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MODELING OF MICRO/NANO CHANNEL FLOWS

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ABSTRACT

This paper reviews the models for the fluid flow in micro/nano channels developed previously. These models include the full MDS (molecular dynamics simulation) model, the quasi-continuum model, the modified Navier-Stokes equation model, the dissipative particle dynamics method, the lattice Boltzman method, the multiscale hybrid model and the flow factor approach model. It was pointed out that most of the models have their own imperfections like huge time and computer storage consumption for simulating a system of realistic size or inaccuracy because of the model limitation. It was also mentioned that the most challenging is to develop efficient models for simulating engineering flows which often occur in much longer channels than currently simulated on a computer. These welcome models should be sufficiently accurate with fast calculation and acceptable computer storage consumption.

Keywords: *Micro/nano channel flow; Model; Continuum; Non-continuum; Molecular dynamics.*

1. INTRODUCTION

With the development of small size equipment like MEMS (micro electromechanical systems), micro fluidics and micro transportation and cooling systems, fluid flows occur in very small channels the heights of which are on the micrometer or nanometer scales(Pham et al., 2007; Senturia, 2001; Squires and Quake, 2005). Such flows often can not be satisfactorily described by continuum theory like the Navier-Stokes equation, because the fluid-wall interaction plays a role in the flow and this interaction makes the fluid become non-continuum across the channel height and/or make the fluid-wall interfacial slippage occur (Bitsanis et al., 1987; Somers and Davis, 1992).

In the past decades, various theoretical and experimental researches were taken on the micro/nano channel flow (Bitsanis et al., 1988; Cheikh and Kopper, 2003; Craig et al., 2001; Jabbarzadeh et al., 1997; Koo and Kleinstreuer, 2003; Takaba et al., 2007; Thompson and Troian, 1997; Whitby et al., 2008; Yang and Zheng, 2010; Zhu and Granick, 2001). Both theory and experiment showed that the fluid-wall interfacial slippage may often occur in micro/nano channel flow, depending on the fluid-wall interaction (Cheikh and Kopper, 2003; Craig et al., 2001; Jabbarzadeh et al., 1997; Takaba et al., 2007; Thompson and Troian, 1997; Zhu and Granick, 2001). A hydrophobic wall frequently results in the interfacial slippage, while a hydrophilic wall alleviates or prevents the interfacial slippage (Cheikh and Kopper, 2003; Craig et al., 2001; Jabbarzadeh et al., 1997; Takaba et al., 2007; Thompson and Troian, 1997; Zhu and Granick, 2001). The MDS results showed that the fluid is ordered to the wall and thus non-continuum across the channel height when the channel height is on the scale of the fluid molecule diameter i.e. on the nanometer scale (Bitsanis et al., 1988; Jabbarzadeh et al., 1997; Takaba et al., 2007; Thompson and Troian, 1997; Yang and Zheng, 2010). The non-continuum effect of the confined fluid is caused by the fluid discontinuity and inhomogeneity across the channel height, contributed by the fluid-wall interaction (Zhang and Lu, 2005; Zhang, 2006). This effect can have a very significant influence on a nano channel flow (Bitsanis et al., 1988; Jabbarzadeh et al., 1997; Sofos et al., 2009 and 2015; Takaba et al., 2007; Thompson and Troian, 1997; Yang and Zheng, 2010). Also, the fluid-wall interaction has a strong influence on the density and viscosity profiles across the channel height, which show that both the density and viscosity of the confined fluid across the channel height are actually inhomogeneous in a nano channel flow. The enhancement of the density and viscosity of the confined fluid due to the fluid-wall interaction should also be considered in the study of a nano channel flow (Meyer et al., 1998).

Conventional (continuum) hydrodynamic theory suffers from obvious shortcomings in describing a micro/nano channel flow, owing to ignoring the fluid-wall interfacial slippage, the fluid non-continuum effect and the enhancement of both the density and viscosity of the confined fluid due to the fluid-wall interaction (Pinkus and Sternlicht, 1961; Temam, 2000). It often fails to predict a micro/nano scale flow (Chan and Horn, 1985; Cheikh and Kopper, 2003; Craig et al., 2001; Liu and Li, 2011; Zhu and Granick, 2001). In this circumstance, a lot of models have been proposed for depicting micro/nano channel flows, include the full MDS model, the quasi-continuum model, the modified Navier-Stokes equation model, the dissipative particle dynamics method, the lattice Boltzman method, the multiscale hybrid model and the flow factor approach model. These models have more or less capabilities to predict micro/nano scale flows. They may be suitable in certain operating conditions. The challenging thing or the existing problem are that most of the models cannot be successfully applied to an engineering modeling of micro/nano channel flow in which the channel length is several orders larger than the channel height, because of the huge computational time and storage consumption or the calculation inaccuracy.

The present paper makes a review on the current existing models for micro/nano channel flows and make discussions about their advantages and shortcomings. This review may be helpful for developing potential models for simulating an engineering micro/nano

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channel flow.

