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A DUAL–SCALE MODELLING APPROACH FOR DRYING HYGROSCOPIC POROUS MEDIA*

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Abstract. A new dual–scale modelling approach is presented for simulating the drying of a wet hygroscopic porous material that couples the porous medium (macroscale) with the underlying pore structure (microscale). The proposed model is applied to the convective drying of wood at low temperatures and is valid in the so–called hygroscopic range, where hygroscopically held liquid water is present in the solid phase and water exits only as vapour in the pores. Coupling between scales is achieved by imposing the macroscopic gradients of moisture content and temperature on the microscopic field using suitably–defined periodic boundary conditions, which allows the macroscopic mass and thermal fluxes to be defined as averages of the microscopic fluxes over the unit cell. This novel formulation accounts for the intricate coupling of heat and mass transfer at the microscopic scale but reduces to a classical homogenisation approach if a linear relationship is assumed between the microscopic gradient and flux. Simulation results for a sample of spruce wood highlight the potential and flexibility of the new dual–scale approach. In particular, for a given unit cell configuration it is not necessary to propose the form of the macroscopic fluxes prior to the simulations because these are determined as a direct result of the dual–scale formulation.

Key words. drying, porous media, multiscale, dual–scale, homogenisation, exponential integrators, Krylov subspace methods, wood

AMS subject classifications. 65F60, 65F20, 65M08, 65M20

1. Introduction. The macroscopic approach for modelling heat and mass transport in a porous medium is well developed (see, e.g., [25, 26]). At this length scale, the method of *volume averaging* [19] can be used to overcome the difficulties associated with the complex geometry of the underlying pore structure. This technique performs a smoothing of highly oscillatory physical quantities (e.g., phase density) via an averaging volume containing (typically) hundreds or thousands of pores. This averaging method produces balance equations (derived from the standard conservation laws) that resemble those of a continuum with the exception that volume–averaged quantities and effective parameters appear in their definitions. The macroscopic approach is schematised in Figure 1.1 via the exchange of macroscopic fluxes (arrows 1) between the accumulation terms (denoted by 2) in the balance equations. The most comprehensive macroscopic formulation for drying of porous media (see, e.g., [15]), which originates from the work of Whitaker [25], forms the basis for our dual–scale approach (see Section 2.1).

One of the main drawbacks of the macroscopic approach is that the effective coefficients must be supplied to the model, most of which are nonlinear functions of moisture content and temperature. Homogenisation theory allows these effective coefficients to be predicted from the microscopic structure of the porous medium (see, e.g., the book chapter [8]). This theory assumes that the underlying pore structure consists of a periodic arrangement of cells, and produces steady-state, uncoupled problems on the unit cell, which must be solved once, prior to the simulation. The

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Fig. 1.1: Possible interactions within and between the macroscopic and microscopic scales for the balance equations.

resulting homogenised coefficient supplied to the macroscopic formulation thereafter consists of two contributions: the average of the microscopic properties, which accounts for the proportion and microscopic coefficients for each phase in the unit cell; and a corrective term, which accounts for the unit cell morphology [10]. Homogenisation is an example of a *scaling* (dual–scale) method: information is supplied in the "microscale to macroscale" direction only (represented by arrows 3 in Figure 1.1). Drying configurations whereby the scaling approach fails are well documented in the literature (see, e.g., [11, 12]) and provide motivation for moving towards two–way dual–scale approaches, such as the approach featured in this work.

Dual-scale approaches for transport in porous media are presented in the book chapter [18] and the references therein. The main idea behind these models is that at each point in the macroscopic domain, there is specified a microcell that represents the pore structure present at that point. A set of (time-dependent) partial differential equations is proposed to describe the global (macroscopic) flow, and a separate set of (time-dependent) equations is used to describe the local (microscopic) flow. In this case, interaction between scales is a true two-way process (represented by arrows 3) and 4 in Figure 1.1) with coupling between scales usually occurring on the boundary of the microcell using various kinds of boundary conditions. The simplest coupling strategy is to impose the macroscopic values via a Dirichlet boundary condition and the average fluxes across the boundary as source terms at the macroscopic level. This works nicely when the microscopic scale acts as a storage phase and the macroscopic scale as a conductive phase (see [11] for a full set equations addressing this situation for the drying of a bed of particles). However, in the majority of porous media, the roles of storage and conduction is shared between scales. In the absence of local thermodynamic equilibrium, one possible way to deal with such a situation is to propose a microscale formulation capable of accounting for the macroscopic fluxes and the microscopic fields simultaneously (represented by arrows 5 in Figure 1.1). For this case, the coupling between scales is more challenging, because the macroscopic variables and their gradients have to be accounted for at the microscale.

The ultimate goal of the dual-scale approach would be to transfer everything at the microscale: the schematic diagram of Figure 1.1 would be reduced to arrows 5 denoting the fluxes, with the accumulative terms (denoted by 2) transferred as a net rate of change of the microscopic field within the unit cell. This approach, while ideal,



Fig. 1.2: Microscopic pore structure of softwood.

is very computationally demanding when the time constants of both scales differ by several orders of magnitude.

The focus of the present article is the formulation of a dual-scale approach (in two-dimensions) for simulating the convective drying of a porous medium at low temperatures. Such a configuration involves a huge contrast between the macroscopic and microscopic time constants. The proposed model applies in the hygroscopic range only, where liquid water is absent from the pores. This assumption avoids tracking the gas-liquid interface in the pore, which is non-trivial. The approach taken in this paper lies somewhere between the scaling and two-way dual-scale approaches mentioned above: interaction between the macroscopic and microscopic scales occurs in both directions but steady-state conditions are assumed on the microscale (see Section 2.2). Referring to Figure 1.1, arrows 1 now disappear as the heat and mass fluxes are computed via an average at the microscopic level (arrows 3), which allows the macroscopic fields to be updated. The coupling is closed because the updated values and gradients of the macroscopic variables are returned to the microscopic level as boundary conditions (arrows 4).

The proposed dual-scale model is applied to a cross-section of spruce wood, a softwood species, in Section 4.2. Softwood is a heterogeneous, anisotropic porous material that is comprised of long tubular cells called tracheids, 90–95% of which are oriented in the direction of the length of the log. These longitudinal tracheids, which are comprised of the cell wall (solid phase) and cell lumen (pore) and pore-connecting pits, are long and narrow — ranging from 3–4 mm in length and 25–50 μ m in diameter [17]. Abrupt changes in the tracheid diameter and cell-wall thickness from earlywood (rapid growth period, thin cell walls) and latewood (slow growth period, thick cell walls) produce the annual growth rings visible at the macroscopic scale (see Figure 1.2). Tracheids found in both earlywood and latewood are investigated in Section 4.1.

2. Model formulation. Consider a bounded macroscopic domain $\mathcal{B} \subset \mathbb{R}^2$, with boundary $\partial \mathcal{B}$, that represents a two-dimensional sample of porous material. We assume that the underlying microstructure present at each point $x = (x_1, x_2)^T \in \mathcal{B}$ takes the form of a periodic arrangement of cells defined by a single unit cell $\mathcal{C}_x =$ $(0, a) \times (0, b) \subset \mathbb{R}^2$ with boundary $\partial \mathcal{C}_x$. Furthermore, the partition $\mathcal{C}_x = \mathcal{C}_x^{(s)} \cup \mathcal{C}_x^{(g)}$ of \mathcal{C}_x is defined, where $\mathcal{C}_x^{(s)}$ and $\mathcal{C}_x^{(g)}$ denote the solid and gaseous phase (pore) regions of the unit cell, respectively (see Figure 2.1). The coordinate variable $y = (y_1, y_2)^T \in \mathbb{R}^2$ denotes the position on the unit cell. We assume that the positive y_1 and y_2 directions align with the positive x_1 and x_2 directions. In the following sections, separate sets of partial differential equations are used to describe the global flow in \mathcal{B} and the local flow within \mathcal{C}_x , where the subscripts \mathcal{B} and \mathcal{C}_x are used to denote the macroscopic and microscopic variable fields, respectively.



Fig. 2.1: Macroscopic domain and unit cell.

