Simulation study on bubble motion in capillaries based on lattice boltzmann method

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Abstract. The lattice Boltzmann method with mesoscopic properties can conveniently describe the interaction of multiphase molecules and has wide application prospects in the field of multiphase flow. In this paper, the improved Shan-Chen pseudo-potential multiphase model in lattice Boltzmann method was used to simulate the process of bubble passing through stenotic capillaries during the pathogenesis of decompression sickness, and the velocity variation of the fluid in the process of flow was studied. According to the research results, it can be concluded that: (1) in the direct channel, the velocity of the fluid slows down with the increase of the gas composition, and the clogging can cause a more obvious trend of deceleration; (2) in the narrow channel, the fluid velocity changes abruptly when the gas enters and leaves the narrow area, and with the increase of the gas composition, the velocity change tends to be stable when the gas can completely fill the narrow area. This research provides a theoretical basis for further understanding the pathogenesis of decompression sickness.

1. Introduction

When the ambient air pressure is reduced too fast or the amplitude is too large, the inert gas dissolved in the body exceeds the safety limit of supersaturation, and escapes to form bubbles, resulting in decompression sickness (DCS) [1]. DCS is a common disease in occupations under abnormal air pressure such as deep water and high altitude environment, which seriously affects the health and life safety of these employees. At present, the study of DCS is mainly divided into two aspects: One is the study of physiological mechanism. It is believed that there are two main influencing factors, one is gas embolism which means after bubble aggregation increases, gas embolus is formed in the blood vessel, which can block blood circulation and cause tissue ischemia, hypoxia, edema and other injuries[1]; the other is the inflammatory reaction which means the surface activity of gas-blood interface can cause a series of biochemical changes such as inflammation, inducing damage to the inner wall of the blood vessel, at the same time, the secondary inflammatory reaction aggravates the disorder of human physiology [2]. The second aspect is the research on decompression sickness prevention and treatment model, including dissolved gas model and bubble model[3], probabilistic decompression model and decisive decompression model[4, 5], and some emerging decompression models[6-11], etc. At present, there is a lack of quantitative analysis in the pathogenesis of DCS and quantitative analysis models for
the formation, transport and dissolution of bubbles in the course of the disease. Especially in the transport process, the mechanism by which bubbles cause damage to the vascular endothelial cell layer is not clear enough, and the corresponding pathogenesis is also not clear[12]. At the same time, although the molecular dynamics simulation has been used to study the mechanism of bubble formation[13], due to the computational scale of molecular dynamics, there are still many limitations in the study of bubble generation processes based on molecular dynamics.

The lattice Boltzmann (LBM) method can conveniently describe the two-phase interface, and is suitable for handling complex geometric boundaries. In recent years, LBM has made remarkable progress in the field of micro-scale multiphase flow[14-16]. The multiphase flow is a science developed on the basis of fluid mechanics, heat transfer and mass transfer. The macroscopic kinetic behavior of multiphase flow system is actually the result of microcosmic interaction between different phases. LBM has mesoscopic properties and can easily describe the interaction of multiphase molecules, and it overcomes the problem of limited computational scale in molecular dynamics research from a new point of view. Due to these properties, LBM multiphase flow model has become an effective numerical simulation method in the field of multiphase flow.

In this paper, the improved Shan-Chen pseudo-potential polyphase model was introduced, and the correctness of the model was verified. Finally, based on the two-dimensional and three-dimensional models, the changes of fluid velocity during the passage of the bubble through the straight channel and the narrow channel were calculated respectively.

2. Mathematical Model
In recent years, lattice Boltzmann multiphase / multicomponent models have developed rapidly. The existing models include color model, pseudo-potential model, free energy model, kinetic theory model and so on [17, 18].

2.1. Improved Shan-Chen pseudo-potential Multiphase Model
Shan[17] et al. proposed a LBM model which could directly describe the interaction between particles in 1993. This model reflects this interaction by establishing a pseudo-potential, so it is called the pseudo-potential model. Each distribution function represents a fluid component and satisfies the following Lattice Boltzmann equation:

\[
f_i^\sigma (x + e_i \delta t, t + \delta t) - f_i^\sigma (x, t) = -\frac{1}{\tau_k} \left[ f_i^\sigma (x, t) - f_i^{\sigma(\sigma)} (x, t) \right] \quad \sigma = 1, 2, \cdots, S
\]

(1)

Among them, the equilibrium distribution function of the \( \sigma \) th component was related to the lattice model. The pseudo-potential model assumed that there was a nonlocal interaction between fluid particles with different components, and its potential energy function was as follows:

\[
V_{\sigma \sigma}(x, x') = \hat{G}_{\sigma \sigma}(\|x-x'\|)\psi_\sigma(x)\psi_\sigma(x')
\]

(2)

Among them, \( \psi \) was the correlation function with component density; \( G \) was called Green function, which determined the interaction strength between different components. Generally, only the influence of the adjacent lattice points was considered.

