LBM-Based Numerical Simulation of Contact Angle on Gradient Sodiophilic Nanostructured Surfaces

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Abstract

Heat pipe cooled reactors have emerged as a research focus in the nuclear energy domain owing to their high safety and efficient heat transfer performance. The wick, as a core component, has surface wetting characteristics that directly influence capillary force and heat transfer efficiency. This study investigates the mechanism by which gradient sodium-philic nanostructured surfaces affect the liquid sodium contact angle using the Lattice Boltzmann method. By enhancing the multi-relaxation-time model and pseudo-potential interaction force model, the effects of geometric parameters including micropillar height, spacing, and width on the liquid sodium contact angle are examined, achieving stable simulation of the wetting and spreading process of liquid sodium on both flat and inclined micropillar-structured surfaces. The research findings provide a theoretical foundation for the optimal design of wick surfaces and hold significant reference value for improving heat pipe heat transfer performance.

Full Text

Preamble

Numerical Simulation of Contact Angle on Gradient Sodium-Philic Nanostructured Surfaces Based on LBM

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Abstract

Heat pipe cooled reactors have emerged as a research focus in nuclear energy due to their inherent safety and efficient heat transfer capabilities. As the core component of heat pipes, the wick structure directly influences capillary force and heat transfer efficiency through its surface wettability. This study investigates the influence mechanism of gradient sodium-philic nanostructured surfaces on liquid sodium contact angles using the Lattice Boltzmann Method (LBM). By improving the Multi-Relaxation-Time (MRT) model and pseudo-potential interaction force model, we examine how geometric parameters—including micropillar height, spacing, and width—affect the contact angle of liquid sodium, achieving stable simulations of wetting and spreading processes on both flat and inclined micropillar-structured surfaces. The results provide a theoretical foundation for optimizing wick surface design and offer valuable insights for enhancing heat pipe thermal performance.

Keywords: Lattice Boltzmann Method; Wettability; Contact Angle; Gradient Nanostructure; Sodium Heat Pipe

Introduction

The development of advanced technologies such as deep-sea exploration and aerospace has created an urgent demand for highly reliable, long-life energy systems. Heat pipe cooled reactors have become an ideal alternative to conventional energy systems owing to their inherent safety, modular design, and efficient heat transfer characteristics [1]. As the core component of heat pipes, the wick drives working fluid circulation through capillary forces, and its performance directly affects reactor heat transfer efficiency and operational stability. Research indicates that the capillary performance of wicks is closely related to the wetting behavior of liquid sodium on their surfaces, making the regulation mechanism of surface micro/nanostructures on wettability a key factor in wick design optimization [2]. However, the high density ratio of liquid sodium in high-temperature sodium heat pipes and the complex solid-liquid-gas interactions make it difficult to precisely characterize the dynamic wetting properties of gradient nanostructured surfaces using traditional experimental methods, necessitating the development of high-precision numerical simulation approaches.

Recent years have witnessed significant progress in surface wettability regulation research. Cansoy et al. [3] prepared square and cylindrical micropillar structures and found that contact angles are largely influenced by surface chemical composition, with the Cassie-Baxter equation being applicable only under specific geometric parameters. Hemeda et al. [4] established a mathematical model revealing the critical pressure mechanism for wetting state transitions on superhydrophobic surfaces. The Lattice Boltzmann Method (LBM) has demonstrated unique value in multiphase flow interfacial dynamics simulations due to its mesoscopic scale advantages [5]. For instance, Hyväluoma et al. [6] employed LBM to conduct two-phase lattice Boltzmann simulations of flow on structured

surfaces with attached bubbles, investigating the effects of geometry, pressure, and shear rate on slip. Lin et al. [7] utilized this method to explore droplet spreading characteristics on stepped microstructured surfaces. Hu et al. [8] combined LBM with three-dimensional simulations of condensation on nanostructured superhydrophobic surfaces, analyzing how geometric dimensions of nanoarrays and local wettability heterogeneity affect nucleation sites and final wetting states of condensate droplets. Fang et al. [9] incorporated temperature fields to perform LBM numerical simulations of droplet spreading and evaporation on surfaces with different wettabilities. However, current LBM-based simulation studies primarily focus on room-temperature working fluids, with relatively few investigations on high-temperature alkali metal sodium. Moreover, traditional single-relaxation-time LBM models are prone to numerical instability under conditions of gradient structures and large density ratios, limiting accurate simulations of complex operating conditions [10-11].

