Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary file

S1. Temperature evolution

The temperature evolution without the temperature gradient is summarized in Fig.S1. Previous studies have reported that the external force will bring artificial energy to fluid, which will lead to unrealistic temperature rise of system. As shown in Fig.S1, the temperature near the surface rises in a small degree, this phenomenon can be also observed in the cases has been induced the temperature gradient. In simulation of this paper, the solid-liquid interaction between the hot sink and fluid is stronger than that of hot source and fluid, which lead to the heat induced by the friction can be dissipated in time. Furthermore, the velocity of simulation driven by the external force is difficult to control, meaning that the velocity in the latter half of the microchannel is usually larger, which will easily lead to unrealistic temperature rise. Therefore, the velocity in our simulation is relatively small. Due to the temperature rise is small, it can be ignored in this research.

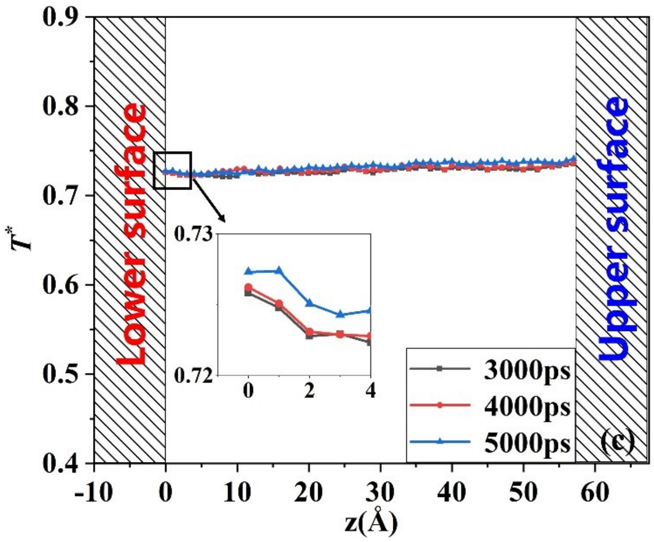

Fig.S1 Temperature profile evolution

S2. Density discussion

Table S1. Phase states of fluid adjacent to lower surface

β	T_h^*	ρ_{f-n}^*	T_{f-n}^*	Phase state
0.2	0.89	0.35	0.73	Gas+Liquid
0.2	1.06	0.63	0.91	Gas+Liquid
0.2	1.22	0.82	1.08	Liquid
0.6	0.89	1.56	0.77	Solid
0.6	1.06	1.58	0.94	Solid
0.6	1.22	1.59	1.12	Solid
1	0.89	2.47	0.83	Solid
1	1.06	2.39	1.00	Solid
1	1.22	2.32	1.17	Solid

As shown in Fig.4, there are 4 layers of fluid atoms with oscillation between the solid surface and bulk fluid when $\beta = 0.2$, and the maximum density is only 0.82 ($T_h^* = 1.22$). When $\beta = 1$, there are 5 layers of fluid atoms with oscillation, the maximum density reaches 2.47 ($T_h^* = 1.22$).

It can be seen that the density near the surface increases as the temperature rises when $\beta = 0.2$, the density of the first layer at $T_{\mathrm{h}}^* = 1.22$ is 134% higher than that at $T_{\mathrm{h}}^* = 0.89$. However, when $\beta = 0.6$, surface temperature has little influence on the density profile. When $\beta = 1$, density near the surface decreases as the temperature rises, the density of the first layer at $T_{\mathrm{h}}^* = 1.22$ is 6.1% lower than that at $T_{\mathrm{h}}^* = 0.89$.

From Tab.S1, it can be seen that the phase of fluid near the lower surface are mixture of gas and liquid ($T_{\mathrm{f-n}}^* = 0.72$ and 0.89) or pure liquid ($T_{\mathrm{f-n}}^* = 1.07$) when $\beta = 0.2$, the density of which is lower than the bulk liquid. When $\beta > 0.6$, the phase of fluid adjacent to the surface is solid.

S3. Velocity and velocity slip

As shown in Fig. 8, comparing the case $T_{\mathrm{h}}^* = 0.89$ with $T_{\mathrm{h}}^* = 1.22$ when $\beta = 0.2$, it can be found that velocity near the lower surface decreases as T_{h}^* rises, but which increases as T_{h}^* rises when solid-liquid interaction stronger ($\beta = 1$). Similar to the velocity profile, the effects of T_{h}^* on l_s are different as β changes. When $\beta = 0.2$, l_s decreases 35Å as T_{h}^* rises from 0.89 to 1.22, but l_s increases 3.5Å When $\beta = 1$. It is worth noting that there is little difference in l_s when $\beta = 0.6$ as T_{h}^* changes, which indicates that $\beta = 0.6$ is a critical point of separating the effects of temperature on velocity. The effects of surface temperature on slip length are in accordance with density.

When $\beta = 0.2$, it can be found that velocity near the lower surface decreases as T_{h}^* rises, but which increases as T_{h}^* rises when solid-liquid interaction stronger ($\beta = 1$). Similar to the velocity profile, the effects of T_{h}^* on l_s are different as β changes. When $\beta = 0.2$, l_s decreases as T_{h}^* rises, but l_s increases When $\beta = 1$.

S4. Temperature profile and Kapitza length

As shown in Tab.S1, the temperature difference ΔT^* between liquid and surface decreases significantly as β increases. In the meanwhile, ΔT^* decreases slightly as T_{h}^* rises. For example, when $\beta = 0.2$, ΔT^* equals 0.16, 0.15 and 0.14 when $T_{\mathrm{h}}^* =$ 0.89, 1.06 and 1.22, respectively. However, when $\beta = 1$, ΔT^* decreases to 0.059, 0.055 and 0.051 when $T_{\mathrm{h}}^* =$ 0.89, 1.06 and 1.22, respectively, indicating that both stronger solid-liquid interaction and higher surface temperature can enhance the heat transfer of the interface.