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# Lattice Boltzmann Modeling of Thermal Conduction in Composites with Thermal Contact Resistance

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**Abstract.** The effective thermal conductivity of composite materials with thermal contact resistance at interfaces is studied by lattice Boltzmann modeling in this work. We modified the non-dimensional partial bounce-back scheme, proposed by Han et al. [*Int. J. Thermal Sci., 2008*. **47**: 1276-1283], to introduce a real thermal contact resistance at interfaces into the thermal lattice Boltzmann framework by re-deriving the redistribution function of heat at the phase interfaces for a corrected dimensional formulation. The modified scheme was validated in several cases with good agreement between the simulation results and the corresponding theoretical solutions. Furthermore, we predicted the effective thermal conductivities of composite materials using this method where the contact thermal resistance was not negligible, and revealed the effects of particle volume fraction, thermal contact resistance and particle size. The results in this study may provide a useful support for materials design and structure optimization.

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**Key words**: Lattice Boltzmann method, partial bounce-back scheme, thermal contact resistance, effective thermal conductivity.

## 1 Introduction

It is well known that the thermal contact resistance (TCR) is caused by the low-conductivity interfacial gap between two contact surfaces, which has significant impact in many en-

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gineering applications, such as electronic packaging [1, 2] and composite materials manufacture and design [3, 4]. Because of the often tiny scale and complex shape involved, experimental investigation is often cumbersome and even impossible, many efforts have been made in developing theoretical model to investigate the TCR, based on two basic surface contact modes: the conforming rough surfaces mode [5] and the nonconforming rough surfaces mode [6, 7]. However, in practical issues there are always a lot surfaces with irregular shapes in contact, such as the particle-particle contact in particle-reinforced composites. Thus comes many difficulties in predicting the thermal properties of these composites when the inner TCR is concerned. To the best of our knowledge, few remedies are available to deal with this thorny problem, and numerical methods have therefore become the alternative.

In recent years, the lattice Boltzmann method (LBM) has been developed into a successful numerical scheme for fluid flow simulation [8, 9]. Compared with the traditional CFD methods, LBM has advantages especially for applications involving large number of interfaces or/and complex geometries. Besides for hydrodynamics, efforts have also been made to apply LBM to solving various fluid transport problems coupled with electrokinetics, magnetic, thermodynamics or even chemical reactions [10–17]. Attempts have been made in using LBM to study the interfacial heat transfer process, and a few models have been developed in the lattice Boltzmann method for simulation of the thermo-hydrodynamics since 1993 [18–25]. More specifically, a single distribution function model was introduced into the lattice Boltzmann method to simulate the Rayleigh-Bénard convection. It was however admitted that with severe numerical instability, the applicable temperature range is limited to a narrow scope [18–20]. To overcome the drawback, a double distribution function model was developed [21–23], in which a density distribution function is introduced to simulate the hydrodynamics (fluid flow), while an internal energy distribution function to tackle the thermodynamics (heat transfer). He et al. [23] proved that such double distribution model can appropriately treat the viscous heat dissipation and compression work done by the pressure. However, Hes method is too complicated to use so that several simplified versions have been subsequently developed. For instance, Peng et al. [24] proposed a simple internal energy function evolution method for cases with negligible heat dissipation and compression work. Wang et al. [25] developed a general scheme for fluid-solid interfacial conjugate heat transfer process. Consequently, this type of method has gained wide application in predictions of effective thermal properties of engineering multiphase materials, with results validated by experimental data [26–30].

Furthermore, in analyzing macroscopic engineering materials, an important assumption is the continuity held at interfaces, i.e., thermal contact resistance is negligible. One result this assumption led to is that the effective thermal conductivity of granular porous materials increases with the decreased pore size for a given porosity [31], which agreed well with experimental data from both natural and engineering materials [32, 33]. However, some recent measurements for nanoporous materials have shown some contradictory results that the effective thermal conductivity actually decreases with the reduced