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Numerical Simulation for Non-Equilibrium Heat and Mass Transfer during Drying by Two User-Defined Scalar Transport Equations in ANSYS Fluent

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Abstract: In this paper, we have discussed one method of non-equilibrium numerical solution of heat and mass transfer processes during drying using UDS and UDF in FLUENT. A mathematical model of fluid flow and non-equilibrium heat and mass transfer in porous media is proposed. The governing equations are presented for fluid, solid and porous region. Special consideration is given to reflect moisture transfer from porous media to surrounding moist air flow. In order to solve these equations by using a commercial CFD package, FLUENT, reforming of type of govern equations into FLUENT's type is presented, accounted for "variation" of physical properties of solid in regard with reforming of equation type. Transient simulation of drying process of porous media placed in 2D channel by using FLUENT is presented. The results demonstrate the mathematical model and reforming of equations' type presented in this work is capable of simulating non-equilibrium heat and mass transfer in porous media. The results show that numerical predictions follow the expected trends with respect to temperature and velocity at inlet.
Keywords: Computational Fluid Dynamics (CFD), non-equilibrium heat and mass transfer, Porous media, Drying, FLUENT

NOMENCLATURE

A_{gs} specific surface area of porous media, m^{-1}
c_E inertia coefficient of porous media
c_p specific heat at constant pressure in fluid region, J/(kgK)
c_{ps} specific heat in solid region, J/(kgK)
D binary diffusivity coefficient, m^2/s
f body force per unit mass, m/s^2
h specific enthalpy, J/kg
h_{fg} latent heat of evaporation at 0°C in fluid region, J/kg
h_{gs} interfacial heat transfer coefficient in porous media, $W/(m^2K)$
h_{gsm} interfacial mass transfer coefficient in porous media, m/s
k thermal conductivity, W/(mK)
K Darcy permeability of porous media, m^2
Le Lewis number
m mass, kg
$\dot{m}$ mass flow rate, kg/s
Nu Nusselt number
P pressure, Pa
Pr Prandtl number
R gas constant, J/(kgK)

Re Reynolds number
t temperature, °C
τ time, s
v fluid velocity [=(u,v,w)], m/s
x distance in x-direction from origin, m
y distance in y-direction from origin, m
Y mass fraction
μ dynamic viscosity, N s/m^2
ρ_s density of solid, kg/m^3
ρ_g density of gas mixture, kg/m^3
ω_{spec} specific humidity, kg of H_2O/kg of dry air
ε porosity

subscripts and superscripts
a air
e energy
eff effective property in porous media
g gas
s solid
t total
v vapour

I. INTRODUCTION

Fluid flow and heat transfer problems in porous media are widely applied in drying, filtration, preservation of agri-food products, fluidized bed reactors etc. Two energy equations for the solid matrix and fluid should be respectively set up due to existent temperature difference between the solid matrix and fluid of porous media for such classes of problems, especially for large porosity porous media such as fluidized bed, textile, metal foams. Today, a significant amount of work has been focused on the numerical simulation of the problems involving non-equilibrium heat and mass transfer. Especially, Computational Fluid Dynamics (CFD) is used to simulate such classes of problems.

Amiri and Vafai[1],Alazmi and Vafai[2] have respectively investigated multi-factors' effects such as local thermal non-equilibrium effect, non-Darcian effect and variable porosity on forced convection flow and free surface flow through porous media, in which they found that local thermal non-equilibrium effect is more pronounced in the presence of thermal dispersion.

Nakayama et al.[3] have made extensive investigations for two-energy equation model, including exact solutions, tortuosity and dispersion effects, local thermal non- equilibrium analysis and so on. Betchen et al.[4]had described a conjugate domain model, based upon the finite- volume approach that accounts for fluid flow and non-equilibrium sensible heat transfer in porous regions. One key contribution of their work was interface treatment between regions of the conjugate domain. Furqan Ahmad Khan et al.[5] proposed a numerical formulation capable of simulating fluid flow and non-equilibrium heat and mass transfer in three-dimensional conjugate fluid/solid/porous domains.

