Thermodynamic analysis of gas flow and heat transfer in microchannels

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ABSTRACT

Thermodynamic analysis, especially the second-law analysis, has been applied in engineering design and optimization of microscale gas flow and heat transfer. However, following the traditional approaches may lead to decreased total entropy generation in some microscale systems. The present work reveals that the second-law analysis of microscale gas flow and heat transfer should include both the classical bulk entropy generation and the interfacial one which was usually missing in the previous studies. An increase of total entropy generation will thus be obtained. Based on the kinetic theory of gases, the mathematical expression is provided for interfacial entropy generation, which shows proportional to the magnitude of boundary velocity slip and temperature jump. Analyses of two classical cases demonstrate validity of the new formalism. For a high-Kn flow and heat transfer, the increase of interfacial transport irreversibility dominates. The present work may promote understanding of thermodynamics in microscale heat and fluid transport, and throw light on thermodynamic optimization of microscale processes and systems.

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1. Introductions

In recent years, with the rapid development of micro- and nanofabrication and nanotechnology [1] and micro-electromechanical systems (MEMS) [2], there are increasing interests and studies on microscale gas flow [3–7] and heat transport [8–11]. The thermodynamics at microscale has attached more and more attentions in theory, such as the non-equilibrium entropy [12–14], or in applications for optimization of thermal efficiency of microsystems. The entropy generation minimization principle [15] or so-called the second-law analysis [16], originated in classical irreversible thermodynamics (CIT) [17], has been extended from the conventional engineering field to microscale systems. Hitherto the second-law analysis of microscale gas heat convections in simple geometries (micro-channels, micro-pipes, micro-ducts, etc.) has been widely performed via either analytical approach [18–24] or numerical simulations [25–28]. All these works followed the traditional methodology: "computing the entropy generation after a resolution of velocity and temperature field distributions" based on the entropy generation formula in terms of velocity and temperature gradients [15,16]. The size effects at microscale were incorporated in obtaining the velocity and temperature distributions by solving the classical hydrodynamic equations with velocity slip and temperature jump boundary conditions. A common conclusion was made that the total

entropy generation decreased with the increase of Knudsen number (*Kn*, defined as the ratio of mean free path to characteristic length) in microscale systems such as in the classical work [18,19].

However, the particular phenomena of velocity slip and temperature jump occur at the gas–solid interface in microscale gas flow [4]. The non-continuous velocity and temperature profiles come from the in-sufficient interactions between gas molecules and solid walls. In other words, the gas-surface interaction near the solid wall cannot reach a local equilibrium state as a fundamental hypothesis in CIT [17]. Such a non-equilibrium effect, non-doubtfully, will bring additional irreversibility and entropy generation. Actually the entropy generation in rarefied gas systems has been declared to consist of two parts [29]: one from the inter-molecular interactions and the other from the gas-surface interactions, which are denoted as the bulk and the interfacial entropy generations, respectively hereafter. The study on interfacial entropy generation originated earlier in formulating fluid–solid interfacial boundary conditions in the frame of non-equilibrium thermodynamics [30,31]. The boundary conditions were obtained as bilinear phenomenological flux-force relations from the non-negative interfacial entropy generation restricted by the second law [30]. The kinetic theory foundations were also investigated rooted in linearized Boltzmann transport equation (BTE) [32–34], where both the boundary conditions and the Onsager reciprocal relations for kinetic coefficients [29,35,36] have been derived. These outstanding works laid a solid basis for interfacial boundary conditions from both thermodynamic and statistical physical perspectives. But they mainly focus on the rarefied gas transport with

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Nomenclature

$\mathbf{c}$ (c_x, c_y, c_z)	molecular velocity [m/s]
$\mathbf{u}$ (u_x)	fluid velocity [m/s]
T	thermodynamic temperature [K]
x, y, r	coordinate components [m]
Pr	Prandtl number [–]
Kn	Knudsen number [–]
Br	Brinkman number [–]
c_p	specific heat capacity at constant pressure [J/(kg·K)]
$\dot{m}$	mass flow rate [kg/s]
A_c	cross-sectional area [m²]
R	radius of the micro-pipe [m]
H	half of the height of the micro-channel [m]
k	thermal conductivity of fluid [W/(m·K)]
P	wetting perimeter [m]
Y	dimensionless value of y [–]
q	heat flux supply [W/m²]
A, B	combinational parameters [–]
f	molecular velocity distribution function [m⁻³(m/s)⁻¹]
$\mathbf{F}$	external force on per unit mass of fluid [m/s²]
k_B	Boltzmann constant [J/K]
p	thermodynamic pressure [Pa]
e	specific internal energy [J/kg]
s	specific entropy or specularity parameter of wall [J/(K·kg)] or [–]
$\mathbf{J}^s$	entropy flux [W/(K·m²)]
S_{gen}	entropy generation rate [W/K]

