



A Randomly Fractal Approach to Calculate the Thermal Conductivity of Moist Soil

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ABSTRACT

Ground coupled heat pump (GCHP) is an energy saving technology that uses the shallow geothermal energy for the building heating and refrigeration systems. An optimized design of ground heat exchangers (GHEs) is the key to minimize the installation fee of GCHP systems. The effective thermal conductivity of soil is an important input parameter in the design of GHEs. This paper proposed a randomly fractal approach to predict the effective thermal conductivity of soil-like materials (quartz sand). The fractal Monte-Carlo method combined with the Quartet Structure Generation Set (QSGS) method was used to reconstruct the random structure of the soil-like materials. Lattice Boltzmann method (LBM) was further applied to the complicated porous structure and compute the effective thermal conductivity. The simulation results were compared to the findings from experiments and other similar models. The impacts of porosity, fractal dimension, size ratio and accumulation structure on the effective thermal conductivity were also analyzed in detail.

INTRODUCTION

Ground coupled heat pump (GCHPs) system is an energy saving technology that utilizes the ground as a steady heating or cooling source. The ground heat exchangers (GHEs) are the key components of GCHPs with high installation fee. A proper design of the GHEs would efficiently improve the performance and decrease the overall cost of the entire system. During the design stage of GHEs, the effective thermal conductivity of soil is an important input parameter to predict the heat transfer between boreholes and the ambient soil. From current literature, the effective thermal conductivity are mainly derived from four types of methods, which are field-testing, empirical correlations [3-5], theoretical modeling [6, 7] and geostatistical simulation. In most GSHP design tools, the effective thermal conductivity are either directly input by considering the findings from field-testing or calculated from empirical correlations with porosity and moisture content. However, from field-testing, it is observed that the measured effective thermal conductivity of moist soil varies differently even at the same location and the neglect of such variations might lead to inappropriate designs; from modelling, most of the models highly depend on the empirical coefficients and other fictitious parameters without physical meanings. A more general form is preferred to

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better predict the variations of the effective thermal conductivity or the heat transfer in the moist soil.

Porosity, thermal conductivity of different phases, size distribution and the pack geometry are some structure related parameters and may affect the effective thermal conductivity of soil-like materials (soil, sand and clay etc.) [1, 2], but such impacts are barely considered in the estimation of the effective thermal conductivity. Experimental and modelling study on the impacts of these structure related parameters would help improve the prediction accuracy of heat transfer belowground. Fractal theory provide a possible way to correlate these structure related parameters [8] with the effective thermal conductivity in porous medium. The fractal models of Sierpinski carpets and sponges are the most simple forms to include structure related parameters during heat transfer analysis [9]. A more realistic structure of soil is required to further investigate the impacts of structural parameters on the effective thermal conductivity of soil. One possible reconstruction technique is to combine the fractal theory with random reconstruction methods, such as Monte-Carlo method [10, 11]. Due to the complex geometries in the realistic structure, it would be difficult to solve the heat and mass transfer by the normally used finite volume or finite element methods. Lattice Boltzmann method (LBM) is a promising mesoscopic method to deal with complex boundaries and has been successfully applied in numerous studies [12-15] of heat and mass transfer in soil-like materials.

Therefore, in this study, a more realistic structure of soil-like materials would be reconstructed by a combined method of MC (Monte-Carlo) [10] and QSGS (Quartet Structure Generation Set) [16], and the effective thermal conductivity of the reconstructed moist soil-like materials would be calculated by LBM algorithm. The factors that would affect the thermal conductivity are analyzed in detail.

NUMERICAL METHOD

Basic concepts

Water film: water accumulates as a layer and covers the exterior surface of the particle, see Figure 1a.

Water bridge: water accumulate locally and form a connection between two particles, see Figure 1a.

Thermal bridge: preferential thermal path with low thermal resistance, see Figure 1a.

Fractal dimension: a characteristic parameter in fractal theory; in this study, it represents the mass proportion of particles in small size, see Figure 1b and c.