The governing transport equations were presented for the fluid, solid, and porous regions, with special consideration given towards the manner in which moisture is accounted for in the air–water vapour mixture. Their approach was physically realistic throughout the domain and at interfaces between conjugate regions. Special attention was given to ensure that heat and mass transfer occurs smoothly across all the interfaces. The unsteady problem of drying of an initially saturated porous material was simulated to demonstrate the non-equilibrium mass transfer feature of the developed formulation.

The results were accurate compared to available experimental results.[6-8].

Recently, there have been several studies investigating the numerical modeling of the diverse problems involving heat and mass transfer including drying problems. In this respect, heat and mass transport equations have been proposed to model different heat and mass transfer problems based on the thermal non-equilibrium assumption [9-11]. On the numerical simulation of the heat and mass transfer inside porous media, an in-house CFD source code and commercial

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software, FLUENT, were applied to simulate the heat and mass transfer inside porous media [12-14]. More sophisticated finite-volume and finite-difference numerical formulations have been proposed to model different types of heat and mass transfer problems inside porous media. [15-18].

The above literature shows that most of these studies have considered local thermal-equilibrium to model heat transfer and treated numerically as a conjugate problem. However, few studies have proposed , specifically formulating non-equilibrium heat and mass transfer models , to predict drying process using commercial software FLUENT.

The aim of present study is to develop a numerical formulation capable of modeling non-equilibrium heat and mass transfer inside porous media and solve the equations by using FLUENT. To achieve the present objective, moisture transport equation and energy transport equation for the solid matrix of porous media will be reformed to user-defined scalar equation type in FLUENT. In addition, the properties of solid and some terms of these equations will be also defined with regarding coefficients and terms of UDS equation in FLUENT. By using UDF(User Defined Function) in FLUENT, these problems can be solved. Then, validation of the predicted values will be carried out by comparing with those obtained experimentally.

II. MATHEMATICAL MODEL

The transport equations to simulate the local non-equilibrium heat and mass transfer in 2D geometry are the mass, momentum, species and energy transport equations as following, wherein moist air is the working fluid. Moist air with a uniform free stream velocity of U_0 is assumed to flow into a 2D channel in which a wet porous material is placed. (Fig.1) Porous media comprise of wet solid matrix and moist air. Moist air passes through the porous zone and fluid zone. Transport properties of porous media, including porosity, permeability, specific surface, inertial coefficient, surface heat transfer coefficient and thermal conductivity of both fluid and solid, moisture diffusivity of solid, critical moisture content were analyzed and developed. moist air refers to a mixture of dry air and water vapor in which the dry air is treated as if it were a pure component. Probably the amount of water vapor changes as a result of the mass exchange between constituents in the porous media. The amount of water vapor can be quantified by the introduction of one additional species transport equation to the mass, momentum and energy transport equations.

The amount of water vapor in the moist air can be specified in various ways. The water vapour mass fraction (Y_v) is used to species transport equation as a variable. The relations between the water vapour mass fraction (Y_v), the dry air mass fraction (Ya) and specific humidity can be respectively expressed as

The specific humidity (ω_{spec}) specifying the amount of water vapour in air is expressed as shown below. [19]

$$\omega_{spec} = \frac{m_v}{m_a} = \frac{(\frac{R_a}{R_v})p_v}{p_a} \tag{1}$$

Where m_v is the mass of water vapour, m_a is the mass of dry air, P_a is the dry air partial pressure, P_v is water vapour partial pressure, and R_a and R_v are the gas constants for air and water vapour, respectively.

The temperature of the moist air is obtained by solving the energy transport equation.

The relation between the vapour mass fraction (Y_v) and specific humidity can be expressed as

$$Y_v = \frac{\omega_{spec}}{1+\omega_{spec}}, \quad Y_a = 1 - Y_v = \frac{1}{1+\omega_{spec}} \tag{2}$$

