Capillary pressure effect on vacuum drying process of porous medium modeling

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Drying is the key process in chemical, food and other related industry process. A lot of modeling methods and simulation technology has been used to reveal the heat and mass transfer process. The parameters of modeling are very important because the simulation results are decided by them. The capillary Pressure is condition boundary that is very difficult to gotten. Based on the theory of heat and mass transfer, a coupled model for the porous medium vacuum drying process is constructed. The model is implemented and solved using COMSOL software. The parameter sensitivity analyses of capillary pressure were then examined. The temperature, and moisture characteristics were shown.

Key words: heat and mass transfer, porous medium, vacuum drying, capillary pressure, COMSOL

INTRODUCTION

As the basic unit operation in chemical engineering, drying is the key process in chemical, food and other related industry process. The vacuum drying has been used to corn in china [1-3]. However, the corn vacuum drying theory remains unclear. Hypothesized that corn is a porous medium, the vacuum drying is a complicated heat and mass transfer process that has been the subject of intensive research [4–7]. All vacuum drying models have to address the water phase change during numerical solving. In one method, the vapor pressure is equal to its equilibrium value [8-11]. Another method is non-equilibrium method [12–16]. As the porous medium, the heat and mass transfer in vacuum drying process has been studied with nonequilibrium method by us [17, 18]. In fact, the parameters of modeling are very important because the simulation results are decided by them. But most of the modeling is gotten by the reference [8-11]. It must be clarify the impact of model parameters on

the model predictions [19]. The intrinsic permeability and mass transfer coefficient has been studied by us, it is shown the obviously effect on simulation results [20,21]. Another parameter, capillary pressure also has the very important parameter [22], the details effect should be given.

In this paper, heat and mass transfer of porous medium in the vacuum drying process is implemented by using a non-equilibrium method. The parameter sensitivity analyses of capillary pressure were then examined.

MODEL DEVELOPMENT

Problem Description

A physical one-dimensional (1D) model that explains the drying process is shown in Fig. 1. The heat and mass transfer is considered only in the y direction. The total height of the porous medium is 1cm. The bottom is the heat surface, and the mass is out of from the top surface.

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Fig. 1. 1D model of porous medium *Assumption*

The porous medium consists of a continuous rigid solid phase, an incompressible liquid phase (free water), and a continuous gas phase that is assumed to be a perfect mixture of vapor and dry air, considered as ideal gases. For a mathematical description of the transport phenomenon in a porous medium, we adopt a continuum approach, wherein macroscopic partial differential equations are achieved through the volume averaging of the microscopic conservation laws. The value of any physical quantity at a point in space is given by its average value on the averaging volume centered at this point.

The moisture movement of the inner porous medium is liquid water and vapor movement; that is, the liquid water could become vapor, and the vapor and liquid water are moved by the pressure gradient. The heat and mass transfer theory could be found in everywhere [8].

The compressibility effects of the liquid phase are negligible, and the phase is homogeneous:

$$\overline{\rho}_{w} = cste \tag{1}$$

The solid phase is rigid and homogeneous:

$$\overline{\rho}_s = cste \tag{2}$$

The gaseous phase is considered an ideal gas. This phase ensures that

$$\overline{\rho}_a = \frac{m_a P_a}{R\overline{T}} \tag{3}$$

$$\overline{\rho}_{v} = \frac{m_{v}P_{v}}{R\overline{T}} \tag{4}$$

$$\overline{P}_g = \overline{P}_a + \overline{P}_v \tag{5}$$

$$\overline{\rho}_g = \overline{\rho}_a + \overline{\rho}_v \tag{6}$$

The assumption of the local thermal equilibrium between the solid, gas, and liquid phases involves

$$\overline{T}_{s} = \overline{T}_{g} = \overline{T}_{w} = \overline{T}$$
(7)

Governing Equations

Mass conservation equations are written for each component in each phase. Given that the solid phase is rigid, the following is given:

$$\frac{\partial \overline{\rho}_s}{\partial t} = 0 \tag{8}$$

The averaged mass conservation of the dry air yields

$$\frac{\partial(\varepsilon \cdot S_g \overline{\rho}_a)}{\partial t} + \nabla \cdot (\overline{\rho}_a \overline{V}_a) = 0$$
⁽⁹⁾

For vapor,

$$\frac{\partial(\varepsilon \cdot S_g \overline{\rho}_v)}{\partial t} + \nabla \cdot (\overline{\rho}_v \overline{V}_v) = \dot{I}$$
(10)