2.1. Macroscopic transport equations. To describe the macroscopic flow, the comprehensive formulation presented in [15] is utilised. Under low temperature drying conditions, the assumption of a fixed gaseous pressure is valid. This assumption produces a two–equation model (a balance equation is not included for the air phase)

of the form (see, e.g., [23])

$$\frac{\partial \psi_{\ell}}{\partial t}(u(x,t)) + \nabla_x \cdot \boldsymbol{q}_{\ell}(u(x,t)) = 0, \quad x \in \mathcal{B}, \quad \ell = \mathrm{w}, \mathrm{e}, \quad (2.1)$$

representing the conservation of water $(\ell = w)$ and energy $(\ell = e)$, where the conserved quantities and flux vectors are given by

$$\psi_{\rm w} = \rho_0 X + \varepsilon_{\rm g} \rho_{\rm v} , \qquad \qquad \psi_{\rm e} = \rho_0 (X h_{\rm b} + h_{\rm s}) + \varepsilon_{\rm g} (\rho_{\rm v} h_{\rm v} + \rho_{\rm a} h_{\rm a}) , \qquad (2.2)$$

$$\boldsymbol{q}_{\mathrm{w}} = \frac{1}{A(\mathcal{C}_{x})} \int_{\mathcal{C}_{x}} \boldsymbol{Q}_{\mathrm{w}} \, dA \,, \quad \boldsymbol{q}_{\mathrm{e}} = \frac{1}{A(\mathcal{C}_{x})} \int_{\mathcal{C}_{x}} \boldsymbol{Q}_{\mathrm{e}} \, dA \,, \tag{2.3}$$

The subscript x on the gradient in Equation (2.1) indicates that the operator is taken with respect to the macroscopic coordinate variable x. Equation (2.3) expresses the macroscopic flux vector as the (area) average of the microscopic flux vector Q_{ℓ} over the unit cell C_x . Recall that in the hygroscopic range, liquid water is absent from the pores and present only as bound water in the solid phase. This explains the two contributions, bound water ($\rho_0 X$) and water vapour ($\varepsilon_g \rho_v$), to the mass variable. The following notation is adopted in this paper: ε (volume fraction), ρ (density), h (enthalpy), g (gas phase), v (vapour phase), a (air phase), s (solid phase) and b (bound water phase). An overline is used to signify a superficially-averaged variable (as opposed to an intrinsically-averaged variable without an overline) and $A(\cdot)$ denotes area. The density of the porous medium ρ_0 denotes the superficial average of the solid phase. The primary variables are chosen as the moisture content X (kg kg⁻¹) and temperature T (°C), with $u(x,t) = (X_{\mathcal{B}}(x,t), T_{\mathcal{B}}(x,t))^T$ in Equation (2.1). All remaining variables are functions of the primary variables (see Section 2.3).

Initially, the porous medium has some prescribed distribution of moisture content and temperature. The boundary conditions applied on the drying surfaces have been discussed in detail previously (see, e.g., [23]). These conditions prescribe the liquid and energy fluxes on $\partial \mathcal{B}$ (i.e., they prescribe $(\boldsymbol{q}_{\ell} \cdot \boldsymbol{n}_{\partial \mathcal{B}})$ for $\ell = w, e$, where $\boldsymbol{n}_{\partial \mathcal{B}}$ is the unit vector normal to $\partial \mathcal{B}$ outward to \mathcal{B}) and depend on the wet– and dry–bulb temperatures, and velocity of the circulating air in the drier.

2.2. Microscopic cell problem. The following steady–state problem is proposed on the unit cell

$$\nabla_y \cdot \boldsymbol{Q}_{\ell}(U(y)) = 0, \quad y \in \mathcal{C}_x, \quad \ell = w, e,$$
(2.4)

where the microscopic variable field $U(y) = (X_{\mathcal{C}_x}(y), T_{\mathcal{C}_x}(y))^T$. In the absence of liquid water, the pore region of the unit cell is comprised of air and water vapour only. Thus, in the hygroscopic range, liquid migration is governed by two different mechanisms: bound water diffusion in the solid phase and water vapour diffusion in the gaseous phase [17]. We assume that these two processes can be represented by the following mass fluxes

$$\boldsymbol{Q}_{\mathrm{w}}^{(\mathrm{s})} = -\rho_{\mathrm{s}} D_{\mathrm{b}} \nabla_{y} X_{\mathcal{C}_{x}}, \qquad y \in \mathcal{C}_{x}^{(\mathrm{s})}, \qquad (2.5)$$

$$\boldsymbol{Q}_{\mathrm{w}}^{(\mathrm{g})} = -\rho_{\mathrm{g}} \frac{D_{\mathrm{v}}}{1 - \omega_{\mathrm{v}}} \nabla_{y} \omega_{\mathrm{v}} , \quad y \in \mathcal{C}_{x}^{(\mathrm{g})} , \qquad (2.6)$$

which together with Fourier's law give the following form for the heat fluxes

$$\boldsymbol{Q}_{\mathrm{e}}^{(\mathrm{s})} = -k_{\mathrm{s}} \nabla_{\boldsymbol{y}} T_{\mathcal{C}_{\boldsymbol{x}}} + h_{\mathrm{b}} \boldsymbol{Q}_{\mathrm{w}}^{(\mathrm{s})}, \quad \boldsymbol{y} \in \mathcal{C}_{\boldsymbol{x}}^{(\mathrm{s})}, \qquad (2.7)$$

$$\boldsymbol{Q}_{\mathrm{e}}^{(\mathrm{g})} = -k_{\mathrm{g}} \nabla_{\boldsymbol{y}} T_{\mathcal{C}_{x}} + h_{\mathrm{v}} \boldsymbol{Q}_{\mathrm{w}}^{(\mathrm{g})}, \quad \boldsymbol{y} \in \mathcal{C}_{x}^{(\mathrm{g})}.$$
(2.8)

In the mass fluxes, $D_{\rm b}$ and $D_{\rm v}$ denote the microscopic diffusion coefficients of bound water and water vapour in air, respectively. We note that the form of the vapour flux (2.6) is derived by assuming the air phase is stagnant [1, §17.2]. Introducing the indicator variable

$$\chi = \begin{cases} 0 \quad y \in \mathcal{C}_x^{(s)} \\ 1 \quad y \in \mathcal{C}_x^{(g)} \end{cases},$$
(2.9)

allows one to define

$$\boldsymbol{Q}_{w} = (1-\chi)\boldsymbol{Q}_{w}^{(s)} + \chi \boldsymbol{Q}_{w}^{(g)}, \qquad (2.10)$$

$$\boldsymbol{Q}_{e} = (1-\chi)\boldsymbol{Q}_{e}^{(s)} + \chi \boldsymbol{Q}_{e}^{(g)}, \qquad (2.11)$$

for all $y \in \mathcal{C}_x$, together with the conserved quantities

$$\Psi_{\rm w} = (1-\chi)\rho_{\rm s}X_{\mathcal{C}_x} + \chi\rho_{\rm v}\,,\tag{2.12}$$

$$\Psi_{\rm e} = (1 - \chi)\rho_{\rm s} \left(X_{\mathcal{C}_x} h_{\rm w} + h_{\rm s} \right) + \chi \left(\rho_{\rm v} h_{\rm s} + \rho_{\rm a} h_{\rm a} \right) \,. \tag{2.13}$$