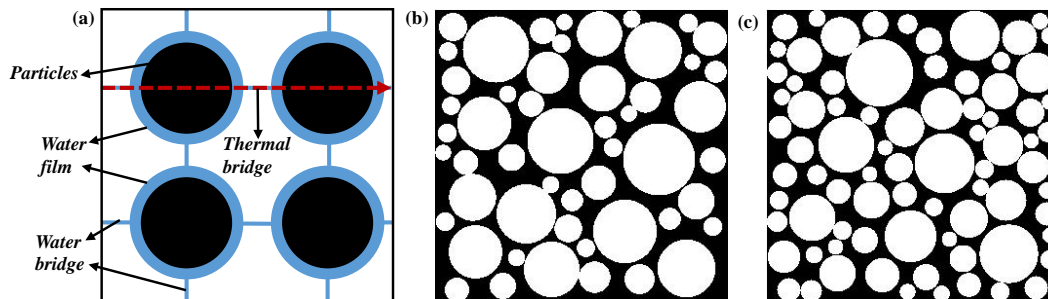


Figure 1. Schematics of (a): water film, water bridge and thermal bridge; (b) and (c): reconstructed soil-like materials when the fractal dimension is 1.1 and 1.7 with the same size ratio and porosity (black - air, white - solids)

Governing equations

In the following analysis, it is assumed that: i) the thermal conductivity of solid is constant; ii) the convective and radiative heat transfer is neglected due to the porous geometry and the low temperature; iii) there are no internal heat sources or body forces; iv) there is no phase change phenomenon; v) heat transfer is two-dimensional. The governing equations are shown in Equations (1) to (3) [16]. The effective thermal conductivity could be calculated by Equation (4).

$$(\rho C_p)_{a/s/w} \left(\frac{\partial T}{\partial t} \right) = k_{a/s/w} \nabla^2 T \quad (1) \quad T_{a,int} = T_{s,int} = T_{w,int} \quad (2)$$

$$k_a \frac{\partial T}{\partial t} \Big|_{a,int} = k_s \frac{\partial T}{\partial t} \Big|_{s,int} = k_w \frac{\partial T}{\partial t} \Big|_{w,int} \quad (3) \quad k_{eff} = \frac{L \cdot \int q \, dA}{\Delta T \cdot \int dA} \quad (4)$$

Reconstruction method

In order to better investigate the impacts of structures on the effective thermal conductivity of moist samples, the geometries are reconstructed by a combined methods of MC (Monte-Carlo) [10] and QSGS (Quartet Structure Generation Set) [16]. MC method is preferred to generate main solid particles in the fractal scale (Equation (5), where λ_i is the radius of the i_{th} particles, R_i is the i_{th} random number ranged from 0 to 1) [8], while QSGS method is added to generate the remains, so the geometries could be more connective (Figure 2b). The reconstruction procedure is summarized in Figure 2a. The generation of water phase would follow the formation of water bridges (when the degree of saturation is lower than 30% [17]) and water films, as shown in Figure 2c, d and e.

$$\lambda_i = \frac{\lambda_{min}}{(1 - R_i)^{1/D_f}} = \left(\frac{\lambda_{min}}{\lambda_{max}} \right) \frac{\lambda_{max}}{(1 - R_i)^{1/D_f}} \quad (5)$$

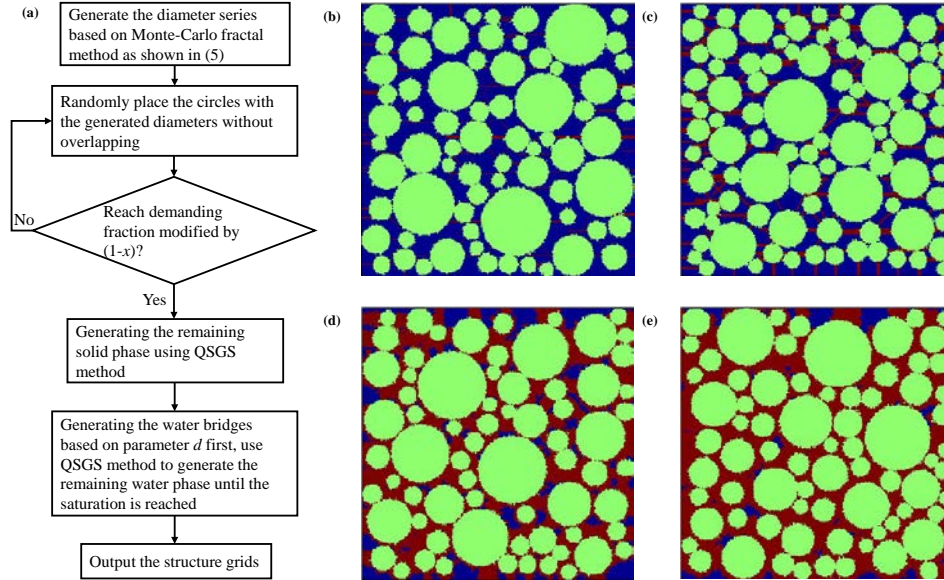


Figure 2. (a) Reconstruction procedures; (b) when the degree of saturation is 0.05; (c) when the degree of saturation is 0.25; (d) when the degree of saturation is 0.5; (e) when the degree of saturation is 0.9 (blue - air, green - solids, red - water)

