Reply to "Comment on 'Heat transfer and fluid flow in microchannels and nanochannels at high Knudsen number using thermal lattice-Boltzmann method'"

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In this reply to the Comment by Li-Shi Luo, we discuss the results of the lattice Bhatnagar-Gross-Krook (LBGK) model for high-Knudsen-number (Kn) flow and heat transfer, in the range of $\text{Kn} \leqslant 1$. We present various studies employing the LBGK model for high-Kn flow and heat transfer simulations. It is concluded that, with the use of the LBGK model in the thermal lattice Boltzmann method for $\text{Kn} \geqslant 0.8$, some approximations appear in the negative pressure deviation from the linear distribution along the channel. But for $\text{Kn} < 0.8$, the velocity and temperature profiles, compressibility effects, Knudsen layer capturing, and Knudsen paradox phenomenon can be predicted by the LBGK model. We also reject Li-Shi Luo's claim about the nonconvergence of our numerical scheme by presenting a velocity profile across the channel corresponding to three different high-resolution meshes.

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First, the authors would like to thank Li-Shi Luo (L.S.L.) for reading and commenting on our work.

L.S.L. [1] points out that our results are erroneous and our claim of "capability of the lattice Boltzmann method to model shear-driven, pressure-driven, and mixed shear-pressure-driven rarefied flows and heat transfer up to $\text{Kn} = 1$ in the transitional regime" is false and our results are erroneous. He states that the lattice Bhatnagar-Gross-Krook (LBGK) model with the bounce-back type of boundary conditions is just an incompressible Navier-Stokes solver and is not valid beyond the slip-flow regime.

In recent years, the LBGK model has frequently been used to simulate pressure- and shear-driven micro- and nanoscale flows successfully. This is not the issue which needs to be proved. So, we propose to have a look at the following works with corresponding Knudsen numbers: [2] up to $\text{Kn} = 0.776$, [3] up to $\text{Kn} = 1.58$, [4] up to $\text{Kn} = 10$, [5] up to $\text{Kn} = 1.58$, [6] up to $\text{Kn} = 1$, [7] up to $\text{Kn} = 10$, [8] up to $\text{Kn} = 0.1303$, [9] up to $\text{Kn} = 2.5$, [10] up to $\text{Kn} = 0.388$, [11] up to $\text{Kn} = 10$, [12] up to $\text{Kn} = 1.13$, [13] up to $\text{Kn} = 5.85$, and [14] up to $\text{Kn} = 0.5$.

This will help to clarify completely how the LBGK model with the bounce-back, diffuse scattering boundary condition or kinetic boundary condition can simulate pressure- and shear-driven flows and heat transfer in the transitional regime. Various verifications of results obtained from the LBGK model with solution of the Boltzmann equation or direct simulation Monte Carlo (DSMC) or experimental results can be found in the mentioned references. So the ability of the LBGK model to simulate gaseous flow and heat transfer in the transitional regime has been shown previously in many papers.

L.S.L. also points out that in our results for $\text{Kn} \geqslant 0.8$, the pressure deviation from the linear distribution along the microchannel becomes negative and concave. He concludes from this fact that the results presented in our paper are erroneous. Of course, this negative pressure deviation from the linear distribution for $\text{Kn} \geqslant 0.8$ is not acceptable and has not been seen in experimental results yet [2]. As we have mentioned in Ref. [17] the paper, similar results were reported previously [2] up to $\text{Kn} = 0.776$. Guo *et al.* [10] have successfully overcome this problem in the LBGK model.

On the other hand, the important point in our results is that the velocity profiles match up to $\text{Kn} = 1$ with the results of the linearized Boltzmann equation and definitely can be further improved by using the higher order D2Q13 velocity model with the LBGK model up to $\text{Kn} = 10$ [4]. So again, it can be concluded that the LBGK model is able to simulate shear-driven and pressure-driven flows accurately for $\text{Kn} < 0.8$, but with some approximations in predicting the pressure distribution along the channel for $\text{Kn} \geqslant 0.8$.

L.S.L. also declares that the LBGK model cannot capture the Knudsen layer in the transitional regime. In order to become more familiar with the physical origins of this method of Knudsen layer capturing, we invite him to have a look at Refs. [3,4,6], and [12]. Also, there are similar works which have simulated the Knudsen layer with the LBGK model using other ideas [8,10]. Engineers always welcome this kind of modeling.

