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Gas flow towards an adsorbing planar wall subject to partial gas-surface thermal accommodation

C. Tantos¹, S. Naris, D. Valougeorgis

Laboratory of Transport Phenomena, Department of Mechanical Engineering
University of Thessaly, Pedion Areos, 38334 Volos, Greece

Abstract

The steady half-space single gas flow driven by an adsorbing planar wall is investigated based on the solution of the BGK kinetic model. The mass and heat transfer between the gas and the plate are characterized by the sticking and thermal accommodation coefficients, the surface temperature and the far upstream velocity and temperature. The work is focused on the influence of partial thermal gas-surface interaction on all flow quantities and mainly on the value of the sticking coefficient. The surface temperature is taken to be equal or lower than the upstream temperature. It has been found that as the gas thermal accommodation on the surface is reduced for prescribed adsorbing flux and temperature difference the sticking coefficient must be increased to sustain the prescribed flux or otherwise for the same sticking coefficient the adsorbing flux is reduced. This behavior is further enhanced as the difference, between the surface and the far upstream temperatures, is increased, which is commonly the case in cryogenic applications. Overall, the effect of the thermal accommodation coefficient is significant in all flow quantities and the type of thermal gas-surface interaction must be accordingly taken into consideration.

¹ Corresponding author: christantos@mie.uth.gr

1. Introduction

Gas adsorption processes are present in many natural, physical, biological, and chemical systems and are widely used in industrial applications such as water purification, air conditioning (adsorption chillers), vapor deposition (CD/DVD metallization) and vacuum pumping (getters and cryogenic pumps). Due to mass transfer a gas adsorption flow is induced. Since in most cases the surface temperature is lower (or much lower) than the gas temperature in the bulk flow, heat transfer is also present. Thus, gas adsorption flow combines both mass and heat transfer. At the gas-surface interface a Knudsen layer is developed and therefore, modeling of such flows is commonly based on kinetic theory by applying the Boltzmann equation or kinetic model equations [1] or alternatively the Direct Simulation Monte Carlo Method (DSMC) [2].

In gas adsorption a fraction of molecules impinging to the surface is adsorbed (stick to the surface), while the remaining fraction is re-emitted (reflected) into the gas. At the surface the so-called sticking coefficient is commonly defined as [3]

$$\alpha_{sc} = \frac{J^- - J^+}{J^-}, \quad (1)$$

where J^- and J^+ are the particle fluxes impinging to and reflected from the surface respectively. The sticking coefficient $\alpha_{sc} \in [0,1]$ is a measure of the probability that a molecule landing on the surface will permanently stick on it and provides an indication of the effectiveness of gas removal from the system. It may be estimated as a free parameter by matching experimental with corresponding computational results characterizing a specific gas-surface set up (surface porosity, gas type, gas and surface temperatures). Then, these estimates may be applied in deriving boundary conditions for the simulation of adsorption processes in similar set-ups.

Following this procedure the sticking coefficients of several gases for cryopanel coated with activated carbon at very low temperatures have been estimated [4, 5] and then, they have been applied in the numerical modeling of cryopumps used in the main pumping systems of magnetic confinement fusion reactors [6, 7]. Also, in a recent theoretical work the half-space adsorption flow problem for single gases and gas mixtures has been solved providing the relationship between the problem parameters [8, 9]. The

problem is solved in dimensionless form based on the DSMC method and it has been found that in the case of single gases the sticking coefficient depends on the Mach number of the flow far upstream and the ratio of the gas temperature far upstream over the surface temperature.

It is noted that all available works are based on the assumption that the emitted particles are in thermal equilibrium with the surface, i.e., the reflected particles have the same temperature with that of the adsorption surface. In cases however, where the temperatures of the surface and of the gas far from the surface differ significantly it is reasonable to argue that the elapse accommodation time for the reflected particles on the surface is not adequate to reach the surface temperature. Then, the reflected particles are not fully thermally accommodated at the surface. This type of gas-surface thermal interaction is modeled by the so-called thermal accommodation coefficient [10], which now is defined for that fraction of the incident molecular stream which is reflected from the surface [11], i.e.,

$$\alpha_{TAC} = \frac{(1 - \alpha_{SC})E^- - E^+}{(1 - \alpha_{SC})E^- - E_w^+}. \quad (2)$$

In Eq. (2), E^- is the incident energy flux, E^+ is the reflected energy flux and E_w^+ is the energy flux that would have been achieved if the reflected molecules were in thermal equilibrium with the surface. For $\alpha_{SC} = 0$, the above definition is reduced to the typical one introduced in purely heat transfer problems [10, 12]. All works cited above [4-9] have been performed assuming $\alpha_{TAC} = 1$.