LBM algorithm

DnQm series are the most commonly used LBM models, and the subscript “n” stands for the dimension of the problem, while the subscript “m” stands for the quantity of the discrete velocities. Due to the relatively large geometry scale of soil-like materials, D2Q5 is selected because of the acceptable accuracy and computation time. Compared to the multiple-relaxation-time (MRT) collision operator (more time consuming) and the single-relaxation-time (SRT) collision operator (less accurate), a twin-relaxation-time (TRT) collision operator is selected because of the accuracy and stability [18, 19]. For conduction problem, the temperature evolution equation with TRT collision operator for D2Q5 could be given in Equation (6) [18].

$$g_i(\vec{r} + \vec{e}_i \delta_t, t + \delta_t) - g_i(\vec{r}, t) = -\omega^+ \delta_t (g_i^+(\vec{r}, t) - g_i^{eq+}(\vec{r}, t)) - \omega^- \delta_t (g_i^-(\vec{r}, t) - g_i^{eq-}(\vec{r}, t)) \quad (6)$$

the subscript “i” represents the discrete directions. The equilibrium population function, the symmetric part and anti-symmetric part of the populations including equilibrium populations could be obtained from Equations (7) to (9).

$$g_i^{eq}(\vec{r}, t) = \begin{cases} 0, & i = 0 \\ T/6, & i = 1 \sim 4 \end{cases} \quad (7) \quad g_i^+(\vec{r}, t) = (g_i(\vec{r}, t) + g_j(\vec{r}, t))/2 \quad (8)$$

$$g_i^-(\vec{r}, t) = (g_i(\vec{r}, t) + g_j(\vec{r}, t))/2 \quad (9) \quad 1/\omega^-_{a/s/w} = 3k_{a/s/w}/((\rho C_p)_{a/s/w} \cdot c^2 \delta t) + 0.5 \quad (10)$$

where the subscript “j” represents the opposite discrete direction of direction “i”. Since energy is conserved in the governing equations, the collision parameter related to the thermal diffusivity is the anti-symmetric one and can be obtained from Equation (10). To assure the temperature and heat flux continuity constrain at interfaces, the volumetric heat capacity (ρC_p) of different phases are assumed to be the same value [20]. c is the lattice constant which equals to δ_x/δ_t , and δ_x is the lattice length step which is commonly set as 1. Once the anti-symmetric collision parameter is determined, the symmetric collision parameter can be computed from Equation (11). The fields of temperature and heat flux can be derived from Equations (12) and (13) [21]. The boundary conditions are specular reflection form for the insulated boundaries and non-equilibrium bounce back form for the isothermal boundaries [22].

$$\Lambda = \left(\frac{1}{\omega_{a/s/w}^+} - 0.5 \right) \left(\frac{1}{\omega_{a/s/w}^-} - 0.5 \right) \quad (11) \quad T(\vec{r}, t) = \sum_i g_i(\vec{r}, t) \quad (12)$$

$$Q(\vec{r}, t) = \sum_i (\vec{e}_i g_i(\vec{r}, t)) \cdot (1 - 0.5\omega_{a/s/w}^-) \quad (13) \quad \vec{e}_i = \begin{cases} (0, 0), & i = 0 \\ ((\cos \theta_i, \sin \theta_i)c, \theta_i = (i-1)\pi/2), & i = 1 \sim 4 \end{cases} \quad (14)$$

where Λ is a magic parameter [18]; it affects the stability and the accuracy of the calculation and this magic parameter is assigned 1/6 in this study [23]. $Q(\vec{r}, t)$ is the heat flux vector and \vec{e}_i is the discrete velocity of the i_{th} direction and is given in Equation (14).