For free water,

$$\frac{\partial(\varepsilon \cdot S_w \overline{\rho}_w)}{\partial t} + \nabla \cdot (\overline{\rho}_w \overline{V}_w) = -\dot{I}$$
⁽¹¹⁾

For water, the general equation of mass conservation is obtained from the sum of the conservation equations of vapor (v) and free water (1). The general equation is written as follows:

$$\frac{\partial W}{\partial t} + \nabla \cdot \left\{ \frac{1}{\overline{\rho}_s} \left(\overline{\rho}_w \overline{V}_w + \overline{\rho}_v \overline{V}_v \right) \right\} = 0$$
(12)

$$W = \frac{\varepsilon \cdot S_w \bar{\rho}_w + \varepsilon \cdot S_g \bar{\rho}_v}{(1 - \varepsilon) \bar{\rho}_s}$$
(13)

For the Darcy flow of vapor,

$$\overline{\rho}_{v}\overline{V}_{v} = \overline{\rho}_{v}\overline{V}_{g} - \overline{\rho}_{g}D_{eff} \cdot \nabla\overline{\varpi}$$
⁽¹⁴⁾

For the Darcy flow of air,

$$\overline{\rho}_{a}\overline{V}_{a} = \overline{\rho}_{a}\overline{V}_{g} + \overline{\rho}_{g}D_{eff} \cdot \nabla\overline{\omega}$$
⁽¹⁵⁾

The vapor fraction in mixed gas is given by

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$$\overline{\omega} = \frac{\rho_v}{\rho_g} \tag{16}$$

The saturation of free water and gas is

$$S_{\sigma} + S_{w} = 1 \tag{17}$$

Where the gas and free water velocity is given by

$$\bar{V}_{g} = -\frac{k_{in,g} \cdot k_{r,g}}{\mu_{g}} \cdot (\nabla \bar{P}_{g} - \rho_{g} \vec{g})$$
(18)

$$\bar{V}_{w} = -\frac{k_{in,w} \cdot k_{r,w}}{\mu_{w}} \cdot (\nabla \bar{P}_{w} - \rho_{w} \vec{g})$$
⁽¹⁹⁾

For bound water,

$$\rho_{w}\bar{V}_{w} = -\rho_{s} \cdot D_{b}\nabla(\frac{\rho_{w}}{\rho_{s}})$$
⁽²⁰⁾

The pressure moving the free water is given by

$$\overline{P}_{w} = \overline{P}_{g} - \overline{P}_{c} \tag{21}$$

By considering the hypothesis of the local thermal equilibrium, the energy conservation is reduced to a unique equation:

$$\frac{\partial \bar{\rho} \bar{T}}{\partial t} + \nabla \cdot (\bar{\rho}_a \bar{V}_a C_a \bar{T}_a + \bar{\rho}_v \bar{V}_v C_v \bar{T}_v$$
(22)

$$+\rho_{w}V_{w}C_{w}T_{w}) = \nabla(k_{e} \cdot \nabla T) - \lambda \cdot I$$

$$k_{e} = (1-\varepsilon)k_{s} + \varepsilon(S_{w} + S_{e}(\omega k_{v} + (1-\omega)k_{e}))$$
(23)

$$\overline{\rho}\overline{T} = \overline{\rho}_{s}\overline{T}_{s} + \varepsilon \cdot S_{g}\overline{\rho}_{a}\overline{T}_{a} + \varepsilon \cdot S_{g}\overline{\rho}_{v}\overline{T}_{v}$$

$$+\varepsilon \cdot S_{w}\overline{\rho}_{w}\overline{T}_{w}$$
(24)

BOUNDARY AND INITIAL CONDITIONS

The model was run for different parameters. It was heated from the bottom, and the air and vapor was escaped from the top surface. The other boundaries of the model are insulated and impermeable. The boundary conditions are then given as:

B.C. for Eq. (9):

$$\rho_{a,top} = \rho_{a,dryer} \tag{25}$$

(25)

(**n** n)

B.C. for Eq. (10) [15]:

$$n_{v,top} = -h_m \varepsilon S_g \left(\rho_{v,top} - \rho_{v,dryer} \right)$$
(26)

B.C. for Eq. (15):

$$n_{w,top} = -h_m \varepsilon S_w (\rho_{v,top} - \rho_{v,drver})$$
(27)

B.C. for Eq. (21) in bottom:

$$T_{bottom} = T_h \tag{28}$$

B.C. for Eq. (21) in top:

$$q_{top} = h(T_{ext} - \overline{T}) + (\lambda + C_w \overline{T}) n_{w,top} + C_v \overline{T} n_{v,top}$$
(29)

The initial moisture of the porous medium is represented by the liquid water saturation; different initial water saturation values are used. To compare the effects, drying base moisture content (d. b.) was also used, as shown in Eq. (12). The water phase change rate is used as 1000 that has been studied before [17].