2. CURRENT MODELS

2.1 Full MDS Model

Various studies have been made on nano channel flow by using molecular dynamics simulation (Bitsanis et al., 1988; Jabbarzadeh et al., 1997; Takaba et al., 2007; Thompson and Troian, 1997; Yang and Zheng, 2010). Here are only listed part references. This scheme belongs to a direct simulation and has the advantage of satisfactory accuracy. It considers the interactions between the fluid molecules and between the fluid and wall molecules by using the Lennard-Jones interaction potential model, the Coulomb interaction potential model or other suitable interaction models (Bitsanis et al., 1988; Jabbarzadeh et al., 1997; Rudyak, 2009; Stillinger and Rahman, 1974; Sun and Ebner, 1992; Takaba et al., 2007; Thompson and Troian, 1997; Yang and Zheng, 2010). The Lennard-Jones potential model is a short-range interaction model and was often used previously because of its convenience in calculation by using the cutoff circle radius. Taking this model will substantially reduce the burden of computational time and storage and thus make the simulation feasible by using thin walls as shown in Fig.1. The Lennard-Jones potential model reads (Allen and Tildesley, 1989):

$$U_{i,j} = 4U_0[(\frac{a}{r_{i,j}})^{12} - (\frac{a}{r_{i,j}})^6] \tag{1}$$

where U_0 is a constant potential energy, a is a characteristic length, and $r_{i,j}$ is the distance between two molecules.

By using the Lennard-Jones potential model in MDS, Liu and Li (2011) showed that the Navier-Stokes equation can be valid for the channel height greater than 50nm, regardless of the fluid-wall interaction; For a nano channel height on the 1nm scale, MDS should normally be used to simulate the fluid flow inside the channel to capture the special flow characteristic; The flow was heavily dependent on the fluid-wall interaction.

The Coulomb interaction model is a long-range interaction model describing ionic interactions. This model is also frequently used for describing a realistic inter-molecular interaction (Dang and Chang, 1997; Lee and Rossky, 1994). Applying this model requires the usage of thick walls as shown in Fig.1. This will cause a heavy increase of the computational time and storage consumption, which sometimes makes the computation unaffordable. The Coulomb interaction model for two charged atoms reads (Allen and Tildesley, 1989):

$$U_{i,j} = K_c \frac{q_i q_j}{r_{i,j}} \tag{2}$$

where q_i and q_j are respectively the charges of the ith and jth atoms and K_c is the Coulomb constant.

In a more general case, the short-range and long-range interactions may simultaneously occur between two molecules. In this case, the inter-molecular potential energy should be calculated by (Allen and Tildesley, 1989):

$$U_{lk} = \sum_{\mu \in l}\sum_{v \in k}\{\frac{q_\mu q_v}{r_{l\mu,kv}}K_c + 4U_{\mu v}[(\frac{a_{\mu v}}{r_{l\mu,kv}})^{12} - (\frac{a_{\mu v}}{r_{l\mu,kv}})^6]\} \tag{3}$$

where q_μ and q_v are respectively the charges of the interacting atoms of the two molecules, $r_{lu,kv}$ is the distance between the interacting atoms of the two molecules, and $a_{\mu v}$ and $U_{\mu v}$ are respectively the same with a and U_0 in Eq.(1).

The heavy burden of computational time and storage currently limits a full MDS only to particular cases with very small channel length and thin walls. In the current circumstance, a full MDS scheme is difficult to carry out for an engineering micro/nano channel flow, which has a significantly larger channel length.

In a normal MDS, the flow velocity in a nano channel should be sufficiently high to reduce the calculation errors caused by the thermal motion of molecules. Zhang and Li (2007) developed an MDS scheme which can calculate the low flow velocity in a nano channel flow.

Altogether, the current challenges to MDS, which arise from engineering, are: (1) the long channel simulation; (2) the inter-molecular interaction model implementation which requires the usage of thick walls; (3) low flow velocity simulation. Overcoming these problems and improving the application of MDS may rely on the developments of new computers and new computational schemes.

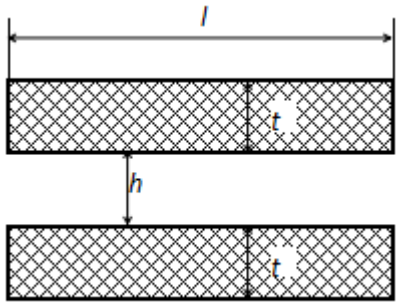

Fig. 1 A nano channel flow. h: the channel height; t: the wall thickness;l: the channel length. In a normal MDS, h, t and l are on the same scale in magnitude. Thin wall: h and t are on the same scale in magnitude. Thick wall: $t >> h$. Long (engineering) channel: $l >> h$.

2.2 The Quasi-Continuum Model

In itself, a continuum hydrodynamic theory is not suitable for a nano channel flow, which is essentially non-continuum. Since a non-continuum theory was not easy to be developed for a nano channel flow, the quasi-continuum model were ever developed for describing this flow. Bhadauria and Aluru (2013) developed a quasi-continuum model for a nanoscale fluid flow which was a transport model using the Cauchy momentum equation as follows:

$$\frac{D\rho u}{Dt} = -\nabla P + \nabla \cdot \tau + f \tag{4}$$

where $D/Dt = \partial/\partial t + u \cdot \nabla$ is the material derivative, u is the velocity field, ρ is the fluid mass density, P is the hydrostatic pressure, f is the body force per unit volume, τ is the deviatoric stress tensor.

