 11 (a) and Figure 12 (b). Note the uneven flux in the  
520 later stages of drying at 64°C is related to the intracellular space moving in relation to the  
521 moisture gradient. When drying at 47°C, P1, P2 and P3 moved 0.62mm, 1.23mm and 1.84mm  
522 respectively towards the center of the domain. For drying at 64°C, P1, P2 and P3 moved  
523 0.4mm, 0.81mm and 1.22mm respectively. The different shrinkage velocity for the two drying  
524 temperatures resulted in slightly different final cell sizes of 119 µm for drying at 47°C and 109  
525 µm for 64°C following the trend uncovered in the X-ray µCT investigation. It should be noted,  
526 the shrinkage velocity approach results in ideal **microscale** shrinkage.

527 **[Figure 11 can be placed here]**

### 528 3.6 Sensitivity Investigation

529 A sensitivity analysis was conducted on a parameter with uncertainty, specifically on  
530 cell wall permeability, which was considered constant. Literature has demonstrate when drying  
531 at 70°C the average cell wall thickness of granny smith apples changes from 9.312µm when  
532 fresh to 4.685µm when dried (Joardder et al., 2015). This change mainly occurs when the FW  
533 content reduces surrounding an intracellular space and ICW begins to transport through the cell  
534 wall. Permeability is the diffusivity of a cell wall over its width, hence as diffusivity and the  
535 wall thickness changes uncertainty exists within permeability. To evaluate the sensitivity of the

536 downscaling model, the cell permeability was investigated by varying the utilized value by  
537  $\pm 10\%$  while drying at  $47^\circ\text{C}$ . This parameter was investigated in relation to the average  
538 macroscale moisture content (kg/kg dry basis), the intracellular water content (kg/kg dry basis)  
539 and the cell wall flux ( $\text{mol}/\text{m}^2\text{s}$ ). Additionally, thermal conductivity has some uncertainty as  
540 multiple functions exist in literature and as a result a brief investigation can be found in  
541 Appendix D of the Supplementary material.

542 The downscaling model's sensitivity to cell wall permeability can be seen in Figure 13.  
543 The macroscale moisture content and the microscale ICW content were not sensitive to the  
544 change in cell wall permeability with their magnitudes and trend not changing. However, as  
545 permeability is key in the cellular boundary condition, the changes in permeability do influence  
546 the magnitude of the cell wall flux. Plus 10% results in an increase to the magnitude of the flux  
547 whereas minus 10% decrease the flux through the cell wall. The difference is significant and  
548 clearly evidenced for P3 but much smaller for P1 and P2. Furthermore, the downscaling model  
549 was also sensitive to cell wall permeability when deformation was not considered  
550 (Supplementary material Appendix C).

551 [Figure 12 can be placed here]

552

#### 553 4. Discussion

554 The downscaling model provides new insight into the transport of ICW while  
555 accurately predicting drying at  $47^\circ\text{C}$  and  $64^\circ\text{C}$ . When drying at lower temperatures ( $47^\circ\text{C}$ ) the  
556 consideration of a constant ICW with the upscaled diffusivity [Equation (16)] creates a fairly  
557 constant diffusivity which was sufficient to accurately predict drying. This finding is consistent  
558 with pre-existing literature (Defraeye & Verboven, 2017; Welsh et al., 2023). When drying at  
559 medium temperatures ( $64^\circ\text{C}$ ), the multiscale downscaling model accurately predicted drying,

560 suggesting that ICW estimation based on cell size changes is suitable to utilize the upscaled  
561 diffusivity property with the rupture threshold. This technique enhances the generalizability of  
562 the modeling approach and differs from previously published work (Welsh et al., 2023).  
563 Notably, the shrinkage velocity approach, based on X-ray  $\mu$ CT data, was employed to estimate  
564 cell size changes. The model could be further refined by incorporating a physics-based  
565 approach to cellular deformation, such as van der Sman et al. (2024)'s recent work on pore  
566 development in viscoelastic foods during drying.

567         The microscales at the three points of interest provided interesting insight, Figure 9 to  
568 Figure 10. Each produced spatially dependent microscales which is different to the previously  
569 published microscale models where a single microscale is used to predict the material's  
570 evolution (Rahman et al., 2018). The flux evolution was very unique for each intracellular  
571 space at each point of interest. The microscale near the outside edge (P3) experienced  
572 significantly more flux throughout the entire duration of drying. The magnitude of the flux also  
573 depended on the drying air temperature and is sensitive to the magnitude of the cell wall  
574 permeability. Additionally, the flux through the cell wall (shown in Figure 12) was very  
575 dependent on how the points of interest (intracellular spaces) are considered in relation to the  
576 macroscale deformation, i.e. do the intracellular spaces remain at the same location within the  
577 macroscale domain when shrinkage occurs, do the intracellular spaces shrink and move as the  
578 macroscale domain shrinks and the material's porosity increases, and/or if the intracellular  
579 spaces do move, at what rate? This is evidence when comparing the flux evolution of the  
580 downscaling model with and without deformation [Figure 12 (a) and Figure 12(b)]. This work  
581 assumed the points of interest and thus intracellular spaces were always equally distributed  
582 along the domain. This assumption results in the intracellular spaces moving towards the center  
583 of the macroscale domain in relation to the shrinkage occurring, mimicking what occurs in  
584 relation to shrinkage and the materials porosity evolution. If a different assumption is

585 **considered, it would likely result in a different evolution of flux.** Literature has demonstrated  
586 when drying at medium temperature (above 50°C), progressive and ultimate cell rupturing  
587 would have occurred (Khan et al., 2018). It is theorized, due to the convective heating profile,  
588 when the surface reaches 50°C the intracellular space near the surface lose their rigidity and  
589 tend to become droopy, hence nearing their rupturing limit (Khan et al., 2018). The intracellular  
590 spaces lose turgor pressure and tend to fail due to the imposed thermal stress of continuous  
591 penetration of heat energy. Though past research on cell rupturing has been conducted using  
592 nuclear magnetic resonance which is only able to produce results of the entire sample (domain  
593 averages) and does not give insight into the spatial propagation of the rupturing mechanism.  
594 Further investigation is needed in the future, but the cell wall flux may provide valuable insight  
595 in predicting when and/or where cell rupturing spatially propagates within PBFMs.

596 One key component of any multiscale model is its temporal coupling. Previous works  
597 within the field (Rahman et al., 2018) have only utilized multiscale modeling to upscale  
598 properties. Such an approach produces a property, often a homogenized property, through  
599 computing the microscale in a steady state condition for specific discrete points of interest (i.e.  
600 when a cell has a moisture content of 3 kg/kg dry basis). However, as the current study is a  
601 multiscale downscaling model, the microscale evolves with time and hence a temporal coupling  
602 is required. Specifically, the HMM approach was utilized. This approach saves on  
603 computational cost but does not simulate the microscale for the entire simulation (as described  
604 in 2.3.1 Macro-micro temporal coupling). Instead, the approach just computes the microscale  
605 for a small period of time after the exchange point. Hence, there is a portion of time (9.16 mins)  
606 which is skipped in between the exchange steps. This saves on computational cost however it  
607 can create a delayed effect on the transport, which will not always be desired. Depending on  
608 the purpose of the model and the available computational resources, this skipped time can be  
609 either reduced or increased. Alternatively, temporal couplings like the continuous HMM

610 simulate the microscale across the entire time period and can be employed based on the model's  
611 purpose.