I.C. for Eq. (9):

$$\rho_a = \rho_{a,0} = \frac{P_{anb,0}M_a}{RT_0} \tag{30}$$

I.C. for Eq. (10):

$$\rho_{v} = \rho_{v,0} = \frac{P_{sat,0}M_{v}}{RT_{c}}$$
(31)

I.C. for Eq. (11):

$$S_w = S_{w,0} \tag{32}$$

I.C. for Eq. (21) :

$$\bar{T} = T_0 \tag{33}$$

PHASE CHANGE

The evaporation rate is a complex function of drying process in porous medium. The phase change can be formulated in two ways, equilibrium and non-equilibrium. Evaporation of water has been implemented using an equilibrium formulation where water in the solid matrix is assumed to be in equilibrium with water-vapor in the surrounding air. However, recent studies have shown that evaporation is not instantaneous and nonequilibrium exists during rapid evaporation between water-vapor in gas phase and water in solid phase [15]. Furthermore, the equations resulting from an equilibrium formulation cannot be implemented in any direct manner in the framework of most commercial software. The more general expression of non-equilibrium evaporation rate used for modeling of phase change in porous media that is consistent with studies on pure water just mentioned, is given by [14,15],

$$\dot{H} = K_r \frac{m_v (a_w P_{sat} - P_v) S_g \varepsilon}{RT}$$
(34)

Here is a parameter signifying the rate constant of evaporation. The non-equilibrium formulation, given by equation (35), allows precisely this, i.e., can express the evaporation rate explicitly and therefore would be preferred in a commercial software and is therefore used in our model.

The phase change rate of water could not be decided by any method for porous medium drying [13, 14]. The rate constant parameter has the dimension of reciprocal time in which phase change occurs. A large value of signifies that phase change occurs in a small time. For the assumption of equilibrium, is infinitely large or phase change occurs instantaneously. A very high value of , however, makes the convergence of the numerical solution difficult.

NUMERICAL SOLUTION

COMSOL Multiphysics 3.5a was used to solve the set of equations. COMSOL is advanced software used for modeling and simulating any physical process described by partial derivative equations. The set of equations introduced above was solved using the relative initial and boundary conditions of each. COMSOL offers three possibilities for writing the equations: (1) using a template (Fick Law, Fourier Law), (2) using the coefficient form (for mildly nonlinear problems), and (3) using the general form (for most nonlinear problems). Differential equations in the coefficient form were written using an unsymmetric-pattern multifrontal method. We used a direct solver for sparse matrices (UMFPACK), which involves significantly more complicated algorithms than solvers used for dense matrices. The main complication is the need to handle the fill-in in factors L and U efficiently.

A two-dimensional (2D) grid was used to solve the equations using COMSOL Multiphysics 3.5a. Given the symmetry condition setting at the left and the right sides, the 2D is applied to the 1D model shown in Fig. 1. The mesh consists of 2×200 elements (2D), and time stepping is 1 (0 s to 100 s of solution), 5 (100 s to 200 s of solution), 20 (200 s to 1000 s of solution), 30 (1000 s to 2000 s of solution), 40 (2000 s to 4000 s of solution), 50 (4000 s to 20000 s of solution) and 100 (20000 s to 50000 s of solution). Several grid sensitivity tests were conducted to determine the sufficiency of the mesh scheme and to ensure that the results are grid-independent. The maximum element size was established as 1e⁻⁴. A backward differentiation formula was used to solve time-dependent variables. Relative tolerance was set to 1e⁻³, whereas absolute tolerance was set to 1e⁻⁴. The simulations were performed using a Tongfang PC with Intel Core 2 Duo processor with 3.0 GHz processing speed, and 4096 MB of RAM running Windows 7.