Here, the steady-state half space single gas adsorption flow, as defined in [8], is solved via kinetic modeling. The aim of the present work is to investigate the effect of the partial wall thermal accommodation on the other flow parameters and mainly on the sticking coefficient α_{SC} by varying the thermal accommodation coefficient as $\alpha_{TAC} \in [0,1]$. Furthermore, the distributions of all macroscopic quantities with practical interest as well as dimensional results for specific gases are provided.

2. Formulation of the gas adsorption flow

Consider a monatomic gas occupying the half space $\hat{x} > 0$ bounded by a planar infinite plate located at $\hat{x} = 0$, with \hat{x} being the coordinate which spans the direction normal to the plate. The gas motion is generated by the adsorbing plate maintained at uniform temperature T_w , while the mass and heat transfer between the gas and the plate are characterized by the sticking coefficient α_{SC} and thermal accommodation coefficient α_{TAC} . Far upstream the gas is at local equilibrium at some temperature $T_\infty \geq T_w$ flowing with some velocity U_∞ in the negative \hat{x} direction. The flow is one-dimensional normal to the plate. In spite of the simplicity of the flow configuration the relationship among the flow parameters and their effect on the flow bulk quantities have not been yet fully investigated.

2.1 Basic equations

The adsorption flow is governed by the steady-state one-dimensional Bhatnagar-Gross-Krook (BGK) kinetic equation [13, 14] given by

$$\xi_x \frac{\partial \hat{f}}{\partial \hat{x}} = \frac{P}{\mu} (\hat{f}^M - \hat{f}). \quad (3)$$

Here, the main unknown is the distribution function $\hat{f} = \hat{f}(\hat{x}, \boldsymbol{\xi})$, with $\boldsymbol{\xi} = [\xi_x, \xi_y, \xi_z]$ being the molecular velocity vector, P is the local pressure, μ is the viscosity at local temperature T and

$$\hat{f}^M = \frac{N}{(2\pi RT)^{3/2}} \exp \left[-\frac{(\xi_x - U)^2 + \xi_y^2 + \xi_z^2}{2RT} \right] \quad (4)$$

the local Maxwellian distribution, with R denoting the gas constant. Also, the number density N , the \hat{x} -component of the bulk velocity U (the other two components are zero) and temperature T are defined by the moments of \hat{f} as follows:

$$N(\hat{x}) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{f} d\xi_x d\xi_y d\xi_z \quad (5)$$

$$U(\hat{x}) = \frac{1}{N(\hat{x})} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \xi_x \hat{f} d\xi_x d\xi_y d\xi_z \quad (6)$$

$$T(\hat{x}) = \frac{1}{3N(\hat{x})R} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [(\xi_x - U)^2 + \xi_y^2 + \xi_z^2] \hat{f} d\xi_x d\xi_y d\xi_z \quad (7)$$

Other macroscopic quantities of some practical interest in the present work are the pressure defined by the equation of state $P = Nk_B T$, where k_B is the Boltzmann constant, the normal pressures

$$P_{xx}(\hat{x}) = m \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\xi_x - U)^2 \hat{f} d\xi_x d\xi_y d\xi_z, \quad P_{yy}(\hat{x}) = P_{zz}(\hat{x}) = m \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \xi_y^2 \hat{f} d\xi_x d\xi_y d\xi_z \quad (8)$$

and the energy and heat fluxes in the x direction given by

$$E(\hat{x}) = \frac{m}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \xi^2 \xi_x \hat{f} d\xi_x d\xi_y d\xi_z \quad (9)$$

and

$$Q(\hat{x}) = \frac{m}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [(\xi_x - U)^2 + \xi_y^2 + \xi_z^2] (\xi_x - U) \hat{f} d\xi_x d\xi_y d\xi_z, \quad (10)$$

respectively, where m is the molecular mass ($R = k_B / m$).