The vapour mass fraction (Y_v) along with the total pressure (P_t) can then be used to calculate the vapour pressure (P_v) by the following expression

$$p_v = \frac{Y_v R_v P_t}{R_a + Y_v (R_v - R_a)} \tag{3}$$

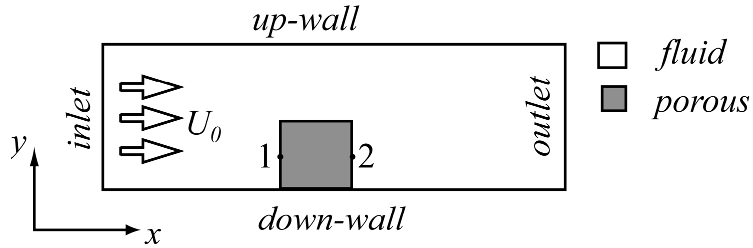

Fig. 1. Schematic diagram of computational domain

A. The Transport Equations for Fluid Region

The conservation of mass and momentum equations, energy transport equation of the air-water vapour mixture(moist air), water vapour transport equation in the pure fluid region given by:

conservation of mass and momentum equations

$$\frac{\partial \rho_g}{\partial \tau} + \nabla \cdot (\rho_g V) = 0 \tag{4}$$

$$\frac{\partial (\rho_g V)}{\partial \tau} + \nabla \cdot (\rho_g V V) = -\nabla P + \mu_g \nabla^2 V + \rho_g f \tag{5}$$

Energy transport equation of the air–water vapour mixture

$$\frac{\partial (\rho_g Y_a h_a + \rho_g Y_v h_v)}{\partial \tau} + \nabla \cdot (\rho_g Y_a h_a V) + \nabla \cdot (\rho_g Y_v h_v V) = k_g \nabla^2 t_g + \nabla \cdot (\rho_g h_a D_g \nabla Y_a) + \nabla \cdot (\rho_g h_v D_g \nabla Y_v) \tag{6}$$

Water vapour transport equation

$$\frac{\partial (\rho_g Y_v)}{\partial \tau} + \nabla \cdot (\rho_g Y_v V) = \nabla \cdot (\rho_g D_g \nabla Y_v) \tag{7}$$

where,h_a is the specific enthalpy of dry air, h_v is the specific enthalpy of water vapour, t_g is the temperature of the air–water vapour mixture.

ha and h_v are through the temperature of the air–water vapour mixture (t_g) as shown below.

$$h_a = C_{pa} t_g \tag{8}$$

$$h_v = h_{fg} + C_{pv} t_g \tag{9}$$

B. The Transport Equations for Porous Region

In the porous region, since there exist a state of local thermal non–equilibrium between the solid matrix and moist air of the porous media,volume-averaged forms of the transport equations are usually described by the following governing equations[5].

Mass and momentum equations of the moist air

$$\varepsilon \frac{\partial \langle \rho_g \rangle^g}{\partial \tau} + \nabla \cdot (\langle \rho_g \rangle^g \langle V \rangle) = 0 \tag{10}$$

$$\frac{\partial (\langle \rho_g \rangle^g \langle V \rangle)}{\partial \tau} + \frac{1}{\varepsilon} \nabla \cdot (\langle \rho_g \rangle^g \langle V \rangle \langle V \rangle) = -\varepsilon \nabla \langle P \rangle^g + \mu_g \nabla^2 \langle V \rangle + \varepsilon \langle \rho_g \rangle^g f - \frac{\varepsilon \mu_g}{K} \langle V \rangle - \frac{\varepsilon \langle \rho_g \rangle^g c_E}{\sqrt{K}} |\langle V \rangle| \langle V \rangle \tag{11}$$

Energy transport equation of the moist air

$$\frac{\partial(\langle\rho_g\rangle^g\langle Y_a\rangle^g\langle h_a\rangle^g+\langle\rho_g\rangle^g\langle Y_v\rangle^g\langle h_v\rangle^g)}{\partial\tau}+\nabla\cdot(\langle\rho_g\rangle^g\langle Y_v\rangle^g\langle h_a\rangle^g\langle V\rangle)+\nabla\cdot(\langle\rho_g\rangle^g\langle Y_v\rangle^g\langle h_v\rangle^g\langle V\rangle)$$
$$=k_{eff,g}\nabla^2\langle t_g\rangle^g+\nabla\cdot(\rho_g h_a D_{eff,g}\nabla\langle Y_a\rangle^g)+\nabla\cdot(\rho_g h_v D_{eff,g}\nabla\langle Y_v\rangle^g)$$
$$+\langle\dot{m}_{evap}\rangle\langle h_{vs}\rangle^s-h_{gs}A_{gs}(\langle t_g\rangle^g-\langle t_s\rangle^s) \tag{12}$$