Coupling between the macroscopic and microscopic variable fields occurs on the boundary of the unit cell

$$X_{\mathcal{C}_x}(a, y_2) = X_{\mathcal{C}_x}(0, y_2) + a \frac{\partial X_{\mathcal{B}}}{\partial x_1}(x, t), \quad 0 < y_2 < b, \qquad (2.14a)$$

$$X_{\mathcal{C}_x}(y_1, b) = X_{\mathcal{C}_x}(y_1, 0) + b \frac{\partial X_{\mathcal{B}}}{\partial x_2}(x, t), \quad 0 < y_1 < a, \qquad (2.14b)$$

$$T_{\mathcal{C}_x}(a, y_2) = T_{\mathcal{C}_x}(0, y_2) + a \frac{\partial T_{\mathcal{B}}}{\partial x_1}(x, t), \quad 0 < y_2 < b, \qquad (2.14c)$$

$$T_{\mathcal{C}_x}(y_1, b) = T_{\mathcal{C}_x}(y_1, 0) + b \frac{\partial T_{\mathcal{B}}}{\partial x_2}(x, t), \quad 0 < y_1 < a, \qquad (2.14d)$$

$$\boldsymbol{Q}_{\ell}(0, y_2) \cdot \boldsymbol{n}_{\partial \mathcal{C}_x} = \boldsymbol{Q}_{\ell}(a, y_2) \cdot \boldsymbol{n}_{\partial \mathcal{C}_x}, \qquad 0 < y_2 < b, \quad \ell = \mathrm{w}, \mathrm{e}, \qquad (2.14\mathrm{e})$$

$$\boldsymbol{Q}_{\ell}(y_1, 0) \cdot \boldsymbol{n}_{\partial \mathcal{C}_x} = \boldsymbol{Q}_{\ell}(y_2, b) \cdot \boldsymbol{n}_{\partial \mathcal{C}_x}, \qquad 0 < y_1 < a, \quad \ell = w, e, \qquad (2.14f)$$

where $n_{\partial \mathcal{C}_x}$ is the unit vector normal to $\partial \mathcal{C}_x$ outward to \mathcal{C}_x , and via the relationship

$$\frac{1}{A(\mathcal{C}_x)} \int_{\mathcal{C}_x} \Psi_\ell(U(y)) \, dA = \psi_\ell(u(x,t)) \,, \quad \ell = \mathbf{w}, \mathbf{e} \,. \tag{2.15}$$

This formulation respects the gradient of the macroscopic variable field at the unit cell level, ensures calibration of the microscopic conserved quantities with the macroscopic conserved quantities and is consistent with the assumption of a periodic arrangement of cells.

Remark. The approach of applying the macroscopic gradient over the unit cell C_x is equivalent to homogenisation if a linear relationship is assumed between the microscopic gradient and microscopic flux. For example, consider the following simple one-dimensional problem

$$\frac{dQ}{dy} = 0$$
, $Q(y) = -k(y)\frac{dU}{dy}$, $0 < y < a$ (2.16a)

subject to

$$U(a) = U(0) + a\frac{du}{dx}, \quad Q(0) = Q(a), \quad \frac{1}{a}\int_0^a U(y)\,dy = u \tag{2.16b}$$

where u is the macroscopic variable. For this problem, it is simple to show that the microscopic flux is constant and given by

$$Q(y) = -\kappa \frac{du}{dx}, \quad \kappa = \frac{a}{\int_0^a \frac{d\tilde{y}}{k(\tilde{y})}}, \quad (2.17)$$

where κ is the classical homogenised coefficient. Following from the definition in Equation (2.3), the macroscopic flux vector takes the form of the homogenised flux

$$q = \frac{1}{a} \int_0^a Q(y) \, dy = -\kappa \frac{du}{dx} \,. \tag{2.18}$$

2.3. Closure conditions for softwood. The following relationships close the model:

(i) The volume fraction of the gaseous phase (i.e., the porosity) in Equation (2.2) is given by $\varepsilon_{\rm g} = 1 - \varepsilon_{\rm s}$, where the solid fraction is assumed to vary with moisture content, temperature and density [13]

$$\varepsilon_{\rm s} = \frac{\rho_0(\rho_{\rm w} + \rho_0 X)}{\rho_{\rm s}(\rho_{\rm w} + \rho_0 (X - X_{\rm fsp}(T)))}, \qquad (2.19)$$

and the fibre saturation value of moisture content decreases linearly with increasing temperature according to the relation $X_{\rm fsp} = 0.325 - 0.001T$ (see, e.g., [21]). We note that $X < X_{\rm fsp}$ denotes the hygroscopic range for wood. This form of $\varepsilon_{\rm s}$ accounts for the swelling and shrinkage of the cell-wall (solid phase) depending on the volume of bound water.

(ii) The gaseous pressure is constant and equal to the atmospheric value P_{atm} and the gaseous phase is assumed to be a binary mixture of two ideal gases (i.e., water vapour and dry air) giving the following relationships:

$$P_{\rm a} + P_{\rm v} = P_{\rm atm} , \quad \rho_{\rm v} = \frac{P_{\rm v} M_{\rm v}}{R(T + 273.15)} , \quad \rho_{\rm a} = \frac{P_{\rm a} M_{\rm a}}{R(T + 273.15)} , \quad (2.20)$$

where

$$P_{\rm v} = P_{\rm v}^{\rm (sat)}\psi, \quad P_{\rm v}^{\rm (sat)} = \exp\left(25.5058 - \frac{5204.9}{T + 273.15}\right),$$
 (2.21)

$$\psi = 1 - \exp\left(-0.764269\left(\frac{X}{X_{\rm fsp}}\right) - 3.67872\left(\frac{X}{X_{\rm fsp}}\right)^2\right).$$
 (2.22)

The gaseous phase density and mass fraction of vapour in the air phase appearing in the definition of the vapour flux (2.6) are given by $\rho_{\rm g} = \rho_{\rm a} + \rho_{\rm v}$ and $\omega_{\rm v} = \rho_{\rm v}/\rho_{\rm g}$, respectively.

(iii) Water and air at 0° C are the reference states for enthalpy, and the specific heat values (J kg $^{\circ}$ C⁻¹) are constant. In addition, the integral and differential heats of sorption are assumed negligible giving the following enthalpy-temperature relationships

$$h_{\rm s} = C_{{\rm p}_s}T, \quad h_{\rm b} = C_{{\rm p}_w}T, \quad h_{\rm s} = C_{{\rm p}_s}T, \quad h_{\rm v} = h_{\rm vap}^0 + C_{{\rm p}_v}T, \quad (2.23)$$

where h_{vap}^0 is the latent heat of water vaporisation at 0°C.

(iv) In the heat flux definitions (2.7) and (2.8), the solid and gaseous conductivities are assumed constant and given by $k_{\rm s} = 0.5 \,\mathrm{W}\,\mathrm{m}^{-1}\,\mathrm{K}^{-1}$ and $k_{\rm g} = 0.023 \,\mathrm{W}\,\mathrm{m}^{-1}\,\mathrm{K}^{-1}$ [14], respectively. In the mass fluxes, the microscopic diffusion coefficients of bound water and water vapour in air, are given by [20, 5]:

$$D_{\rm b} = \exp\left(-12.8183993 + 10.8951601X - \frac{4300}{T + 273.15}\right), \qquad (2.24)$$

$$D_{\rm v} = 0.0000226 \left(\frac{T + 273.15}{273.15}\right)^{1.81}.$$
 (2.25)

3. Computational considerations. One has to keep in mind that the dual– scale approach proposed in this paper is significantly more demanding in computational resources than a classical macroscopic approach. The microscopic variable field needs to be updated each time the macroscopic field is updated. Thus, sophisticated numerical techniques are imperative for an efficient simulation.

3.1. Mesh terminology. Both the porous medium (macroscopic domain \mathcal{B}) and unit cell (microscopic domain \mathcal{C}_x) are meshed using triangular-shaped elements. It must be noted that for the unit cell configurations presented in this work (see Section 4.1) one could use structured (rectangular) elements, however, it is our aim to develop a general tool able to deal with any configuration for the unit cell (e.g., irregular geometries coming from actual wood images).

We denote by $\mathcal{T}_{\mathcal{D}}$ and $\mathcal{N}_{\mathcal{D}}$ the set of triangles and nodes that together describe a triangulation over a given domain \mathcal{D} . For each node $i \in \mathcal{N}_{\mathcal{D}}$, we define a control volume Ω_i with boundary $\partial\Omega_i$. We denote by $\mathcal{E} = \bigcup_{i \in \mathcal{N}_{\mathcal{D}}} \partial\Omega_i$, the set of edges that define the control volume boundaries and introduce the partition $\mathcal{E} = \mathcal{E}_{int} \cup \mathcal{E}_{ext}$ of \mathcal{E} into the set of interior edges \mathcal{E}_{int} (the edges located in \mathcal{D}) and the set of boundary edges \mathcal{E}_{ext} (the edges located on $\partial\mathcal{D}$). The interior edges are constructed by connecting the centroid of each triangle to the midpoint of its edges. Furthermore, for each node $i \in \mathcal{N}_{\mathcal{D}}$, we denote the set of its control volume edges by $\mathcal{E}_i = \{\sigma \in \mathcal{E} \mid \sigma \subset \partial\Omega_i\}$ and the set of its interior control volume edges by $\mathcal{E}_{i,int} = \{\sigma \in \mathcal{E} \mid \sigma \subset \partial\Omega_i\} = \mathcal{E}_i \cap \mathcal{E}_{int}$. The unit vector, normal to the control volume edge σ and outward to the control volume Ω_i , is denoted by $\mathbf{n}_{i,\sigma}$. The notations $A(\cdot)$ and $L(\cdot)$ are used to represent area and length, respectively.