In their model, the fluid-wall interfacial slippage was considered, the density variation along the confinement was calculated to facilitate the computation of viscosity profile across the channel height; the viscosity was a density dependent property. Their treatment was reasonable according to the MDS results. They showed that their model for a Poiseuille flow well agreed with the MDS results for certain operating conditions.

Giannakopoulos et al. (2014) proposed a quasi-continuum model for self-diffusion and fluid ordering in nano channel flows, which is based on the following basic constitutive equation:

$$J = -M\nabla\mu \tag{5}$$

where J is the diffusional flux, M is the diffusional mobility, and μ is the local chemical potential.

In their model, the fluid-wall interaction was introduced; the model was of Schrodinger type. Their model was capable of capturing

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the fluid ordering and the density variation across the channel height in a nano channel flow as found by MDS. The shortcoming of their model is that it still requires an MDS calculation to extract fluid parameters. Compared to a full MDS, their model requires a smaller computational cost, and it can also be easily implemented to two and three dimensional domains, by using various boundary conditions (Giannakopoulos et al., 2014).

There actually are a lot of the similar models for a nano scale flow. Here are only discussed limited references. The advantage of a quasi-continuum model is that it can greatly facilitate the computation for an engineering nano channel flow by largely reducing the computational time and storage cost. However, the shortcoming of such a model is that the model can suffer from inaccuracy and it is often applicable for certain operating conditions.

2.3 The Modified Navier-Stokes Equation Model

The Navier-Stokes equation is a continuum equation, which should fail for a non-continuum flow. Liu and Li showed that when the channel height was sufficiently large, the Navier-Stokes equation was still valid; While for a very small channel height, the Navier-Stokes equation failed (Liu and Li, 2011). Roohi and Darbandi (2009) modified the Navier-Stokes equation for solving the velocity distribution in micro/nano channel flows by using the slip boundary conditions and the viscosity coefficient (i.e. effective viscosity). It is a problem in this scheme that the velocity profile and the mass flow rate often can not be correctly solved simultaneously. For solving this problem, the Knudsen number should be limited to a certain range.

A lot of other people also ever used the modified Navier-Stokes equation to predict a nano channel flow by considering the fluid-wall interfacial slippage. Some found the success of this equation for giving the flow velocity profile in certain operating conditions. In itself, such an equation is essentially continuum and should not cover all nano channel flows.

2.4 The Dissipative Particle Dynamics Method

The dissipative particle dynamics method is like a coarse grain method. Kasiteroupoulou et al. (2011) used this method to simulate a nano channel flow. The method incorporates the parameters of the fluid-wall interaction, the wall number density, the cutoff circle radius and the external driving force. The model considers the force exerted on the ith particle by the jth particle to be consisted of three components, i.e. (Kasiteroupoulou et al., 2011) :

$$\vec{F}_{ij} = \vec{F}^{C}_{ij} + \vec{F}^{D}_{ij} + \vec{F}^{R}_{ij} \tag{6}$$

where $\vec{F}^{C}_{ij}$ is the conservative force, $\vec{F}^{D}_{ij}$ is the dissipative force, and $\vec{F}^{R}_{ij}$ is the random force. These three forces are respectively expressed as:

$$\vec{F}^{C}_{ij}(r_{ij}) = \begin{cases} \alpha_{ij}(1-\frac{r_{ij}}{r_c})\hat{r}_{ij} & , \text{ for } r_{ij} \le r_c \\ 0 & , \text{ for } r_{ij} > r_c \end{cases} \tag{7}$$

where α_{ij} is the maximum repulsion between the ith and jth particles, r_{ij} is the distance between these two particles, $\hat{r}_{ij} = \vec{r}_{ij}/r_{ij}$, and r_c is the cutoff circle radius.

$$\vec{F}^{D}_{ij} = -\gamma\omega^{D}(r_{ij})(\vec{v}_{ij}\cdot\hat{r}_{ij})\hat{r}_{ij} \tag{8}$$

where γ is the coefficient determining the magnitude of the dissipative force, $\vec{v}_{ij}$ is the velocity of the ith particle relative to the jth particle, and ω^{D} is the weight function providing the range of interaction for the dissipative force.

$$\vec{F}^{R}_{ij} = \sigma\omega^{R}(r_{ij})\xi_{ij}\hat{r}_{ij} \tag{9}$$

where σ is the coefficient determining the magnitude of the random force, ω^{R} is the weight function providing the range of interaction for the random force, and ξ_{ij} is a random variable with Gaussian statistics. All forces between the ith and jth particles vanish for $r_{ij} > r_c$.

Duong-Hong et al. (2008) also ever used the dissipative particle dynamics method to simulate a nanoscale flow and suggested that this method would be more capable of handling a complex system compared to a full MDS. Although this method may be faster and more efficient than a full MDS in treating a complex system, its calculation accuracy may be lowered compared to a full MDS. For simulating a big size system, this method may also face the problem of massive computational time and storage consumption. Regarding this method, more references can be found.

