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Drying of porous media: an algorithm to determine effective parameters

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Abstract:

The drying process plays an important role in various industries such as chemical engineering, food, agriculture, and construction. The drying process is a complex one due to the phenomena of heat and mass transfer, which take place simultaneously. In principle, these transport processes can be modelling using continuous and discrete approaches. Following the continuous approach, porous media was simulated as continuous, and effective parameters for heat and mass transfer were employed. In this continuous model, the effective diffusivity and effective thermal conductivity parameters had strong effects on the results. The purpose of this research was to develop an algorithm to determine the effective parameters of the drying of porous media by using a continuous model.

Keywords: **continuous model, drying, effective diffusivity, numerical model.**

Classification numbers: **2.2, 2.3**

Introduction

Drying is a separation process in solid-liquid systems. In practice, the drying process plays an important role in various industries. In principle, these transport phenomena in porous media can be modelled by using two approaches: continuous and discrete, as mentioned by D. Michel, et al. (1987) [1]. By using the continuous model, porous media is simulated to be continuous and effective parameters for heat and mass transfer are used.

Following the continuous approach, Whitaker used a volume averaging technique to obtain a set of macroscopic transport equations from a system of basic transport laws at a microscopic level for the three phases (gas, liquid, and solid). Details of the above technique can be found in Whitaker's works [2-4]. According to Whitaker's model, porous media is assumed to be continuous, and a system of conservation equations of heat, mass, and motion is developed through the main state variables. The model developed by Whitaker has been widely applied in the study of the drying of porous media, for example, in the drying analysis of sand [5-8], glass beads [9], sandstone [10], porous insulators [11], brick [12], cellular materials [13], wood [14-17], and light concrete [18-20]. In these mentioned works, the model is usually quite successfully matched against experimental data. As a result, the above research works highlight the acceptance of the complete theory.

Among other methods, [21, 22] used a control volume finite element method (CV-FEM) [23] to solve the numerical problem. The advantage of this method is that the coupled heat and mass transfer is modelled using effective parameters, which have a physical meaning and are not lumped parameters. The model developed by Whitaker, Perré, and Turner very effectively solves the drying problem of porous media because the heat and mass transfer happen simultaneously, and these phenomena are simulated using effective parameters. However, the most difficult point when solving the problem is the determination of the model parameters as pointed out by H.T. Vu, et al. (2016) [24]. According to [25, 26], these parameters must either be experimentally determined or must be modelled from the microstructure of the material. In fact, these parameters are functions of state variables, e.g., moisture content, temperature, and pressure. These parameters should be determined with

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great care concerning the microscopic material structure as they have decisive effects on simulated drying characteristics. By solving the so-called inverse problem, one can find a way to determine these parameters.

Experimental methods such as magnetic resonance imaging (MRI) have used to obtain the drying kinetics of porous materials, for example, the moisture content, X_{exp}, can be obtained as function of space and time. By using experimental data such as this, effective transport parameters such as diffusivity can be obtained by progressively modifying the transport parameters until the simulated drying kinetics (X_{sim}) match the experimental ones (X_{exp}). Therefore, the purpose of this research is to develop an algorithm to determine the effective parameters of drying of porous media by using a continuous model. However, due to the lack of experimental data, we use the forward problem to generate the data for the inverse problem by employing the control volume method and some known material parameters. Then, the algorithm of the inverse problem is presented, and numerical examples are considered to demonstrate the accuracy of the computed parameters. In this study, we consider the problem in one-dimensional space as well.

Governing equations

There are four equations that govern the drying process in a porous medium. The first is the conservation equation for water in liquid and gas phases. The second is the conservation equation for air in the gas phase. The third is the conservation equation of energy, and the fourth are the sets of equations of motion for the liquid phase and for the gas phase [3, 21].

The conservation equation for water in both liquid and gas phase is:

$$\frac{\partial}{\partial t}\left(\rho_w\varepsilon_w+\varepsilon_g\rho_v\right)+\nabla\cdot\left(\rho_w\mathbf{v}_w+\rho_v\mathbf{v}_g\right)=\nabla\cdot\left[\rho_g\mathrm{D}_{eff}\cdot\nabla\left(\frac{\rho_v}{\rho_g}\right)\right] \qquad (1)$$

where ρ_w, ρ_v, and ρ_g are the mass density of the liquid, vapor, and gas phases, respectively, ε_w and ε_v are the volume fractions of the liquid and gas phase, respectively, v_w and v_w are the velocities of the liquid and gas phase, respectively, and D_{eff} is the effective diffusivity tensor.