INPUT PARAMETER

For capillary pressure, it has some different presentation,

It was as [8],

 $\overline{P}_{c1} = (aS_w \exp(-bS_w) + c(1 - S_w)S_w^{-d})(1 - 2.79 \times 10^{-3}(T - 273.16)) \times 10^5$ a = 1.937, b = 3.785, c = 0.093, d = 1.400 (35) it also was as [11],

$$\overline{P}_{c2} = 1.24 \times 10^4 (S_w + 1 \times 10^{-4})^{-0.61}$$
(36)

In the reference [12],

$$\overline{P}_{c3} = 56.75 \times 10^3 (1 - S_w) \exp(\frac{1.062}{S_w})$$
(37)

The air pressure in the surface or dryer,

$$P_{a,dry} = \begin{cases} (101325 - 1700t) + 2400 & t < 61s \\ 25 & t >= 61s \end{cases}$$
(38)

The parameter details are given in Table 1 and Table 2.

Table 1. Boundary and initial condition

Initial temperature	T_0	273+25	K
Initial air pressure	$P_{atm,0}$	101325	Pa
Initial saturation	$S_{_{w,0}}$	0.3	
Vapor pressure of dryer	$P_{v,dry}$	2000	Pa
Air pressure of dryer	$P_{a,dry}$	Eq.(45)	Pa
Temperature of dryer	T_{ext}	273+28	Κ

RESULTS AND DISCUSSION

Fig.1 is the results of different capillarity pressure parameter effect moisture and temperature

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Parameter	Value or	Source	Unit	
$ ho_l$	998	[12]	kg m ⁻³	
$ ho_v$	Ideal gas		kg m ⁻³	
$ ho_{ m a}$	Ideal gas		kg m ⁻³	
$ ho_S$	476	[8]	kg m ⁻³	
C_{w}	4187	[12]	J kg ⁻¹ K ⁻¹	
C_v	1840	[12]	J kg ⁻¹ K ⁻¹	
C_a	1000	[12]	J kg ⁻¹ K ⁻¹	
Cs	1400	[8,12]	J kg ⁻¹ K ⁻¹	
k_w		[15]	$W m^{-1} K^{-1}$	
k_{v}	0.026	[15]	$W m^{-1} K^{-1}$	
k_a	0.026	[15]	$W m^{-1} K^{-1}$	
k_s	0.21		$W m^{-1} K^{-1}$	
$k_{n,w}$	4×10 ⁻¹⁴		m ²	
$k_{in,g}$	4×10 ⁻¹⁴		m ²	
$k_{,in,l}$		[14]		
$k_{,r,g}$		[14]		
μ_l	0.988×10 ⁻³	[15]		
μ_g	1.8×10 ⁻⁵	[15]	Pa s	
h	2.5	[11]	Pa s	
h_m	10	[15]	W m ⁻² K ⁻¹	
λ	2.26×10^{6}	[15]	m s ⁻¹	
ε	0.615	[8]	J kg ⁻¹	
$D_{e\!f\!f}$		[8]	m^2	
Sr	0.08	[14]		
D_b		[8]	$m^2 s^{-1}$	
M_a	29×10 ⁻³	[12]	kg mol ⁻¹	
M_{ν}	18×10 ⁻³	[12]	kg mol ⁻¹	
P_c		[8],[11],[12]	Pa	

Table 2. Parameters used in the simulation process

curves when intrinsic permeability = 4×10^{-13} . The drying time is obviously different with different capillarity pressure model. The drying time is longest when capillarity pressure model Pc-2 used, and the drying time is lest when capillarity pressure model Pc-3 used. The moisture change is almost in direct proportion to the time when Pc-3 used in most drying time. But other capillarity pressure models are not

The temperature curve is also shown the obviously different. The temperature is increased at the drying initial stage because the heat and mass transfer is from bottom to up more than phase change. But model Pc-3 is with longer time temperature maintains and Pc-1 is with shorter time temperature maintains. The model Pc-1 is no obviously maintains time. Fig.3 is the results of different capillarity pressure parameter effect moisture and temperature curves when intrinsic permeability = 4×10^{-14} . The drying time is obviously different with different capillarity pressure model.



Fig.2. Capillarity pressure model effect when intrinsic permeability $k = 4 \times 10^{-13}$, (a) Moisture vs. time, (b) Temperature vs. time for model Pc-1, (c) Temperature vs. time for model Pc-2, (d) Temperature vs. time for model Pc-3.



Fig.3. Capillarity pressure model effect when itrinsic permeability $k = \times 10^{-14}$, (a) Moisture vs. time, (b) Temperature vs. time for model Pc-1, (c) Temperature vs. time for model Pc-2, (d) Temperature vs. time for model Pc-3.



