ELSEVIER

International Journal of Biological Macromolecules 41 (2007) 260–265

INTERNATIONAL JOURNAL OF
Biological
Macromolecules
STRUCTURE, FUNCTION AND INTERACTIONS

www.elsevier.com/locate/ijbiomac

A study of local effect and global effect on the microthermal bio-flows by molecular dynamics

David T.W. Lin *

Department of Mechanical Engineering, Far East University, No. 49, Chung Hua Road, Hsin-Shih, Tainan County 744, Taiwan, ROC

Received 27 February 2007; received in revised form 9 March 2007; accepted 9 March 2007
Available online 16 March 2007

Abstract

This study develops a hybrid numerical scheme based on a molecular dynamics (MD) algorithm and the GROMACS protein data bank to analyze the thermal bio-flow of alanine molecules in a microchannel. The numerical results show that the velocity profiles in the microchannel are highly dependent on both global effects, i.e. the effective channel width and local effects, i.e. the thermal boundary conditions. Specifically, the magnitude of the fluctuations observed in the velocity profiles increase as the channel width decreases or as the thermal boundary temperature increases. The results presented in this study provide useful information regarding suitable microchannel widths and operational temperatures for bio-chip devices and contribute a further understanding of basic human thermal bio-flow phenomena, particularly, regarding the correlation between the rate of local metabolism, burn and frostbite events, respectively.

Keywords: Alanine; GROMACS; MD; Thermal bio-flow

1. Introduction

In constructing a thermal bio-flow model to analyze heat and mass transfer phenomena, a key requirement is to establish the correlation between the flow fields established in body fluids and the thermal gradient at fluid's contact boundary. The flow field of the body fluid on the bio-chip and the local metabolism, burn and frostbite will be disclosed as the thermal bio-flow model can be detected. Researchers have employed a variety of bio-heat models to investigate heat transfer phenomena in bio-tissue, including the Pennes equation, Keller and Seiler's analytical method, molecular dynamics (MD) simulations and so forth [1–3]. In general, researchers have considered both micro- and nano-scale thermal flow problems. For example, Niu et al. [4] studied the microthermal flow problem using the thermal lattice Boltzmann model and found that the numerical results were consistent with those obtained under conventional velocity slip and temperature jump boundary conditions. Han [5] investigated the problem of thermophoresis in liquids using a MD approach and showed that the nature of the phenomena induced during thermophoresis is determined principally by the characteristic size of the system involved. Khare et al. [6] employed MD simulations to examine the heat and momentum transfer at a solid–liquid interface characterized by laminar shear flow conditions.

MD simulations are characterized by a fine temporal resolution and therefore, make possible an accurate modeling of the rapid variations inherent in natural molecular systems. Furthermore, the elevation of the protein's force field is the key process in MD. Therefore, MD simulation is one of the most promising methods for acquiring the basic phenomena in the protein system. These phenomena are of great interest to bio-chemical researchers attempting to compile a complete understanding of the roles played by various protein materials in common biomedical problems. Therefore, the protein data banks, which play the important role in the calculation of the molecular dynamics, have been studied in most of the recent papers. Increasingly, these data banks have been used as the basis for MD studies aimed at exploring the basic properties and phenomena of bio-molecules.

For example, El-Bastawissy et al. [7] have studied the protein material at normal and elevated temperature in MD. Suenaga [8] investigated a small-sized protein folding with implicit solvent. The comparison of sampling efficiency between the molecular dynamics and the Monte Carlo method in protein is investigated

* Fax: +886 6 5977510.
E-mail address: david@cc.feu.edu.tw.

0141-8130/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.ijbiomac.2007.03.003

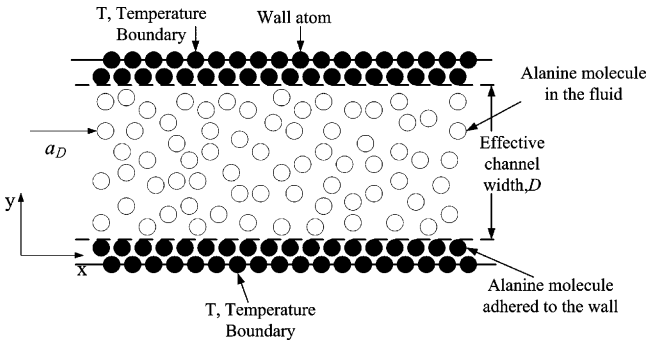

Fig. 1. Schematic diagram of simulation geometry.

by Yamashita et al. [9]. In addition, the development of softcore potential functions for overcoming steric barriers is reported by Hornak and Simmerling [10]. As well, Komeiji et al. [11] studied the protein simulation by parallel molecular dynamics. Zal and Gascoigne [12] use the live FRET imaging to reveal early protein–protein interactions.