L.S.L. proposes using the multirelaxation time (MRT)-LBM instead of the LBGK model to overcome the so-called "defects of the lattice BGK model." The MRT approach is more flexible in tuning some physical parameters [e.g., Prandtl number (Pr)] and has been shown to be numerically more stable than the popular LBGK collision operator [15]. But it is interesting that a comparison of the pressure deviations along the channel and velocity profiles across the channel obtained from the MRT-LBM [16], our LBGK model [17], and DSMC results [16] for $\text{Kn} = 0.388$ shows that our results are closer to the DSMC results than the MRT-LBM results. No more data are presented for $\text{Kn} > 0.388$ in Ref. [16].

On the other hand, it is important to point out that engineering applications need new LBGK models which can

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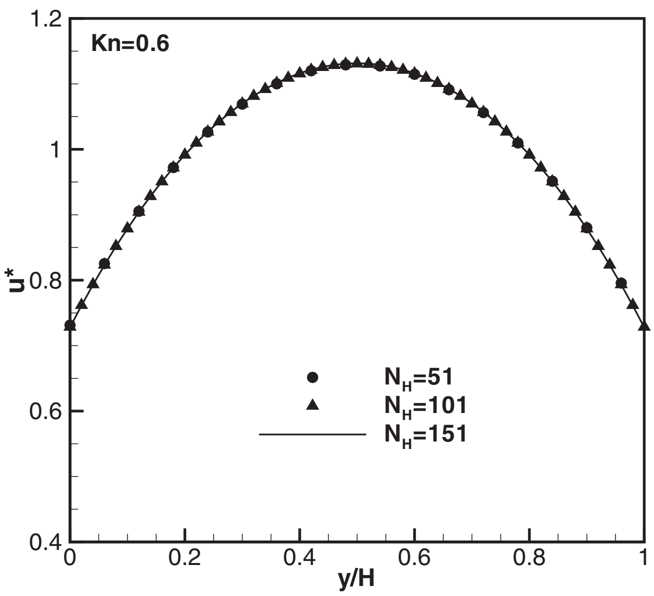

FIG. 1. Comparison of the dimensionless velocity profiles obtained from the LBGK model for Kn = 0.6 and $N_H = 51$, 101, and 151.

simulate simultaneously the developing velocity and temperature profiles considering the temperature-dependent properties, compressibility effects, and Knudsen layer capturing in the transitional regime as our model does. The negative pressure deviation along the channel for Kn $\geqslant 0.8$ is an acceptable approximation of the method. We must mention that from the engineering point of view, these kinds of deviations are called "approximations" not "errors." Then we will try to improve the approximations.

So the next step forward will be to improve the model in our paper, in order to predict the pressure distribution correctly for Kn numbers >0.8. But this does not mean that the results obtained from the LBGK model are false and this model is not able to simulate pressure- and shear-driven flows on the micro- and nanoscales. One method for improving the approximation of our model could be to employ the MRT-LBM, which must be studied and developed more in the future. Another choice would be to modify the dependence of viscosity on density in the LBGK model as presented in Ref. [2] and to use a higher order velocity discretization model.

On the other hand, capturing the correct nonlinear pressure distribution along the channel for Kn < 0.8 shows the ability of our method to simulate compressibility effects. This fact rejects the claim that the LBGK is an "incompressible" solver.

L.S.L. makes another digressive claim in stating that the LBM cannot even reproduce the Knudsen paradox [18]. This claim was rejected later in Refs. [7,13], and [19]. The prediction of the Knudsen paradox by the LBGK model shows that this model certainly is something beyond a Navier-Stokes solver.

L.S.L. states that a few studies on high-Kn simulations with the LBGK model demonstrate the convergence of the results, as the mesh resolution N_H is increased. Figure 1 shows a comparison of the dimensionless pressure-driven velocity profile obtained from our LBGK model for Kn = 0.6 and $N_H = 51$, 101, and 151. A similar convergence was also seen in all other velocity and temperature profiles in our paper. Figure 1 obviously shows that the results of our model converge excellently.

In conclusion, L.S.L.'s claims that our results are erroneous and the lattice Boltzmann method which was presented in our paper is not "capable of modeling shear-driven, pressure-driven, and mixed shear-pressure-driven rarefied flows and heat transfer up to Kn = 1 in the transitional regime" are false is erroneous. His report should be corrected to state that for Kn > 0.8 the results of our paper have some approximations in predicting the pressure distribution along the channel. Consequently, we propose to use higher order velocity discretizations such as the D2Q13 model [4], or a way to omit the negative pressure deviation for Kn > 0.8 as done in Ref. [10], or any other method to improve the approximations in our results for the range of Kn > 0.8.

Finally, the LBGK models are the beginning of a long road, not the end. In other words, extending our work to go beyond Kn = 1 considering different aspects of small-scale flow and heat transfer with the LBGK model still more concern.

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