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A dissipative particle dynamics algorithm for fluid-solid conjugate heat transfer

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ABSTRACT

Dissipative particle dynamics with energy conservation (eDPD) is developed to simulate fluid-solid conjugate heat transfer in a microchannel. A temperature reset region placed ahead of a parallel-plate microchannel and a periodic boundary condition with a body force applied in the streamwise direction are used to generate the hydrodynamically developed, thermally developing flow. To insure the temperature and heat flux continuities at the fluid-solid interface, heat transfer in the fluid zone and solid zone is solved entirely, and an equivalent mesoscopic heat friction coefficient is proposed in the eDPD simulation. The results by eDPD method with the new numerical schemes agree well with those by the finite volume method (FVM) for the predictions of heat transfer in a thick-wall microchannel.

1. Introduction

Fluid flow and heat transfer through microchannels has become a popular research topic in the last two decades due to many applications in bioengineering, micro-and nanoelectromechanical systems (MEMS and NEMS) [1]. As the size of channels falls in order of micro scale ranges, the experiential formulas in convectional heat transfer theories can hardly be used to predict the heat transfer at boundaries between fluid and solid. This is because the heat transfer in such microchannels is influenced by various effects such as axial conduction in the wall and temperature dependent properties [2,3].

The hydraulic radii of microchannels we refer to here are about 10–1000 μm. Conjugate effects become more critical in these microchannels than in macro-channels because the microchannels wall thickness become comparable to the small hydraulic radius. The axial heat conduction in the solid wall is very pronounced. Therefore, the channel wall cannot be treated as thin wall. The simple boundary condition impositions, such as constant wall temperature or constant heat flux, are not suitable for such microchannels. A fluid-solid conjugate heat transfer condition is the reasonable boundary condition at the interface, which demands temperature and heat flux continuities. With such a boundary condition, macroscopic numerical methods like the classical finite volume method (FVM) and finite difference method (FDM) have been widely used to study various conjugate heat transfer problems. Toh et al. [4] used the FVM to study the three-dimensional fluid flow and heat transfer phenomena inside heated channels. Li et al. [5] investigated the influence of geometric parameters of the channel and the thermophysical properties of liquid on the flow and heat transfer with the FDM. Recently, Avci et al. [3] performed a numerical simulation of conjugate heat transfer with viscous dissipation in a microtube using the FVM. Their results indicated that axial conduction in the wall decreases the Nusselt number in the entrance region. Aydin et al. [6] applied the FVM to study the conjugate heat transfer in a duct with an axially varying heat flux. Their results obtained for some limiting cases are found to be in a good agreement with those given in the literature. Apart from the macroscopic methods like the FVM and FDM, lattice Boltzmann method (LBM), as a mesoscopic statistics based method booming in these years, has also been used to model the conjugate heat transfer problems. Wang et al. [2] proposed a "half lattice division" treatment for the fluid-solid interaction. They simulated the fluid flow and heat transfer in a heated thick-wall microchannel and the results agree well with the FVM with less mesh number and less computational costs. Cai et al. [7] applied the LBM to simulate fluid-solid coupling heat transfer in fractal porous medium. Tarokh et al. [8] investigated the heat transfer between hot and cold streams separated by a finite thickness and finite thermal conductivity wall using the LBM. More recently, Hu et al. [9] proposed a full Eulerian lattice Boltzmann model for the conjugate heat transfer with complex interfaces. Based on reformulating the lattice Boltzmann equation for solving the conservative form of the energy equation, Karani et al. [10] proposed an approach for studying conjugate heat transfer in

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Nomenclature

u	flow velocity
H	height of the channel
T	temperature
c_p	heat capacity in physical units
Q	internal heating source
t	time
r_c	cutoff radius
r	distance
v	particles velocity
m	mass of DPD particles
f	force
a	repulsion force parameter
e	unit vector
q	heat flux
w	weighting function
C_v	heat capacity in DPD units
k_B	Boltzmann constant
g	body force
D	thermal diffusivity
Pr	Prandtl number
Pe	Peclet number
Re	Reynolds number
s	exponent of weighting function
T^*	dimensionless temperature
Nu	Nusselt number