It is convenient to rewrite the governing equations in dimensionless form using the far upstream ($\hat{x} \rightarrow \infty$) macroscopic distributions as reference quantities. Thus, the dimensionless number density, velocity, temperature, normal stresses, pressure, energy flux and heat flux are defined as

$$n = N / N_{\infty}, \quad u = U / v_{\infty}, \quad \tau = T / T_{\infty}, \quad p_{ii} = P_{ii} / (2P_{\infty}), \quad p = P / P_{\infty} \\ e = E / (P_{\infty} v_{\infty}), \quad q = Q / (P_{\infty} v_{\infty}) \quad (11)$$

Respectively. All quantities with the subscript “ ∞ ” are the reference quantities, with $v_{\infty} = \sqrt{2RT_{\infty}}$ being the most probable molecular speed far upstream. The equation of state now reads $p = n \times \tau$. The mean free path far upstream, defined as

$$\lambda_{\infty} = \frac{2}{\sqrt{\pi}} \frac{\mu_{\infty} v_{\infty}}{P_{\infty}}, \quad (12)$$

is taken as the characteristic length. The dimensionless distribution function is given by $f(x, \mathbf{c}) = \hat{f}(\hat{x}, \boldsymbol{\xi}) v_{\infty}^3 / N_{\infty}$, where $x = \hat{x} / \lambda_{\infty}$ and $\mathbf{c} = \boldsymbol{\xi} / v_{\infty}$ are the dimensionless length and molecular velocity vector respectively.

Furthermore, the computational effort is significantly reduced by eliminating, based on the well-known projection procedure, the y - and z -components of the molecular velocity vector $\mathbf{c} = [c_x, c_y, c_z]$. This is achieved by introducing the reduced distributions [15]:

$$F(x, c_x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f dc_y dc_z \quad \text{and} \quad G(x, c_x) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (c_y^2 + c_z^2) f dc_y dc_z. \quad (13)$$

Next, operating successively with the integral operators $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\cdot) dc_z dc_y$ and $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (\cdot) (c_y^2 + c_z^2) dc_z dc_y$ on the dimensionless form of Eqs. (3-10), yields a system of two integro-differential equations for the reduced distributions functions

$$c_x \frac{\partial F}{\partial x} = \frac{2}{\sqrt{\pi}} \rho \sqrt{\tau} [F^M - F], \quad c_x \frac{\partial G}{\partial x} = \frac{2}{\sqrt{\pi}} \rho \sqrt{\tau} [G^M - G] \quad (14)$$

with the reduced Maxwellians given by

$$F^M = \frac{\rho}{(\pi\tau)^{1/2}} \exp\left[-\frac{(c_x - u_x)^2}{\tau}\right], \quad G^M = \frac{\rho\tau}{(\pi\tau)^{1/2}} \exp\left[-\frac{(c_x - u_x)^2}{\tau}\right] \quad (15)$$

coupled with the associated moments

$$\begin{aligned} n(x) &= \int_{-\infty}^{\infty} F dc_x, & u(x) &= \frac{1}{n} \int_{-\infty}^{\infty} c_x F dc_x, \\ \tau(x) &= \frac{2}{3n} \int_{-\infty}^{\infty} [(c_x - u)^2 F + G] dc_x, & P_{xx}(x) &= \int_{-\infty}^{\infty} (c_x - u)^2 F dc_x, \\ E(x) &= \int_{-\infty}^{\infty} c_x (c_x^2 F + G) dc_x, & q_x(x) &= \int_{-\infty}^{\infty} (c_x - u) [(c_x - u)^2 F + G] dc_x \end{aligned} \quad (16)$$

In the formulation of the basic equations presented here the hard-sphere intermolecular interaction model has been applied.

2.2 Boundary conditions

The adsorption process on the planar surface at $\hat{x} = 0$ is modeled by prescribing the distribution of reflected molecules according to

$$\hat{f}(0, \xi) = \frac{N_w}{(2\pi RT_A)^{3/2}} \exp\left(-\frac{\xi_x^2 + \xi_y^2 + \xi_z^2}{2RT_A}\right), \quad \xi_x > 0, \quad (17)$$

where the parameters N_w and T_A may be defined as follows.