Fig. 4. Capillarity pressure model effect when Intrinsic permeability $k = 4 \times 10^{-15}$, (a) Moisture vs. time, (b) Temperature vs. time for model Pc-1, (c) Temperature vs. time for model Pc-2, (d) Temperature vs. time for model Pc-3.

The drying time is longest when capillarity pressure model Pc-2 used, and the drying time is lest when capillarity pressure model Pc-3 used. The moisture change is almost in direct proportion to the time when Pc-3 used in most drying time. But other capillarity pressure models are only in drying initial stage. It is different with Fig. 2. The temperature is increased and then maintains some time, and then increased. The different is the capillarity pressure model Pc-2 is with second temperature maintains time.

Fig.4 is the results of different capillarity pressure parameter effect moisture and temperature curves when Intrinsic permeability $=4 \times 10^{-15}$. The drying time is obviously different with different capillarity pressure model.

The drying time is longest when capillarity pressure model Pc-2 used, and the drying time is lest when capillarity pressure model Pc-3 used. The moisture change is almost in direct proportion to the time when Pc-3 used in most drying time. The

temperature is increased and then maintains some time, and then increased only for model Pc-3.

Fig.5 is the results of different capillarity pressure parameter effect moisture and temperature curves when Intrinsic permeability $=4 \times 10^{-16}$. The drying time is obviously different with different capillarity pressure model. In our simulation time, the drying is not gotten end for model Pc-1 and Pc-1.

The moisture change is almost in direct proportion to the time when Pc-3 used in most drying time. The temperature is increased and then maintains some time, and then increased only for model Pc-3.

The difference above is because the mass and heat transfer process different when used different capillarity pressure model. From Eq. (21), the mass of free water transfer is decided by capillarity pressure. The effect is not only shown in moisture change but also shown in temperature characterizes.



Fig.5. Capillarity pressure model effect when Intrinsic permeability $k = 4 \times 10^{-16}$, (a) Moisture vs. time, (b) Temperature vs. time for model Pc-1, (c) Temperature vs. time for model Pc-2, (d) Temperature vs. time for model Pc-3.

CONCLUSION

A coupled model of porous medium vacuum drying based on the theory of heat and mass transfer was implemented in this paper. The parameter sensitivity analyses of capillarity pressure model were then examined. The moisture and temperature characteristic is gotten. The results are shown that the capillarity pressure model has obviously effect on drying process. It would be affect the mass and heat transfer, and then the temperature curve is shown obviously different. The results has some meaningful for vacuum drying of food and chemical material for heat sensitivity.

NOMENCLATURE

R diagonal tenso	R	diagonal tensor
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- D diffusivity (m²s⁻¹)
- D_{eff} diffusion tensor (m²s⁻¹)
- g gravity vector (m s⁻²)
- *h* intrinsic averaged enthalpy (J kg⁻¹)
- *I* water phase rate (kg s⁻¹m⁻³)
- k intrinsic permeability (m²)
- k_r relative permeability
- *m* mass (kg)
- *n* outer unit normal to the product
- *P* pressure (Pa)
- P_c capillary pressure (Pa)
- *R* universal Gas constant (J kmol⁻¹K⁻¹)
- *S* saturation
- t time (s)
- T temperature (K)
- *W* moisture content (in dry basis)

Greek letters

- ΔH latent of phase change (J kg⁻¹)
- λ_{ef} effective thermal conductivity tensor (W

 $m^{-1} K^{-1}$)

- μ viscosity (kg m⁻¹ s⁻¹)
- ρ density (kg m⁻³)
- ω vapor fraction

Subscripts

- *a* dry air
- g gas
- w water
- s solid
- v vapor
- sat vapor saturation
- *in* intrinsic
- *r* relative

Mathematical operators

- Δ gradient operator
- ∇ divergence operator

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МОДЕЛИРАНЕ НА ЕФЕКТА НА КАПИЛЯРНОТО НАЛЯГАНЕ ВЪРХУ ВАКУУМ-СУШЕНЕТО В ПОРЬОЗНА СРЕДА

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(Резюме)

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Сушенето е ключов процес в химичната, хранителната и други сходни индустрии. Използвани са много методи за моделиране и симулиране за изучаване на топло и масообменните процеси при сушенето. Капилярното налягане трудно се определя в тези случаи. Съставен е модел на процеса на вакуум-сушенето на базата на теорията на топло-масообмена. Моделът е приложен с помощта на софтуер COMSOL. Изследвана е параметричната чувствителност спрямо капилярното налягане. Показани са температурните характеристики и влажността.