## 612 **5. Conclusion**

613 The multiscale model accurately described the drying process at both low and medium  
614 temperatures (47°C and 64°C). Furthermore, the integration of downscaling coupling in the  
615 model provided valuable insights into the microscale evolution during drying. When drying at  
616 medium temperatures, the rupturing threshold was reached and the ICW of the sample was  
617 predicted considering the changes in the cells size. To demonstrate the capacity of the approach,  
618 microscales at three points of interest were investigated. Each microscale evolved differently  
619 depending on the applied drying conditions and their spatial location within the domain. The  
620 ICW trend through the cell wall provided important insight into what the cell wall experiences  
621 at different locations and was also unique for each microscale location and drying temperature.  
622 Additionally, the convective drying temperature significantly influenced the magnitude of the  
623 flux the cell wall experienced due to the moisture migration. Further investigating is required  
624 but such a multiscale approach could be utilized to investigate how cell rupturing propagates  
625 within a domain. The model could also be refined to calculate cellular deformation through a  
626 more mathematical approach with deformation on both spatial scales coupled with some  
627 consideration of cell rupturing. **Additionally, the microscale could be extended to 3D.** The  
628 multiscale downscaling approach, coupled with Welsh et al. (2023) upscaling technique will  
629 facilitate the construct of an in-depth concurrent multiscale model being developed in the  
630 future.

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636

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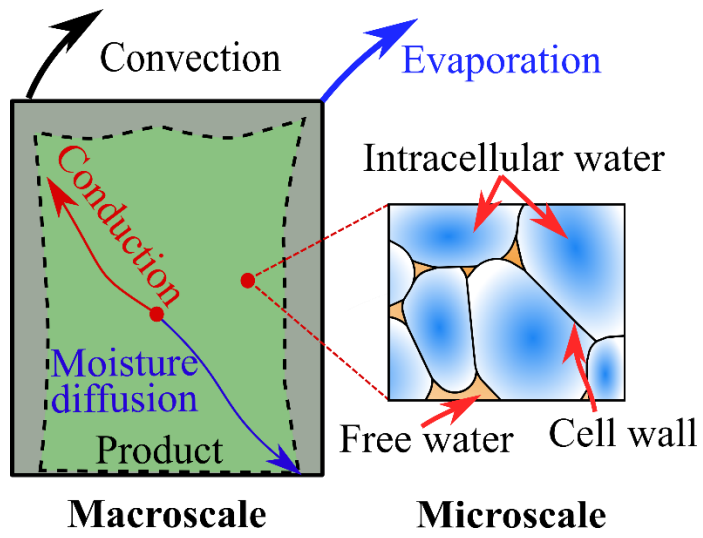
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779 **Figures:**



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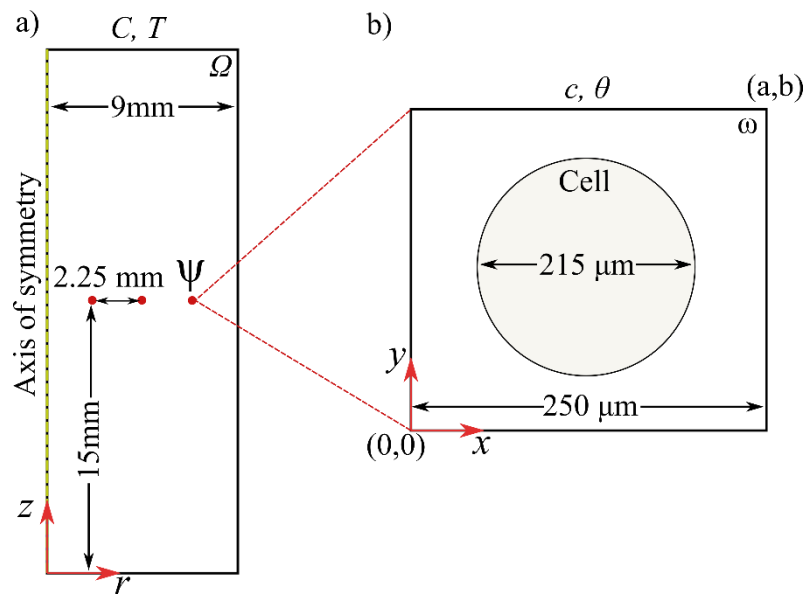
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Figure 1. Cellular structure of plant-based food material

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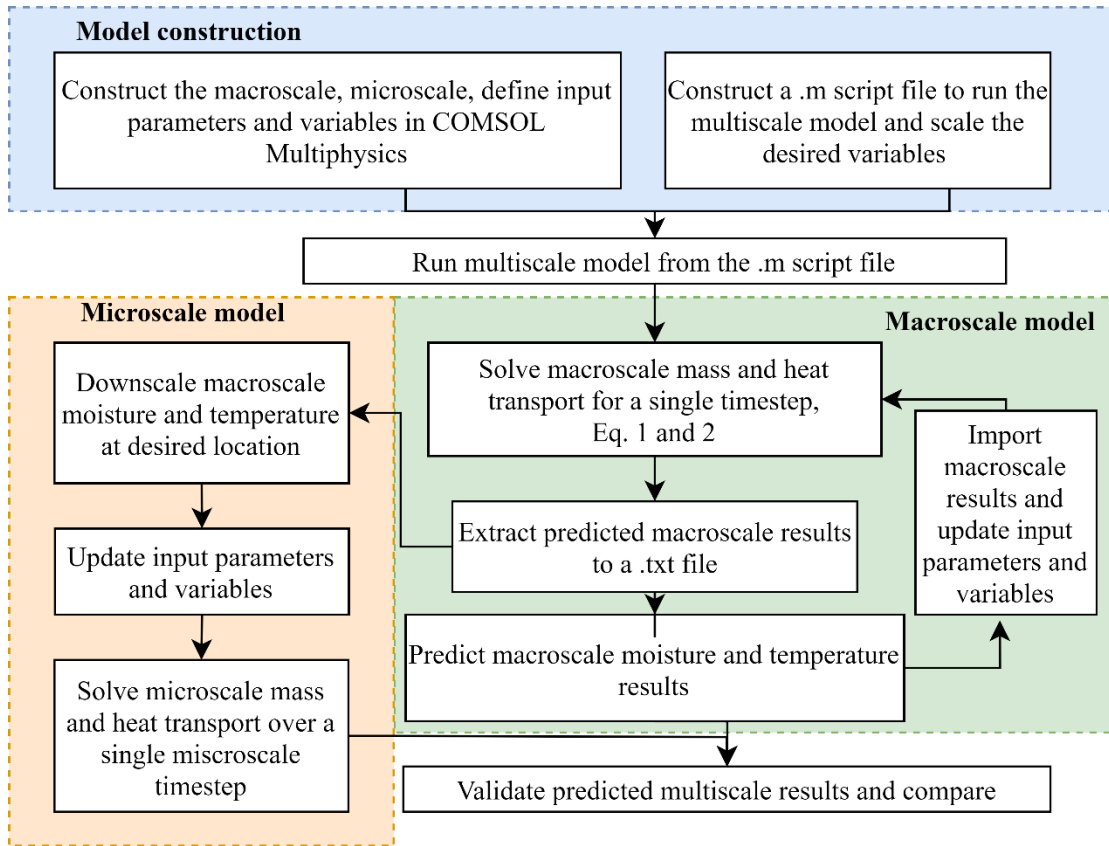
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Figure 2. Domains, a) axisymmetric macroscale domain with the three locations of interest marked by red dots, and b) microscale domain.