Based on these considerations, this study improves the S-C pseudo-potential model and constructs a parametric model of gradient micropillar structures to systematically investigate the influence of micropillar spacing, width, and height on contact angles, revealing the dynamic mechanism of wetting state regulation by gradient structures. The research findings provide theoretical support for nanostructure optimization of high-temperature sodium heat pipe wicks.

1.1 MRT-LBM Model

For multiphase flow problems, numerous models are available in the Lattice Boltzmann Method. This study employs an improved pseudo-potential model to simulate gas-liquid two-phase flow with large density ratios [12]. The single-relaxation-time model is replaced with a Multi-Relaxation-Time (MRT) model, which ensures computational stability by adjusting multiple relaxation times, making program modifications controllable [13]. The standard lattice Boltzmann equation with the collision matrix incorporated is:

$$f_i(\mathbf{r} + \mathbf{c}_i\Delta t, t + \Delta t) - f_i(\mathbf{r}, t) = -\mathbf{M}^{-1}\mathbf{S}\mathbf{M}[f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)]$$

where $\mathbf{r}$ represents a lattice point in the computational flow field; Δt is the time step; $\mathbf{c}_i$ is the discrete velocity of fluid particles; $\mathbf{M}^{-1}\mathbf{S}\mathbf{M}$ constitutes the collision matrix operator, which can be expressed as $\Omega = \mathbf{M}^{-1}\mathbf{S}\mathbf{M}$; $\mathbf{M}$ is the orthogonal transformation matrix, and $\mathbf{M}^{-1}$ is its transpose, both related to the selection of the velocity discretization model; $\mathbf{S}$ is a diagonal matrix; f_i is the velocity distribution function of fluid particles; and f_i^{eq} is the equilibrium distribution function, expressed as:

$$f_i^{eq} = w_i\rho\left[1 + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{|\mathbf{u}|^2}{2c_s^2}\right]$$

where $\mathbf{u}$ is the macroscopic fluid velocity at the node, c_s is the lattice sound speed (taken as $c_s = \sqrt{3}/3$ in the D2Q9 model), and each direction has corresponding weight coefficients w_i. For the D2Q9 model [14], the weight coefficients are:

$$w_i = \begin{cases} 4/9 & i = 0 \\ 1/9 & i = 1,2,3,4 \\ 1/36 & i = 5,6,7,8 \end{cases}$$

The collision process is difficult to implement in velocity space, requiring mapping of particle functions to moment space. To better satisfy thermodynamic consistency, this study adopts the new external force term proposed by Li et al. [15] and introduces an additional term to conveniently adjust surface tension while ensuring program stability. The modified evolution equation takes the form:

$$\mathbf{m}(\mathbf{r} + \mathbf{c}_i\Delta t, t + \Delta t) = \mathbf{m}(\mathbf{r}, t) - \mathbf{S}[\mathbf{m}(\mathbf{r}, t) - \mathbf{m}^{eq}(\mathbf{r}, t)] + \delta_t(\mathbf{I} - \frac{\mathbf{S}}{2})\mathbf{F}_L$$

The equilibrium distribution function in moment space is:

$$\mathbf{m}^{eq} = \rho\left(1, -2 + 3|\mathbf{u}|^2, 1 - 3|\mathbf{u}|^2, u_x, -u_x, u_y, -u_y, u_x^2 - u_y^2, u_x u_y\right)^T$$

The diagonal matrix $\mathbf{S}$ contains multiple relaxation times:

$$\mathbf{S} = \mathrm{diag}(1, 1.5, 1.5, 0, \tau_\nu^{-1}, 0, \tau_\nu^{-1}, \tau_\zeta^{-1}, \tau_\zeta^{-1})$$

The relaxation times are set as $\tau_\rho^{-1} = \tau_j^{-1} = 1.0$, $\tau_e^{-1} = \tau_\zeta^{-1} = 0.8$, and $\tau_q^{-1} = 1.1$. The parameter τ_ν represents the relaxation time related to kinematic viscosity, with $\tau_\nu = 3\nu + 0.5$.