Water vapour transport equation

$$\varepsilon\frac{\partial(\langle\rho_g\rangle^g\langle Y_v\rangle^g)}{\partial\tau}+\nabla\cdot(\langle\rho_g\rangle^g\langle Y_v\rangle^g\langle V\rangle)=\nabla\cdot(\langle\rho_g\rangle^g D_{eff,g}\nabla\langle Y_v\rangle^g)+\langle\dot{m}_{evap}\rangle \tag{13}$$

Moisture transport equation and energy transport equation of the solid matrix.

$$(1-\varepsilon)\langle\rho_s\rangle^s\frac{\partial\langle Y\rangle^s}{\partial\tau}=\nabla\cdot(\langle\rho_s\rangle^s D_{eff,s}\nabla\langle Y\rangle^s)-\langle\dot{m}_{evap}\rangle \tag{14}$$

$$(1-\varepsilon)\langle\rho_s\rangle^s\frac{\partial\langle h_s\rangle^s}{\partial\tau}=\nabla\cdot(k_{eff,s}\nabla\langle t_s\rangle^s)-\langle\dot{m}_{evap}\rangle\langle h_{vs}\rangle^s+h_{gs}A_{gs}(\langle t_g\rangle^g-\langle t_s\rangle^s) \tag{15}$$

where, $\langle h_s\rangle^s$ is the intrinsic volume-averaged specific enthalpy of solid matrix, $\langle h_{vs}\rangle^s$ is the intrinsic-averaged specific enthalpy of water vapour in intrinsic volume-aver aged temperature of solid matrix which are represented as follow.

$$\langle h_s\rangle^s=(C_s+\langle Y\rangle^s C_w)\langle t_s\rangle^s \tag{16}$$

$$\langle h_{vs}\rangle^s=h_{fg}+C_{pv}\langle t_s\rangle^s \tag{17}$$

C. Initial and Boundary Conditions

Initially the moist air of fluid region, solid matrix and moist air of the porous media are assumed to be at same temperature, uniform vapour mass fraction and moisture content(d.b)
Also, overall gas phase is assumed to be at stop.
Boundary conditions are:

$$t_g=t_{gin},Y_v=Y_{vin},u=u_{in},v=0 \quad \text{at inlet} \tag{18}$$

$$\frac{\partial t_g}{\partial x}=\frac{\partial Y_v}{\partial x}=0,P=0 \quad \text{at outlet} \tag{19}$$

Up and down walls are assumed to be no-slip, adiabatic and impermeable.

D. Define UDS equations in FLUENT.

FLUENT provides comprehensive modeling capabilities for a wide range of incompressible and compressible, laminar and turbulent fluid flow , heat transfer, species transport and other problems in 2D and 3D. Steady-state or transient analyses can be performed. And FLUENT is able to solve these problems in porous media.
In handling of energy equation in porous media, FLUENT assumes, by default, that multi phase fluid and the solids are in thermal equilibrium. Non -equilibrium between fluid and solid can be considered as a user-defined scalar (UDS) equation. Physical quantities such as temperature and moisture content of solid in non-equilibrium porous region, which are unsupported in FLUENT basically, are considered as UDSs. Using UDS is a method capable of considering heat and mass transfer in solid in non-equilibrium porous region in FLUENT model, with combining the external drying process that the water vapor evaporated from surface of material spread out by convective and diffusive mass transfer.

In order to use the UDS equations of heat and mass transfer in solid in porous region in FLUENT, equations(14),(15)for the solid matrix must be reformed because FLUENT can solve just the equation like only this(below,follow) type[20]

$$\frac{\partial \rho \phi_k}{\partial \tau} + \frac{\partial}{\partial x_i}(\rho u_i \phi_k - \Gamma_k \frac{\partial \phi_k}{\partial x_i}) = S_{\phi_k} \qquad k=1,\ldots,N \qquad (20)$$

Where Γ_k, S_{ϕ_k} is diffusivity and source term of the kth scalar respectively.