3.2. Macroscale solution approach. A discrete representation of the balance law (2.1) over Ω_i is given by

$$\frac{d}{dt}\psi_{\ell}^{(i)} + \frac{1}{A(\Omega_i)}\sum_{\sigma\in\mathcal{E}_i}\int_{\sigma} (\boldsymbol{q}_{\ell}\cdot\boldsymbol{n}_{i,\sigma}) \, ds = 0 \,, \quad i\in\mathcal{N}_{\mathcal{B}} \,, \quad \ell = \mathrm{w}, \mathrm{e} \,, \tag{3.1}$$

where $\psi_{\ell}^{(i)}$ denotes evaluation of the conserved quantity at node *i*. We approximate the line integral along the edge σ using a midpoint quadrature rule via the numerical flux

$$q_{\ell,i,\sigma} = \left(\boldsymbol{q}_{\ell,\sigma} \cdot \boldsymbol{n}_{i,\sigma}\right) L(\sigma), \qquad (3.2)$$

where $q_{\ell,\sigma}$ represents evaluation of the flux vector at the midpoint of σ . This produces the following control volume equation

$$\frac{d}{dt}\psi_{\ell}^{(i)} + \frac{1}{A(\Omega_i)}\sum_{\sigma\in\mathcal{E}_i}q_{\ell,i,\sigma} = 0, \quad i\in\mathcal{N}_{\mathcal{B}}.$$
(3.3)

For a boundary edge ($\sigma \in \mathcal{E}_{i,\text{ext}}$), one simply uses the boundary flux expressions in the definition of the numerical flux $q_{\ell,i,\sigma}$.

For an internal edge ($\sigma \in \mathcal{E}_{i,\text{int}}$), the flux vector $\boldsymbol{q}_{\ell,\sigma}$ is assumed constant within a given macroscopic element and computed via a discretised version of the integrals (2.3). To do this, a unique unit cell problem, with unit cell domain \mathcal{C}_{ϵ} , is associated with each macroscopic element $\epsilon \in \mathcal{T}_{\mathcal{B}}$ and the corresponding macroscopic flux vector computed as an element area-weighted average of the numerical microscopic flux vectors (see Section 3.3).

Applying a chain rule to the left-hand side of (3.3) gives

$$\frac{d}{dt} \begin{bmatrix} X_{\mathcal{B}}^{(i)} \\ T_{\mathcal{B}}^{(i)} \end{bmatrix} = \frac{-1}{A(\Omega_i)} \begin{bmatrix} (\psi_{\mathbf{w}})_{X_{\mathcal{B}}} & (\psi_{\mathbf{w}})_{T_{\mathcal{B}}} \\ (\psi_{\mathbf{e}})_{X_{\mathcal{B}}} & (\psi_{\mathbf{e}})_{T_{\mathcal{B}}} \end{bmatrix}^{-1} \sum_{\sigma \in \mathcal{E}_i} \begin{bmatrix} q_{\mathbf{w},i,\sigma} \\ q_{\mathbf{e},i,\sigma} \end{bmatrix} \equiv \begin{bmatrix} g_{\mathbf{w}}^{(i)} \\ g_{\mathbf{e}}^{(i)} \end{bmatrix}, \quad i \in \mathcal{N}_{\mathcal{B}}, \quad (3.4)$$

where, for example, $(\psi_w)_{X_{\mathcal{B}}}$ denotes the partial derivative of ψ_w with respect to $X_{\mathcal{B}}$. This allows the full macroscopic discretisation to be expressed as a system of differential equations in the form

$$\frac{d\boldsymbol{u}}{dt} = g(\boldsymbol{u}), \quad \boldsymbol{u}(0) = \boldsymbol{u}_0 \tag{3.5}$$

where $\boldsymbol{u} = (X_{\mathcal{B}}^{(i)}, T_{\mathcal{B}}^{(i)})_{i \in \mathcal{N}_{\mathcal{B}}}$ and $g(\boldsymbol{u}) = (g_{w}^{(i)}(\boldsymbol{u}), g_{e}^{(i)}(\boldsymbol{u}))_{i \in \mathcal{N}_{\mathcal{B}}}$. We approximate the solution of the initial value problem (3.5) via a linearisation around $t = t_{n}$ of the form

$$\frac{d\boldsymbol{u}}{dt} = g(\boldsymbol{u}_n) + J_g(\boldsymbol{u}_n)(\boldsymbol{u} - \boldsymbol{u}_n), \quad \boldsymbol{u}(t_n) = \boldsymbol{u}_n, \quad (3.6)$$

where J denotes the Jacobian matrix with function-identifying subscript. The solution of (3.6) is given by

$$\boldsymbol{u}(t_n + \tau) = \boldsymbol{u}_n + \tau \varphi(\tau J_g(\boldsymbol{u}_n)) g(\boldsymbol{u}_n), \qquad (3.7)$$

where $\varphi(z) = (e^z - 1)/z$ and $\tau = t - t_n$. The linearisation strategy presented above and the resulting time-stepping formula (3.7) with stepsize τ is an example of an exponential integrator (see, e.g., [3, 7, 22]). The attraction of using this method over implicit methods (e.g., the backward differentiation formulae (BDF)) is that Krylov subspace methods for approximating the φ -function matrix-vector product perform well without the overhead associated with preconditioning. In our algorithm, the stepsize is controlled via local error estimation (i.e., estimation of the error incurred during a single time step) using the estimate proposed in [3] for (3.7), which has performed well at controlling the stepsize in recent case studies involving transport in porous media (see, e.g., [3, 4]).

3.3. Microscopic solution approach. Linear interpolation is used to supply the macroscopic information required for the unit cell problem on C_{ϵ} . For example, if $\mathcal{I}_{\epsilon}\varphi(x)$ denotes the standard linear interpolant of a variable φ over a triangle $\epsilon \in \mathcal{T}_{\mathcal{B}}$ (i.e., $\mathcal{I}_{\epsilon}\varphi(x)$ is linear in x_1 and x_2 and $\mathcal{I}_{\epsilon}\varphi(x) = \varphi$ at the vertices of ϵ), then evaluation of $\mathcal{I}_{\epsilon}X_{\mathcal{B}}(x)$ and $\mathcal{I}_{\epsilon}T_{\mathcal{B}}(x)$ at the centroid of ϵ provides the macroscopic values used to evaluate ψ_{ℓ} in Equation 2.15. The macroscopic gradients appearing in the boundary conditions (2.14a)–(2.14d) are given by $\nabla_x \mathcal{I}_{\epsilon}X_{\mathcal{B}}$ and $\nabla_x \mathcal{I}_{\epsilon}T_{\mathcal{B}}$, which are constant across the element.

A discrete representation of the balance law (2.4) over Ω_i is given by

$$\sum_{\sigma \in \mathcal{E}_i} Q_{\ell,i,\sigma} = 0, \quad i \in \mathcal{N}_{\mathcal{C}_{\epsilon}}, \quad \epsilon \in \mathcal{T}_{\mathcal{B}}, \quad \ell = \mathbf{w}, \mathbf{e},$$
(3.8)

where the numerical flux is again defined using the midpoint approximation

$$Q_{\ell,i,\sigma} = (\boldsymbol{Q}_{\ell,\sigma} \cdot \boldsymbol{n}_{i,\sigma}) L(\sigma) \,. \tag{3.9}$$

The vector $\boldsymbol{Q}_{\ell,\sigma} = (1-\chi)\boldsymbol{Q}_{\ell,\sigma}^{(\mathrm{s})} + \chi \boldsymbol{Q}_{\ell,\sigma}^{(\mathrm{g})}$ featured in the approximation (3.9) represents evaluation of the flux vector at the midpoint of the edge σ . It is important that the mesh is constructed so that the element edges (and hence nodes) are aligned with the interface between the solid phase and pore. This ensures that each edge is located in homogeneous material (solid phase or pore), that is, the phase indicator variable $\chi = 0$ ($\sigma \subset C_{\epsilon}^{(\mathrm{s})}$) or $\chi = 1$ ($\sigma \subset C_{\epsilon}^{(\mathrm{g})}$).