2.5 The Lattice Boltzman Method

The lattice Boltzman method (LBM) has been widely used in simulating both gas and fluid dynamics. It is like a coarse grain method. LBM models a fluid as consisted of various particles which move with lattice velocity. The particle dynamics is expressed by the lattice Boltzman equation (Zhang, 2011):

$$f_i(x + c_i\Delta t, t + \Delta t) - f_i(x,t) = \Omega_i(f) \tag{10}$$

where $f_i(x,t)$ is the probability of finding a particle at lattice cite x at time t, $\Omega_i(f)$ is the collision operator, and c_i is the moving velocity of the particle.

For macroscopic (bulk) flow, LBM is actually the numerical discretization of the Navier-Stokes equation. This method is not only valid for low Knudsen numbers such as in macro scale flow, but also valid for high Knudsen numbers, for which micro/nano channel flows occur. It can deal with the slip flow and the fluid-solid interaction (Hartings et al., 2009).It is a natural tool for studying rarefied gas dynamics. The method has the advantage of easily treating the boundary condition (Zhang, 2011). It was proposed that LBM is able to reach experimental time and length scales, and is suitable for modeling microfluidic application in contrast to MDS (Hartings et al., 2009). Although LBM may be remarkably faster in computation than MDS for a nanoscale simulation (Zhang, 2011), when simulating a long channel nanoscale flow, simply using LBM may still encounter the similar problems in computational time and storage consumption as in MDS.

2.6 The Multiscale Hybrid Model

The multiscale hybrid models were developed for solving a micro channel flow in which the channel height is relatively large while the fluid-wall interfacial phenomena should be considered (Atkas and Aluru, 2002; Liu et al., 2007; Nie et al., 2004; Sun et al., 2010; Yang and Zheng, 2010; Yen et al., 2007). In this case, close to the wall is implemented an MDS or MCS (Monte Carlo simulation) scheme, while away from the wall is implemented a continuum model. By this way, the calculation can not only be fast and computer-storage saved, but also give correct results. Across the channel height, there is a coupling subzone which is a transition zone of the two different schemes. Yen et al. (2007) proposed that the height of the pure MDS region should be at least 12σ for validity and sufficiently accuracy of the hybrid

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simulation. Better convergence can be obtained with an overlap region of at least 10σ in height (σ is the diameter of the fluid molecule) (Yen et al., 2007).

Besides the MDS or MCS-continuum hybrid schemes, there is the MDS-LBM hybrid scheme. In a hybrid simulation, LBM can handle the continuum flow, while MDS computes a nanoscale flow. It was said that by the appropriate mapping of length and time units from LBM to MDS, the velocity field obtained from MDS can be reproduced by LBM (Zhang, 2011). This implies a feasible way of an MDS-(multigrid) LBM hybrid simulation for a multiscale complex flow (Zhang, 2011). In this hybrid scheme, LBM can be coupled with MDS at the finest scale such as near the boundary, and then progressively increase the LBM mesh size in the bulk flow by using a multigrid method(Zhang, 2011). This can efficiently save the computational time and storage while successfully solve a multiscale flow.

For a long micro channel flow, the above mentioned multiscale hybrid schemes may also face the problems of huge computational time and storage consumption which is unaffordable. For overcoming this kind of problem, Borg et al. (2013) proposed the internal multiscale method (IMM) for simulating micro/nano channel flows. In this method, the channel was divided into separated micro sub-domains and macro sub-domains. In the micro sub-domain, MDS was implemented, while in the macro sub-domain, conventional hydrodynamic conservation equation was employed. The method optimized the use of the MDS by applying it only at a limited number of streamwise-distributed cross sections of the macroscale geometry. This method is more capable of handling longer channels with faster calculation compared to a full MDS. The accuracy of the method depends on the number of the separated micro sub-domains in the whole channel. IMM on the (i-1)th molecule across the channel height, $\delta\tau_i$ is the shear stress difference between the two molecules, D is the fluid molecule diameter, p is the hydrodynamic pressure, and x is the coordinate in the direction of the confined film flow. The model treats the fluid as non-continuum and incorporates the fluid discontinuity and inhomogeneity across the channel height, which are dependent on the density profile.

This model gives the flow equation for a nanoscale fluid flow as (Zhang, 2016a):

$$q_{m,bf} = \bar{lu}\, h\rho_{bf}^{eff} + \frac{S\rho_{bf}^{eff} h^3}{12\eta_{bf}^{eff}}\frac{dp}{dx} \tag{13}$$

where $q_{m,bf}$ is the mass flow rate of the confined fluid through the nano channel, h is the channel height, $\bar{lu} = (\bar{u}_a + \bar{u}_b)/2$, ρ_{bf}^{eff} and η_{bf}^{eff} are respectively the average density and effective viscosity of the confined fluid across the channel height, and S is the parameter depicting the non-continuum effect of the confined fluid ($-1 \le S < 0$);

Here, $\bar{u}_a$ and $\bar{u}_b$ are respectively the velocities of the confined fluid at the upper and lower channel walls.

As Eq. (13) shows, the model also incorporates the fluid-wall interfacial slippage and is an equivalent continuum model. For a sufficient large value of h, Eq. (13) is reduced to a continuum Reynolds equation. This model was validated by comparison with the MDS results (Zhang, 2015a and b, 2016a, b and c). It not only can give the correct velocity profiles across the channel height but also can calculate the correct mass flow rates through the channel, for both the Couette and Poiseuille flows (Zhang, 2015a and b, 2016a, b and c). The model transforms a non-continuum flow as an equivalent continuum problem.