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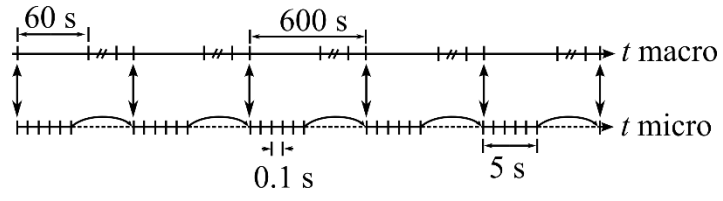
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Figure 3. Simulation Methodology

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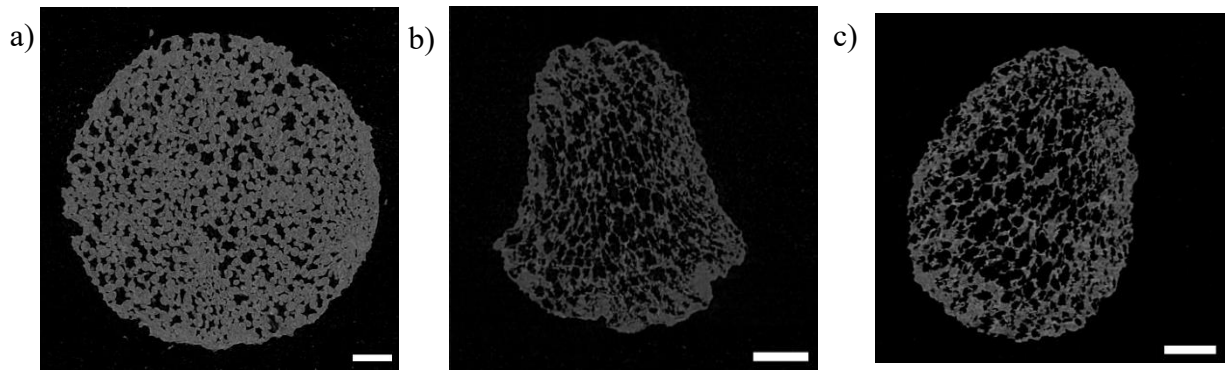
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Figure 4. Multiscale temporal coupling.

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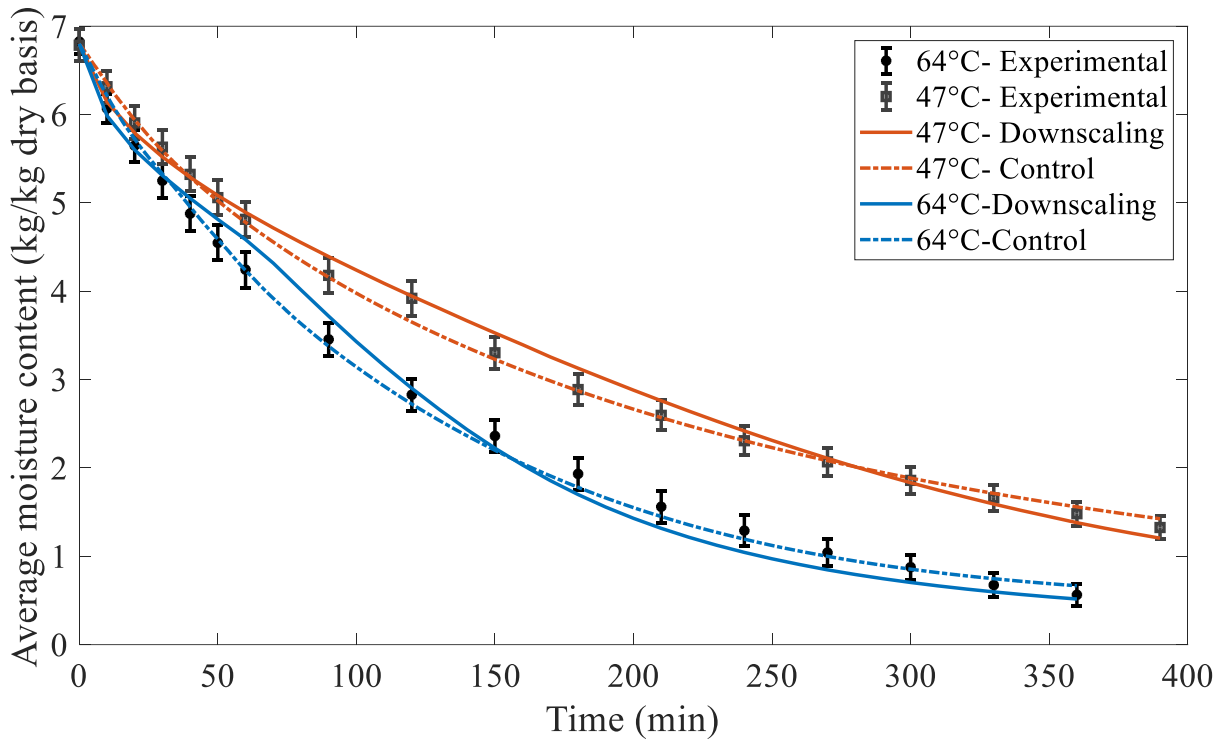
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801 Figure 5. X-ray  $\mu$ CT images of, (a) fresh, (b) dried at 45°C at 0.8 kg/kg dry basis, (b)  
802 dried at 60°C at 1.23 kg/kg dry basis. **The white scalebar represents 1mm in each**  
803 **corresponding image.**

