



Bound water diffusivity effect on vacuum drying process of porous medium modeling

Lili Zhao¹, Zhentian Sun¹, Zhijun Zhang^{2*}, Shiwei Zhang² and Wenhui Zhang²

¹School of Mechanical Engineering, Shenyang University, Shenyang, P. R. China

²School of Mechanical Engineering and Automation, Northeastern University, Shenyang, China

ABSTRACT

As the basic unit operation in chemical industry, 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 bound water diffusivity is important parameter in drying latter stage 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 bound water diffusivity were then examined. The temperature, pressure and moisture characteristics were shown.

Key words: heat and mass transfer; porous medium; sensitivity analyses; vacuum drying; COMSOL.

INTRODUCTION

As the basic unit operation in chemical industry, drying is the key process in chemical, food and other related industry process. The corn drying is used the air drying usually, but the vacuum drying has been used to corn in china [1-3]. Hypothesized the corn as the porous medium, the vacuum drying of corn is a complicated heat and mass transfer process. It has been the subject of intensive research [4-7]. A lot of modeling methods and simulation technology has been used to reveal the heat and mass transfer process [8-16]. As the porous medium, the heat and mass transfer in vacuum drying process has been studied with non-equilibrium method by us [17, 18]. In fact, the parameters of modeling are very important because the simulation results are decided by them. The mass transfer coefficient is condition boundary that is very difficult to gotten. 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].

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 bound water diffusivity were then examined.

EXPERIMENTAL SECTION

PROBLEM DESCRIPSTION

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 heat transfer is through the bottom surface of medium and mass transfer is through the top surface of medium. The total height of the porous medium is 1 cm.

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].

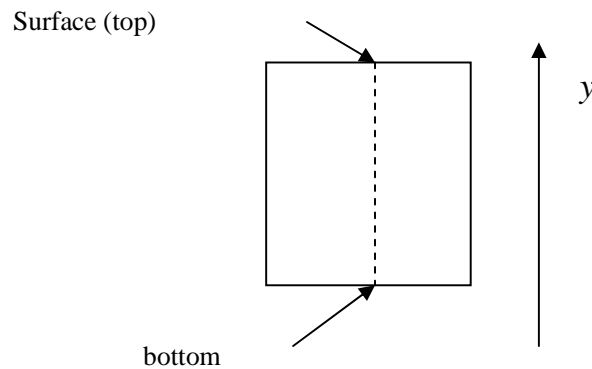


Figure 1. 1D model of porous medium with cortex

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

$$\bar{\rho}_l = cste \quad (1)$$

The solid phase is rigid and homogeneous:

$$\bar{\rho}_s = cste \quad (2)$$

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

$$\bar{\rho}_a = \frac{m_a \bar{P}_a}{R\bar{T}} \quad (3)$$

$$\bar{\rho}_v = \frac{m_v \bar{P}_v}{R\bar{T}} \quad (4)$$

$$\bar{P}_g = \bar{P}_a + \bar{P}_v \quad (5)$$

$$\bar{\rho}_g = \bar{\rho}_a + \bar{\rho}_v \quad (6)$$

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

$$\bar{T}_s = \bar{T}_g = \bar{T}_w = \bar{T} \quad (7)$$

GOVERNING EQUATIONS**Mass balance equation**

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

$$\frac{\partial \bar{\rho}_s}{\partial t} = 0 \quad (8)$$

The averaged mass conservation of the dry air yields

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

For vapor,

$$\frac{\partial(\varepsilon \cdot S_g \bar{\rho}_v)}{\partial t} + \nabla \cdot (\bar{\rho}_v \bar{V}_v) = \dot{m}_l + \dot{m}_b \quad (10)$$

For free water,

$$\frac{\partial(\varepsilon \cdot S_l \bar{\rho}_l)}{\partial t} + \nabla \cdot (\bar{\rho}_l \bar{V}_l) = -\dot{m}_l \quad (11)$$

For bound water,

$$\frac{\partial(\varepsilon \cdot \bar{\rho}_b)}{\partial t} + \nabla \cdot (\bar{\rho}_b \bar{V}_b) = -\dot{m}_b \quad (11)$$