The convective term $\rho u_i \phi_k$ can be ignored if no convective mass transfer. Diffusivity may be set as a constant or function of temperature and moisture content by using the UDF(user defined function).
Accordingly, equation (14), (15) have to be reformed. their type is reformed like these

$$\frac{\partial \langle \rho_s \rangle^s \langle Y \rangle^s}{\partial \tau} = \nabla \cdot (\frac{\langle \rho_s \rangle^s D_{eff,s}}{(1-\varepsilon)} \nabla \langle Y \rangle^s) - \frac{\langle \dot{m}_{evap} \rangle}{(1-\varepsilon)} \qquad (21)$$

$$\frac{\partial \langle \rho_s \rangle^s \langle h_s \rangle^s}{\partial \tau} = \nabla \cdot (\frac{k_{eff,s}}{(1-\varepsilon)} \nabla \langle t_s \rangle^s) - \frac{\langle \dot{m}_{evap} \rangle \langle h_{vs} \rangle^s}{(1-\varepsilon)} + \frac{h_{gs} A_{gs} (\langle t_g \rangle^g - \langle t_s \rangle^s)}{(1-\varepsilon)} \qquad (22)$$

FLEUNT uses above equations, and so source terms and physical properties of solid region must be changed. The source terms of heat and mass respectively converted to these:

$$S_s = -\frac{\langle \dot{m}_{evap} \rangle \langle h_{vs} \rangle^s}{(1-\varepsilon)} + \frac{h_{gs} A_{gs} (\langle t_g \rangle^g - \langle t_s \rangle^s)}{(1-\varepsilon)}$$

$$S_{Ys} = -\frac{\langle \dot{m}_{evap} \rangle}{(1-\varepsilon)} \qquad (23), (24)$$

These source terms are the function of temperature and mass ratio, which are the basic variables in FLEUNT and negative terms of these must be inserted to energy and species transport equations as source terms ,based on the energy and mass balance. source terms of energy and species transport equations(12), (13) are like these:

$$S_t = \frac{\langle \dot{m}_{evap} \rangle \langle h_{vs} \rangle^s}{(1-\varepsilon)} - \frac{h_{gs} A_{gs} (\langle t_g \rangle^g - \langle t_s \rangle^s)}{(1-\varepsilon)}$$

$$S_Y = \frac{\langle \dot{m}_{evap} \rangle}{(1-\varepsilon)} \qquad (25), (26)$$

Thermal conductivity converts to $\frac{k_{eff,s}}{(1-\varepsilon)}$.

Also, mass diffusivity converts to $\frac{\langle \rho_s \rangle^s D_{eff,s}}{(1-\varepsilon)}$

In FLUENT, unsteady term of UDS equation is defined as $\frac{\partial(\rho t_s)}{\partial \tau}$, so this is also modified as $\frac{\partial(\langle\rho_s\rangle^s \langle h_s\rangle^s)}{\partial \tau}$ that is $\frac{\partial(\langle\rho_s\rangle^s (C_s+\langle Y\rangle^s C_w)\langle t_s\rangle^s)}{\partial \tau}$

In other hands, these UDS equations are available only in porous region, and density of fluid is originally used in these equations in FLUENT, instead of solid density. Therefore, the unsteady terms should be reset. Density in unsteady term of energy equation of solid in porous region is changed to $\langle\rho_s\rangle^s \langle c_s\rangle^s$ where the density and specific heat of solid is the function of moisture content (d.b) of solid in porous region.

As you see, these UDS equations are added in the basic FLUENT equations , so the properties of solid and some terms of the equations are changed to satisfy the need of basic equation. By using UDF(User Defined Function) in FLUENT, these problems can be solved. DEFINE_DIFFUSIVITY is used to specify the the diffusivity for species transport equations such as thermal conductivity, mass diffusivity and so on. DEFINE_SOURCE is used to specify the source term for different type of solved equation in FLUENT. DEFINE_UDS_UNSTEADY can be used to specify the unsteady terms of UDS equations. DEFINE_PROPERTY is used to specify the properties of working media such as density and thermal conductivity.