For the set of nodes $\mathcal{N}_{C_{\epsilon}}$ we distinguish between those located on the north $(y_2 = b)$, east $(y_1 = a)$, south $(y_2 = 0)$ and west $(y_1 = 0)$ boundaries of \mathcal{C}_{ϵ} , denoted by the subsets \mathcal{N}_N , \mathcal{N}_E , \mathcal{N}_S and \mathcal{N}_W respectively, and the set of internal nodes \mathcal{N}_{int} . The mesh is also constructed to ensure alignment of nodes on opposing boundaries of \mathcal{C}_{ϵ} , i.e., nodes located on the east boundary are horizontally aligned (having equal y_2 coordinates) with the west boundary nodes and nodes located on the north and south boundaries are aligned vertically (having equal y_1 coordinates). This alignment is used to enable the implementation of the periodic boundary conditions described in Equation 2.14. With alignment, the solution along the east and north boundaries can be computed from the solution along the west and south boundaries, respectively, (or vice versa) via the boundary conditions (2.14a)-(2.14d). This means we can restrict our attention to the subset of nodes not located on the north or east boundaries, which we will denote by $\mathcal{N}_V = \mathcal{N}_{\mathcal{C}_{\epsilon}} \setminus (\mathcal{N}_E \cup \mathcal{N}_N)$. In this case, the full microscopic discretisation leads to an overdetermined system of nonlinear equations (the number of equations outnumber the number of unknowns by two) that can be expressed as

$$G(\boldsymbol{U}) = \begin{bmatrix} f(\boldsymbol{U}) \\ r(\boldsymbol{U}) \end{bmatrix} = 0, \qquad (3.10)$$

where $\boldsymbol{U} = (X_{\mathcal{C}_{\epsilon}}^{(i)}, T_{\mathcal{C}_{\epsilon}}^{(i)})_{i \in \mathcal{N}_{V}} \in \mathbb{R}^{2n}, f(\boldsymbol{U}) = (f_{w}^{(i)}(\boldsymbol{U}), f_{e}^{(i)}(\boldsymbol{U}))_{i \in \mathcal{N}_{V}} \in \mathbb{R}^{2n}, r(\boldsymbol{U}) = (r_{w}(\boldsymbol{U}), r_{e}(\boldsymbol{U}))^{T} \in \mathbb{R}^{2}$ and $G(\boldsymbol{U}) \in \mathbb{R}^{2n+2}$, and *n* denotes the number of nodes not situated on the north or east boundaries of \mathcal{C}_{ϵ} (i.e., the cardinality of \mathcal{N}_{V}). The two coordinate functions of $r(\boldsymbol{U})$ are given by

$$r_{\ell}(\boldsymbol{U}) = \psi_{\ell}(\mathcal{I}_{\epsilon}X_{\mathcal{B}}(x), \mathcal{I}_{\epsilon}T_{\mathcal{B}}(x)) - \frac{1}{A(\mathcal{C}_{\epsilon})} \sum_{i \in \mathcal{N}_{\mathcal{C}_{\epsilon}}} \Psi_{\ell}^{(i)}, \quad \ell = \mathrm{w}, \mathrm{e}.$$

The form of the function $f_{\ell}^{(i)}(U)$ for a node $i \in \mathcal{N}_{V}$, which is given by the discrete representation of the balance law (2.4), is distinguished between the following four cases:

Case 1 (Internal nodes). For an internal node $i \in \mathcal{N}_{int}$, the control volume boundary is entirely described by the set of internal edges $\mathcal{E}_{i,int}$, giving

$$f_{\ell}^{(i)}(\boldsymbol{U}) = \sum_{\sigma \in \mathcal{E}_{i,\text{int}}} Q_{\ell,i,\sigma}, \quad \ell = \text{w,e}.$$
(3.11)

Case 2 (East and west boundary nodes). Excluding corner nodes, the solution at an east boundary node $k \in \mathcal{N}_{\mathrm{E}} \setminus (\mathcal{N}_{\mathrm{N}} \cup \mathcal{N}_{\mathrm{S}})$ is computed from the solution at its opposite west boundary node $i \in \mathcal{N}_{\mathrm{W}} \setminus (\mathcal{N}_{\mathrm{N}} \cup \mathcal{N}_{\mathrm{S}})$ (both nodes have equal y_2 coordinate) using the boundary conditions (2.14a) and (2.14c). This allows computation of the numerical fluxes for the internal edges associated with the east boundary node k (edges contained in \mathcal{E}_k). In this case, a control volume equation is written down for the west boundary node only. Under the periodic flux condition (2.14e), one incorporates the numerical fluxes entering the control volume of the east boundary node, giving

$$f_{\ell}^{(i)}(\boldsymbol{U}) = \sum_{\sigma \in \mathcal{E}_{i,\text{int}}} Q_{\ell,i,\sigma} + \sum_{\sigma \in \mathcal{E}_{k,\text{int}}} Q_{\ell,k,\sigma}, \quad \ell = \text{w,e.}$$
(3.12)

Case 3 (North and south boundary nodes) This case is identical to the previous one, in that the resulting control volume equation for the south boundary node incorporates the numerical fluxes entering the control volume of the north boundary node, i.e., one obtains Equation 3.12 with $i \in \mathcal{N}_S \setminus (\mathcal{N}_W \cup \mathcal{N}_E)$ and $k \in \mathcal{N}_N \setminus (\mathcal{N}_W \cup \mathcal{N}_E)$ where both nodes having equal y_1 coordinate.

Case 4 (Corner nodes). The solution at the north–west, north–east and south– east corner nodes can all be computed from the solution at the south–west corner node via the boundary conditions (2.14a)–(2.14d). In this case, a control volume equation is written down for the south–west boundary node only $i \in \mathcal{N}_S \cap \mathcal{N}_W$, which incorporates the numerical fluxes entering the control volumes of all four corner nodes:

$$f_{\ell}^{(i)}(\boldsymbol{U}) = \sum_{j \in \mathcal{N}_{c}} \sum_{\sigma \in \mathcal{E}_{j, \text{int}}} Q_{\ell, j, \sigma} = 0, \quad \ell = \text{w, e.}$$
(3.13)

where $\mathcal{N}_c = (\mathcal{N}_N \cap \mathcal{N}_E) \cup (\mathcal{N}_N \cap \mathcal{N}_W) \cup (\mathcal{N}_S \cap \mathcal{N}_W) \cup (\mathcal{N}_S \cap \mathcal{N}_E)$ denotes the set of corner nodes.

In summary, to evaluate the function g(u) in the macroscopic discretisation (3.5) one must solve the microscopic discretisation (3.10) for each macroscopic element. The fast solution of the overdetermined system of nonlinear equations (3.10) is therefore crucial to a fast dual-scale simulation.

We employ a Newton strategy to solve the overdetermined nonlinear system (3.10), with initial solution approximation $U_0 \in \mathbb{R}^{2n}$, by defining the following sequence of iterates

$$\boldsymbol{U}_{k+1} = \boldsymbol{U}_k + \delta \boldsymbol{U}_k, \quad k = 1, 2, \dots,$$
(3.14)

where the correction vector δU_k satisfies the overdetermined linear system

$$\begin{bmatrix} J_f \\ J_r \end{bmatrix} \delta \boldsymbol{U}_k = -\begin{bmatrix} f \\ r \end{bmatrix} \quad \Leftrightarrow \quad J_G \delta \boldsymbol{U}_k = -G \tag{3.15}$$

where $\boldsymbol{U}_k \in \mathbb{R}^{2n}$, $J_f \equiv J_f(\boldsymbol{U}_k) \in \mathbb{R}^{(2n) \times (2n)}$, $J_r \equiv J_r(\boldsymbol{U}_k) \in \mathbb{R}^{2 \times (2n)}$, $J_G \equiv J_G(\boldsymbol{U}_k) \in \mathbb{R}^{(2n+2) \times (2n)}$, $f \equiv f(\boldsymbol{U}_k) \in \mathbb{R}^{2n}$, $r \equiv r(\boldsymbol{U}_k) \in \mathbb{R}^2$, $G \equiv G(\boldsymbol{U}_k) \in \mathbb{R}^{2n+2}$.

