Proceedings World Geothermal Congress 2020+1
Reykjavik, Iceland, April - October 2021

Simulation of Migration of Leaked Contaminants of Buried Tubes under Periodic Temperature Boundaries Using Lattice Boltzmann Method

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Keywords: Buried tube, underground contaminants, periodic temperature boundary, lattice-Boltzmann simulation

ABSTRACT

The risk of underground environmental pollution caused by the surface contaminants of buried tubes and the leakage of its internal working fluid is increasing with the large-scale application of borehole heat exchangers. Previous studies have shown that periodic freezing and melting processes can cause redistribution of contaminants concentration. Similarly, the periodic heat injection and heat extraction of buried pipes can also cause redistribution of contaminants concentration. However, fewer related studies can be found presently. In this paper, the Multiple-relaxation–time lattice Boltzmann model (MRT-LBM) is used to simulate the contaminants migration in porous media under periodic temperature boundaries. By regarding the contaminants leakage point as the continuous injection point source and the accumulative flow rate of contaminants as an additional item of source term, the mathematical model of solute migration and the Darcy velocity model are established; the unsteady heat conduction and convection equations were established by regarding the heat injection and heat extraction in summer and winter time as a various cylindrical heat source. Coupling the above equations and combined with the D3Q7 model of lattice Boltzmann methods (LBM), the relationship between the contaminants concentration front and the periodic temperature period is obtained, thus the accumulation position of the contaminants can be determined.

1. INTRODUCTION

With the large-scale application of borehole heat exchangers, the risk of contamination of the underground environment caused by the leakage of the working fluid in the buried pipe and the contamination of tube after its life expectancy is also increasing. Previous simulations of contaminants were mostly focus on the contaminants migration under formation temperature conditions, while the simulation under the operating conditions of buried pipes (periodic temperature boundaries) has not been found. The migration of underground contaminants under normal temperature boundary is mainly based on the convection-dispersive Nielson equation and the Richards equation, which includes source terms of adsorption and desorption. Even for one-dimensional problems, the equation solving is quite complicated. Therefore, Leo and Booker (1999) proposed semi-analytic solutions of contaminants transport from deeply buried cylindrical repository surrounded by zoned media. The migration of underground contaminants under periodic temperature boundaries can be considered as the double-diffusion mixed convection in porous media. When heat and mass transfer simultaneously occur in the double diffusive flow, the fluid flow is not only driven by the temperature gradient but also by the concentration gradient. The energy flux caused by the concentration gradient is called Dufour effect and the mass flux caused by the temperature gradient is Soret effect. Previous numerical methods have focused on finite difference methods, finite element methods, finite volume methods and the popular lattice-Boltzmann (LBM) method in recent years. The LBM method is easy to handle complex solid boundary and multi-component fluid problems. However, a disadvantage of the commonly used Lattice-Bhatnagar-Gross-Krook (LBGK) model is that numerical instability and permeability dependence on fluid viscosity, while the LBM multiple-relaxation–time lattice Boltzmann model (MRT) can overcome the above defects by constructing appropriate collision operators to accurately achieve the fluid-solid boundaries independent of fluid viscosity and independently adjust the relaxation time. Many researchers have studied double-diffusion mixed convection in porous media with LBM method. Bettaibi and Kuznik (2016) used hybrid LBM-MRT model coupled with finite difference method for double-diffusive mixed convection in rectangular enclosure with insulated moving lid. Kefayati (2018) simulated double-diffusive natural convection and entropy generation of Carreau fluid in a heated enclosure with an inner circular cold cylinder. Zhao Kai (2010) used lattice Boltzmann method to investigate the convective heat and mass transfer with double diffusive effect inside a complex porous medium. Yoshino and Inamuro (2003) analyzed Lattice Boltzmann simulations for flow and heat/mass transfer problems in a three-dimensional porous structure. Yoshida and Nagaoka (2010) proposed the Multiple-relaxation-time lattice Boltzmann model for the convection and anisotropic diffusion equation. Liu (2018) applied the Multiple-relaxation-time lattice Boltzmann model to simulate double-diffusive convection in fluid-saturated porous media; Rahimi and Kasaeipoor (2018) studied the Lattice Boltzmann method based on Dual-MRT model for three-dimensional natural convection and entropy generation in CuO–water nanofluid filled cuboid enclosure included with discrete active walls.