Greek symbols

ζ^e	random number for the energy
ζ	random number for the momentum
κ	collisional heat flux parameter
κ_o	mesoscopic heat friction
σ	random force parameter
γ	dissipative force parameter
α	random heat flux parameter
λ	thermal conductivity
ρ	density
ν	kinetic viscosity

Subscripts

i,j	indices
s	solid
f	fluid
int	interface
equ	equivalent
m	mean
w	wall
max	maximum

Superscripts

C	conservative
D	dissipative
R	random
$Coll$	collision
$Visc$	viscous
$Rand$	random

heterogeneous media. Compared with macroscopic methods like the FVM and FDM, it seems that the mesoscopic method like LBM is more efficient when dealing with conjugate heat transfer problems with complex geometry [2,7–10].

In this paper, we develop dissipative particles dynamics with energy conservation (eDPD) for the investigation of conjugate heat transfer problems. Dissipative particle dynamics (DPD) is a particle-based mesoscopic method introduced by Hoogerbrugge and Koelman [11]. A single DPD particle represents a cluster of actual molecules or atoms and has soft interactions with other DPD particles. These characteristics ensure that the computational costs of DPD simulations are much less than MD simulations [12]. Although the DPD method is a powerful simulation tool, this method behaves unpredictably to clearly correlate the input simulation parameters to the outputs of interest such as physical properties (viscosity, diffusion, compressibility, thermal conductivity) [13–17]. DPD users have to perform preliminary computation runs to exclude the unpredictability. For example, DPD researchers need to perform a simulation of Poiseuille flow to know the exact values of viscosity though the kinetic theory can relate viscosity to model input parameter. The choices of model parameters influence the simulation greatly and we need to parameterize the simulations carefully. For instance, Moshfegh et al. [13] showed changing weighting functions can adjust system viscosity up to three times higher than theoretical value. Their study also found that the greater values of cut-off radii may lead to the instability of the simulation system. Another problem is that the calibration process is indispensable for using DPD to simulate the real system and this process may be difficult because of the poor scalability inherent in DPD method. The smoothed dissipative particle dynamics (SDPD) may be promising because it allows the simulation with physical properties known as a *priori* [14–16]. However, the SDPD method is actually the smoothed particle dynamics method (SPH) with fluctuation dissipation, which may limit its application compared with DPD. On the other hand, some progress to rectify this scalability problem of DPD method has been made. Recently Moshfegh et al. [17] established clear unit conversion formulas to facilitate the calibration of DPD setting parameters to SI units in their study of electroosmotic flow in nanochannels. The standard DPD method is also limited to isothermal problems. Español [18] and Avalos and Mackie [19] proposed an energy conservative DPD version (eDPD) by introducing internal energy to every single DPD particle. So far eDPD has been utilized to study various heat transfer problems. Ripoll et al. [20] and Abu-Nada [21] applied the eDPD to heat conduction problems. Willemsen et al. [22] developed a numerical model to simulate conduction melting by combing the eDPD with the enthalpy method. Recently Johansson et al. [23] examined a convection solidification problem with the schemes proposed by Willemsen [22]. Natural convection and mixed convection in closed cavities were well modeled by eDPD [24–28]. It is worth mentioning that Cao et al. [26] made a comparison between eDPD and LBM when dealing with the mixed convection in an eccentric annulus. Their results indicated that the simulations conducted by eDPD can have the same accuracy as LBM. Yamada et al. [29] investigated the forced convection in a parallel-plate channel with constant wall temperature and constant wall heat flux. Other studies modified the eDPD for multicomponent heat transfer [30] and heat transfer with temperature dependent properties [31]. There are also some applications to heat transfer in nanocomposite [32] and nanofluids [33,34]. Yamada et al. [35] applied the eDPD to simulate ballistic-diffusive heat transfer in thin films. However, the computational cost is huge. Recently Zhang et al. [36] improved their work by treating the phonons scattering as heat fluxes among DPD particles.