MODEL VALIDATION

The proposed LBM model is validated by two basic two-phase (air-solid) conjugate heat transfer models (named the series and the parallel models). The thermal conductivity of air (k_1) is set as 0.026W/m-K and the higher

thermal conductivity of solid (k_2) is set as a multiple of k_1 . The size of the grids is 200 by 200. The collision parameter of air phase, which is correlated to the thermal diffusivity, is assigned 1.2 based on the comparison with the theory results and this value remains constant in this study. The comparisons between analytical and numerical results derived from the D2Q5 model combined with TRT collision operator are shown in Table 1. It shows that all the relative deviations are lower than 0.5% even when there is a large difference between the values of k_1 and k_2 , which is accurate enough for this study. It should be noted that the relative deviations could be further decreased by adjusting the collision parameters.

Table 1. Comparisons between analytical and numerical results

$k_1: k_2$	Series model			Parallel model		
	Analytical (W/m-K)	Numerical (W/m-K)	Deviations (%)	Analytical (W/m-K)	Numerical (W/m-K)	Deviations (%)
1:5	0.043333	0.043468	0.311831	0.078000	0.078378	0.484423
1:10	0.047273	0.047503	0.487672	0.143000	0.143683	0.477902
1:100	0.051485	0.051736	0.487682	1.313000	1.318126	0.390404
1:1000	0.051948	0.052030	0.157215	13.013000	13.021614	0.100976

RESULTS AND DISCUSSIONS

Comparisons between experimental and simulated results

Quartz sand was selected as the test material and the experimental results of four groups of moist samples (Table 2) were derived by using a thermal conductivity probe. The test procedures followed the standard ASTM D5334-14 and the uncertainty of the thermal probe is $\pm 12\%$ (see the error bars in Figure 3). In order to further investigate the impacts of structural parameters on the thermal conductivity of sand, these four moist samples were varied in porosity, fractal dimension and size ratio. Considering the fact that higher size ratio required less fine grids, grid independency tests was required to minimize the error caused by the accuracy of grids.

Table 2. Structural parameters of four experimental groups

Group No.	Porosity	Fractal Dimension	Size Ratio	Solid Thermal Conductivity
1	0.393	1.7	1:5	1.5W/m-K
2	0.452	1.7	1:5	
3	0.393	1.7	1:23	
4	0.393	1.1	1:23	

The comparisons between the simulation and experimental results with corresponding uncertainty range are indicated in Figure 3. It should be noted that the simulation results were the average values derived from more than 10 randomly reconstructed geometries with the same structural parameters and the experimental results were the average values derived from three locations and three times measurements in each location. From the plot, it was observed that generally the experimental results increased rapidly when the degree of saturation was low (20% in Group 1 and 3,

16% in Group 2 and 32% in Group 4) and then slowed down as the degree of saturation increased. This might be explained by the fact that water bridges among adjacent particles tend to provide preferential thermal paths due to the higher thermal conductivity of solid phase than that of water and air. As the degree of saturation increased, water film started to form and grow, but the impact were less than that of the formally formed thermal path.

Compared to the experimental results, the simulation values indicated similar asymptotic trends. However, the simulation results were 5% to 60% lower than the experimental results and the deviations reached the maximum when the degree of saturation ranged from 10% to 30%. There are four possible reasons to explain such differences. First, the simulated moisture distribution might still be deviated from experimental cases and the regeneration of water distribution should be considered based on the theory of hydromechanics. Second, instead of regular circles, the shape of particles would be random polygon, which could be easier to form water bridges. Third, it was observed that cracks exist in the solid particles of quartz sand, which may lead to a variation on the solid thermal conductivity if water diffuse into the solid particles with small cracks; fourth, when the degree of saturation is low, the heating element in the thermal probe would result in water evaporation and moisture redistribution, which could lead to higher values of test results.