The previous studies are mainly concentrated on the natural convection in porous media for the representative elementary volume (REV) scale, while fewer simulations of the heat and mass transfer process of binary mixture fluid in porous medium. In order to study the coupling heat-mass diffusion in porous media at the pore scale, this paper uses D3Q7-MRT model coupled with flow solute transport and heat transfer to simulate the concentration field of the leaked contaminants of a single buried pipe under the periodic temperature boundaries.

2. MATHEMATICAL MODEL

2.1 Conceptual model and mathematical description

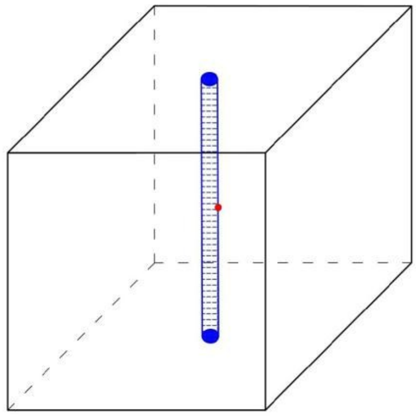


Figure 1: Conceptual model of underground contaminants migration

As shown in Figure 1, the square cavity filled with uniform sand is used to simulate the underground environment (31cm × 31cm × 31cm). The cylindrical heat source with periodic changes is placed in the cavity center (simulating the periodic heat injection and extraction of the buried pipe). There is a continuous leaking concentration point source on the right side of the middle section of the line heat source. All surfaces of the square cavity are well insulated and the initial concentration gradient is zero.

Assuming that the porous medium is uniform and isotropic, the dynamic properties of the fluid and the porous medium are constant, ignoring the viscous dissipation of the porous medium, the Boussinesq hypothesis is used to satisfy the local thermal equilibrium condition between the fluid and the solid. Based on the Brinkman-Darcy-extended model, the governing equations for the double-diffusion natural convection in the cavity filled with porous media are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (1)$$

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)\left(\frac{u}{\varepsilon}\right) = -\frac{1}{\rho}\nabla(\varepsilon p) + \nu_e \nabla^2 u + F \quad (2)$$

$$\frac{\partial T}{\partial t} + \nabla \cdot (uT) = \alpha_e \nabla^2 T \quad (3)$$

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = D_e \nabla^2 C \quad (4)$$

$$F = -\frac{\varepsilon \nu_e}{K} u - \frac{\varepsilon F_\varepsilon}{\sqrt{K}} |u| u + \varepsilon G \quad (5)$$

The dimensionless parameters in the model are defined as

$$X = \frac{x}{H}, Y = \frac{y}{H}, Z = \frac{z}{H}, U = \frac{u}{\sqrt{3}c_s}, V = \frac{v}{\sqrt{3}c_s}, W = \frac{w}{\sqrt{3}c_s}$$
$$\theta = \frac{T - T_c}{T_h - T_c}, \varphi = \frac{C - C_c}{C_h - C_c}, \mathrm{Pr} = \frac{\nu}{\alpha}, Le = \frac{\alpha}{D}, P = \frac{p}{3\rho {c_s}^2}, Da = \frac{K}{H^2}$$
$$Ra_t = \frac{g\beta_T (T_h - T_c) H^3 \,\mathrm{Pr}}{\nu^2}, Ra_s = \frac{g\beta_C (C_h - C_c) H^3 Le}{\nu^2} \quad (6)$$

2.2 Lattice Boltzmann model

D3Q7 model is used in this paper and its discrete velocity and weight coefficient are as follows

$$[e_0, e_1, e_2, e_3, e_4, e_5, e_6] = \begin{bmatrix} 0\,1 -1\,0 & 0 & 0 & 0 \\ 0\,0 & 0 & 1 -1\,0 & 0 \\ 0\,0 & 0 & 0 & 0 & 1 -1 \end{bmatrix} c$$