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

$$\frac{\partial W}{\partial t} + \nabla \cdot \left\{ \frac{1}{\bar{\rho}_s} (\bar{\rho}_l \bar{V}_l + \bar{\rho}_v \bar{V}_v + \bar{\rho}_b \bar{V}_b) \right\} = 0 \quad (12)$$

$$W = \frac{\varepsilon \cdot S_l \bar{\rho}_l + \varepsilon \cdot S_g \bar{\rho}_v + \varepsilon \cdot \bar{\rho}_b}{(1 - \varepsilon) \bar{\rho}_s} \quad (13)$$

For the Darcy flow of vapor,

$$\bar{\rho}_v \bar{V}_v = \bar{\rho}_v \bar{V}_g - \bar{\rho}_g D_{eff} \cdot \nabla \bar{\omega} \quad (14)$$

For the Darcy flow of air,

$$\bar{\rho}_a \bar{V}_a = \bar{\rho}_a \bar{V}_g + \bar{\rho}_g D_{eff} \cdot \nabla \bar{\omega} \quad (15)$$

For bound water,

$$\rho_b \bar{V}_b = -\rho_s \cdot D_b \nabla \left(\frac{\rho_b}{\rho_s} \right) \quad (20)$$

The vapor fraction in mixed gas is given by

$$\bar{\omega} = \frac{\rho_v}{\rho_g} \quad (16)$$

The saturation of free water and gas is

$$S_g + S_l = 1 \quad (17)$$

Momentum balance equation

Where the gas and free water velocity is given by

$$\bar{V}_g = -\frac{k_{in,g} \cdot k_{r,g}}{\mu_g} \cdot (\nabla \bar{P}_g - \rho_g \bar{g}) \quad (18)$$

$$\bar{V}_w = -\frac{k_{in,l} \cdot k_{r,l}}{\mu_l} \cdot (\nabla \bar{P}_l - \rho_l \bar{g}) \quad (19)$$

The pressure moving the free water is given by

$$\bar{P}_l = \bar{P}_g - \bar{P}_c \quad (20)$$

Energy balance equation

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

$$\frac{\partial \bar{\rho} \bar{T}}{\partial t} + \nabla \cdot (\bar{\rho}_a \bar{V}_a C_a \bar{T}_a + \bar{\rho}_v \bar{V}_v C_v \bar{T}_v + \bar{\rho}_l \bar{V}_l C_l \bar{T}_l + \bar{\rho}_b \bar{V}_b C_b \bar{T}_b) = \nabla (k_e \cdot \nabla \bar{T}) - \lambda \cdot \dot{i} \quad (21)$$

$$k_e = (1 - \varepsilon)k_s + \varepsilon(S_l k_l + k_b + S_g(\omega k_v + (1 - \omega)k_a)) \quad (22)$$

$$\bar{\rho} \bar{T} = \bar{\rho}_s \bar{T}_s + \varepsilon \cdot S_g \bar{\rho}_a \bar{T}_a + \varepsilon \cdot S_g \bar{\rho}_v \bar{T}_v + \varepsilon \cdot S_l \bar{\rho}_l \bar{T}_l + \varepsilon \cdot \bar{\rho}_b \bar{T}_b \quad (23)$$

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):

$$\rho_{a,top} = \rho_{a,dryer} \quad (24)$$

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

$$n_{v,top} = -h_m \varepsilon S_g (\rho_{v,top} - \rho_{v,dryer}) \quad (25)$$

B.C. for Eq. (15):

$$n_{l,top} = -h_m \varepsilon S_l (\rho_{v,top} - \rho_{v,dryer}) \quad (27)$$

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

$$T_{bottom} = T_h \quad (29)$$

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

$$q_{top} = h(T_{ext} - \bar{T}) + (\lambda + C_l \bar{T})n_{l,top} + C_v \bar{T}n_{v,top} \quad (30)$$

The initial moisture of the porous medium is represented by the liquid water saturation. And other initial condition is as follows.

I.C. for Eq. (9):

$$\rho_a = \rho_{a,0} = \frac{P_{amb,0}M_a}{RT_0} \quad (31)$$

I.C. for Eq. (10):

$$\rho_v = \rho_{v,0} = \frac{P_{sat,0}M_v}{RT_0} \quad (32)$$

I.C. for Eq. (11):

$$S_l = S_{l,0} \quad (33)$$

I.C. for Eq. (21):

$$\bar{T} = T_0 \quad (34)$$

The detail value of boundary and initial condition is show in Table 1.