The conservation equation for air in the gas phase can be formulated as:

$$\frac{\partial}{\partial t}\left(\varepsilon_g\rho_a\right)+\nabla\cdot\left(\rho_a\mathbf{v}_g\right)=\nabla\cdot\left[\rho_g\mathrm{D}_{eff}\cdot\nabla\left(\frac{\rho_a}{\rho_g}\right)\right] \qquad (2)$$

The most complex one is the conservation equation of energy and it is given as:

$$\begin{aligned}&\frac{\partial}{\partial t}\left(\varepsilon_s\rho_sh_s+\varepsilon_w\rho_wh_w+\varepsilon_g\rho_vh_v+\varepsilon_g\rho_ah_a\right)+\nabla\cdot\left[\rho_wh_w\mathbf{v}_w+\left(\rho_vh_v+\rho_ah_a\right)\mathbf{v}_g\right]\\&=\nabla\cdot\left[\rho_gh_a\mathrm{D}_{eff}\nabla\left(\frac{\rho_a}{\rho_g}\right)\right]+\nabla\cdot\left[\rho_gh_v\mathrm{D}_{eff}\nabla\left(\frac{\rho_v}{\rho_g}\right)\right]+\nabla\cdot\left(\boldsymbol{\lambda}_{eff}\nabla T\right)\end{aligned} \qquad (3)$$

where ε_s and ρ_s are the volume fraction and the mass density of the solid phase, respectively, h_s, h_w, h_v, and h_a are the enthalpies per unit mass of the solid, water, vapor, and air, respectively, and λ_{eff} is the effective thermal conductivity tensor.

The equation of motion for the liquid phase can be written as:

$$v_w=-\frac{Kk_w}{\eta_w}\nabla P_w \qquad (4)$$

and the equations of motion for the gas phase are given as:

$$v_g=-\frac{Kk_g}{\eta_g}\nabla P_g \qquad (5)$$

where K is absolute permeability tensor, k_w and k_g are the relative permeability tensors for liquid and gas phase, respectively, η_w and η_g are the dynamic viscosity of water and gas, respectively, P_w is the pressure of the liquid phase, and P_g is the pressure of the gas phase.

In addition, the boundary conditions for mass and heat transfer at the external drying surfaces of the porous medium must be specified. The gas pressures at the external drying surfaces are fixed at the pressure of the bulk drying air. Sorption isotherm, capillary pressure, ideal gas laws, and enthalpy-temperature relations will complete the set of equations (1-8) by facilitating the expression of all variables as functions of the three state variables. Finally, initial conditions are needed to close the sets of equations. These conditions can be found from the work of H.T. Vu (2006) [27].

Material properties

For our calculations, a light concrete reference material is considered. More information about this material can be found in these works of [21, 22]. The porosity is ψ=0.8. The solid density is $\rho_s=2500\,\mathrm{kg.m^{-3}}$

and the heat capacity is $\overline{\rho C_p} = \varepsilon_s \rho_s (840 + 4185X)$ J.kg^{-1}.K^{-1}. The fully saturated material has a moisture content X_{sat}=1.6.

The sorption isotherm is given as:

$$\varphi(X,T) = \frac{P_v}{P_v^*(T)} = \begin{cases} 1 & , \text{ if } X > X_{irr} \\ \frac{X}{X_{irr}}\left(2 - \frac{X}{X_{irr}}\right), & \text{if } X \le X_{irr} \end{cases} \tag{6}$$

where X_{irr}=0.07, which is the irreducible content and $P_v^*(T)$ is the saturation pressure.

Parameters of real material and parameters to be determined

The following table presents the parameters of the real material and the parameters to be determined (Table 1). The first column is the parameters of the real material, which is light concrete in this case. Based on these values, we can derive the unknown parameters, i.e., the parameters to be determined, as functions of state variables.