III. RESULTS AND DISCUSSION

A numerical calculation had done by using FLUENT16.2,based on the presented method in this paper.
h_{gs} in Eqs.(12) and (15) is computed using the expression [21,24,25]

$$Nu = 2.0 + 1.1\mathrm{Re}^{0.6}\,\mathrm{Pr}^{0.33} \tag{27}$$

The $\langle \dot{m}_{evap} \rangle$ term in Eqs. (12-15) can be expressed as [22]

$$\langle \dot{m}_{evap} \rangle = \langle\rho_g\rangle^g h_{gsm} A_{gs} (\langle Y_v\rangle^{gs} - \langle Y_v\rangle^g) \tag{28}$$

where, $\langle Y_v\rangle^{gs}$ refers to the vapour mass fraction occurring at the interface the porous media, computed using Eqs.(1)–(3), and by assuming that the relative humidity at surface of solid matrix is equal to 100%. Saturation pressure of water vapor was estimated by the relationships given by Mohsen Ranjbaran [16]. The interfacial mass transfer coefficient (h_{gsm}) appearing in Eq. (28) is found from the following expression [23]

$$h_{gsm} = h_{gs}\left(\frac{DLe^{-\frac{2}{3}}}{k}\right) \tag{29}$$

Properties of solid in porous region and structural characters of porous region are presented in Table 1.

Table 1. porous media properties[24, 25]

density	350kg/m^3	K	4.00×10^{-6}m^2
specific heat	1590/kg℃	Specific area	917.7m^2/m^3
thermal conductivity	0.25w/mk	critical moisture content	0.25
Porosity	0.7	equilibrium moisture content	0.05
cE	0.244		

It is assumed that initially 40% of the solid-constituent volume of the porous material is occupied by water, and temperature is 23℃ overall region.

Air flow is considered to enter the channel at temperature 80℃, vapor mass fraction 0.01 and velocity 5m/s. As you can see from Fig.2, variation rate of moisture content at point 1 and 3 is not equal ,so it arrived at equilibrium state in different times. From curve 2 in Fig. 2, drying rate of solid in porous region retains constant until 1500s, and decrease until 4500s, and after 4500s, arrived equilibrium state, that is, there is no mass transfer from solid to air.

although moisture content (d.b) of solid in porous region arrives at equilibrium moisture content, temperature difference between centre point in inlet and outlet is 40℃, we are known from Fig. 3. This is because velocity of air in porous region is very low, so thermal capacity of air is much less than solid in porous region and also thermal conductivity of solid is very low.

volume averaged temperature and moisture content (d.b) of solid in porous region at different inlet velocity are shown in Fig. 4, 5 respectively. It is found that drying rate increases when air velocity at inlet increase ,and drying time in which the moisture content (d.b) of solid in porous region arrived equilibrium state decrease by about 250s at every velocity steps, and critical moisture content (d.b) of solid in porous region varies at each cases.

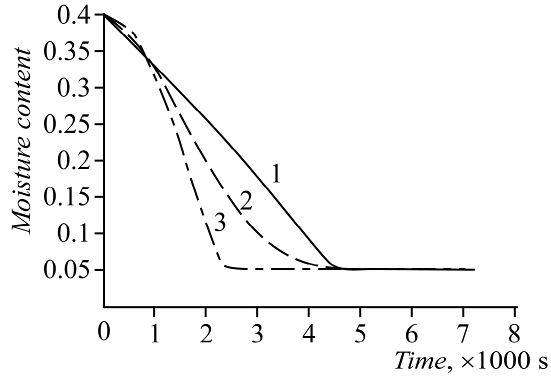

Fig. 2. Volume averaged moisture content (d.b) of solid in porous region along drying time.