Table 1. Boundary and initial condition

Parameter	Symbol	Value	Unit
Initial temperature	T_0	273+25	K
Initial air pressure	$P_{atm,0}$	101325	Pa
Initial saturation	$S_{l,0}$	0.3	
pressure of dryer	P_g	$P_g = \begin{cases} (101325-1700t) & t < 58s \\ 2725 & t \geq 58s \end{cases}$	Pa
Relative moisture of gas		0.01	
Temperature of dryer	T_{ext}	273+28	K

NUMERICAL SOLUTION

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 2×100 elements (2D), and time stepping is 0.1 (0 s to 10 s of solution), 1 (10 s to 100 s of solution), 10 (100 s to 10000 s of solution), 20 (10000 s to 20000 s of solution), 50 (20000 s to 20000 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 $1e^{-6}$, whereas absolute tolerance was set to $1e^{-6}$. 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

The parameter is listed in Table 2. The most parameter is gotten from the reference. The Intrinsic permeability is input for four groups in order to study the sensitivity.

Table 2. Parameters used in the simulation process

Parameter	Symbol	Value 1	Unit	Source
<i>Density</i>				
Water	ρ_l	998	kg m ⁻³	[12]
Vapor	ρ_v	Ideal gas	kg m ⁻³	
Air	ρ_a	Ideal gas	kg m ⁻³	
Solid	ρ_s	476	kg m ⁻³	[8]
<i>Specific heat capacity</i>				
Water	C_l	4187	J kg ⁻¹ K ⁻¹	[12]
Vapor	C_v	1840	J kg ⁻¹ K ⁻¹	[12]
Air	C_a	1000	J kg ⁻¹ K ⁻¹	[12]
Solid	C_s	1400	J kg ⁻¹ K ⁻¹	[8,12]
<i>Thermal conductivity</i>				
Water	k_l		W m ⁻¹ K ⁻¹	[15]
Vapor	k_v	0.026	W m ⁻¹ K ⁻¹	[15]
Air	k_a	0.026	W m ⁻¹ K ⁻¹	[15]
Solid	k_s	0.21	W m ⁻¹ K ⁻¹	
<i>Intrinsic permeability</i>				
Water	$k_{in,l}$	4×10 ⁻¹³	m ²	
Vapor and air	$k_{in,g}$	4×10 ⁻¹³	m ²	
<i>Relative permeability</i>				
Water	$k_{r,l}$			[11]
Vapor and air	$k_{r,g}$			[11]
<i>Viscosity</i>				
Water	μ_l	0.988×10 ⁻³	Pa s	[15]
Vapor and air	μ_g	1.8×10 ⁻⁵	Pa s	[15]
<i>Heat transfer coefficient</i>				
	h	2.5	W m ⁻² K ⁻¹	[11]
<i>Mass transfer coefficient</i>				
	h_m	10	m s ⁻¹	[15]
<i>Latent heat of vaporization</i>				
	λ	2.26×10 ⁶	J kg ⁻¹	[15]
<i>Porosity</i>				
	ϵ	0.615	m ²	[8]
<i>Effective diffusivity of gas</i>				
	D_{eff}		m ² s ⁻¹	[8]
<i>Bound water diffusivity</i>				
	D_b	10 ⁻¹⁰ , 10 ⁻⁹ , 10 ⁻⁸ , 10 ⁻⁷ , 10 ⁻⁶	m ² s ⁻¹	
<i>Capillarity Pressure</i>				
	P_c		Pa	[8]
<i>Critical Saturation of free water</i>				
	S_r	0.08		[14]
<i>Molar mass of air</i>				
	M_a	29×10 ⁻³	kg mol ⁻¹	[12]
<i>Molar mass of air</i>				
	M_v	18×10 ⁻³	kg mol ⁻¹	[12]

RESULTS AND DISCUSSION

The moisture curve of different bound water diffusivity is shown in Figure 1. The moisture of bound water diffusivity $D_b=10^{-10}$ or 10^{-9} m² s⁻¹ is similar in moisture curve. It just has a little different. It is shown that the different bound

water diffusivity has little effect on drying process when it lowers than 10^{-9} . When $D_b=10^{-8}$, the moisture curve has larger different. But when $D_b=10^{-7}$ or $10^{-6} \text{ m}^2 \text{ s}^{-1}$, the moisture curve is also similar. The reason is that the mass transfer is controlled by heat transfer or mass transfer rate to outside.