Table 1. Parameters of real material and parameters to be determined.

Parameters of real material	Unknown (parameters to be determined)
$\overline{\rho C_p} = \rho_0 (840 + 4185X) \left(\mathrm{Jkg^{-1}K^{-1}}\right)$	$\overline{\rho C_p} = \rho_0 (C_1 + C_2 X)$
$K_{eff} = (0.142 + 0.46X)$	$K_{eff} = (K_1 + K_2 X)$
$D_{eff} = 0.2 D_v k_{rg}$	$D_{eff} = D_1 D_v k_g$
$K_w = 2 \times 10^{-13}$ $[m^2]$	K_w
$K_g = 2 \times 10^{-13}$ $[m^2]$	K_g
$k_w = \begin{cases} 0 \; if \; X \le X_{irr} \\ S_{fw}^3 \;\; other \end{cases}$	$k_g = \begin{cases} 0 \; if \; X \le X_{irr} \\ 1 + (2S_{fw} - 3)S_{fw}^2 \;\; other \end{cases}$
$k_g = \begin{cases} 0 \; if \; X \le X_{irr} \\ 1 + (2S_{fw} - 3)S_{fw}^2 \;\; other \end{cases}$	$k_g = \begin{cases} 0 \; if \; X \le X_{irr} \\ k_{rg1} + (k_{rg2} S_{fw} + k_{rg3}) S_{fw}^2 \;\; other \end{cases}$

The problem

The problem can be stated as follows:

1. Vector $\boldsymbol{f}_{x0}$ is the vector containing experimental data. For example, moisture content *X*, temperature *T* and pressure *P* at different measurement points during the drying time t_{dry}. Vector $\boldsymbol{f}_{x0}$ depends on vector $\boldsymbol{x}$, which contains the material properties.

2. We can model the drying process of porous media and calculate the vector $\boldsymbol{f}_{xc}$ that contains *X, V,* and *P* at measurement points. With different values of $\boldsymbol{x}$, we have different values of f_{xc}, respectively, so we can write: $f_{xc} = f_{xc}(x)$.

3. If we do not know the material properties *x*, but we have f_{x0} and find a certain vector $\hat{x}$ such that, after inserting into the model ($f_{xc}(x)$) we have a vector $f_{xc}(x)$ and vector f_{x0} that are the same (or almost the same), we can state that vector $\hat{x}$ is the vector containing the material properties we are looking for.

In practice, it is difficult to find $\hat{x}$ such that vector $f_{xc}(x)$ and vector f_{x0} are identical. Therefore, we will determine $\hat{x}$ so that the two mentioned vectors are nearly identical. This means we need to determine $\hat{x}$ such that $[f_{xc}(x)$ - $f_{x0}]^T[f_{xc}(x)$ - $f_{x0}]$ is a minimum, i.e., to solve the optimal problem. This problem can be summarized as follows:

$$\min r(x)$$

$$r(x) = \frac{1}{2}[f(x)]^T f(x) = \sum_{i=1}^{m} \frac{1}{2}[f_i(x)]^2 \tag{7}$$

where *m* is the length of vector *f*.

In this research, we use the Levenberg-Marquardt [28] method to solve the optimal problem. FORTRAN and MATLAB are employed to solve the equations.

Levenberg-Marquardt method

More details of the Levenberg-Marquardt method can be found from the research work of D.W. Marquardt [28]. The Levenberg-Marquardt steps, $\boldsymbol{s}_k$, can be defined by:

$$\min\left(\frac{1}{2}\left\|f'(x_k)s_k + f(x_k)\right\|_2^2\right) \tag{8}$$

$$subjected\ to: \left\|D_k s_k\right\|_2 \le \Delta_k$$

where: $\boldsymbol{f}'(\boldsymbol{x}_k) = \left.\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\boldsymbol{x}}\right|_{x=x_k}$, vector Δ_k is a given vector, and D_k is a matrix.

Note that x_k is the value of vector x_k at step *k* and s_k is a vector of the same length as x_k. The length of $\boldsymbol{x}$ is the number of parameters. For example, if we need to determine one parameter (d_{v1}), the length of $\boldsymbol{x}$ is 1 and the length of Δ_k is 1 as well. The size of the matrix D_k is 1x1, but the length of *f(x)* is 3*n*, where *n* is the number of measurement points. In our model, we have 3 elements, so then there are 3 measurement points. Then, the length of *f(x)* is 9 and, similarly, the length of $f'(x_k)$ is 9.