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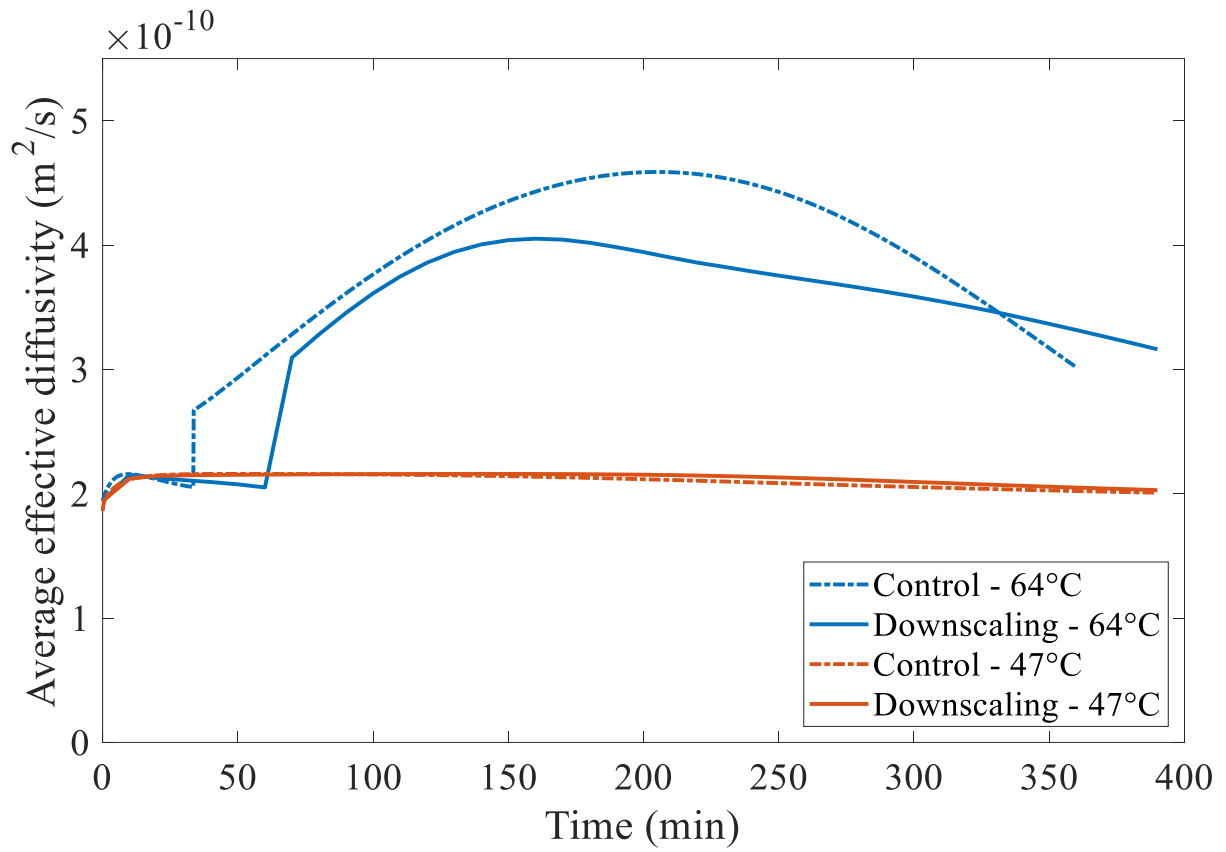
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Figure 6. Average macroscale moisture content (kg/kg dry basis) at low and medium

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temperature drying.

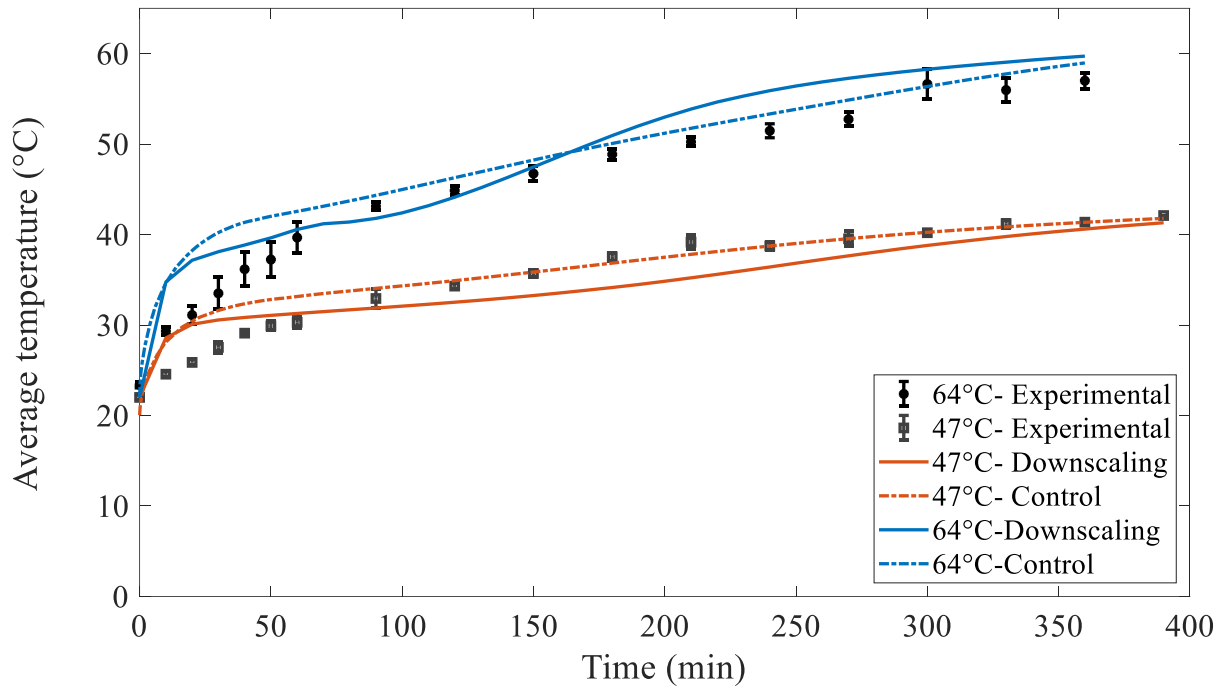
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810 Figure 7. Average macroscale diffusivity (m<sup>2</sup>/s), Equation (16), for both drying temperatures.

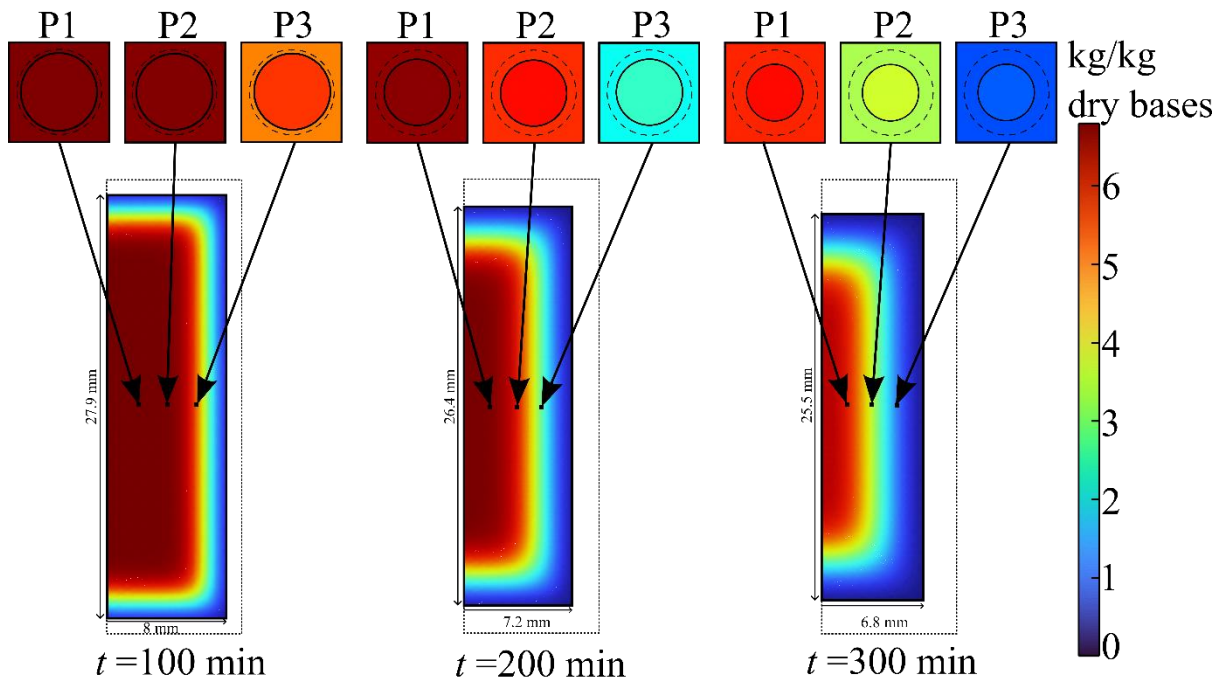
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813 Figure 8. Average macroscale surface temperature (°C) for both drying temperatures.