The temperature curve of different bound water diffusivity at different height of 5mm was shown in Figure3. When $D_b=10^{-10}$ or 10^{-9} , and $D_b=10^{-7}$ or 10^{-6} the temperature curve is almost the same. But the obviously the $D_b=10^{-8}$ is very different. In All Figures, the temperature is lift up and maintains some time. At last, the temperature is slowly lift up and gotten the end temperature.

The pressure curve of different bound water diffusivity at different height of 5mm was shown in Figure4. When $D_b=10^{-10}$ or 10^{-9} , and $D_b=10^{-7}$ or 10^{-6} the pressure curve is almost the same. But the obviously the $D_b=10^{-8}$ is very different. In All Figures, the pressure is lift up and maintains some time. At last, the pressure is slowly down and gotten the end pressure.

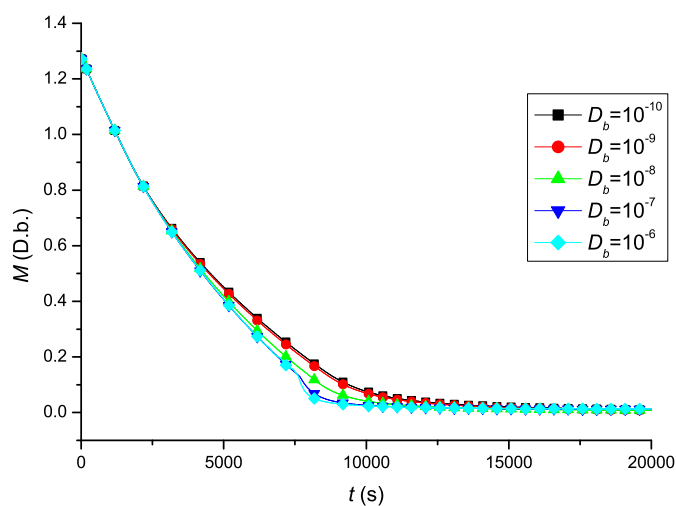


Figure 2. Moisture curve (d. b.) of bound water diffusivity

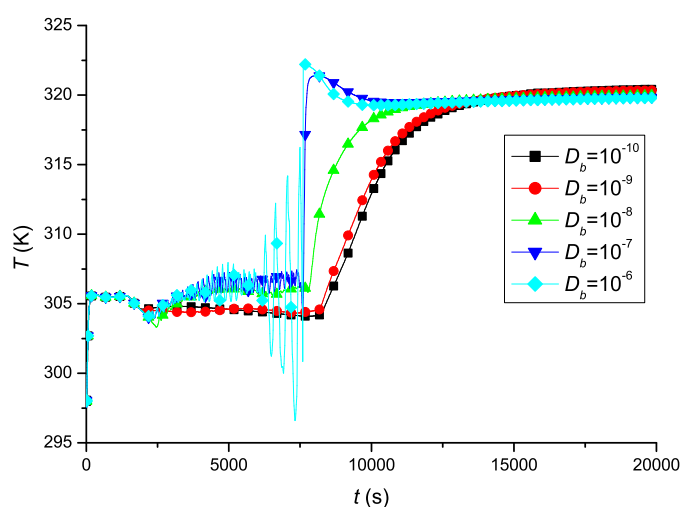


Figure 3. Temperature curve of bound water diffusivity at height of 5mm

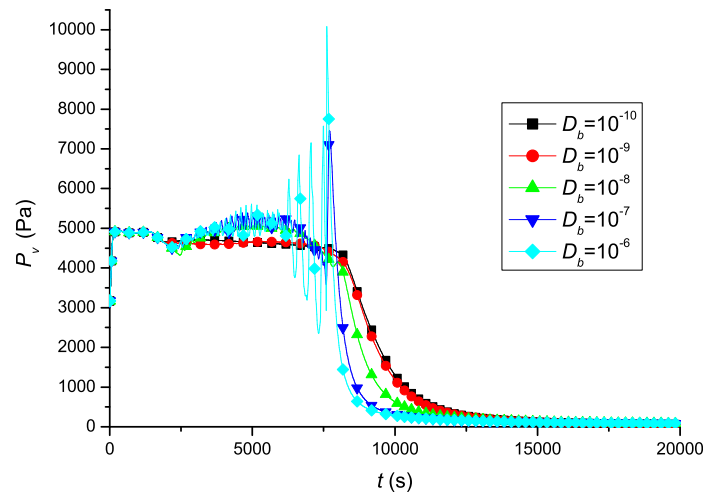


Figure 4. Pressure curve of bound water diffusivity at height of 5mm

CONCLUSION

A coupled model of porous medium vacuum drying with cortex effect based on the theory of heat and mass transfer was implemented in this paper. The parameter sensitivity analyses of mass transfer coefficient were then examined. The moisture and temperature characteristic is gotten. The results are shown that bound water diffusivity 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