We have $\|a\|_2$ as the norm matrix of vector a, which can be calculated as: $\|a\|_2 = \sqrt{a^T a}$ In addition, we have $\|a\|_2^2 = a^T a$. For example:

$$\begin{aligned} &\|f'(x_k)s_k + f(x_k)\|_2 = \sqrt{[f'(x_k)s_k + f(x_k)]^T [f'(x_k)s_k + f(x_k)]} \\ &\|f'(x_k)s_k + f(x_k)\|_2^2 = [f'(x_k)s_k + f(x_k)]^T [f'(x_k)s_k + f(x_k)]. \end{aligned} \tag{9}$$

The trust region changes between the number of iterations corresponding to the real value and the assumed value of the target function. Then, we have:

$$\rho_k = \frac{r(x_k) - r(x_k + s_k)}{r(x_k) - \frac{1}{2}\|f'(x_k)s_k + f(x_k)\|_2^2} \tag{10}$$

This value must be greater than an extremely small positive number (normally 0.0001). In case the loop is not satisfied, we must reduce the trust region and repeat the iteration. When the ratio is close to 1, we can proceed to the next steps.

In the Levenberg-Marquardt algorithm, the condition of Eq. (8) must be satisfied with

$$\left[f'(x_k)^T f'(x_k) + \lambda_k D_k^T D_k\right] s_k = -f'(x_k)^T f(x_k) \tag{11}$$

where $\lambda_k \geq 0$.

Algorithm to determine the effective parameters

An algorithm to determine the effective parameters is presented in Fig. 1.

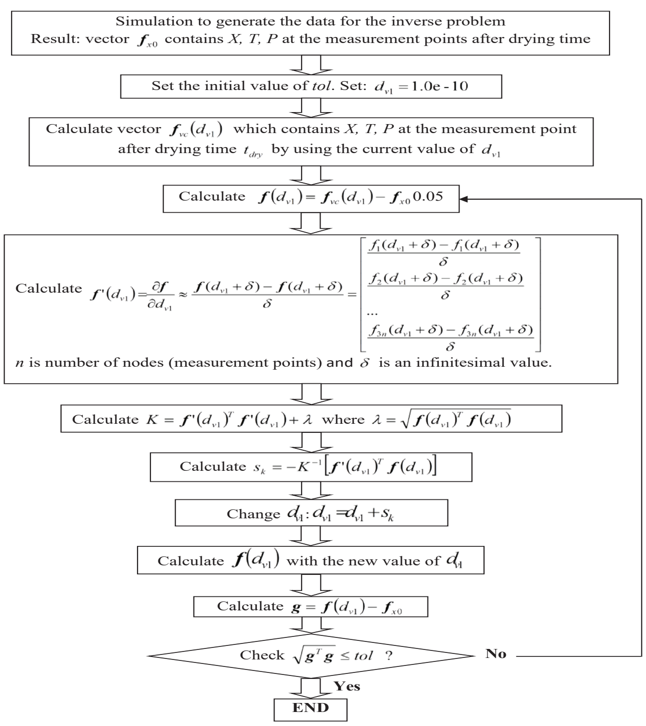

Fig. 1. Algorithm to determine the effective diffusivity.

Results and discussion

The convergence of the inverse problem is illustrated in Fig. 2. From this figure, we can see that after four iterations, the problem is converged. This result also shows that d_{v1} from the calculation is very consistent with the initial assumption value of d_{v1}. This result is very important because it determines the convergence of the inverse problem and also confirms the correctness of the algorithm.

Furthermore, we will apply this algorithm to determine the effective diffusivity. This parameter is calculated as follows:

$$D_{eff} = 0.2 \cdot \delta_{va} \cdot k_g \tag{12}$$

where δ_{va} [m^2s^{-1}] is the binary diffusivity of vapor in air, and

$$\delta_{va}(T,P) = D_{v1} \cdot \left(\frac{T}{T_R}\right)^{D_{v2}} \frac{P_R}{P_g} \tag{13}$$

where D_{v1}=2.26.01^{-5}, D_{v2}=1.81, and k_g is the relative permeability of gas.