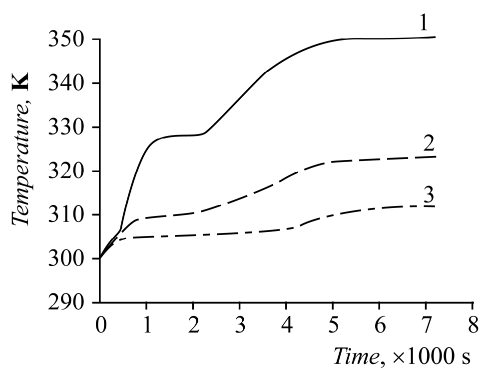

Fig. 3. Volume averaged temperature of solid in porous region along drying

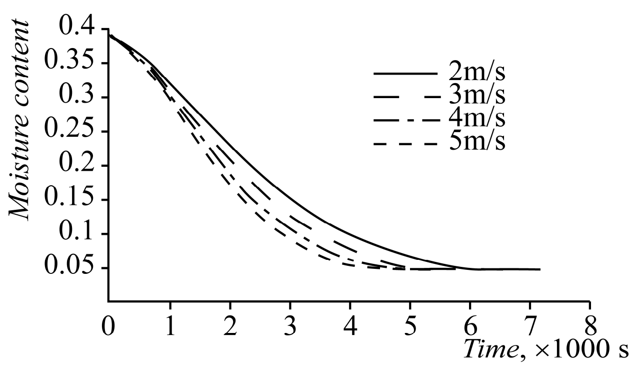

Fig. 4. Volume averaged moisture content (d.b) of solid in porous region at air velocity at inlet.

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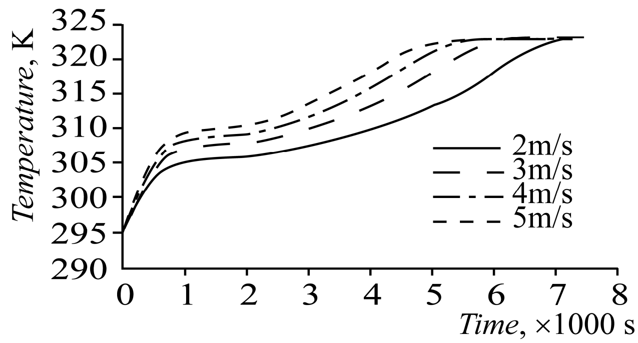

Fig. 5. Volume averaged temperature of solid in porous region at air velocity at inlet.

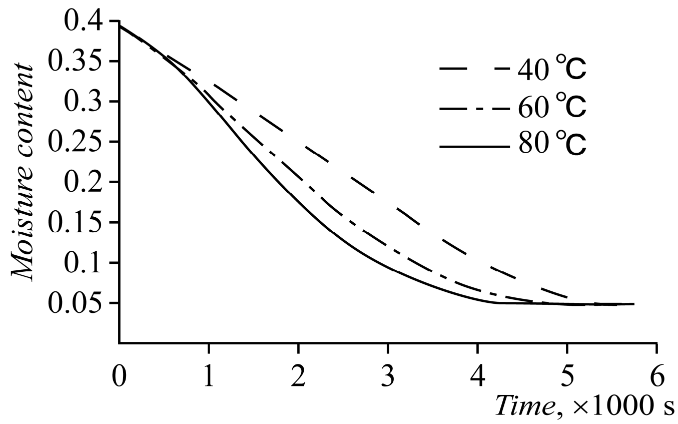

Fig. 6. Volume averaged moisture content (d.b) of solid in porous region at air temperature at inlet.

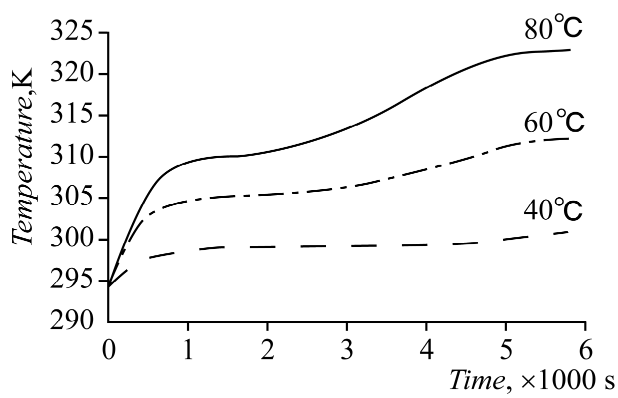

Fig. 7. Volume averaged temperature of solid in porous region at air temperature at inlet.

Fig. 6, 7 show that volume averaged moisture content and temperature of solid in porous region at air temperature at inlet respectively.
We can see that when air temperature at inlet increase, drying rate increase, but critical moisture content decrease.

IV. CONCLUSION

In the present study, CFD method for analyzing non-equilibrium heat and mass transfer in regular constructional porous media was proposed. A formulation capable of simulating non-equilibrium heat and mass transfer in porous domains was presented, with special consideration towards reforming the heat and mass transfer equations in order to make it possible in FLEUNT.