B	diagonal tensor
D	diffusivity (m^2s^{-1})
D_{eff}	diffusion tensor (m^2s^{-1})
g	gravity vector (m s^{-2})
h	intrinsic averaged enthalpy (J kg^{-1})
I	water phase rate ($\text{kg s}^{-1}\text{m}^{-3}$)
k	intrinsic permeability (m^2)
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 ($\text{J kmol}^{-1}\text{K}^{-1}$)
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 ($\text{W m}^{-1}\text{K}^{-1}$)

μ	viscosity (kg m ⁻¹ s ⁻¹)
ρ	density (kg m ⁻³)
ω	vapor fraction
<i>Subscripts</i>	
<i>a</i>	dry air
<i>g</i>	gas
<i>w</i>	water
<i>s</i>	solid
<i>v</i>	vapor
<i>sat</i>	vapor saturation
<i>in</i>	intrinsic
<i>r</i>	relative
<i>Mathematical operators</i>	
Δ	gradient operator
$\nabla \cdot$	divergence operator

Acknowledgments

This research was supported by the National Natural Science Foundation of China (Grant Nos. 31000665, 51176027, 31371873 and 31300408).

REFERENCES

- [1] CH Xu, ZJ Zhang, SW Zhang and X He, Proceedings of the 5th Asia-Pacific Drying, **2007**, 1261-1267.
- [2] ZJ Zhang, CH Xu, SW Zhang and X He, Proceedings of the 5th Asia-Pacific Drying Conference, **2007**, 330-337.
- [3] ZJ Zhang, CH Xu, and SW Zhang, Proceedings of the International Conference on Computer Science and Information Technology, **2008**, 534-538
- [4] Y Ichikawa, A.P.S. Selvadurai, *Transport Phenomena in Porous Media, Aspects of Micro / Macro Behaviour*, **2012**.
- [5] AK Haghi, *Theor. Found. Chem. Eng.*, **2006**, 40(1), 14-26.
- [6] SJ Kowalski, *Drying of porous materials*, Springer, **2007**
- [7] J Bear, Y Bachmat, *Introduction to Modeling of Transport Phenomena in Porous Media*, Springer, **1990**.
- [8] A Erriguible, P Bernada, F Couture, and MA Roques, *Chem. Engin. Process.*, **2007**, 46., 1274-1285.
- [9] A Erriguible, P Bernada, F Couture and MA Roques, *Drying Technol.*, **2005**, 23(3), 455-472.
- [10] K Murugesan, HN Suresh, K. N.Seetharamu, and PA Aswatha NarayanaT Sundararajan, *Int. J. Heat Mass Tran.*, **2001**, 44(21), 4075-4086.
- [11] P Perré and IW Turner, *AIChE Journal*, **2006**, 52(9), 3109-3117.
- [12] SS Torres, W Jomaa, JR Puiggali and S Avramidis, *Appl. Math. Model.*, **2011**, 35(10), 5006-5016.
- [13] SS Torres, JR Ramírez and LL Méndez-Lagunas, *Chem. Biochem Engin. Quart.*, **2011**, 25(3), 327-334.
- [14] A Warning, A Dhall, D Mitrea and AK Datta, *J. Food Engin.*, **2012**, 110(3), 428-440.
- [15] A Halder, A Dhall, and AK Datta, *Food Bioprod. Process.* **2007**, 85(3), 209-219.
- [16] A Halder, A Dhall, and A K Datta, *Food Bioprod. Process.*, **2007**, 85(3), 220-230.
- [17] ZJ Zhang and NH Kong, *Math. Probl. Engin.*, **2012**, Article ID 347598, 18 pages.
- [18] ZJ Zhang, SW Zhang, TY Su, and SS Zhao, *Math. Probl. Engin.*, **2013**, Article ID 120736, 9 pages.
- [19] M Jalili, A Anca-Couce, and N Zobel, *Energ. Fuel.*, **2013**, 27, 6705-6717.