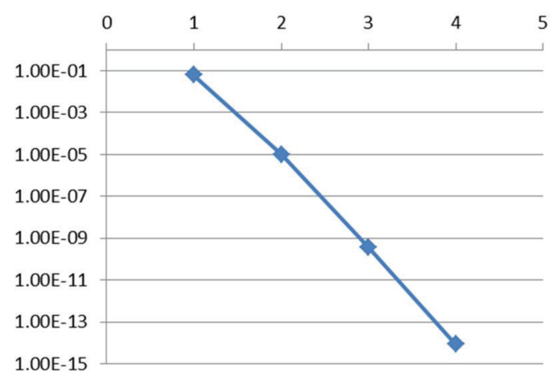

Fig. 2. Illustration of the convergence of the inverse problem.

In the inverse problem, we assume that both material parameters D_{v1} and D_{v2} are unknown. The inverse problem is then to retrieve the values D_{v1}= 2.26.10^{-5} and D_{v2}=1.81 given above. We then use the Levenberg-Marquardt algorithm first by assigning D_{v1} and D_{v2} to some initial values $D_{v1}=D_{v1}^0$ and $D_{v2}=D_{v2}^0$. After that, we solve the inverse problem to determine the computed parameters, which are denoted by D_{v1}^C and D_{v2}^C. In our calculation, we use a 20-node mesh (*N=20*) and 51 sampling points (*S=51*) for the forward problem. In the inverse problem, we choose the initial values D_{v1}^0=3.0.10^{-5} and D_{v2}^0=3.0. By solving the inverse problem, we get D_{v1}^C=2.26.10^{-5} and

D^C_{v2}=1.81. These values are very close to the value of D_{v1} and D_{v2} above.

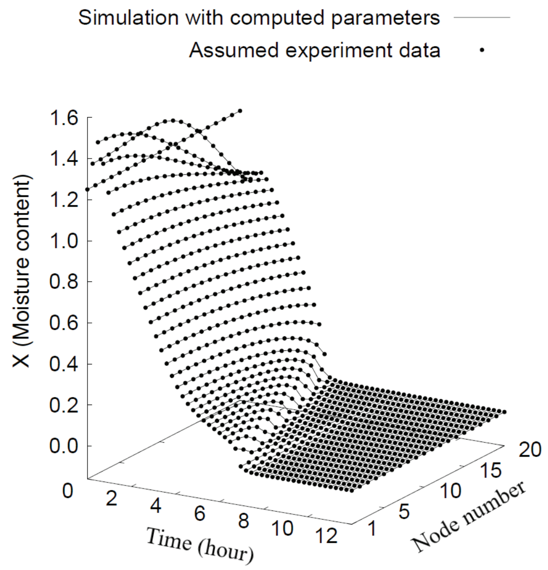

Fig. 3. Simulation of drying using data computed from solving the inverse problem *(N=20, S=51).*

The use of these two computed parameters in the forward problem is presented in Fig. 3. In this figure, the result of the inverse problem is shown, and the assumed input is presented by dotted lines (assumed experimental data) taken from a spherical specimen. From these data, the inverse problem is solved by iteratively changing the material parameters D_{v1} and D_{v2}. With each new set of material parameters, a simulation is done, and the moisture profiles (solid lines) are computed and compared with the assumed input data. The process is repeated until the simulated result (solid lines) matches the input data (dotted lines). In Fig. 3, the solid lines are the simulation result computed with the final values of material parameters D_{v1} and D_{v2}. It shows that, in this case, the drying kinetics are computed with good accuracy.

Conclusions

In this research, an algorithm to determine the effective parameters of the drying of porous media is presented. By solving the inverse problem, we obtained very reasonable results. However, more numerical tests should be realized to understand and improve the solution of the inverse problem. In the next step of our research, the model will be extended into two- and three-dimensional space. In addition, the use of real experimental data to evaluate the model will also be within the scope of our future research.

COMPETING INTERESTS

The authors declare that there is no conflict of interest regarding the publication of this paper.

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