The results show that our predictions follow the expected trends with respect to temperature and velocity at inlet. As such, the present model reforming is shown to be capable of simulating a large class of problems associated with non-equilibrium heat and mass transfer in porous media by using FLUENT.

In the future these problems will be investigated with regarding the change of pore space in porous media during drying.

Declaration of Competing Interests

The authors have no financial conflict for this paper.

V. ACKNOWLEDGMENTS

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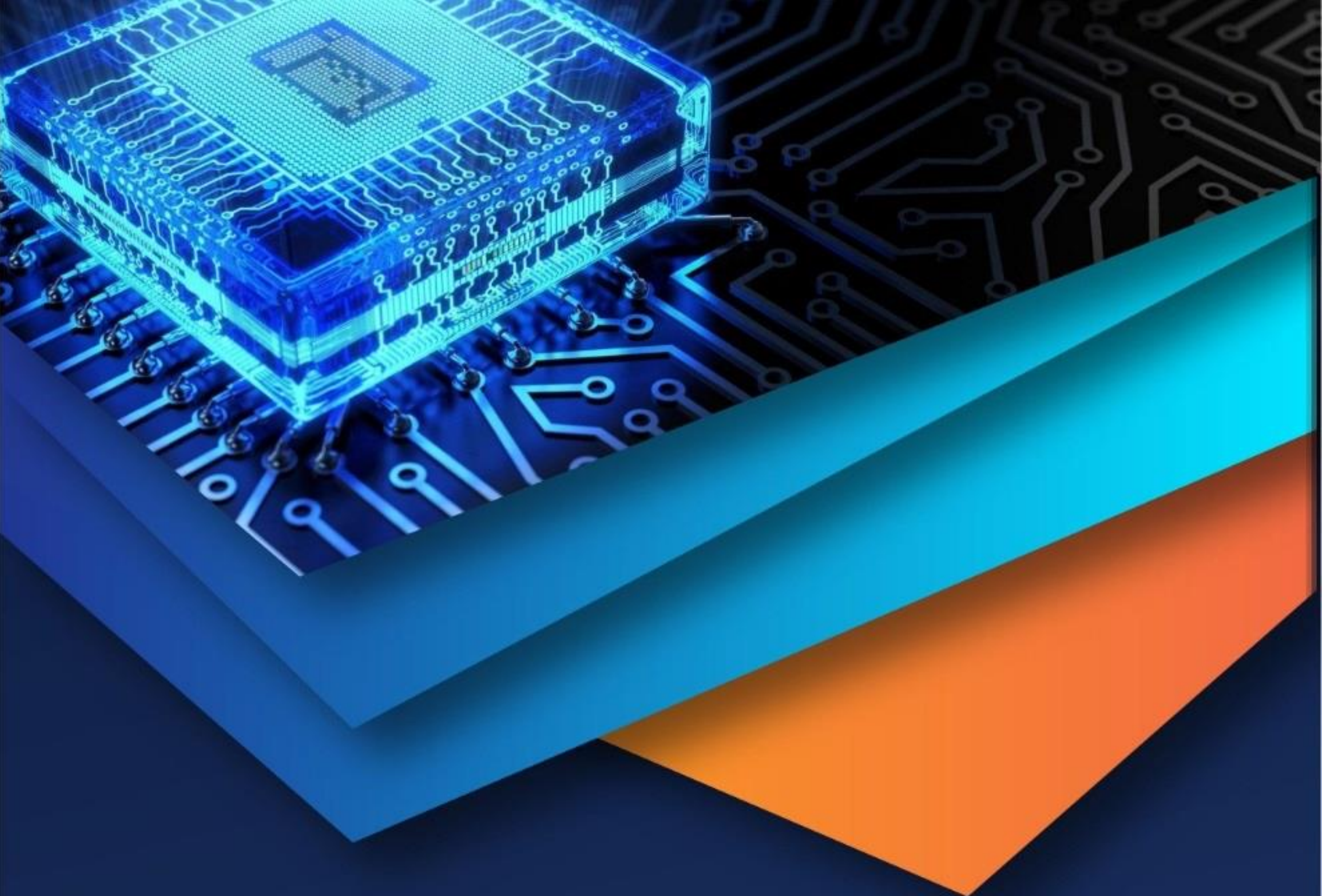

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