The introduced term $\mathbf{C}$ takes the form:

$$\mathbf{C} = \xi \begin{pmatrix} 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0 \end{pmatrix}$$

The variables Q_{xx}, Q_{yy}, and Q_{xy} are calculated as:

$$Q_{xx} = \sum_{i=1}^{8} w_i c_{ix}^2 \psi(\mathbf{r}+\mathbf{c}_i\Delta t) Q_{yy} = \sum_{i=1}^{8} w_i c_{iy}^2 \psi(\mathbf{r}+\mathbf{c}_i\Delta t) Q_{xy} = \sum_{i=1}^{8} w_i c_{ix} c_{iy} \psi(\mathbf{r}+\mathbf{c}_i\Delta t)$$

where parameter κ adjusts surface tension.

The external force term $\mathbf{F}_L$ is expressed as:

$$\mathbf{F}_L = \left(0, 6\mathbf{u}\cdot\mathbf{F} + \frac{12\mathbf{F}^2}{\psi^2(\rho)}, -6\mathbf{u}\cdot\mathbf{F} - \frac{12\mathbf{F}^2}{\psi^2(\rho)}, F_x, -F_x, F_y, -F_y, 2(u_{xF}x - u_{yF}y), u_{xF}y + u_{yF}x\right)^T$$

where σ is a parameter for adjusting thermodynamic stability, taken as 0.12.

The force $\mathbf{F}$ is calculated as:

$$\mathbf{F} = \mathbf{F}_{int} + \mathbf{F}_{ads} + \mathbf{F}_g$$

The interparticle interaction force takes the form:

$$\mathbf{F}_{int}(\mathbf{r}) = -G_{int}\psi(\mathbf{r}) \sum_{i=1}^{8} w_i \psi(\mathbf{r} + \mathbf{c}_i\Delta t)\mathbf{c}_i$$

where G_{int} is a constant and w_i are the weight coefficients for directional forces, which for D2Q9 can be expressed as:

$$w_i = \begin{cases} 1/3 & i = 0 \\ 1/12 & i = 1,2,3,4 \\ 1/12 & i = 5,6,7,8 \end{cases}$$

The interaction potential ψ is primarily determined by particle density ρ and pressure p:

$$\psi(\rho) = \sqrt{\frac{2(p - c_0^2\rho)}{c_0^2 G_{int}}}$$

where c_0 is a force coefficient taken as $c_0 = 6$.

The fluid-solid interaction force is:

$$\mathbf{F}_{ads}(\mathbf{r}) = -G_{ads}\psi(\mathbf{r}) \sum_{i=1}^{8} w_i \psi(\rho_w) s(\mathbf{r} + \mathbf{c}_i\Delta t)\mathbf{c}_i$$

where $s(\mathbf{r}+\mathbf{c}_i\Delta t)$ is an indicator function with value 1 for solid nodes and 0 for fluid nodes.

Gravity $\mathbf{F}_g$ is expressed as:

$$\mathbf{F}_g = \rho\mathbf{g}$$

where $\mathbf{g}$ is gravitational acceleration.

Within the simulated temperature range, the Peng-Robinson (P-R) equation of state provides satisfactory results:

$$p = \frac{\rho RT}{1-b\rho} - \frac{a\alpha(T)\rho^2}{1+2b\rho-b^2\rho^2}$$

where $a = 0.45724(RT_c)^2/p_c$, $b = 0.0778RT_c/p_c$, and ω is the acentric factor (for sodium, $\omega = -0.10546$). In practice, we take $a = 3/49$, $b = 2/21$, and $R = 1.0$.

Fluid density and macroscopic velocity are calculated as:

$$\rho = \sum_i f_i \rho\mathbf{u} = \sum_i f_i \mathbf{c}_i$$

1.2 Model Validation

The Lattice Boltzmann Method employs particle groups consistent with statistical mechanics to simulate actual fluid motion. For computational convenience, all physical parameters—including velocity, viscosity, length, surface tension, and pressure—exist in dimensionless lattice units. The lattice units used in numerical simulations are shown in Table 1 , with other lattice parameters listed in Table 2 .