\[
\hat{G}_{\sigma \sigma}(\|x-x'\|) = \begin{cases} 
0 & \|x-x'\| > \delta x \\
G_{\sigma \sigma} & \|x-x'\| = \delta x
\end{cases}
\]

(3)
The interaction strength coefficient $G$ represented the magnitude of the force between the fluid particles. For the two non-miscible fluid particles, there should be mutual repulsive force between them, then $G$ was a positive value at this time, and it needed to be large enough to separate the two phases. At the same time, $G$ could also determine the magnitude of interfacial tension. According to the form of potential energy function, the force applied to this component was defined by the following formula.

$$ F_\sigma = -\psi_\sigma(x) \sum_\sigma G_{\sigma\tau} \sum_i w_i \psi_\tau(x + \varepsilon_i \delta t) e_i $$ (4)

In the pseudo-potential model, the effect of the interaction force $F_\sigma$ on the distribution function $F_{eq}$ was reflected in the equilibrium velocity $U_{eq}$, and this form of the interaction force introduced some errors. After the Shan-Chen pseudo-potential model was proposed, Shan et al. [19] improved it and redefined the equilibrium velocity $u$ in the equilibrium distribution function. At the same time, the velocity $u$ of the mixed fluid was defined as the average value of the velocity before and after the collision. This definition of the flow velocity could greatly reduce the error of the corresponding macroscopic equation.

2.2. Calculation Steps

1. Initializing macro variables
2. Calculating equilibrium distribution function
3. Using standard collision migration process
4. Dealing with the boundary nodes by the bouncing and periodic boundary conditions
5. Calculating macro parameters (density, velocity)
6. Outputing results

3. Verification and Validation

3.1. Simplified Conditions

In LBM, the treatment of phase interface problem could be simply transformed into controlling the interaction force between fluid particles and between fluid and wall. This simplified method could reduce the cost of calculation resources and describe the interface position in detail. The essence of this model was the gas-liquid two-phase flow in the vessel and its interaction with the wall of the vessel. In order to simplify the physical process of the flow, the following assumptions were made: the vessel wall was rigid; the initial bubble shape was cylindrical; the internal gas and liquid were Newtonian fluid; the fluid motion was incompressible flow; the simulation did not consider gravity action; In addition, the scope of this study belonged to the micro-flow range, and the Reynolds number (Re) of the fluid was very small (< 1), so the single relaxation factor LBM method could be used. In this paper, the D3Q19 (3-D space, 19 discrete speeds) model of lattice Boltzmann method was used as the basic model.

The geometric model of capillary action was shown in Figure 1. The upper and lower wall were non-slip boundary conditions, and the entrance and outlet were periodic boundary conditions.

![Figure 1. Geometric model diagram](image-url)
3.2. Model Validation

3.2.1. Validation of Contact Angle. The contact angle referred to the tangent of the gas-liquid interface at the intersection of gas, liquid and solid, fluid 1 and fluid 2 represented two kinds of fluids, and the tangent angle $\theta$ between the liquid side and the solid-liquid boundary was a measure of wettability, as shown in Figure 2.

![Figure 2. Contact angle diagram](image)

In order to verify the correctness of the model, the relaxation process of the cuboid droplets was simulated. The calculation process was as follows: a 40*20*17 cuboid drop was placed in the cavity region of 121*20*70. The change process of contact angle under different numerical conditions of G1, ads was calculated. The results were in good agreement with the analytical solution of contact angle calculation formula (5), which showed that the model in this paper was consistent with the contact angle calculation formula, and the correctness of the model in the contact angle was verified.

$$\cos \theta = \frac{G_{1,\text{ads}} - G_{2,\text{ads}}}{G \rho_1 - \rho_2}$$  \hspace{1cm} (5)

In equation(5), G1,ads was the interaction coefficient between liquid and solid, G2,ads was the interaction coefficient between gas and solid, $\rho_1$ was the density of liquid and $\rho_2$ was the density of gas.

3.2.2. Validation of Grid Independence. In order to further verify the grid independence of the proposed model, the relaxation process of different scale models was simulated. The calculation process was as follows: The cuboid droplets of 28*14*12, 40*20*17 and 52*26*22 were respectively placed in the cavity of 85*14*49, 121*20*70 and 157*26*91 (with the exception of the bottom, all being periodic boundary conditions). The relationship between G1, ads and the contact angle was calculated when the cuboid droplets were relaxed into semi-cylindrical droplets under the condition of different G1, ads values. The calculation results were shown in Figure 3.
It could be obtained from Figure 3 that the contact angle is basically unchanged under different model scales and was well consistent with the analytical solution of formula (5), which verified the mesh independence of the model in calculating the contact angle.