This model has been successfully applied in the analysis of engineering nano channel flow problems such as nano bearings, in which the bearing width is far larger than the nanometer scale film thickness (Zhang, 2013, 2015c and d). The model has the advantages of fast calculation and normal computer storage consumption even for engineering nano channel flows.

seems only capable of solving the flow problem in a particular long channel with required geometrical configuration. However, it still cannot solve the flow problem in a general long micro channel, which may have the same cross section everywhere. In this case, the fluid-wall interfacial phenomena along the whole channel length may need to be modeled, and IMM is not applicable.

2.7 The Flow Factor Approach Model

The author and his colleague proposed the flow factor approach model for describing a nanoscale flow (Zhang and Lu, 2005; Zhang, 2006). The model treats the fluid molecule as a rigid particle and formulates the particle dynamics in equilibrium state by the following two equations (Zhang and Lu, 2005; Zhang, 2006):

$$\tau_{i-1} = \frac{\eta_{line,i-1}\delta u_i}{\Delta_{i-1}} \tag{11}$$

and

$$\delta\tau_i = \frac{\partial p}{\partial x} D \tag{12}$$

where i and (i-1) are respectively the order numbers of the two molecules across the channel height, δu_i, $\eta_{line,i-1}$ and Δ_{i-1} are respectively the velocity difference, the local viscosity and the separation between the two molecules, τ_{i-1} is the shear stress acting

3. CHALLENGES TO CURRENT SIMULATION

Micro/nano channel flows in the past simulation were mostly idealistic and simplified. For example, in MDS, a simple fluid such as liquid argon was often used, both the channel wall and the fluid-wall interaction were often modeled by the Lennard-Jones interaction potential model, and the channel wall was often a "thin wall" (Bitsanis et al.,1988; Jabbarzadeh et al., 1997; Takaba et al., 2007; Thompson and Troian, 1997; Yang and Zheng, 2010). However, in practice, the flowing fluid in a micro/nano channel may be more complicated and can be composed of charged atoms such as water (Mao and Zhang, 2014) and alcohol(Kinugawa and Nakanishi, 1988), the channel wall may also be more complicated and consisted of charged atoms, the fluid-wall interaction may be required to be modeled by a more complicated interaction potential model such as shown by Eq.(3), and the channel wall may often be a "thick wall". These will substantially increase the complexity and difficulty of the simulation for a micro/nano channel flow, since both the computational time and storage are greatly increased. Moreover, other factors in engineering micro/nano channel flows will construct challenges to most of current existing simulation models, described as follows:

(a) Length of a channel and thickness of the wall

In an engineering micro/nano channel flow, the channel length is far larger than the channel height and even on the millimeter scale. It is a "long channel" flow, as shown in Fig.1. Also, the thickness of a channel wall is also much greater than the channel height. Both the long channel and a thick channel wall currently often make most of the simulation models mentioned above unaffordable because of the huge computational time and storage consumption and also the confronting simulation convergence problem.

(b) Irregularly rough channel wall

In previous simulations, for simplicity, the roughness of a channel wall were taken as periodic and of particular configuration such as rectangular shaped (Kasiteropoulou et al., 2013; Sofos et al., 2009). In an actual micro/nano channel flow, the roughness of a channel wall is often irregular and its influence on the flow needs to be considered. This is a challenge to an MDS or most of the current simulation

models. In the simulation, one problem is how to model the irregular wall roughness, and the second problem is to include the whole channel length for simulation, which is too large to take for most of the simulations on a current computer.

(c) Inhomogeneous wall surface

In a nano channel flow, inhomogeneous wall surface was found to be beneficial for the mass transfer through the channel whenever the Poiseuille flow or the Couette flow occur (Zhang, 2016d and e). For inhomogeneous wall surfaces, an MDS or most of the other models may also encounter the problem, since each type of wall surface occupies a channel length which is far larger than the channel height and the channel is actually a "long channel".

All the above mentioned factors in a realistic micro/nano channel flow construct challenges to most of current simulations. Although the flow factor approach model appears capable to handle the above mentioned simulation problems, its validity for more complex liquid molecules needs to be further examined. In the future, potent models and computational schemes need to be developed for solving the existing problems and make the simulation of an engineering micro/nano channel flow feasible.

4. CONCLUSIONS

The current modeling methods for micro/nano channel flows are reviewed in this paper. The characteristic, advantages and shortcomings of these methods were pointed out. Challenges to these methods were also mentioned. A good model should find a satisfactory balance between calculation accuracy, computational time and storage consumption. Most of the current models are not well satisfactory in solving the problem of an engineering micro/nano channel flow, either because of calculation inaccuracy or because of huge computational time and storage consumption.

The most challenge to current simulation arises from engineering micro/nano channel flows, because of the following factors: (a) Channel length or/and channel wall thickness far larger than the channel height; (b) Irregularly rough channel wall; (c) The use of inhomogeneous wall surface. These factors require a calculation scheme must consider the whole length of an engineering micro/nano channel, which makes a molecular dynamic simulation or most of the current simulation models often unaffordable on current computers. A potential model should solve the existing problems of the simulation of engineering micro/nano channel flows.