1.2.1 Laplace Validation

The Laplace law states that when surface tension remains constant, the pressure difference across a droplet is inversely proportional to its curvature radius R at steady state. This section initializes elliptical droplets of different shapes, setting the semi-major axis $a = 2R$ and semi-minor axis $b = R/2$ based on mass conservation. The final droplet radius ranges from 15 to 35 lu with an increment of 1 lu. The computational domain is 150×150 lu, with $G_{int} = -1$ and $\kappa = 0.5$. After the droplet becomes spherical and reaches steady state, simulation results are fitted to a straight line as shown in Figure 1 [Figure 1: see original paper]. The slope satisfies the Laplace formula, demonstrating a linear relationship between additional pressure and the reciprocal of droplet radius. The fitted relationship is $\Delta P = 5.04 \times 10^{-4}/R + 2.71 \times 10^{-7}$, yielding a surface tension of $\sigma = 5.04 \times 10^{-4}$ mu $\cdot$ ts^{-2}.

By adjusting the surface tension coefficient, we can vary the droplet's surface tension. Calculating fluid surface tension under multiple κ values reveals the relationship between parameter κ and surface tension, as shown in Figure 2 [Figure 2: see original paper], which follows a linear trend: $\sigma = -0.0016\kappa + 0.00129$.

1.2.2 Smooth Wall Contact Angle Validation

The droplet radius is set to 30 lu with its center at $(x = n_x/2, y = r/2)$. For solid wall setup, the lower boundary is designated as a smooth wall while all other boundaries employ half-bounce-back conditions. By varying G_{ads} and recording the contact angle when the droplet reaches stable state, data points are fitted to obtain the final result shown in Figure 3 [Figure 3: see original paper]. The contact angle exhibits a linear relationship with the fluid-solid interaction coefficient, consistent with previous studies, following the relation $\theta = 275.314G_{ads} + 238.207$.

2 Results and Analysis

Based on the theoretical analysis in Section 2, the modified MRT-SC model is employed to simulate the wetting characteristics of liquid sodium on micro/nanostructured surfaces, with the entire simulation implemented through C++ programming.

2.1 Spreading Process of Liquid Sodium on Micropillar-Structured Surfaces

This section simulates surfaces with micropillar structures where a represents micropillar width, b spacing, and h height. The parameters are set as $a = b =$ 2 lu and $h = 10$ lu, with droplet radius at 35 lu. The spreading process is illustrated in Figure 4 [Figure 4: see original paper]. Initially, the liquid sodium just contacts the micropillars. By 200 ts, droplet attraction due to liquid-solid interaction becomes observable. During 500–2000 ts, bottom liquid sodium continuously spreads laterally and penetrates into micropillar gaps, while the upper droplet collapses downward due to internal liquid-phase forces, unable to maintain its original spherical shape. At 3500 ts, the liquid sodium has spread into an approximately hemispherical droplet in the Cassie-Baxter state. From 5500 ts until stable equilibrium, vertical oscillations occur as surface tension and pressure difference reach balance, requiring an extended period to achieve stability.

Figure 5 [Figure 5: see original paper] shows the dynamic spreading process of liquid sodium on inclined micropillar surfaces. With $h = 6$ lu, $a = 3$ lu, and $b = 5$ lu, the liquid sodium contacts the micropillar structure at $T = 250$ ts, initiating penetration into gaps. At $T = 500$ ts, an asymmetric wetting region forms at the droplet bottom, with greater extension on the left side. As time progresses, the droplet shifts overall in the inclined direction, with the

upper portion accelerating collapse due to gravity, transforming the shape from an initially symmetric sphere to a left-leaning ellipse. By $T = 5000$ ts, the droplet bottom completely covers micropillar gaps, entering the Wenzel state. During $T = 7500$–15000 ts, the droplet essentially stabilizes under the balance of surface tension and gravity, finally forming a left-deflected hemispherical shape that exhibits contact angle asymmetry induced by gravity.

2.2 Effect of Micropillar Spacing on Liquid Sodium Contact Angle

Micropillar geometry is set with $h = 4$ lu and $h = 10$ lu, $a = 2$ lu, and spacing b ranging from 2 to 10 lu. Figure 6 [Figure 6: see original paper] shows the wetting and spreading states on micropillar structures with various gaps. Combined with Figure 7 [Figure 7: see original paper], when $h = 4$ lu, micropillar spacing significantly affects the final contact angle. As spacing increases, the contact area where liquid sodium fully immerses into gaps enlarges, strengthening solid-liquid interaction forces and creating greater resistance to lateral spreading, ultimately increasing the contact angle and reducing wettability. When $h = 10$ lu, the contact angle variation follows the same trend, but the static contact angle undergoes a transition process, with $b = 5$ lu serving as the inflection point. For spacing less than 5 lu, the contact angle remains in a Wenzel-Cassie intermediate state, while for spacing greater than 5 lu, it completely transitions to the Cassie state.