(7)

$$\omega_i = \begin{cases} 1/4(i=0) \\ 1/8(i \neq 0) \end{cases}$$

(8)

Based on the general seepage LBE model, a lattice Boltzmann model of REV scale for simulating double-diffusion natural convection coupled with temperature field and concentration field of porous media are proposed.

$$f_i(r + c_i\delta t, t + \delta t) - f_i(r,t) = -[M^{-1}SM]_{ij}[f_i(r,t) - f_i^{eq}(r,t)] + \delta t F_i$$

(9)

$$g_i(r + c_i\delta t, t + \delta t) - g_i(r,t) = -[M^{-1}SM]_{ij}[g_i(r,t) - g_i^{eq}(r,t)]$$

(10)

$$h_i(r + c_i\delta t, t + \delta t) - h_i(r,t) = -[M^{-1}SM]_{ij}[h_i(r,t) - h_i^{eq}(r,t)]$$

(11)

The corresponding equilibrium functions are expressed as

$$f_i^{eq} = \omega_i \rho \left[1 + \frac{c_i \cdot u}{c_s^2} + \frac{(c_i \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right]$$

(12)

$$F_i = \omega_i \rho \left[M^{-1}\left(I - \frac{S}{2} \right) M \right]_{ij} \left[\frac{c_i \cdot F}{c_s^2} + \frac{uF : (c_i c_i - c_s^2 I)}{\varepsilon c_s^4} \right]$$

(13)

$$g_i^{eq} = \omega_i T \left[1 + \frac{c_i \cdot u}{c_s^2} \right]$$

(14)

$$h_i^{eq} = \omega_i C \left[1 + \frac{c_i \cdot u}{c_s^2} \right]$$

(15)

The density, velocity, temperature, and concentration in the flow field are defined as

$$\rho = \sum_i f_i, \rho u = \sum_i c_i f_i + \frac{\delta t}{2} \rho F, T = \sum_i g_i, C = \sum_i h_i$$

(16)

3. NUMERICAL SIMULATION OF UNDERGROUND CONTAMINANT MIGRATION

3.1 Program verification

Supposing that the groundwater has a flow velocity along the X and Y axes, there is a concentration point at the initial moment of a certain position, the concentration distribution of this point at a given time can be obtained. The dimensionless parameters are set as: u_x=0.04, u_y=0.02, c(5,5,20)=4, t=400, and the physical model is as follows