The parameter N_w is specified by substituting Eq. (17) into the expression of the reflected particle flux $J^+ = \int_{\xi_x > 0} \xi_x \hat{f}(0, \xi) d\xi$ to deduce $J^+ = N_w \sqrt{RT_A} / \sqrt{2\pi}$. In this expression the definition of the sticking coefficient given by Eq. (1) is introduced, to find

$$N_w = (1 - \alpha_{SC}) \sqrt{\frac{2\pi}{RT_A}} J^-, \quad (18)$$

where $J^- = -\int_{\xi_x < 0} \xi_x \hat{f}(0, \xi) d\xi$ is the incident particle flux.

The parameter T_A , which has been introduced in the boundary condition in order to take into account partial thermal accommodation, is defined by substituting Eq. (17) into the expression for the reflected energy flux $E^+ = \frac{m}{2} \int_{\xi_x > 0} \xi_x \xi^2 \hat{f}(0, \xi) d\xi$. In the resulting expression, Eq. (18) is introduced to yield $E^+ = 2(1 - \alpha_{SC}) J^- k_B T_A$. Operating similarly in the case of full thermal accommodation (now T_A is replaced by T_w) is readily deduced that $E_w^+ = 2(1 - \alpha_{SC}) J^- k_B T_w$. These two expressions for E^+ and E_w^+ are substituted into Eq. (2) for the thermal accommodation coefficient to find

$$T_A = \alpha_{TAC} T_w + (1 - \alpha_{TAC}) \frac{E^-}{2k_B J^-} \quad (19)$$

where $E^- = -\frac{m}{2} \int_{\xi_x < 0} \xi_x \xi^2 \hat{f}(0, \xi) d\xi$ is the incident energy flux. Thus, boundary condition (17) for the reflected molecules is fully defined in terms of the impinging distribution, which is part of the solution.

Far upstream ($\hat{x} \rightarrow \infty$) the gas flow is described by a Maxwellian written as

$$\hat{f}_\infty(\xi) = \frac{N_\infty}{(2\pi RT_\infty)^{3/2}} \exp\left(-\frac{(\xi_x - U_\infty)^2 + \xi_y^2 + \xi_z^2}{2RT_\infty}\right). \quad (20)$$

At that end the distribution function and the resulting macroscopic quantities should not depend on the spatial variable \hat{x} .

Next, the boundary conditions are non-dimensionalized and the projection procedure is introduced in the same manner as in the basic equations. Following this routine manipulation at $x=0$ the emitted reduced distributions are

$$F(0, c_x) = \frac{n_w}{\sqrt{\pi\tau_A}} \exp\left[-\frac{c_x^2}{\tau_A}\right], \quad G(0, c_x) = \frac{n_w\sqrt{\tau_A}}{\sqrt{\pi}} \exp\left[-\frac{c_x^2}{\tau_A}\right], \quad c_x > 0 \quad (21)$$

where the parameters are given by

$$n_w = (1 - \alpha_{SC}) \frac{2\sqrt{\pi}}{\sqrt{\tau_A}} j^-, \quad \tau_A = \alpha_{TAC}\tau_w + (1 - \alpha_{TAC}) \frac{e^-}{2j^-}, \quad (22)$$

with the incident particle and energy fluxes computed as

$$j^- = - \int_{c_x < 0} c_x F(0, c_x) dc_x, \quad e^- = - \int_{c_x < 0} c_x [c_x^2 F(0, c_x) + G(0, c_x)] dc_x, \quad (23)$$

while at $\hat{x} \rightarrow \infty$ the Maxwellian takes the form

$$F_\infty = G_\infty = \frac{1}{\sqrt{\pi}} \exp\left[-(c_x - u_\infty)^2\right], \quad (24)$$

In Eqs. (21-24), the dimensionless quantities are $n_w = N_w / N_\infty$, $u_\infty = U_\infty / v_\infty$, $\tau_A = T_A / T_\infty$, $\tau_w = T_w / T_\infty$, $j^- = J^- / (v_\infty N_\infty)$ and $e^- = E^- / (P_\infty v_\infty)$.