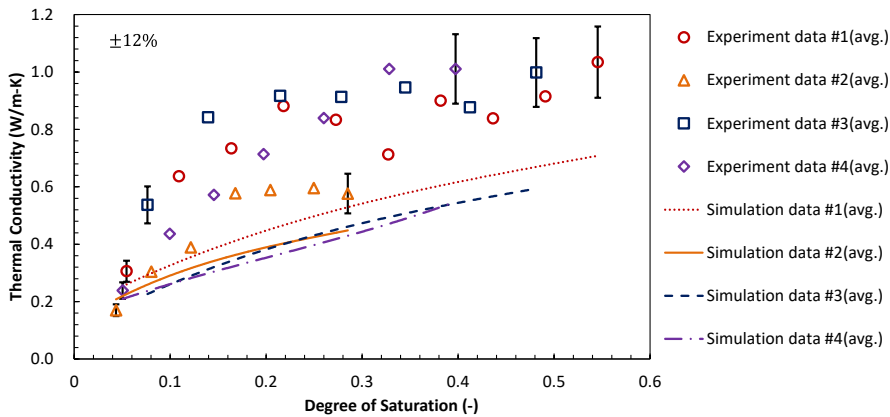


Figure 3. Comparisons between simulation and experimental results with corresponding uncertainty range

Impacts of structural parameters

The impacts of structural parameters on the effective thermal conductivity are indicated in Figure 3. Group 1 and 2 were samples with different porosity. Both experimental and simulated results showed that the values derived in group 1 were always higher than those in group 2 at the same degree of saturation. Therefore, it was verified that porosity would be a dominant factor during the prediction of the effective thermal conductivity of soil-like materials. Group 3 and 4 were samples with different fractal dimensions. Both the experimental and simulated results indicated faster increasing rates in samples with higher fractal dimension (more small size particles). Therefore, the particle size distributions might affect the effective thermal conductivity at low moisture region because it may change the presence of water bridges and would heavily affect thermal path. Group 1 and 3 were samples with different size ratios. The experimental results showed that the thermal conductivity of group 1 were slightly lower than that of

group 3. This was because more conductive thermal bridges were formed among particles with large size differences (small particles filled in the gaps among large particles). However, the simulated values showed opposite conclusion and the thermal conductivity of group 1 were much higher than that of group 3. Such difference might come from the reconstruction stage. The small particles were not only filled in the narrow gaps, but also suspended in the wide space formed among large particles, which deviated from the real cases. Therefore, the impact of size ratio on the effective thermal conductivity still need to be further investigated.

Impact of randomness in accumulation structures

Due to the randomness, the samples would form different accumulation structures even with identical parameters (porosity, fractal dimension and size ratio). Minor differences in the accumulation pattern of particles would vary the effective thermal conductivity of the moist composite. Figure 4 illustrates the uncertainty caused by different accumulation structures. The uncertainty bands were derived from the computation based on more than ten accumulation structures which were randomly generated with identical parameters. It seemed that the uncertainty reached the maximum (ranged from -11.5% to 24.7% based on the average value) when the degree of saturation varied between 20% to 25% and then the uncertainty started to decrease. If all the four groups are considered, then the uncertainty ranges from -25.0% to 40.0%. This was because the variations in accumulation structures would lead to different contact conditions (including both the contact thermal resistance and the formation of water bridges) which might significantly affect heat transfer. The impacts of contact conditions gradually reduced after the fully generation of water bridges. Therefore, the uncertainty bands observed from the plot decreased with the amount of water increased. Quantify the variations caused by the accumulation structures would help explain the results derived from field testing and improve the prediction of ground heat transfer.

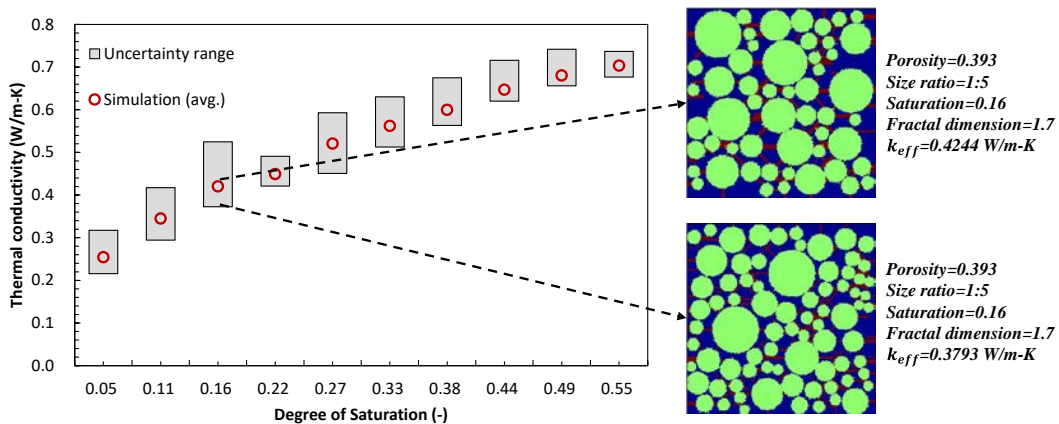
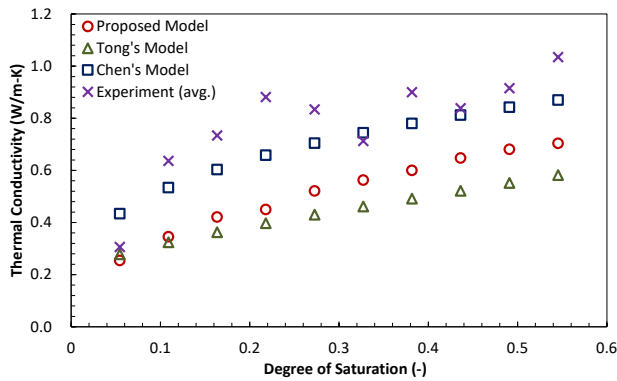