Despite the contributions of the studies above, a review of literature reveals that the micro-scale thermal bio-flow problem has received comparatively little attention. Accordingly, the current study combines the GROMACS protein data bank with MD simulations to investigate the flow field characteristics of alanine protein thermal bio-flows in a microchannel. The simulations focus specifically on the respective effects of the effective microchannel width and the thermal boundary conditions at the liquid–solid interface on the velocity profiles of the alanine molecules. The results of the simulations are intended to provide a further understanding of basic human thermal bio-flow phenomena and to provide useful information regarding a suitable design and operational parameters for bio-chip microchannels.

In this present study, MD is used to calculate the micro-scale bio-flow problem, the reason is that the ratio of the microchannel diameter and the bio-molecule diameter is similar as the ratio of the nano-channel diameter and the water molecule diameter.

The remainder of this paper is organized as follows. Section 2 presents a high-level overview of the current simulation procedure and introduces the relevant mathematical formulations. Section 3 describes the detailed steps involved in the simulation procedure and presents the relevant simulation parameters. Section 4 presents and discusses the numerical results obtained for the velocity flow fields under various effective microchannel width and thermal boundary conditions. Finally, Section 5 summarizes the overall contributions and findings of the study.

2. Mathematical model

As discussed above, the simulations conducted in this study consider the thermal bio-flow of alanine (NHC_2H_4CO) molecules in a microchannel under various microchannel width and thermal boundary conditions. Fig. 1 presents a schematic illustration of the simulation system. The simulations are performed using a hybrid iterative scheme comprising a MD algorithm and the GROMACS protein data bank.

The velocities and positions of the alanine molecules are computed using the leap-frog method [13,14] (i.e. a modified Verlet algorithm), while the effect of the thermal boundary conditions on the protein molecules are modeled using the Andersen thermobath method [15]. The instantaneous velocities of the alanine molecules adhering to the microchannel wall are corrected at each time step in order to maintain the wall temperature at the required value, i.e.

$$T_a = \frac{1}{3N}\left\langle \sum_i v_i^2 \right\rangle, \quad v_i^{new} = v_i\sqrt{\frac{T_s}{T_a}} \tag{1}$$

where N is the number of molecules in the specified region, T_a the instantaneous temperature of the specified region following all of the colliding processes at each time step, T_s the initial temperature of the specified region, v_i the velocity of the ith molecule following all of the colliding processes at each time step and v_i^{new} is the corrected molecular velocity of the ith molecule.

The simulations commence by performing an equibration process in which Eq. (1) is used to adjust the velocities of the molecules when the system is maintained to be in a particular temperature. From basic statistical thermodynamic principles, it is known that the initial velocities of the molecules in an equilibrium system are distributed in accordance with a Maxwell–Boltzmann velocity distribution provided that the temperature of the isolated system is constant. In addition, in a Maxwell–Boltzmann velocity distribution with a system temperature of T, the probability of the ith molecule having a velocity value between v and $v + dv$ is given by

$$p(v)\,dv = \sqrt{\frac{m}{2\pi k_B T}}\exp\left(-\frac{m}{2k_B T}v^2\right)dv \tag{2}$$

In addition, the net momentum of the system must be equal to zero in order to guarantee that the system will not move due to an external force. The conservation conditions for the momentum are described as below.

$$v_i^{new} = v_i - \frac{1}{N}\sum_{i=1}^{N} p_i \tag{3}$$

where p_i is the momentum of the ith molecule. As well, the heat current J [16] is

$$J = \frac{1}{2}\left(\sum_{i=1}^{N} m v_i^2 \vec{v}_i + \sum_{i=1}^{N}\sum_{j\neq i}^{N}\left(\phi(r_{ij})\vec{v}_i - w(r_{ij})\frac{\vec{r}_{ij}}{r_{ij}}\vec{v}_i\frac{\vec{r}_{ij}}{r_{ij}}\right)\right) \tag{4}$$

where $\phi(r_{ij})$ is the potential between molecule i and j. Additionally, $w(r_{ij})$ is the pair virial function and defines as

$$w(r_{ij}) = r_{ij}\frac{d\phi(r_{ij})}{dr_{ij}} \tag{5}$$

The objective of the current flow problem is to establish the gross fluid motion rather than the instantaneous velocity. The average dimensionless velocity $v_{i,k,z}$ of the gross fluid motion