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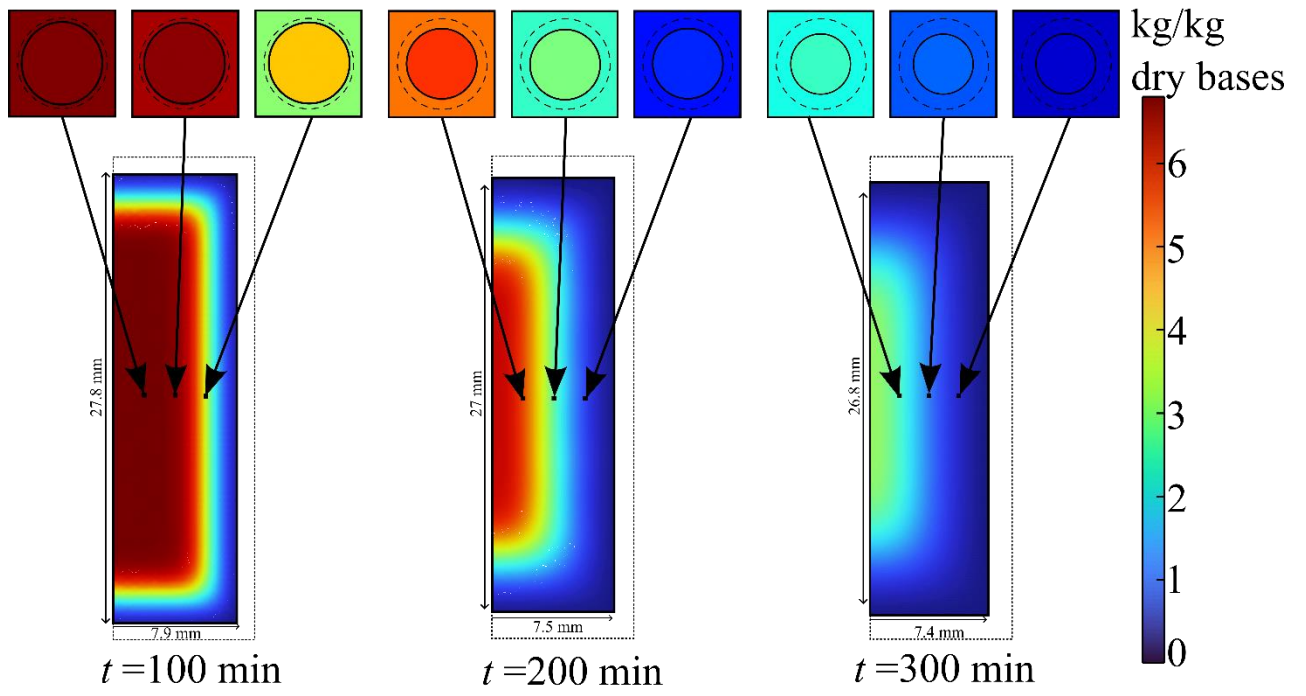


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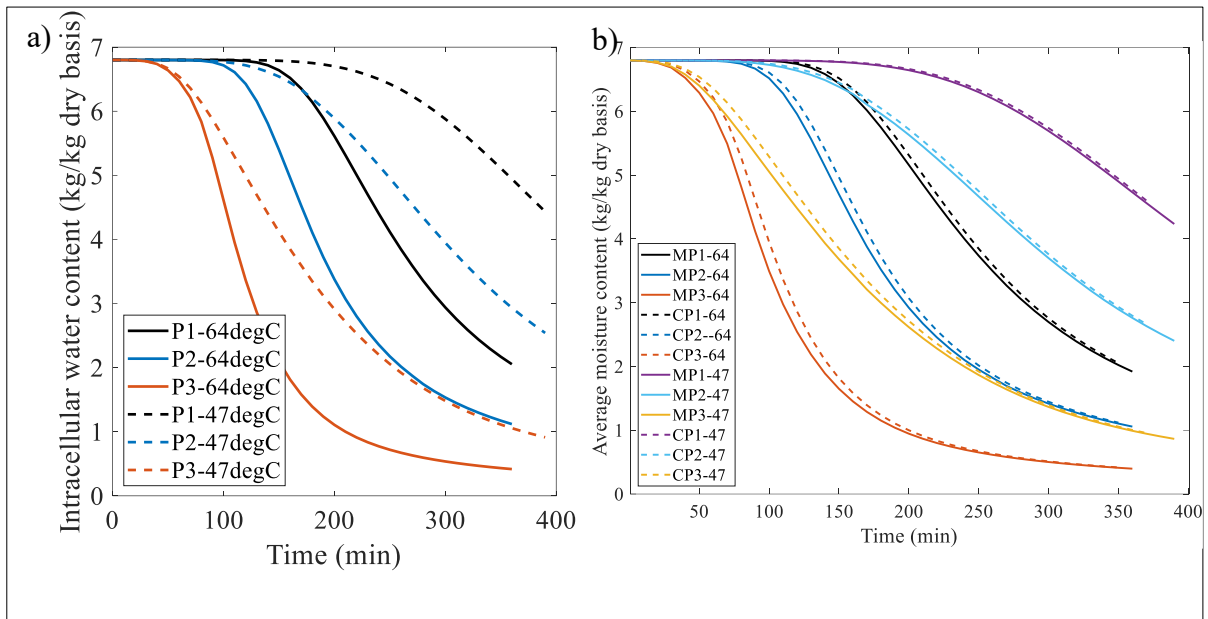
816 Figure 9. Multiscale moisture distribution (kg/kg dry basis) for drying at 47°C. **Original cell**

817 **and macroscale geometries visually represented by the dashed circle and dashed rectangle.**

818



820 Figure 10. Multiscale moisture distribution (kg/kg dry basis) for drying at 64°C. Original cell  
821 and macroscale geometries visually represented by the dashed circle and dashed rectangle.