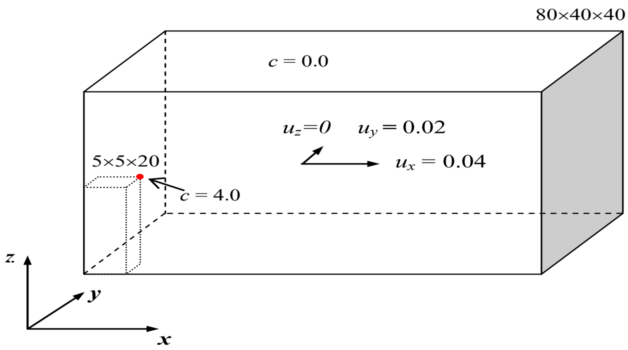


Figure 2: Physical model of the solute transport problem

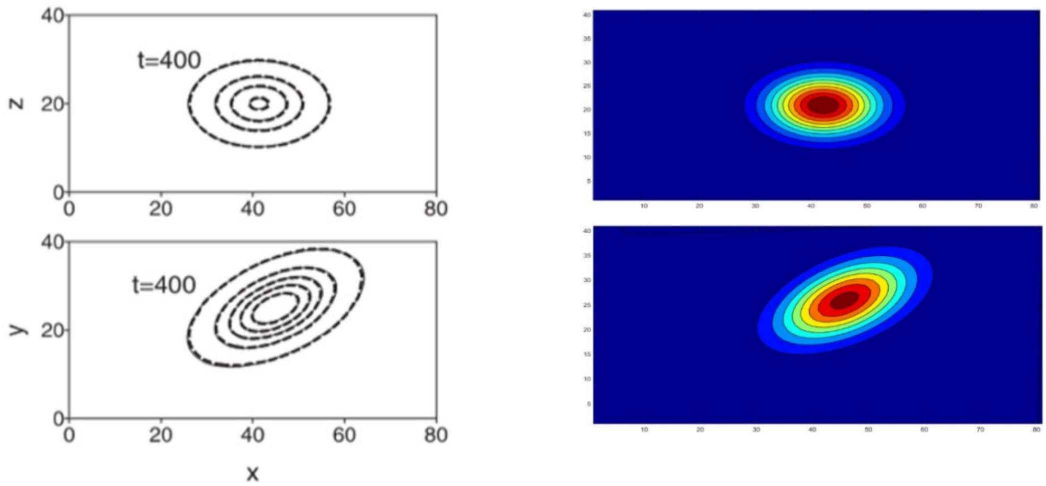
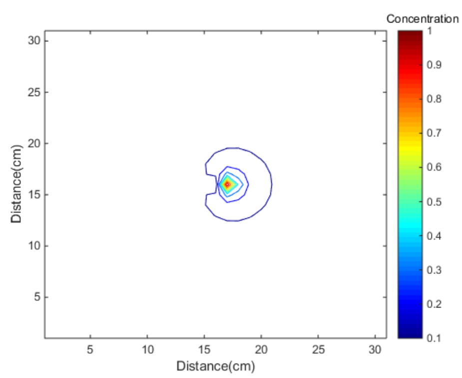


Figure 3: Program verification of solute transport problem

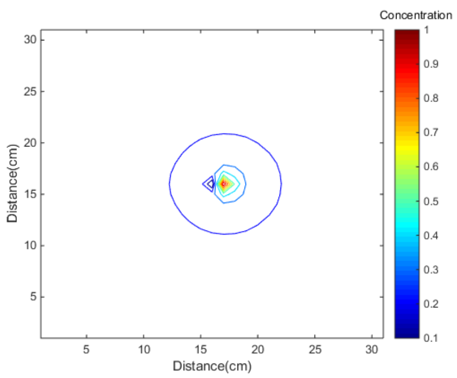
Figure 3 shows the comparison of the results of BGK-D3Q19 model by Zhang (2002) and the results of the MRT-D3Q7 in this paper. It can be seen that on the XY interface and the XY interface, the solute diffusion distribution by the D3Q7 model agrees well with the D3Q19 model, indicating that the method used in this paper is reliable.

3.2 Simulation results

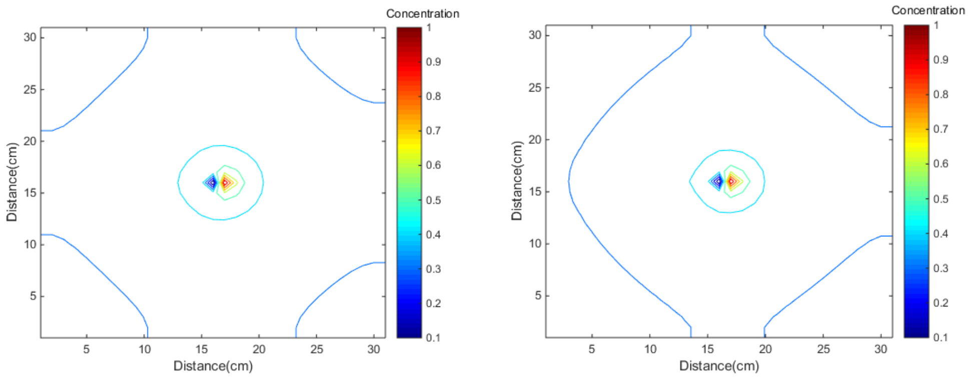
The dimensionless parameters are set as follows: Pr=7, Le=2, Da=5×10^{-4}, Ras=1×10^6, Rat=1×10^5, ε=0.4, simulation period is 40 hours and the temperature boundary changes every 10 hours, including heating period (T=1), heat recovery period (T=T_0), cooling period (T=0), heat recovery period (T=T_0). The maximum absolute residuals of the speed and temperature are both less than 10^{-7}.