REFERENCES

Allen, M. P., and Tildesley, D. J., 1989, *Computer Simulation of Liquids*, Clarendon, Oxford.

Atkas, O., and Aluru, N. R., 2002, "A Combined Continuum/DSMC Technique for Multiscale Analysis of Microfluidic Filters," *Journal of Computational Physics*, **178**, 342-372.
http://dx.doi.org/10.1006/jcph.2002.7030

Bhadauria, R., and Aluru, N. R., 2013, "A Quasi-Continuum Hydrodynamic Model for Slit Shaped Nanochannel Flow," *Journal of Chemical Physics*, **139**, 074109.
http://dx.doi.org/10.1063/1.4818165

Borg, M. K., Lockerby, D. A., and Reese J. M., 2013, "A Multiscale Method for Micro/nano Flows of High Aspect Ratio," *Journal of Computational Physics*, **233**, 400-413.
http://dx.doi.org/10.1016/j.jcp.2012.09.009

Bitsanis, I., Magda, J. J., Tirrell, M., and Davis, H. T., 1987, "Molecular Dynamics of Flow in Micropores," *Journal of Chemical Physics,* **87**, 1733-1750.
http://dx.doi.org/10.1063/1.453240

Bitsanis, I., Vanderlick, T. K., Tirrell, M., and Davis, H. T., 1988, "A Tractable Molecular Theory of Flow in Strongly Inhomogeneous Fluids," *Journal of Chemical Physics*, **89**, 3152-3162.
http://dx.doi.org/10.1063/1.454972

Chan, D. Y. C., and Horn, R. G., 1985, "The Drainage of Thin Liquid Films Between Solid Surfaces," *Journal of Chemical Physics*, **83**, 5311-5324.
http://dx.doi.org/10.1063/1.449693

Craig, V. S. J., Neto, C., and Williams, D. R. M., 2001, "Shear-Dependent Boundary Slip in an Aqueous Newtonian Liquid," *Physical Review. Letters*, **87**, No.054504.
http://dx.doi.org/10.1103/PhysRevLett.87.054504

Cheikh, C., and Koper, G., 2003, "Stick-Slip Transition at the Nanometer Scale," *Physical Review Letters*, **91**, No.156102.
http://dx.doi.org/10.1103/PhysRevLett.91.156102

Dang, L. X., and Chang, T. M., 1997, "Molecular Dynamics Study of Water Clusters, Liquid and Liquid-Vapor Interface of Water with many Body Potentials," *Journal of Chemical Physics*, **106**, 8149-8154.
http://dx.doi.org/10.1063/1.473820

Duong-Hong, D., Wang, J., Liu, G. R., Chen, Y. Z., Han, J., and Hadjiconstatinou, N. G., 2008, "Dissipative Particle Dynamics Simulations of Electoosmotic Flow in Nano-Fluidic Devices," *Microfluidics and Nanofluidics*, **4**, 219-225.
http://dx.doi.org/10.1007/s10404-007-0170-7

Giannakapoulos, A. E., Sofos, F., Karakasidis, T. E., and Liakopoulos, A., 2014, "A Quasi-Continuum Multi-Scale Theory for Self-Diffusion and Fluid Ordering in Nanochannel Flows," *Microfluidics and Nanofluidics*, **17**, 1011-1023.
http://dx.doi.org/10.1007/s10404-014-1390-2

Hartings, J., Kunert, C., and Hyvaluoma, J., 2009, "Lattice Boltzman Simulations in Microfluidics: Probing the No-Slip Boundary Condition in Hydrophobic, Rough, and Surface Nanobubble Laden Microchannels," *Microfluidics and Nanofluidics*, **8**, 1-11.
http://dx.doi.org/10.1007/s10404-009-0506-6

Jabbarzadeh, A., Atkinson, J. D., and Tanner, R. I., 1997, "Rheological Properties of Thin Liquid Films by Molecular Dynamics Simulations," *Journal of Non-Newtonian Fluid Mechanics*, **69**, 169-193.
http://dx.doi.org/10.1016/S0377-0257(96)01520-0

Kasiteropoulou, D., Karakasidis, T. E., and Liakopoulos,A., 2011, "Dissipative Particle Dynamics Investigation of Parameters Affecting Planar Nanochannel Flows," *Materials Science and Engineering,* B, **176**, 1574-1579.
http://dx.doi.org/10.1016/j.mseb.2011.01.023

Kasiteropoulou, D, Karakasidis, T. E., and Liakopoulos, A., 2013, "Mesoscopic Simulation of Fluid Flow in Periodically Grooved Microchannels," *Computers & Fluids* ,**74**, 91-101.
http://dx.doi.org/10.1016/j.compfluid.2013.01.010

Kinugawa, K., and Nakanishi, K., 1988, "Molecular Dynamics Simulation on the Hydration of Fluoroalcohols," *Journal of Chemical Physics*, **89**(9), 5834-5842.
http://dx.doi.org/10.1063/1.455534