Greek symbols

λ	molecular mean free path [m]
μ	dynamic viscosity of fluid [kg/(m·s)]
ρ	mass density of fluid [kg/m³]
γ	specific heat ratio [–]
τ	molecular relaxation time [s]
θ	dimensionless temperature [–]
η	dimensionless value of r [–]
σ	entropy generation rate per unit volume [W/(K·m³)]
Φ_q	dissipation function [s⁻²]
Φ, ϕ	deviational part of velocity distribution function [–]
α, β	dummy index [–]

Subscripts

s	variables of gas at the wall
w	variables of the wall
m	mean value of variables
1	parameters of micro-pipe
2	parameters of micro-channel
eq	equilibrium state
b	bulk region
i	interface region

Acronyms

CIT	classical irreversible thermodynamics
BTE	Boltzmann transport equation

a finite Kn resulting from enhanced mean free path. Theoretical foundation of the entropy generation is seldom explored in microscale gas flow and heat transport, where the reduced system size contributes to the finite Kn. It will be shown that the interfacial entropy generation obtained in rarefied gas transport is not available directly to analysis of microscale gas flows due to a finite portion of Knudsen layer (a thin layer with a thickness about one mean free path near the wall) across the microchannel. On the other hand, the interfacial entropy generation has never been incorporated into the second-law analysis of microscale gas heat convections in the previous work [18–28], to the authors' best knowledge. With the miniaturization of system and increase of Kn, the entropy generation at the interface may become comparable to or even dominant over that in the bulk region. The thermodynamic performance of microscale system will thus be inadequately or erroneously evaluated when neglecting the interfacial irreversibility. It will be shown that the total entropy generation may increase with increasing Kn when both the bulk and interfacial entropy generations are counted.

Therefore, the present work aims at a systematic second-law analysis of microscale gas flow and heat transport with special attention on the role of interfacial entropy generation. Two classical cases are taken for demonstration: heat convections in micro-pipe [37] and in micro-channel [38]. The remainder of this article is organized as: in Section 2, the mathematical expressions of bulk and interfacial entropy generation are derived respectively in the frame of CIT and gas kinetic theory, as the theoretical foundation of second-law analysis. In Section 3, the analytical solutions and then the specific entropy generation formulations of heat convections in micro-pipe and micro-channel are presented. In Section 4, we provide the results of second-law analysis of the two cases of microscale heat convection in Section 3, with the role of interfacial irreversibility to be illustrated and discussed. Concluding remarks are finally made in Section 5.

2. Theoretical foundation of second-law analysis

The theoretical evaluation of thermodynamic irreversibility in microscale gas flow is intimately related to its hydrodynamic modeling, as is shown in Fig. 1. The microscale gas flow within the slip regime ($0.001 \leqslant Kn \leqslant 0.1$) is considered throughout the present work, modeled by the Navier–Stokes equation (or Fourier's law) with a velocity slip (or temperature jump) boundary condition [4]. Although in principle the gas behaviors within the Knudsen layer should be described through a solution of BTE, the present modeling has been proved to yield sufficiently accurate results within the slip regime [4,7]. Accordingly, the total entropy generation includes twofold shown in Fig. 1(b): the bulk part in the microchannel due to the fluid flow (or heat transport) and the interfacial part at the wall induced by velocity slip (or temperature jump). The interfacial entropy generation has been calculated for rarefied gas transport based on kinetic theory of gases, as the difference between the entropy fluxes at the gas side and the solid one [32–34]. The velocity distribution function of gases obtained by the Chapman–Enskog solution to BTE in the bulk region (outside the Knudsen layer) was used to evaluate the entropy flux at the gas side. From the authors' perspective, the obtained entropy generation is actually that within the Knudsen layer, as shown in Fig. 1(c). As the Knudsen layer is modeled approximately by continuum equation, the entropy generation within this layer has been accounted in the bulk part, as indicated in Fig. 1(b). Direct application of previous interfacial entropy generation here will duplicate the entropy generation in the Knudsen layer. Thus in the present work, the interfacial entropy generation is derived as the difference between entropy flux of gas at the wall and entropy flux in the solid wall. The former one is evaluated based on the velocity distribution functions of incident gases (f^-) and reflecting gases (f^+) at the wall, which are related by the Maxwell gas-surface interaction model, as shown in Fig. 1(d). The obtained interfacial entropy