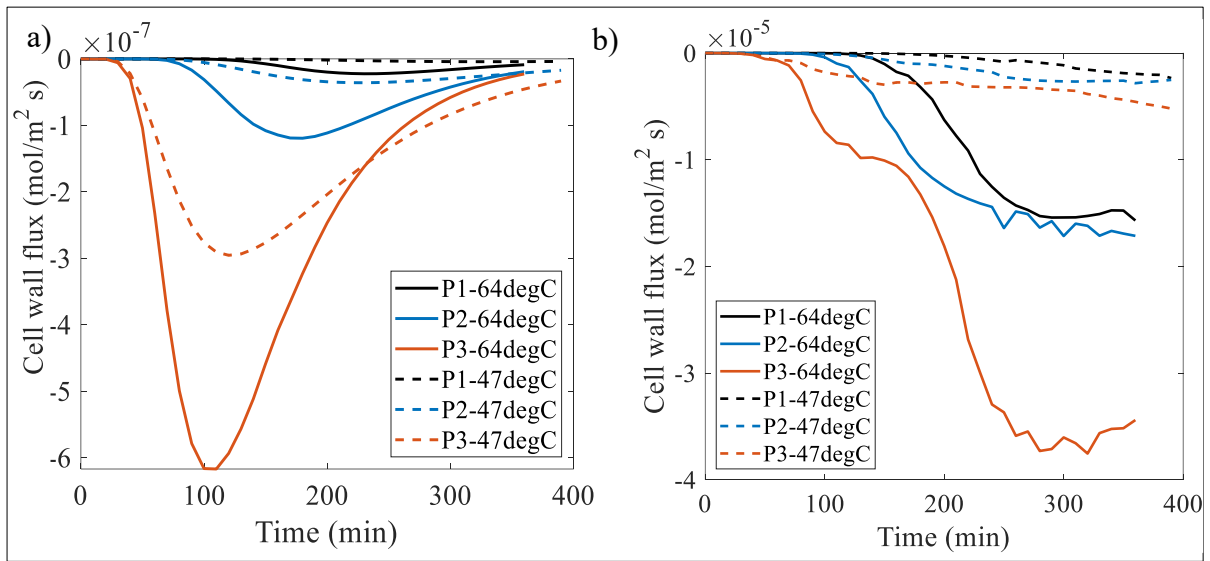


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824 Figure 11. Intracellular water evolution for both drying temperatures, (a) concentration within  
825 each intracellular space at the points of interest (kg/kg dry basis), (b) comparing the  
826 intracellular water content and the macroscale water content (kg/kg dry basis) at each point of  
827 interest where M denotes the macroscale and C denote the intracellular water content.

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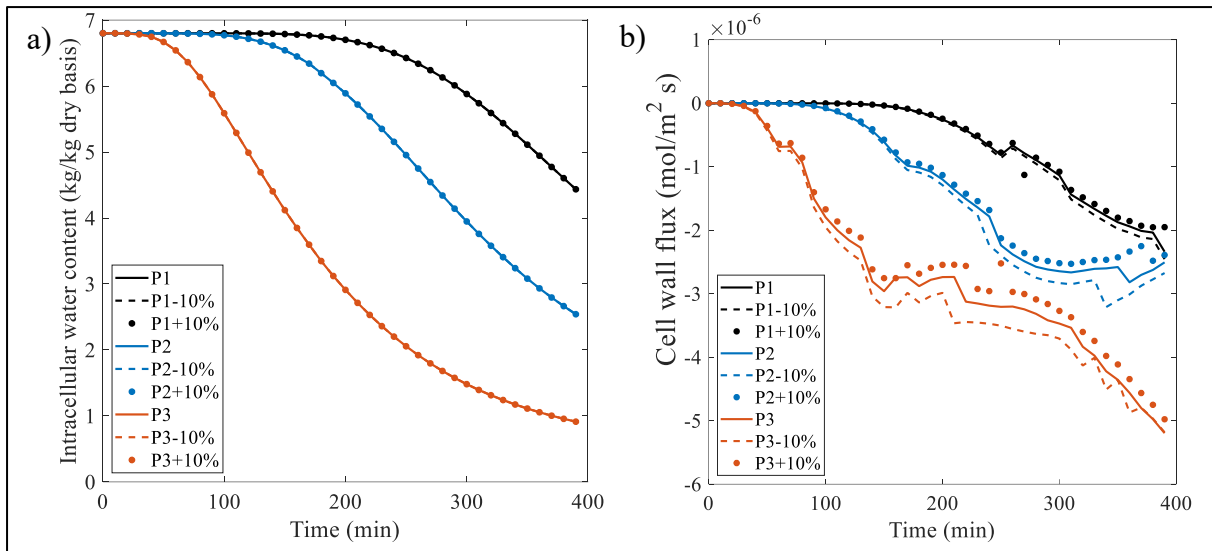
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831 Figure 12. Flux evolution of the intracellular water through the cell wall ( $\text{mol m}^{-2} \text{s}^{-1}$ ) at the  
832 points of interest for both drying temperatures, (a) without macroscale deformation (b) with  
833 macroscale deformation.

834



835

836 Figure 13. Sensitivity investigation for the cell wall permeability  $\pm 10\%$ , a) moisture content

837 (kg/kg dry basis), at each point of interest b) cell wall flux (mol/m<sup>2</sup>s) at each point of interest.

838

839 **Tables:**

840 Table 1. Input parameters

Parameter	Value (unit)	Reference
Density of apple, $\rho$	$-7.301M_{db}^2+92.552M_{db}+450.53$	(Mbarek & Mihoubi, 2019)
Density of water, $\rho_w$	995 (kg m <sup>-3</sup> )	Cengel (2003)
Specific heat of apple, $c_p$	1000(1.4+3.22 $M_{wb}$ ) (J kg <sup>-1</sup> K <sup>-1</sup> )	Białobrzewski (2006)
Thermal conductivity of apple, $k$	0.49-0.443exp(-0.206 $M_{db}$ ) (W/(m·K))	Mattea et al. (1986)
Initial moisture content, $M_0$	6.8 (kg kg <sup>-1</sup> dry basis)	This study
Initial sample temperature, $T_0$	296 (K)	This study
Glass transition temperature of water, $T_{gw}$	138.15 (K)	(Joardder & Karim, 2019)
Initial glass transition temperature, $T_{g0}$	165 (K)	(Joardder & Karim, 2019)
Gordon and Taylor constant, $k_c$	3.4	(Joardder & Karim, 2019)
Initial wet basis moisture content, $M_{0,wb}$	0.86 (kg kg <sup>-1</sup> wet basis)	This study
Latent heat of evaporation, $h_{fg}$	2358600 (J kg <sup>-1</sup> )	Cengel (2003)
Universal gas constant, $R$	8.314 (J mol <sup>-1</sup> K <sup>-1</sup> )	Cengel and Boles (2002)

Molar mass of water, $M_w$	0.018016 (kg mol <sup>-1</sup> )	Cengel and Boles (2002)
Partial vapor pressure, $p_{v \text{ air}}$	1250 (Pa)	(Welsh et al., 2023)
Heat transfer coefficient, $h_T$	18 (W m <sup>-2</sup> K <sup>-1</sup> )	This study
Cell wall permeability	2 x 10 <sup>-5</sup> (m s <sup>-1</sup> )	(Ferrando & Spiess, 2001; Moshelion et al., 2004)

## Supplementary Material

### Appendix A - Converting concentrations to wet and dry bases.

The wet and dry moisture contents were considered as,

$$M_{wb} = \frac{C M_w}{\rho} \quad (\text{A.1})$$

$$M_{db} = \frac{M_{wb}}{1 - M_{wb}} \quad (\text{A.2})$$

where  $M_{wb}$  is the wet bases moisture content (kg/kg wet basis),  $M_{db}$  is the dry bases moisture content (kg/kg dry basis),  $C$  is the instantaneous moisture concentration (mol/m<sup>3</sup>),  $\rho$  is the density of the material (kg/m<sup>3</sup>) and  $M_w$  molar mass of water (kg/mol).