Koo, J., and Kleinstreuer, C., 2003, "Liquid Flow in Microchannels: Experimental Observations and Computational Analyses of Microfluidics Effects," *Journal of Micromechanics and Microengineering*, **13**, 568-577.
http://dx.doi.org/10.1088/0960-1317/13/5/307

Lee, S. H., and Rossky, P. J., 1994, "A Comparison of the Structure and Dynamics of Liquid Water at Hydrophobic and Hydrophilic Surfaces-a Molecular Dynamics Simulation Study," *Journal of Chemical Physics*, **100**, 3334-3340.

http://dx.doi.org/10.1063/1.466425

Liu, C., and Li, Z., 2011, "On the Validity of the Navier-Stokes Equations for Nanoscale Liquid Flows: The Role of Channel Size," *AIP Advances*, **1**, 032108.
http://dx.doi.org/10.1063/1.3621858

Liu, J., Chen, S., Nie, X., and Robbins, M. O., 2007, "A Continuum-Atomistic Simulation of Heat Transfer in Micro- and Nano- Flows," *Journal of Computational Physics*, **227**, 279-291.
http://dx.doi.org/10.1016/j.jcp.2007.07.014

Mao, Y., and Zhang, Y., 2014, "Molecular Dynamics Simulation on Rapid Boiling of Water on a Hot Copper Plate," *Applied Thermal Engineering*, **62**(2), 607-612.
http://dx.doi.org/10.1016/j.applthermaleng.2013.10.032

Meyer, E., Overney, R. M., Dransfeld, K., and Gyalog, T., 1998, *Nanoscience-Friction and Rheology on the Nanometer Scale*, World Scientific Press, River Edge, NJ.

Nie, X. B., Chen, S., and Robbins, M. O., 2004, "A Continuum and Molecular Dynamics Hybrid Method for Micro- and Nano- Fluid Flow," *Journal of Fluid Mechanics*, **500**, 55-64.
http://dx.doi.org/10.1017/S0022112003007225

Pham, P. H., Dao, D. V., and Sugiyama, S., 2007, "A Micro Transportation System with Large Movement of Containers Driven by Electrostatic Comb-Drive Actuators,"*Journal of Micromechanics and Microengineering,* **17**, 2125-2131.
http://dx.doi.org/10.1088/0960-1317/17/10/026

Somers, S. A., and Davis, H. T., 1992, "Microscopic Dynamics of Fluids Confined Between Smooth and Atomically Structured Solid Surfaces," *Journal of Chemical Physics,* **96**, 5389-5407.
http://dx.doi.org/10.1063/1.462724

Squires, T. M., and Quake, S. R., 2005, "Microfluidics: Fluid Physics at the Nanoliter Scale,"*Review of Modern Physics,* **77**, 977-992.
http://dx.doi.org/10.1103/RevModPhys.77.977

Stillinger, F. H., and Rahman, A., 1974, "Improved Simulation of Liquid Water by Molecular Dynamics," *Journal of Chemical Physics*, **60**, 1545-1550.
http://dx.doi.org/10.1063/1.1681229

Sun, J., He, Y., and Tao, W. Q., 2010, "Scale Effect on Flow and Thermal Boundaries in Micro-/Nano- Channel Flow Using Molecular Dynamics-Continuum Hybrid Simulation Method," *International Journal of Numerical Methods in Engineering*, **81**, 207-228.
http://dx.doi.org/10.1002/nme.2683

Sun, M., and Ebner, C., 1992, "Molecular Dynamics Study of Flow at a Fluid-Wall Interface," *Physical Review Letters*, **69**, 3491-3494.
http://dx.doi.org/10.1103/PhysRevLett.69.3491

Takaba, H., Onumata, Y., and Nakao, S., 2007, "Molecular Simulation of Pressure-Driven Fluid Flow in Nanoporous Membranes," *Journal of Chemical Physics*, **127**, 054703.
http://dx.doi.org/10.1063/1.2749236

Temam, R., 2000, "Navier-Stokes Equations: Theory and Numerical Analysis," AMS Chelsea Publishing, Rhode Island.

Thompson, P. A., and Troian, S. M., 1997, "A General Boundary Condition for Liquid Flow at Solid Surfaces,"*Nature*, **389**, 360-362.
http://dx.doi.org/10.1038/39475

Whitby, M., Cagnon, L., Thanou, M., and Quirke, N., 2008, "Enhanced Fluid Flow through Nanosacle Carbon Pipes," *Nano Letters*, **8**, 2632-2637.

Yang, X., and Zheng, Z. C., 2010, "Effects of Channel Scale on Slip Length of Flow in Micro/Nano Channels," ASME *Journal of Fluids Engineering*, **132**, 061201.
http://dx.doi.org/10.1115/1.4001619

Pinkus, O., and Sternlicht, B., 1961, "Theory of Hydrodynamic Lubrication," McGraw-Hill, New York.

Roohi, E., and Darbandi, M., 2009, "Extending the Navier-Stokes Solutions to Transition Regime in Two-dimensional Micro- and Nanochannel Flows Using Information Preservation Scheme," *Physics of Fluids*, **21**, 082001.
http://dx.doi.org/10.1063/1.3177351

Rudyak, V. Y., Belkin, A. A., Egorov, V. V., and Ivanov, D. A., 2009, "Molecular Dynamics Simulation of Plane Poiseuille Flow in Nanochannels," *2nd Micro and Nano Flows Conference* , **1-7**,West London, UK.