The overdetermined linear system (3.15) possesses the following properties:

(i) The odd- and even-numbered entries of f sum to zero. This is a direct result of an important property of the control volume method, namely, the local balance of fluxes: if the control volumes surrounding nodes i and j share a common edge σ then $Q_{\ell,i,\sigma} = -Q_{\ell,j,\sigma}$ since $\mathbf{n}_{i,\sigma} = -\mathbf{n}_{j,\sigma}$. This gives a physical balance of numerical fluxes across all internal edges, i.e.,

$$\sum_{i \in \mathcal{N}_{\mathcal{C}_{\ell}}} \sum_{\sigma \in \mathcal{E}_{i, \text{int}}} Q_{\ell, i, \sigma} = 0.$$
(3.16)

It follows then that

$$\sum_{i \in \mathcal{N}_{\mathcal{V}}} f_{\ell}^{(i)} = \sum_{i \in \mathcal{N}_{\mathcal{C}_{\ell}}} \sum_{\sigma \in \mathcal{E}_{i, \text{int}}} Q_{\ell, i, \sigma} = 0, \quad \ell = \text{w, e}.$$
(3.17)

(ii) Both $v_{\mathbf{w}} = (1, 0, 1, 0, \dots, 1, 0)^T \in \mathcal{N}(J_f^T)$ and $v_{\mathbf{e}} = (0, 1, 0, 1, \dots, 0, 1)^T \in \mathcal{N}(J_f^T)$. Verification follows directly from (i):

$$v_{\ell}^{T} J_{f} = \sum_{i \in \mathcal{N}_{\mathcal{V}}} \nabla_{U} f_{\ell}^{(i)} = \nabla_{U} \sum_{i \in \mathcal{N}_{\mathcal{V}}} f_{\ell}^{(i)} = 0^{T}, \quad \ell = w, e.$$
 (3.18)

To motivate an approach for solving (3.15) the following example is included that applies a control volume discretisation to the simple one-dimensional problem presented in the remark of Section 2.2.

Example. Consider a spatial discretisation of Equation (2.16) using a control volume method with n + 1 nodes, where $y_i \in [0, a]$ denotes the position of node i (with $y_1 = 0$ and $y_{n+1} = a$) and $U_i = U(y_i)$ denotes the unknown at node i. Assume that the control volume edges are located midway between two neighbouring nodes. For simplicity, we assume that the nodes are equally spaced (i.e., $y_{i+1} - y_i = h$ for all i = 1, ..., n) and further that $k(y) = k_1$ for all $y \in [0, a]$, which gives the exact solution

$$U(y) = \frac{du}{dx} \left(y - \frac{a}{2} \right) + u \,, \quad 0 < y < a \,. \tag{3.19}$$

Using a central-difference approximation for the spatial-derivative of U and a controlvolume weighted approximation to the integral constraint in Equation (2.16b), the spatial discretisation of Equation (2.16) is given by

$$\frac{k_1(U_2 - U_1)}{h} - \frac{k_1(U_{n+1} - U_n)}{h} = 0, \qquad (3.20a)$$

$$\frac{k_1(U_{i+1} - U_i)}{h} - \frac{k_1(U_i - U_{i-1})}{h} = 0, \quad i = 2, .., n - 1,$$
(3.20b)

$$\frac{k_1(U_{n+1} - U_n)}{h} - \frac{k_1(U_n - U_{n-1})}{h} = 0, \qquad (3.20c)$$

$$\frac{1}{a} \left(\frac{h}{2} U_1 + h \sum_{i=2}^n U_i + \frac{h}{2} U_{n+1} \right) = u , \qquad (3.20d)$$

Note that a control volume equation is not written down for node n + 1 (east boundary node) since $U_{n+1} = U_1 + a \frac{du}{dx}$ via the boundary condition in Equation (2.16b). Note further that the numerical flux entering the control volume for node n + 1 is incorporated into the control volume equation for node 1 (west boundary node).

Using appropriate scaling, the system (3.20) can be expressed as an overdetermined system of linear equations in the form

$$\begin{bmatrix} A \\ r^T \end{bmatrix} \boldsymbol{U} = \begin{bmatrix} b \\ \beta \end{bmatrix} \quad \Leftrightarrow \quad \tilde{A}\boldsymbol{U} = \tilde{b}, \qquad (3.21)$$

with $\boldsymbol{U} = (U_1, U_2, \dots, U_n)^T \in \mathbb{R}^n$ where

$$A = \begin{bmatrix} 2 & -1 & 0 & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & 0 & -1 & 2 \end{bmatrix} \in \mathbb{R}^{n \times n},$$

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 $b = a \frac{du}{dx} (-1, 0, \dots, 0, 1)^T \in \mathbb{R}^n, r^T = (1, 1, \dots, 1) \in \mathbb{R}^{1 \times n}$ and $\beta = (n-1)u - \frac{a}{2} \frac{du}{dx}$. In what follows, we show that the overdetermined linear system (3.21) is consistent and has a unique solution. Observe that $e = (1, 1, \dots, 1)^T$ satisfies $e^T A = 0^T$ and therefore $e \in \mathcal{N}(A^T)$. A direct result of this observation is that $(e^T, 0)\tilde{A} = e^T A + 0r^T = 0^T$ and therefore $v = (e^T, 0)^T \in \mathcal{N}(\tilde{A}^T)$. Now, applying Gaussian elimination

one can show that $A \sim \begin{bmatrix} -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & n & -n \\ 0 & \dots & 0 & 0 & 0 & 0 \end{bmatrix} = PA, \quad P = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \\ 0 & 1 & 2 & \dots & n-2 & 1 \\ 1 & 1 & 1 & \dots & 1 & 1 \end{bmatrix},$

which leads to the conclusion that $\dim(\mathcal{R}(A^T)) = n - 1$ and hence $\dim(\mathcal{N}(A^T)) = n - \dim(\mathcal{R}(A^T)) = n - (n - 1) = 1$. The latter result, together with the observation that $e \in \mathcal{N}(A^T)$, implies that $\mathcal{N}(A^T) = \operatorname{span}\{e\}$. Given $r^T e \neq 0 \Rightarrow r \notin \mathcal{N}(A^T)^{\perp} \Rightarrow r \notin \mathcal{R}(A^T) \Rightarrow \mathcal{R}(A^T) \cap \operatorname{span}\{r\} = \emptyset$. Using the dimension theorem one can then show that $\dim(\mathcal{R}(\tilde{A}^T)) = \dim(\mathcal{R}(A^T)) + \dim(\operatorname{span}\{r\}) = (n - 1) + 1 = n$ and hence $\dim(\mathcal{N}(\tilde{A}^T)) = (n + 1) - \dim(\mathcal{R}(\tilde{A}^T)) = (n + 1) - n = 1$. Again, the latter result, together with the observation the $v \in \mathcal{N}(\tilde{A}^T)$, implies that $\mathcal{N}(\tilde{A}^T) = \operatorname{span}\{v\}$. Finally, since $v^T \tilde{b} = 0 \Rightarrow \tilde{b} \perp \mathcal{N}(\tilde{A}^T) \Rightarrow b \in \mathcal{R}(\tilde{A})$ and $\dim(\mathcal{N}(\tilde{A})) = n - \dim(\mathcal{R}(\tilde{A})) = 0$, the overdetermined system (3.21) is consistent and has a unique solution.

For this simple example $A = A^T$ and therefore $\mathcal{N}(A) = \mathcal{N}(A^T) = \text{span}\{e\}$, that is the solution of of $A\mathbf{U} = b$ is unique only up to an additive constant (i.e., $\mathbf{U} = \mathbf{U}_p + ce$, where c is arbitrary and \mathbf{U}_p is a particular solution). Since $r^T e \neq 0$, substitution of $\mathbf{U} = \mathbf{U}_p + ce$ into the equation $r^T \mathbf{U} = \beta$, allows c (and hence \mathbf{U}) to be uniquely identified.

The results presented above suggest that solving the overdetermined linear system (3.21) reduces to solving a square system, which consists of those equations corresponding to the n linearly independent rows of \tilde{A} .

PROPOSITION 1. Any set consisting of the vector r^T together with (n-1) unique row vectors of A is linearly independent.