## Appendix B – Experimental drying set up

The experimental drying set up used within this work can be seen in Figure B.1. Within this experimental set up the sample experiences perpendicular airflow along the x-y plane due to the location of the inlet and outlet locations in relation to the sample (inlet is on the samples left and outlet is at its back). It should be noted, the experimental dryer also has microwave capabilities which was not active during the convective drying experiments.

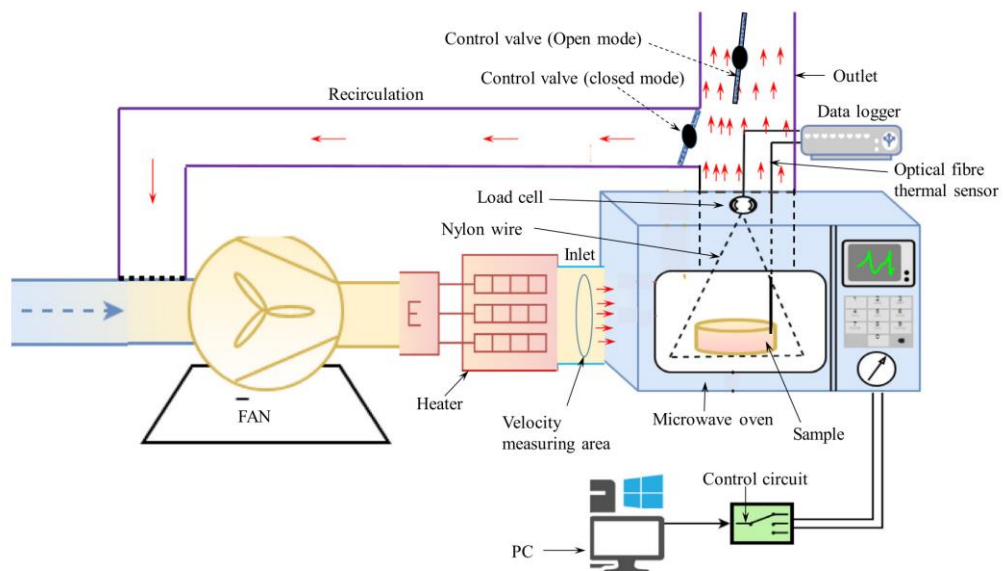


Figure B.1 Schematic diagram of the experimental drying setup used

## Appendix C – Moisture distribution of the downscaling model without deformation

The moisture distribution at both scales of the downscaling model without macroscale deformation can be seen in Figure C.1 and Figure C.2.

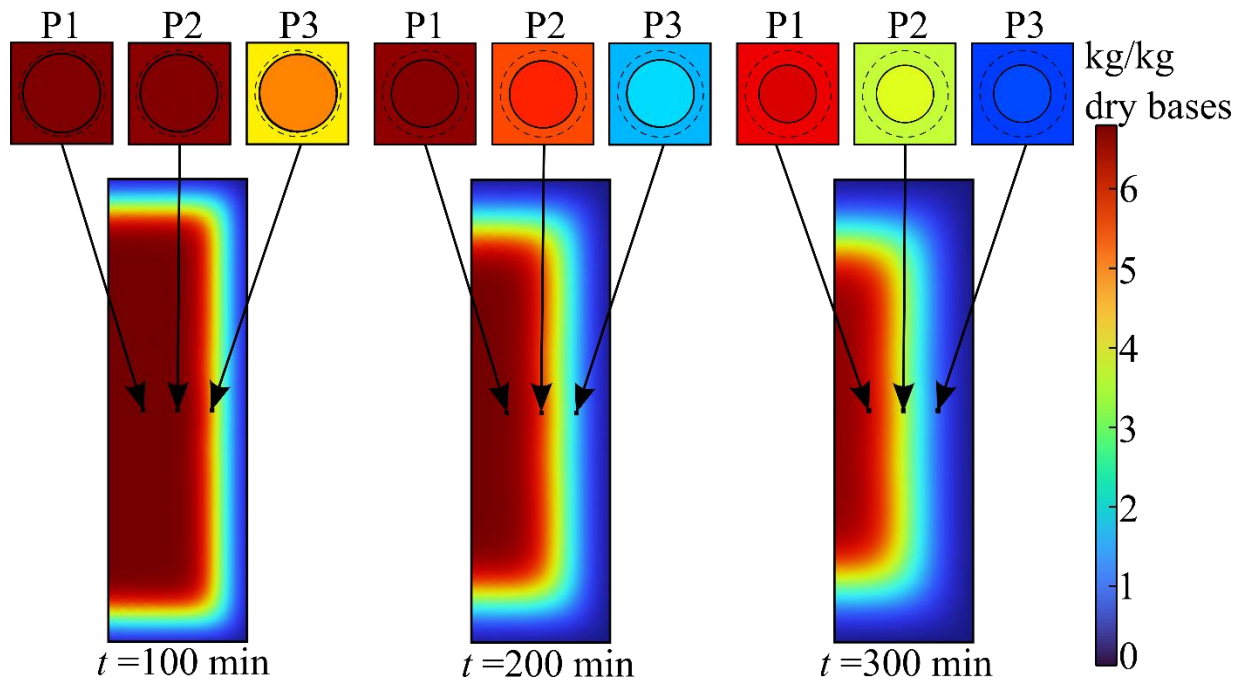


Figure C.1. Multiscale moisture distribution (kg/kg dry bases) for drying at 47°C. Original cell geometry visually represented by the dashed circle.

