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# EVALUATION OF WALL HEAT FLUX BOUNDARY CONDITION IN DSMC IMPLEMENTED IN OPENFOAM

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## KEYWORDS

Wall heat flux boundary condition, Nanochannel, Nanocavity, DSMC.

## ABSTRACT

Cooling and heating play a major role in micro/nano-devices and rarefied gases [1]. In this paper, we report the validation of a wall heat flux boundary condition, implemented in the direct simulation Monte Carlo (DSMC) solver of the OpenFOAM package. We used an enhanced version of OpenFOAM 2.4.0 called OpenFOAM 2.4-MNF. The DSMC solver in this release has enhanced features such as transient adaptive subcells, chemical reaction modules, and defined pressure inlet/outlet boundary conditions. The modified iterative technique (MIT), which was recently introduced by Akhlaghi and Roohi [2] was used in this implementation. This approach implements a desired wall heat flux distribution over the walls of the geometry for rarefied gas simulations.

In this technique, the local wall temperature is modified iteratively in such a way that the desired wall heat flux is achieved. The wall temperature is updated using:

$$\Delta T_w = \alpha \left( q_w^* - q_{des}^* \right) T_w \;, \qquad (1)$$

where $\alpha$ is a parameter controlling convergence, $T_w$ is the current wall temperature, $\Delta T_w$ is the change in wall temperature required to iterate towards the desired heat flux, and $q_{des}^*$ and $q_w^*$ denote the desired and obtained local wall heat flux, respectively. The heat fluxes are normalized as follows:

$$q_w^* = \frac{q_w}{q_f} \qquad (2)$$

where $q_f$ is a macroscopic characteristic heat flux defined as

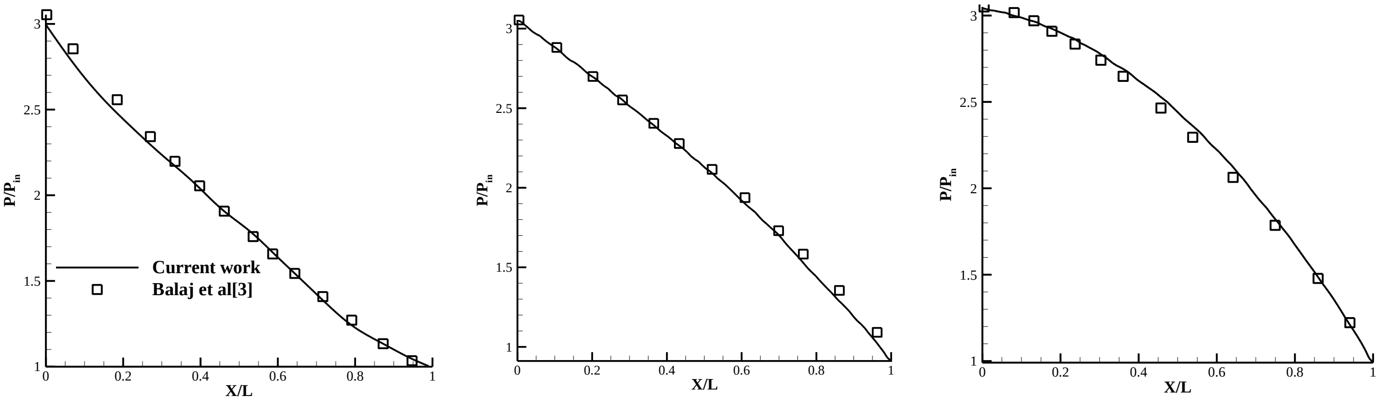
$$q_f = C_P \rho_0 U_0 T_0$$

where $C_p$, $\rho_0$, $U_0$, and $T_0$ are reference values of specific heat capacity, density, velocity and temperature, respectively. (3)

Here, we validate the implementation of equation (1) in dsmcFoam. The working gas is argon in a 2D pressure-driven nanochannel. Fig. 1 shows the normalized center-line pressure distribution under three

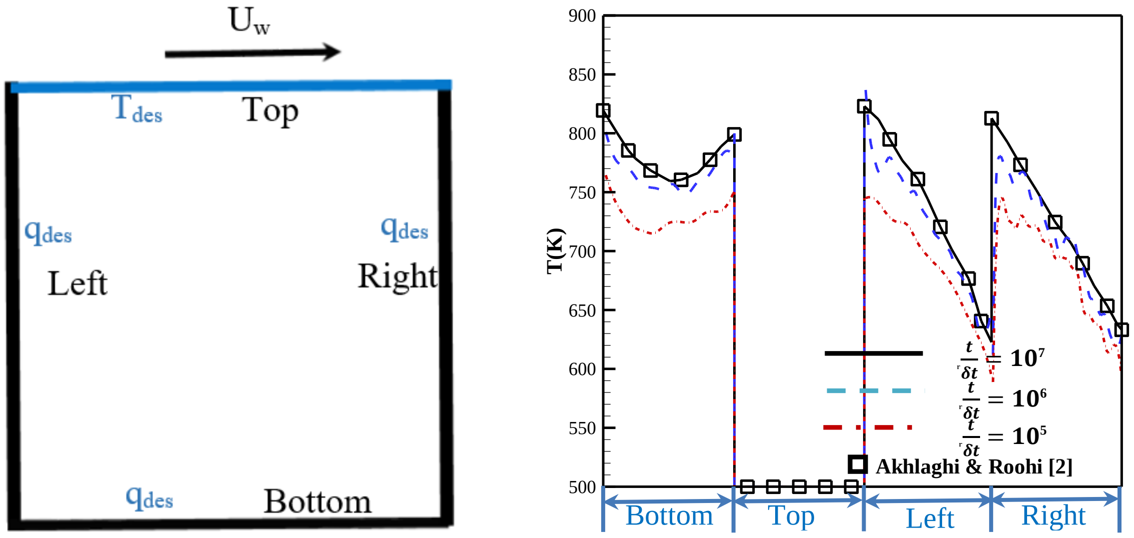
different wall boundary conditions; cooling, adiabatic, and heating wall boundary conditions. Our dsmcFoam solutions are compared with the DSMC solution of Balaj et al. [3] under the same wall conditions and good agreement is found. As is shown, heating or cooling affects the pressure distribution. Cooling results in a concave pressure distribution, and heating increases the convex nature of the pressure profile.

Fig. 2 demonstrates the effect of the heating condition on the wall temperature distribution of the nanocavity. The Knudsen number, *Kn*, is 0.1, the top wall is set at a constant temperature of 500 K, and the three other walls at a constant heat flux of $q^*$=-0.1. The right frame in the figure shows temporal variations of the wall temperature and matches the DSMC solution reported in [2] . Consequently, results shown in Figs. 1-2 indicate that our implementation of the MIT technique is accurate. The next stage will consider wall heat flux effects on the flow and thermal field behavior in complex geometries.



(a) (b) (c)

**Figure 1**: Flow in a microchannel a) Cooling condition (Kn=0.04, $q^*$=-0.3), b) Adiabatic (Kn=0.03, $q^*$=0), and c) Heating (Kn=0.02, $q^*$=+0.3)



(a) (b)

**Figure 2**: a) Schematic geometry of cavity, and b) Temperature profile over four sides of the cavity, Kn=0.1, $q^*$=-0.1.

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