Figure 4. Uncertainty caused by the differences in the accumulation structures

Comparison among similar models

The proposed approach were also compared to other similar prediction models [3, 24] as indicated in Figure 5. The standard deviation is 0.016 for Chen’s model, 0.078 for the proposed model and 0.130 for Tong’s model.

Considering the entire range, Chen's model matched best with the experimental results: the deviations were within 16% when the degree of saturation is higher than 25%. The deviation reached over 25% in the proposed model and over 30% in Tong's model. However, when the degree of saturation is lower than 6%, Chen's model would overestimate the effective thermal conductivity by 41.8%, Tong's model reached the smallest deviation of 9.1% and the proposed model had a deviation of 16.9%. It should be noted that Chen's model is an empirical correlation, which is highly restricted to the test conditions and materials. The proposed model still require further improvements by including the theory of hydromechanics during the reconstruction of water distributions..



Model	Type	Input Parameters
Chen's model	Empirical model	Porosity, degree of saturation and two empirical parameters
Tong's model	Numerical model	Porosity and degree of saturation
Proposed model	Numerical model	Porosity, fractal dimension, size ratio and degree of saturation

Figure 5. Comparisons among similar models

CONCLUSIONS

This paper proposed a randomly fractal approach to predict the effective thermal conductivity of moist soil-like materials and further investigate the impact parameters. Three main findings are summarized as follows:

- (1) Results showed that the proposed model could indicate similar asymptotic trends as the experimental findings, but at lower increasing rates in the low moisture region. Such deviations were possibly caused by the inappropriate moisture distributions reconstructed. Compared to other models, the proposed approach has the potential to reflect more fundamental mechanism of the heat transfer in the soil-like materials with moist.
- (2) Porosity is verified as the dominant parameter on the effective thermal conductivity of moist soil-like materials. Fractal dimension would more affect heat transfer in the low moisture region: higher fractal dimension represents samples with more small size particles and behaves more conductive with the same amount of moisture. Size ratio would also affect the thermal conductivity and materials with larger size ratio seem to behave more conductive. However, the effect of size ratio still needs to be further verified.
- (3) Randomness in the accumulation structures affect the contact conditions among particles and could lead to uncertainties varying from -25.0% to 40.0% of the average values. Such uncertainty bands were observed to reach the maximum with 20% to 25% degree of saturation and then decrease with the amount of water. Quantify the variations caused by the accumulation structures would help explain the results from field testing and improve the prediction of ground heat transfer.

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NOMENCLATURE

Variables			Superscripts and subscripts
A	Heat transfer area	\vec{r}	The location vector
c	Lattice constant	T	Temperature
D_f	Fractal dimension	t	Time
\vec{e}_i	Discrete velocity	Greek symbols	
$g_i(\vec{r}, t)$	Population function of temperature	ΔT	Temperature difference over L
k	Thermal conductivity	δ_t	Time step
L	Thickness	δ_x	Lattice length
$Q(\vec{r}, t)$	Heat flux vector	Λ	Magic parameter
q	Heat flux density	λ	Particle radius
R	Random number ranged from 0 to 1	ρC_p	Volumetric heat capacity
		ω	The collision parameter
		+	symmetric part
		-	anti-symmetric part
		eq	equilibrium populations
		a	air
		s	solid
		w	water
		eff	effective parameters
		int	interface
		max	Maximum value
		min	Minimum value

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