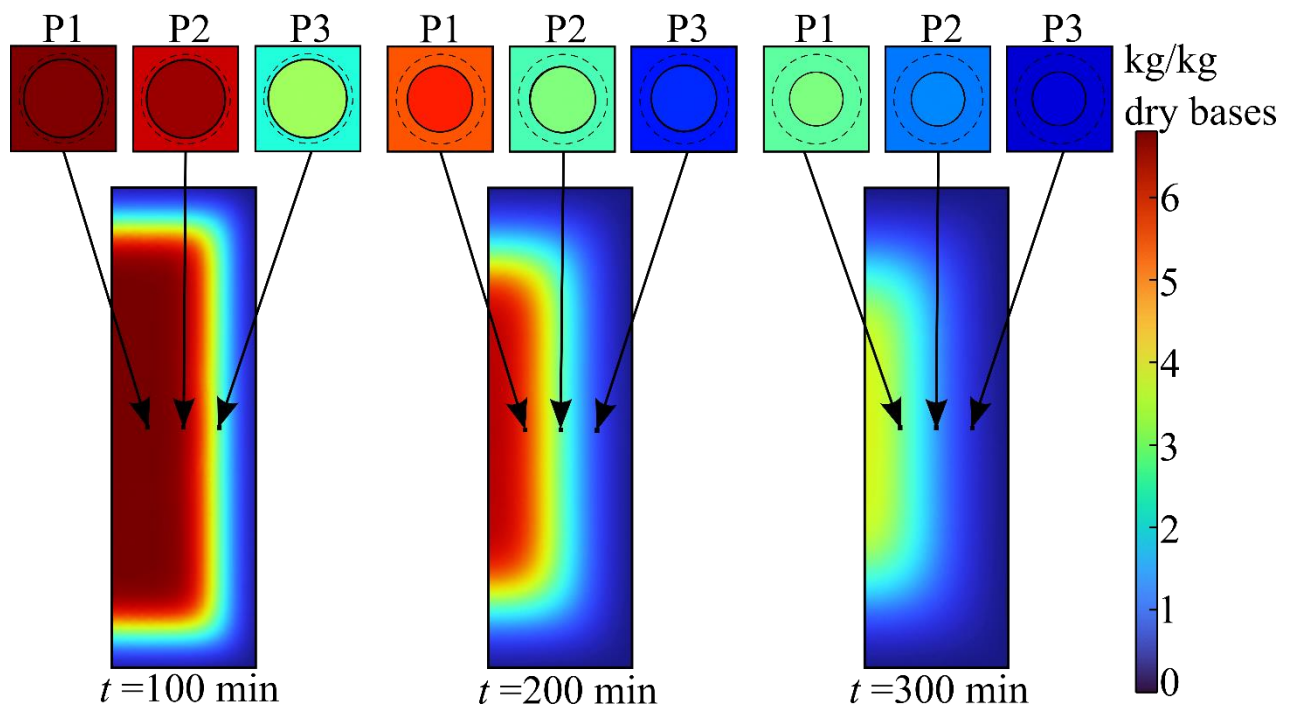


Figure C.3. Multiscale moisture distribution (kg/kg dry bases) for drying at 64°C. Original cell geometry visually represented by the dashed circle.

The sensitivity investigation for the downscaling model without considering deformation can be seen in Figure C.3.

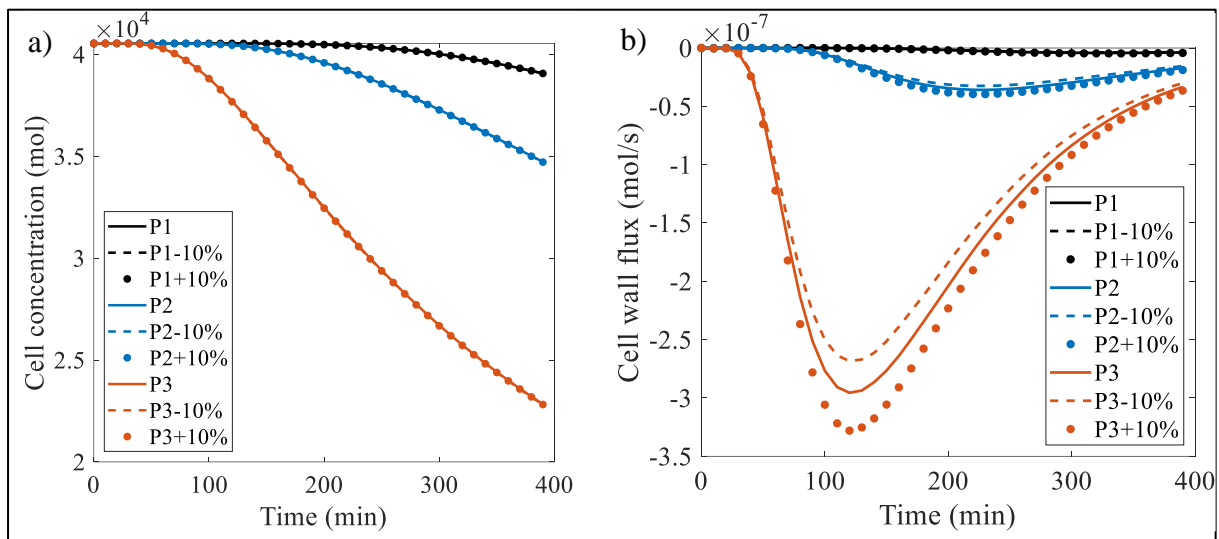


Figure C.3. Sensitivity investigation for the cell wall permeability  $\pm 10\%$ , a) moisture concentration (mol), at each point of interest b) cell wall flux (mol/s) at each point of interest.

## Appendix D - Alternative function for thermal conductivity

Multiple function exists in literature for the thermal conductivity for granny smith apple. To investigate this uncertainty two common functions were investigated, and the results can be seen in Figure D.1. The functions resulted in the same MRE for the average moisture content and temperature. The functions investigated were,  $0.490-0.443 \cdot \exp(-0.206 \cdot M_{db})$  (Mattea et al., 1986), and  $0.148+0.493 \cdot M_{db}$  (SWEAT, 1974).

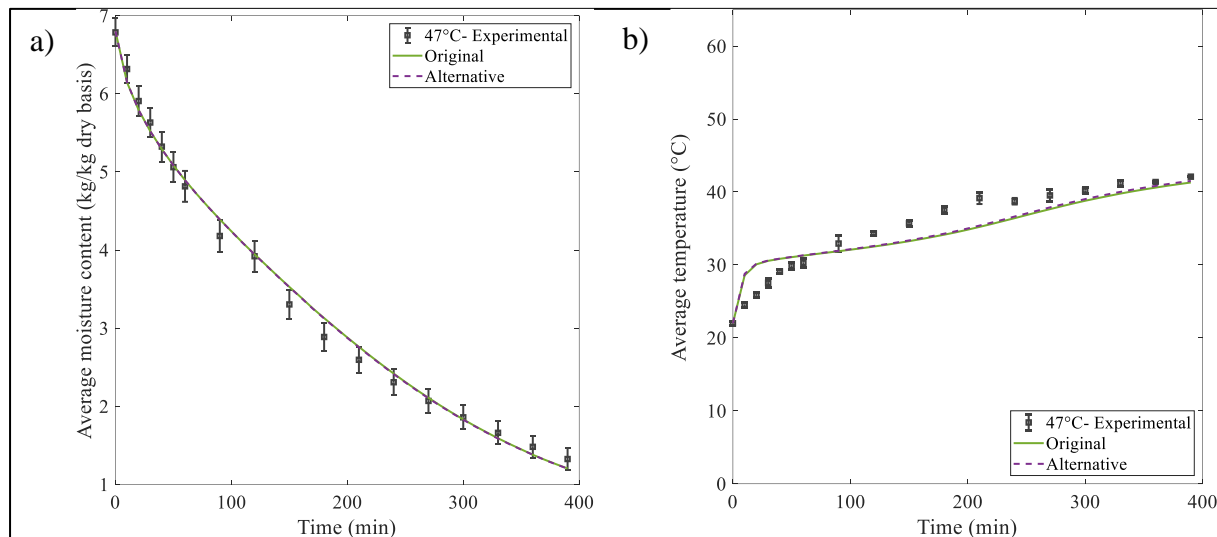


Figure D.1. Comparing different function for thermal conductivity for drying at 47°C, a) average moisture content (kg/kg dry basis) b) Average surface temperature (°C).

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