Further investigation on inclined surfaces employs different left-right micropillar spacings with $h = 6$ lu, $a = 3$ lu, $b_1 = 4$ lu, and $b_2 = 8$ lu. Figure 8 [Figure 8: see original paper] presents the wetting characteristics of liquid sodium on gradient micropillar inclined surfaces. Initially, the droplet center is positioned at the junction between left and right structures. The left side, with smaller spacing, experiences rapid liquid-phase penetration and continuous liquid film formation, while the right side with larger spacing exhibits higher penetration resistance and limited film extension. At $T = 500$ ts, the left liquid film coverage is significantly larger than the right, causing the droplet to shift leftward to balance gravity. During $T = 1000$–2500 ts, the left side enters the Wenzel state with enhanced wettability, while the right side remains in the Cassie-Wenzel state due to excessive spacing, showing obvious gas-liquid interface protrusion. By $T = 5000$–10000 ts, gravity and surface tension jointly drive the droplet to migrate left-downward, forming a wetting gradient.

2.3 Effect of Micropillar Width on Liquid Sodium Contact Angle

In this subsection, micropillar geometry is set with $h = 4$ lu and $h = 10$ lu, $b = 2$ lu, and width a ranging from 2 to 10 lu. Figure 9 [Figure 9: see original paper] illustrates wetting and spreading states on micropillars of various widths, with the line plot shown in Figure 10 [Figure 10: see original paper]. Results indicate that increasing micropillar width tends to increase the contact angle of liquid sodium on structured surfaces. When width increases sufficiently, the contact angle stabilizes around 96.5°. As micropillar width increases, fewer micropillars

are covered at the liquid sodium bottom, reducing solid-liquid contact area and hindering lateral spreading. When width becomes very large, the structured surface can be approximated as a flat plane, and further width increases produce negligible changes in contact angle.

Additionally, a left-right width gradient is established with $h = 6$ lu, $b = 5$ lu, $a_1 = 2$ lu, and $a_2 = 5$ lu. Liquid sodium initially spreads on both sides, but over time, the right side with larger micropillar width experiences reduced solid-liquid contact area and slower spreading. By $T = 5000$ ts, the right side of the droplet ceases forward spreading while the left side maintains the Wenzel state. At final equilibrium, the droplet slides downward as a whole in the inclined direction.

2.4 Effect of Micropillar Height on Liquid Sodium Contact Angle

Micropillar geometry is set with $a = b = 2$ lu and height ranging from 2 to 15 lu with an increment of 1 lu. Figure 12 [Figure 12: see original paper] shows wetting and spreading states on micropillar structures of various heights. Figure 13 [Figure 13: see original paper] presents the contact angles for all different heights. The line plot reveals that when micropillar height is between 2–6 lu, the contact angle gradually decreases with increasing height, as the concave gas-liquid interface more easily contacts the gap bottom, forming the Wenzel state. With increasing micropillar height, the actual contact surface area between liquid sodium and solid walls increases, resulting in smaller contact angles. This height modification can render the structured surface sodium-philic. When micropillar height reaches 6 lu, the contact angle gradually stabilizes around 80°, with liquid sodium on the microstructured surface entering the Cassie-Wenzel intermediate state, indicating that beyond a certain height, further increases have minimal impact on the contact angle.

3 Conclusions and Outlook

This study employs the Lattice Boltzmann Method with an improved multi-relaxation-time pseudo-potential model to simulate liquid sodium contact angles on flat and inclined gradient sodium-philic nanostructured surfaces. Program accuracy is validated through Laplace's law and smooth wall contact angle tests. Results demonstrate that inclined surfaces cause droplets to become asymmetric and left-leaning elliptical. Additionally, the effects of micropillar geometric parameters on wetting characteristics are investigated: increasing micropillar spacing enlarges the liquid sodium contact angle, potentially transforming the surface from sodium-philic to sodium-phobic; micropillar width exhibits similar trends to spacing changes, but when width becomes sufficiently large to approximate a flat plane, contact angle changes become insignificant; for micropillar height, appropriately increasing height in the Wenzel state reduces liquid sodium contact angle and improves wettability. This work provides theoretical support for optimizing heat pipe wick design.

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Note: Figure translations are in progress. See original paper for figures.