(a) T=T_0



(b) T=T_0



(c) T=0 (d) T=T_0

Figure 4: Contaminants concentration fields under periodic temperature boundaries

It can be seen from Figure 4 that at first due to the high temperature of the heat source during heating period(T=1), the natural convection in the porous media is strengthened and the leaked contaminants diffuse faster; when the heat source temperature drops to the normal value (T=T_0), the leaked contaminants diffuse slowly, and the concentration filed tends to be uniform; when the cooling period starts (T=0), the contaminants concentration shrinks and accumulates near the point source, which is due to the negative temperature gradient increasing the flow resistance of the fluid; once the cold source stops working (T=T_0), the point source diffuses more slowly and the concentration gathers near the cold source.

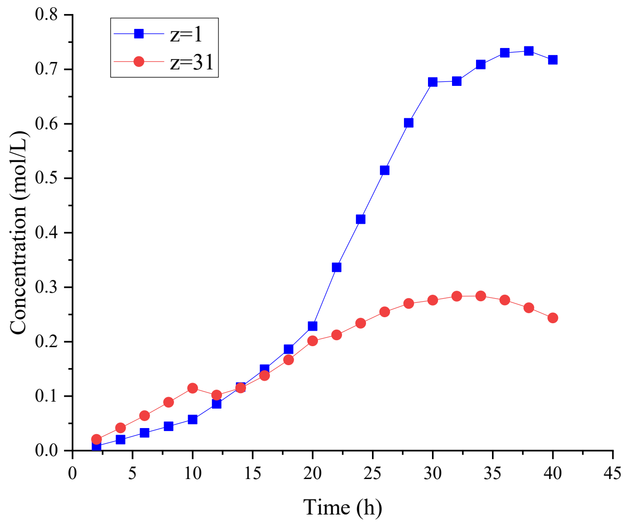


Figure 5: Concentration profile at different depth under periodic temperature boundaries

By comparing the concentration at Z=1cm (the bottom layer) and Z=31cm (the top layer), it can be found that during heating period (1-10h), the contaminants diffusion is affected by the opposite direction of buoyancy lift and gravity and the buoyancy lift is dominant, thus the concentration diffusion of the contaminants at the top layer is two times faster than that of the bottom layer. After the heat source stops working (11-20h), the concentration diffusion of the contaminants at the top layer and the bottom layer is basically the same. After that, under the influence of cold source (21-30h), the contaminants concentration in the bottom layer is more than twice that of the top layer. It is obvious that there is a sharp rise of concentration in the bottom layer near the cold source, while the concentration on the top layer does not show this accumulation trend, which is because the gravity is dominant at this time, the natural convection at the bottom layer is significantly enhanced and the mass transfer is accelerated. After the cold source stops working (31-40h), the concentration at both top and bottom layer diffuses slower, and the concentration at the top layer attends to decrease, which probably because the low temperature causes the fluid flow resistance increases, thus the natural convection is weakened, and the heat and mass transfer are corresponding weakened.

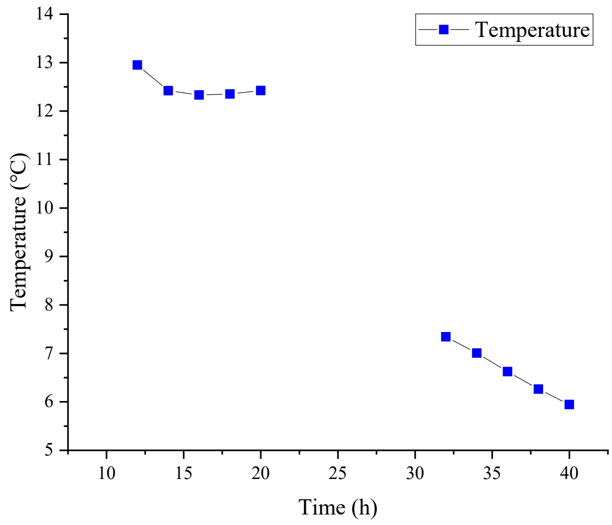
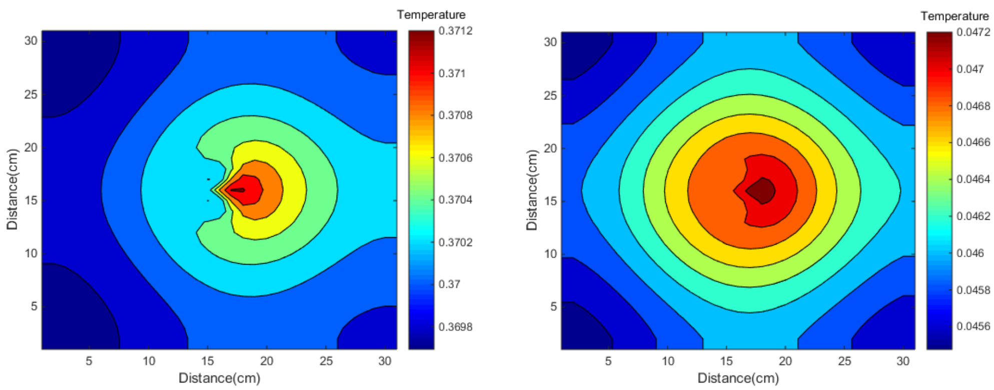