Proof. Assume the set $S = \{r^T\} \cup (\{A_{1,*}, \ldots, A_{n,*}\} \setminus \{A_{k,*}\})$, where $A_{i,*} \in \mathbb{R}^{1 \times n}$ denotes the *i*th row vector of A and $k \in \{1, 2, \ldots, n\}$, is linearly dependent. Under this assumption, there exists $c_i \in \mathbb{R}$ and $\gamma \in \mathbb{R}$, not all equal to zero, such that

$$\sum_{i \neq k}^{n} c_i A_{i,*} + \gamma r^T = 0^T \Rightarrow (c_1, \dots, c_{k-1}, 0, c_{k+1}, \dots, c_n, \gamma)^T \tilde{A} = 0^T$$
(3.22)

It follows that $(c_1, \ldots, c_{k-1}, 0, c_{k+1}, \ldots, c_n, \gamma)^T \in \mathcal{N}(\tilde{A}^T)$, which is a contradiction since $\mathcal{N}(\tilde{A}^T) = \operatorname{span}\{v\} = \operatorname{span}\{(1, 1, \ldots, 1, 0)^T\}$. Hence, it must be that the original hypothesis is false and \mathcal{S} forms a linearly independent set of vectors. \Box

In conclusion, one can replace any equation of $A\mathbf{U} = b$ with the equation $r^T\mathbf{U} = \beta$, that is, solving the overdetermined linear system (3.21) is equivalent to solving the following square linear system

$$\left[(I - e_k e_k^T) A + e_k r^T \right] \boldsymbol{U} = (I - e_k e_k^T) \boldsymbol{b} + e_k \beta , \qquad (3.23)$$

for any k = 1, ..., n, where e_k is the kth column of the $n \times n$ identity matrix I.

Following this example and given that v_w and v_e defined above are linearly independent left-hand nullspace vectors of J_f , we conjecture similar properties for the system (3.15), namely:

CONJECTURE 2. $\dim(\mathcal{N}(J_f^T)) = \dim(\mathcal{N}(J_G^T)) = 2.$

Using identical arguments to those presented in the example above, under Conjecture 2 one can show that the overdetermined linear system (3.15) is consistent and has a unique solution that can be obtained by solving

$$\left[\left(I - PP^{T}\right)J_{f} + PJ_{r}\right]\delta\boldsymbol{U}_{k} = \left(PP^{T} - I\right)f - Pr, \qquad (3.24)$$

with $P = [e_i, e_j] \in \mathbb{R}^{(2n) \times 2}$, where e_i denotes the *i*th column of the $2n \times 2n$ identity matrix I, and i and j index any odd and even row of J_f , respectively. This result is useful because iterative methods designed for square coefficient matrices can be employed to system (3.24).

In our code, we use a right-preconditioned GMRES method to solve (3.24) with an incomplete LU factorisation selected as the preconditioner. In this case, the choices i = 2n - 1 and j = 2n within the permutation matrix P ensure the dense rows of r are located at the bottom of the matrix during factorisation, which produces a minimal fill-in of zero entries.

Remark. An alternative to solving the square linear system (3.24) is to apply a Gauss–Newton strategy to the overdetermined nonlinear system (3.10), where the correction vector is the solution of the (linear) least squares problem

$$\delta \boldsymbol{U}_k = \arg\min_{\boldsymbol{x}\in\mathbb{R}^{2n}} \|\boldsymbol{G} + \boldsymbol{J}_{\boldsymbol{G}}\boldsymbol{x}\|_2.$$
(3.25)

The application of GMRES to such problems has received notable attention in the literature (see e.g. [2, 6, 9, 16, 24, 27]). Since GMRES cannot be applied directly for a rectangular coefficient matrix, these papers have studied strategies that circumvent this problem. These include appending zero columns to obtain a square singular coefficient matrix [16] or introducing a mapping matrix that converts the coefficient matrix from rectangular to square when multiplied on the left or right [6]. However, our numerical experiments indicated that the unique minimiser of (3.25) is indeed the solution of (3.15) and (not surprisingly) applying GMRES to solve the square linear system (3.24) was more efficient.

4. Results for softwood and discussion.

4.1. Unit cell configurations. Two different configurations for the unit cell are investigated in this section, namely a radial/tangential cross-section of a softwood tracheid cell with and without pore-connecting pits. We use the rectangular tracheid model given in [13] with fixed cell-wall thickness t_v (see Figure 4.1). The tangential and radial directions are assumed to extend in the y_1 and y_2 axis directions, respectively.

The radial length a_R and tangential length a_T of the tracheid, which describe the dimensions of the unit cell $(0, a_T) \times (0, a_R)$, are assumed to vary with the density ρ_0 :

$$a_T = 50 \quad (\mu \mathbf{m}), \tag{4.1}$$

$$a_R = 57.5 - 0.0375\rho_0 \quad (\mu m),$$
 (4.2)

for $\rho_0 \in [200, 1000]$ (kg m⁻³) [13]. These relations, which agree well with observation [13], define a fixed radial length and a linearly decreasing tangential length for increasing density ρ_0 . With these definitions, it follows that a relation for the cellwall thickness t_v can be derived by ensuring the solid fraction of C_x matches the macroscopic value (2.19):

$$1 - \frac{(a_R - 2t_v)(a_T - 2t_v)}{a_R a_T} = \varepsilon_s \quad \left(= \frac{A(\mathcal{C}_x^{(s)})}{A(\mathcal{C}_x)} \right).$$
(4.3)

Taking the root of (4.3) that produces the correct physical behaviour (i.e., t_v increasing for increasing ρ_0) gives the following formula

$$t_v = \frac{1}{4}(a_R + a_T) - \frac{1}{4}\sqrt{(a_R + a_T)^2 - 4a_R a_T \varepsilon_s} \quad (\mu m).$$
(4.4)

For the tracheid (pits) configuration, a fixed width equal to $\gamma = 4 \,\mu$ m is assumed for the pore–connecting pits (see Figure 4.1b). In summary, for a given value of the density ρ_0 , and given macroscopic values of moisture content and temperature (which appear in the definition of ε_s given in Equation 2.19), the dimensions of the unit cell for both configurations are fully defined.

Firstly, we assess the effect of the macroscopic moisture content gradient (i.e., $\nabla_x X$) on the macroscopic mass flux (i.e., \boldsymbol{q}_{w} defined in Equation 2.3) in the absence of a temperature gradient. The microscopic fields of moisture content and temperature for $\nabla_x X = (0, 100)$ and $\nabla_x X = (100, 0)$ are exhibited in Figures 4.2 and 4.3. In this case, only the moisture content in the y_1 or y_2 directions (respectively tangential or radial direction) differs in value on opposing boundaries of the unit cell. The nonuniform temperature fields in the absence of a macroscopic temperature gradient are due to the different enthalpy values of bound water and water vapour (see Equation 2.23). A source term is generated due to the condensation of water vapour on the cell wall to continue its migration as bound water. On the contrary, a sink term appears when bound water has to evaporate to continue its diffusion in the porous phase. In the case of a tracheid with pits, both heat and mass fluxes have to pass though the pits either along the cell wall (radial flux) or perpendicular to the cell wall (tangential flux). As the gaseous phase is conductive regarding mass flux, but resistive regarding the thermal flux, a clear anisotropic macroscopic behaviour emerges from the presence of pits. In the tangential direction, the gaseous phase is connected (as it crosses the unit cell boundaries), which eases the total moisture flux, with a factor 6 to 7 evident in Figure 4.4. With a radial gradient, the presence of pits is hardly visible.

The effect of density on the mass flux is evident in Figure 4.5. In this figure, two values of the density are tested, namely $\rho_0 = 400 \text{ kg m}^{-3}$ and $\rho_0 = 800 \text{ kg m}^{-3}$, which are typical of the wood found in the earlywood and latewood components of a growth ring of softwood, respectively. These values produce an earlywood cell of height 42.5 μ m with 3.6790 μ m cell walls and a flatter latewood cell of height 27.5 μ m with thicker 6.9618 μ m cell walls. Due to the conductive behaviour of the gaseous phase, the magnitude of the mass flux is greater for the smaller value of ρ_0 .