Senturia, S. D., 2001, "Microsystem Design*"*,Springer .

Sofos, F., Karakasidis, T. E., and Liakopoulos, A., 2009, "Non-Equilibrium Molecular Dynamics Investigation of Parameters Affecting Planar Nanochannel Flows," *Contemporary Engineering Science*, **2**, 283-298.

Sofos, F., Karakasidis, T. E., and Liakopoulos, A., 2009, "Effects of Wall Roughness on Flow in Nano Channels," *Physical Review E*, **79**, 026305.
http://dx.doi.org/10.1103/PhysRevE.79.026305

Sofos, F., Karakasidis, T. E., and Liakopoulos,A., 2015,"Fluid Structure and System Dynamics in Nanodevices for Water Desalination," *Desalination Water Treatment*, **55**, 1-11.
http://dx.doi.org/10.1080/19443994.2015.1049966

Yen, T. H., Soong, C. Y., and Tzeng, P. Y., 2007, "Hybrid Molecular Dynamics-Continuum Simulation for Nano/Mesoscale Channel Flows," *Microfluidics and Nanofluidics*, **3**, 665-675.
http://dx.doi.org/10.1007/s10404-007-0154-7

Zhang, J., 2011, "Lattice Boltzman Method for Microfluidics: Models and Applications," *Microfluidics and Nanofluidics*, **10**, 1-28.
http://dx.doi.org/10.1007/s10404-010-0624-1

Zhang, W., and Li, D., 2007, "Simulation of Low Speed 3D Nanochannel Flow," *Microfluidics and Nanofluidics*, **3**, 417-425.
http://dx.doi.org/10.1007/s10404-006-0133-4

Zhang, Y. B., and Lu, G. S., 2005, "Flow Factor for Molecularly Thin Fluid Films in One-Dimensional Flow due to Fluid Discontinuity.,"*Journal of Molecular Liquids*, **116**, 43-50.
http://dx.doi.org/10.1016/j.molliq.2004.06.002

Zhang, Y. B., 2006, "Flow Factor of Non-Continuum Fluids in One-Dimensional Contact," *Industrial Lubrication and Tribology*, **58**, 151-169.
http://dx.doi.org/10.1108/00368790610661999

Zhang, Y. B., 2013, "The Reynolds Equation for Boundary Film Considering the Non-Continuum Effect and Its Application to the One-Dimensional Micro Step Bearing: Part II-Calculation for Boundary Slippage," *Journal of Computational and Theoretical Nanoscience*, **10**, 609-615.
http://dx.doi.org/10.1166/jctn.2013.2742

Zhang, Y. B., 2015a, "The Flow Factor Approach Model for the Fluid Flow in a Nano Channel," *International Journal of Heat and Mass Transfer*, **89**, 733-742.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.05.092

Zhang, Y. B., 2015b, "A Quantitative Comparison between the Flow Factor Approach Model and the Molecular Dynamics Simulation Results for the Flow of a Confined Molecularly Thin Fluid Film," *Theoretical and Computational Fluid Dynamics*, **29**, 193-204.

Global Digital Central
ISSN: 2151-8629

http://dx.doi.org/10.1007/s00162-015-0348-7

Zhang, Y. B., 2015c, "Novel Nano Bearings Constructed by Physical Adsorption," *Scientific Reports*, **5**, 14539
http://dx.doi.org/10.1038/srep14539

Zhang, Y. B., 2015d, "An Analysis of a Concentric Micro/Nano Journal Bearing Constructed by Physical Adsorption," *Journal of the Balkan Tribological Association*, **21**, 937-951.

Zhang, Y. B., 2016a, "The Flow Equation for a Nanoscale Fluid Flow," *International Journal of Heat and Mass Transfer*, **92**, 1004-1008.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.09.008

Zhang, Y. B., 2016b, "Calculating the Maximum Flowing Velocity of the Poiseuille Flow in a Nano Channel by the Flow Factor Approach Model," *International Communications in Heat and Mass Transfer,* **73**, 111-113.
http://dx.doi.org/10.1016/j.icheatmasstransfer.2016.02.014

Zhang, Y. B., 2016c, "An Additional Validation of the Flow Factor Approach Model," *International Journal of Heat and Mass Transfer*, **95**, 953-955.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.01.016

Zhang, Y. B., 2016d, "Effect of Wall Surface Modification in the Combined Couette and Poiseuille Flows in a Nano Channel," *International Journal of Heat and Mass Transfer*, **100**, 672-679.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.05.010

Zhang, Y. B., 2016e, "Poiseuille Flow in a Nano Channel for Different Wall Surface Patterns," *International Journal of Heat and Mass Transfer*, **95**, 243-248.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.12.006

Zhu, Y., and Granick, S., 2001, "Rate-Dependent Slip of Newtonian Liquid at Smooth Surfaces," *Physical Review Letters*, **87**, No.096105.
http://dx.doi.org/10.1103/PhysRevLett.87.096105