Figure 6: Temperature curve after heat source and cold source stop working



(a) Heat source stops working (b) Cold source stops working

Figure 7: Isotherm distribution in porous medium during recovery period

Figures 6 and 7 show that after the heat source stops working (11~20h), the temperature field of the contaminants is initially uniform, and then the temperature contour is significantly shifted to one side owing to the concentration point source. Moreover the temperature first decreased and then increased. This is because the temperature drops at the beginning and then the natural convection is strengthened by the buoyancy lift, and the temperature increases. After the cold source stops working (31~40h), the temperature field tends to be uniform. The isotherm distribution has an offset trend but not obvious and the temperature drops. This is because the temperature difference decreases and the heat convection is weakened.

4. CONCLUSION

Based on the lattice-Boltzmann D3Q7-MRT model, this paper simulates the double-diffusion natural convection in the square cavity filled with porous medium under the periodic temperature boundaries, the results indicate 1) The temperature gradient causes natural convection in the porous media. The heat source strengthens natural convection and the concentration diffusion of contaminants accelerates. On the contrary, the cold source increases the flow resistance, so the contaminants accumulate near the cold source; 2) Influenced by the temperature and concentration, the concentration diffusion of contaminants at the top and bottom layers of the square cavity is different. The natural convection at the top layer is enhanced by the buoyancy lift, thus the concentration diffusion is accelerated. Contaminants at the bottom layer of the cavity are affected by the gravity, which leads to the concentration accumulation near the cold source; 3) Due to the Soret and Dufour effects, after the heat source stops, the temperature contour has a significant shift near the concentration point source, while the temperature field tends to be uniform after the cold source stops.

ACKNOWLEDGEMENTS

This work is financially supported by the National Natural Science Foundation of China (Grant No. 41672234) and the National Key Research and Development Program of China (Grant No. 2018YFC0604305)

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Nomenclature

ρ	Density (kg/m^3)
t	Time (s)
u	Velocity (m/s)
p	Pressure (Pa)
ε	Porosity
F	External force (N)
T	Temperature (K)
C	Concentration (mol/L)
v_e	Effective kinematic viscosity
α_e	Effective thermal diffusivity
D_e	Effective mass diffusivity
K	Permeability
F_ε	Structure function
G	Body force
H	Height of cavity
u	Velocity in x-direction
U	Dimensionless velocity in x-direction
v	Velocity in y-direction
V	Dimensionless velocity in y-direction
w	Velocity in z-direction
W	Dimensionless velocity in z-direction
c	Lattice speed
c_s	Sound speed
θ	Dimensionless temperature
ψ	Dimensionless concentration
Pr	Prandtl number
Le	Lewis number
Da	Darcy number
Ra_t	Temperature Rayleigh number
Ra_s	Concentration Rayleigh number
β_T	Thermal expansion coefficient
β_C	Solute expansion coefficient
g	Gravitational acceleration (m/s^2)
ω_i	Value factor for velocity
f_i	Density distribution functions
g_i	Temperature distribution functions
h_i	Concentration distribution functions
M	Transform matrix for density distribution
S	Collision matrix for density distribution