4.2. Dual–scale simulations. Simulation results for the dual–scale approach are reported for the drying of a small sample of softwood. The wood sample is taken as a rectangle of width 5 cm and height 2.5 cm (i.e., $\mathcal{B} = [0,5] \times [0,2.5]$ cm) and is assumed to be homogeneous with $\rho_0 = 441 \text{ kg m}^{-3}$ for all $x \in \mathcal{B}$. It follows from the homogeneity and geometry of \mathcal{B} , that the solution has two lines of symmetry (i.e., $x_1 = 2.5 \text{ cm}$ and $x_2 = 1.25 \text{ cm}$). Taking all fluxes of mass and heat equal to zero at these symmetry lines, allows the computational domain to be reduced to one quarter of



Fig. 4.1: Microcell configurations.



(a) Tracheid (closed)



(b) Tracheid (pits)

Fig. 4.2: Moisture content and temperature fields corresponding to $\rho_0 = 800 \text{ kg m}^{-3}$, $X = 0.2 \text{ kg kg}^{-1}$, $T = 50 \degree \text{C}$, $\nabla_x X = (0, 100)$ and $\nabla_x T = (0, 0)$.



(a) Tracheid (closed)



(b) Tracheid (pits)

Fig. 4.3: Moisture content and temperature fields corresponding to $\rho_0 = 800 \text{ kg m}^{-3}$, $X = 0.2 \text{ kg kg}^{-1}$, $T = 50 \circ \text{C}$, $\nabla_x X = (100, 0)$ and $\nabla_x T = (0, 0)$.



Fig. 4.4: Macroscopic mass flux computed over the unit cell in the absence of a temperature gradient. The macroscopic moisture content gradient is applied in the (a) tangential or y_1 direction only and (b) radial or y_2 direction only and the mass flux plotted in that direction.



Fig. 4.5: Macroscopic mass flux computed over the unit cell in the absence of a temperature gradient. The macroscopic moisture content gradient is applied in the tangential or y_1 direction only and the mass flux plotted in that direction.

the size of the full macroscopic domain (i.e., the rectangle $[0, 2.5] \times [0, 1.25]$). Initially, the moisture content field is flat and equal to the fibre saturation value (computed using the initial temperature of 50 °C). All parameters used in the simulations are listed in Table 4.1.

Initial Moisture Content	$0.275{ m kgkg^{-1}}$
Initial Temperature	50 °C
Density	$441\mathrm{kg}\mathrm{m}^{-3}$
Wet–bulb temperature	$45^{\circ}\mathrm{C}$
Dry–bulb temperature	$60^{\circ}\mathrm{C}$
Velocity of circulating air in kiln	$2\mathrm{ms}^{-1}$
Drying time	$100\mathrm{hrs}$
Macroscale domain	$5\times2.5\mathrm{cm}$
Microscale domain	$50\times42.5\mu\mathrm{m}$

Table 4.1: Drying and initial conditions used in all dual-scale simulations.

Recall that the dimensions of the unit cell configurations (Figure 4.1) depend, not only on the density ρ_0 , but also the macroscopic moisture content and temperature via the definition of the solid fraction stated in Equation 2.19. This latter dependence is impractical in a dual-scale setting because meshing of the unit cell would be required each time the macroscopic solution changes (i.e., a re-meshing of the unit cell would need to be performed for each macroscopic element every time the macroscopic values are changed). For this reason, in [13] it is suggested to fix $X = 0.15 \text{ kg kg}^{-1}$ and $T = 25 \,^{\circ}\text{C}$ when computing the solid fraction throughout the length of the drying simulation. This approach is followed for all dual-scale simulations reported in this section. Using this strategy with $\rho_0 = 441 \text{ kg m}^{-3}$ one obtains a solid fraction equal to 0.3291. Since ρ_0 is fixed for all $x \in \mathcal{B}$, a single unit cell with radial length $a_T =$ 40.963 μ m, tangential length $a_T = 50 \,\mu$ m, and cell-wall thickness $t_v = 6.9619 \,\mu$ m is defined. Essentially, the geometry of the unit cell does not vary spatially or temporally during the drying simulation: mesh generation on the microscale is performed once



Fig. 4.6: Macroscopic moisture content fields after 0.5, 5 and 12 hours of drying for the two different unit cell configurations.



(a) Surface moisture content (at x = (0, 1.25) cm) (b) Core moisture content (at x = (2.5, 1.25) cm)



Fig. 4.7: Surface and core and surface evolution of moisture content and temperature.

prior to the commencement of the simulation and stored thereafter.

All simulations were performed with a macroscopic mesh containing 928 elements and 552 nodes in total (however using symmetry only one quarter of these are computed on). Each microscopic mesh consists of 1062 elements and 576 nodes. Both functions $g(\boldsymbol{u})$ and $G(\boldsymbol{U})$, defined in Equations (3.5) and (3.10), were written in the C programming language and called as if they were MATLAB functions using the MEX-files feature. The computation time is around 5 hours compared with less than 1 minute for the classical macroscopic formulation on the same macroscopic mesh.

Macroscopic moisture content fields produced using the dual-scale approach are given in Figure 4.6. These figures demonstrate the substantial effect of the unit cell configuration on the macroscopic solution behaviour. As previously explained, the inclusion of pits at the microscale eases the moisture migration along the tangential direction. This effect is clearly depicted by the evolution of the moisture content over time (Figure 4.7a and b). In particular, one can observe that the tangential diffusion is able to propagate the boundary conditions up to the core of the section after 5 hours of drying in spite of the longer distance (width = $2 \times$ height). This effect is obvious when comparing Figures 4.6c and 4.6d. This efficient diffusion results in a quasi flat moisture content field after 12 hours of drying (Figure 4.6f). Consistently, this leads to significantly faster drying, with the equilibrium moisture content (approximately equal to 0.08 kg kg^{-1}) attained after 25 hours, compared with more than 100 hours for the closed tracheid configuration (see Figure 4.7b). Interestingly, the trend is opposite at the surface (Figure 4.7a). This is simply explained by the balance between internal and external transfer. In this case, the presence of pits accelerates the internal transfer using the same external heat and mass transfer coefficients: in order to drive the moisture arriving to the surface, the external driving force is forced to be higher in the presence of pits, which can only be obtained by a larger surface moisture content.

At first glance, the evolution of the temperature field is consistent: a faster drying rate means more heat to be supplied for evaporation, hence a lower temperature for the fastest drying (Figure 4.7c and d). Once the fastest drying is finished (around 20 hours), the curves consistently cross each other, as the temperature field of the dried sample tends rapidly towards the dry bulb temperature.

However, a detailed insight in the temperature evolution is more informative. In the case of the *Tracheid (closed)* configuration and even during the first stages of drying, when the drying rate is large, no significant temperature difference can be observed between the surface and core (4.7c and d). This is just because evaporation takes place at the exchange surface. However, in the case of the *Tracheid (pits)* configuration, it is obvious that the core temperature remains lower than the surface temperature during most of the drying process (up to about 10 hours). This is a consequence of a connected porous (gaseous) phase. This feature allows bound water to evaporate inside the sample without further evaporation/condensation at the microscopic scale, as is the case for the closed unit cell. The energy required for evaporation has therefore to be supplied inside the product by thermal conduction, which needs a temperature gradient and explains the lower core temperature.

These simulations demonstrate the potential of the present dual–scale approach, where the macroscopic partition between the bound water and water vapour flux does not need to be set prior to the computation, but is simply an objective result of the unit cell configuration.

5. Conclusions. A new dual–scale approach for simulating the drying of porous media in the hygroscopic range was presented. The proposed dual–scale model couples the macroscopic scale of the porous medium with the microscopic scale of an individual cell.

This model allows the macroscopic mass and thermal fluxes to be computed from the microscopic structure of the porous medium via an average of the microscopic fluxes. More importantly, the model explicitly considers the coupling between heat and mass transfer at the microscopic level.

The drying example proposed in the last section demonstrates the potential of the formulation. In particular, the form of the macroscopic bound water and water vapour fluxes do not need to be set prior to the simulation – they are simply the objective result of the intricate coupling arising at the microscopic scale.

A future application of this dual–scale model would be to consider the case of a unit cell varying in space (heterogenous wood sample) or varying in time, depending on the local history at the corresponding macroscopic position. This would find application in, for example, biofilm development, and modelling shrinkage and cell collapse.

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