3.2.3. Verification of Relative Stability for Fluid Volume. It is known that the Shan-Chen model is an approximate model, which will cause some errors in the case of phase transition. In this paper, the variation of gas volume and liquid volume under different model scales were calculated. When the example was stable, the volume of liquid was almost unchanged and the change of gas volume was less than 0.5%. The error was within acceptable range, so the fluid volume of the model used in this paper was relatively stable.

4. Results and Discussion

4.1. Three-Dimensional Direct Channel Model
The calculation process was as follows: a cylindrical bubble with a radius of 25 and a length of h was placed in a straight channel with a radius of 25 and a length of H. While ensuring that the volume of the liquid in the channel remained the same, we modified the bubble length h and the channel length H. In this paper, several examples were selected to calculate the velocity of the fluid in the channel when the system was stable. When Step = 5000 ts (ts is a dimensionless time step), the bubble form of eight of the examples was shown in Figure 4.
Figure 4. The shape of bubble in the channel with different h values when Step=5000

The velocity of the center point in the steady state of each example was calculated, and the results were shown in Figure 5.

Figure 5. The steady velocity of liquid measured at the center of the straight channel. U1 is the velocity at the center of the channel when the fluid motion was stable; Gas Component is the volume of gas in the channel as a percentage of the volume of the fluid.
As it was shown in Figure 5, the steady velocity of the fluid decreased with the increase of the gas composition when the same force was applied on the liquid. When the gas did not block the channel, the fluid velocity was relatively large and the fluid velocity was reduced obviously as the gas component increased. And the fluid velocity was relatively small when the gas had blocked the channel. In that condition, it was worth noting that with the increase of gas composition, the decreasing trend of fluid velocity slowed down.

4.2. Three-Dimensional Narrow Channel Model

In view of the irregularity of the blood vessels and the fact that the vasospasm was still maintained when the bubble flowed through the site of vasospasm under the action of blood pressure, the rigid model of vessels with stenosis could be simplified.

The calculation process was as follows: a cylindrical bubble with a radius of 25 and a length of \( h \) was placed in a narrow channel with a radius of 25 and a length of \( H \) (\( H-h=425 \)). The formula for calculating the radius of the narrow part was (6), and the variation of the radius was shown in Figure 6.

\[
R = 25 - 10 \times \left( \frac{x}{2000} \right)^{1.3}
\]

(6)

![Figure 6. Variation of narrow channel radius](image)

While ensuring that the volume of the liquid in the channel remained the same, we modified the bubble length \( h \) and the channel length \( H \), and calculated the velocity of the fluid in the channel during the operation of the system (Select two points A, B on the centerline at the radius of 25 in the narrow channel).

In this paper, a number of numerical examples were calculated. The morphological changes of bubble with different step values while passing through narrow channels were observed (\( h=160 \)), as shown in Figure 7.
The stable velocity of the measuring points A and B was basically consistent with each other. And the velocity of points A and B fluctuated when bubble passed through the narrow region. In order to further study the influence of bubble size on the velocity variation as bubble passing through the narrow region, these cases were drawn together for comparison in one figure. At the same time, in order to study the influence better, the velocity curves of each example were processed by Smooth function in MATLAB R2016b, the results were shown in Figure 8.

![Figure 7. The shape of bubble in the channel with different step values when h=160](image)

![Figure 8. Velocity curves of each example treated by Smooth](image)
It was known that the length of the narrow region was fixed under the conditions of different numerical examples. As it was shown in Figure 8: when the bubble entered the narrow region (from wide area to narrow area), the velocity decreased, and the decreasing trend of each example was basically the same. When the bubble basically entered the narrow channel, the change of velocity decreased. The velocity increased when bubble moved from the narrow region to the straight channel region (from narrow area to wide area), and in this condition a velocity range larger than the stability value appeared in each example. According to the difference of several examples, when the bubble became bigger (the gas component increased), the bubble could gradually block the whole narrow area. In the process of motion, when the bubble was big enough to completely block the narrow area, the velocity in the process of maintaining complete blockage was basically stable.

5. Conclusion
In this paper, the improved Shan-Chen pseudo-potential multiphase model in lattice Boltzmann method was used to simulate the process of bubble traversing narrow capillaries in the process of decompression sickness, and the velocity variation of fluid in the process of flow was studied. The conclusions of this study were as follows:
(1) In the case of the same volume of liquid, the change of bubble volume hindered the movement of fluid. Under the same force, the larger the bubble, the slower the velocity of the fluid.
(2) When the bubble volume increased to a certain extent, the bubble adhered to the wall, which obviously hindered the movement of the fluid.
(3) For narrow channels, bubble size had a significant effect on the velocity of bubble while passing through narrow regions. Relative to the size of the narrow area, the larger the bubble volume, the more obvious the blockage of the channel flow.

The above studies supplemented the study of decompression sickness from a quantitative point of view, which could provide a theoretical basis for further understanding in the pathogenesis of decompression sickness.

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