Based on the above dimensionless formulation the flow parameters involved in the present one-dimensional adsorption flow problem are four, namely the coefficients α_{SC} and α_{TAC} , the temperature ratio τ_w and the velocity u_∞ . Commonly, the dimensionless velocity at infinity u_∞ is presented via the Mach number far upstream defined as $Ma_\infty = |U_\infty| / c_\infty$, where $c_\infty = \sqrt{\gamma RT_\infty}$ is the corresponding sound speed [8]. Since for a monatomic gas the ratio of the specific heats is $\gamma = 5/3$ it is seen that $Ma_\infty = |u_\infty| \sqrt{6/5}$.

2.3 Numerical scheme

The governing equations (14) with the associated expressions (15) and (16) subject to boundary conditions (21-24) are solved numerically in an iterative manner. More specifically for prescribed values of α_{SC} , α_{TAC} and τ_w the iteration map starts by assuming all needed macroscopic quantities including the far upstream velocity u_∞ as well as the parameters n_w and τ_A . The kinetic equations (14) are solved to yield the

reduced distributions F and G , which are introduced into the moment equations (16) as well as in the flux equations (23) to find the new estimates of all bulk quantities which are now introduced in the next iteration. The iteration process is terminated when the imposed convergence criteria is fulfilled. Upon convergence the correct value of u_∞ is recovered. Thus, the present problem is properly defined only when three out of the four involved parameters are given. If all parameters both at the plane surface and far upstream are defined no steady-state flow conditions may be reached. Here, we have chosen to compute u_∞ (or the associated Mach number Ma_∞) as a function of the remaining three parameters, i.e.,

$$u_\infty = u_\infty(\alpha_{SC}, \alpha_{TAC}, \tau_w) \quad (25)$$

The discretization of the kinetic equations is based on the discrete velocity method in the molecular velocity space. In the physical space a second order control volume approach is applied using non-uniform grid spacing which follows the geometric sequence $\Delta x_i = \Delta x_1 \times r^{i-1}$, with $\Delta x_1 = 4 \times 10^{-7}$ and $r = 1.0009$ (the subscript $i = 1, \dots, K$ refers to the nodes in the physical space). The macroscopic quantities are computed by Gauss quadrature. This numerical scheme has been extensively applied in the solution of rarefied gas flows with considerable success [16]. The results presented in the next section have been obtained with about 15000 nodes in the physical space and 16 molecular velocities, while the convergence criteria to be fulfilled is

$$\frac{1}{3K} \sum_{i=1}^K \left[\left| n_i^{(t+1)} - n_i^{(t)} \right| + \left| \tau_i^{(t+1)} - \tau_i^{(t)} \right| + \left| u_i^{(t+1)} - u_i^{(t)} \right| \right] < \varepsilon. \quad (26)$$

In (26) the superscript t denotes the iteration index and $\varepsilon = 10^{-5}$ is the tolerance parameter. For $\alpha_{SC} = 0$ the corresponding half-space purely heat transfer problem is recovered.

3. Results and discussion

A validation of the accuracy of the results is displayed in Section 3.1. In Section 3.2, results are presented and discussed for the macroscopic velocity and the Mach number far upstream, as well as for the half space distributions of density, velocity, temperature and pressure in terms of the sticking and thermal accommodation coefficients varying

between zero and one and for various values of the temperature ratio $\tau_w = T_w / T_\infty$. The dependency of the thickness of the Knudsen layer on the flow parameters is also discussed. Finally, in Section 3.3 some dimensional results for specific gases are presented.

At this point it is useful to note that since the upstream quantities are taken as the reference quantities, $n_\infty = 1$ and thus $|u_\infty| = j_\infty = \alpha_{SC} j^-$, i.e. is equal to the upstream net particle flux and to the adsorbed particle flux (all in dimensionless form) and therefore characterizes the intensity of the adsorption process.

3.1 Benchmarking

The accuracy of the results has been confirmed in several ways. In all cases the length L of the computational domain, i.e., the distance between the plate and the position on the x -axis, where the far upstream boundary condition is imposed, has been computationally checked to be long enough to properly recover space independent quantities at that end. Several runs have been performed for the same set of parameters by increasing L until no variation in the numerical results is observed. Grid independency of the results is also confirmed. Furthermore, in all cases tested, the computed macroscopic distributions fulfill the conservation laws derived in the Appendix.

To further validate the accuracy of the results a comparison with available corresponding results in the literature is performed. As it is pointed in the introduction, the same flow configuration has been studied in [8] for $\alpha_{TAC} = 1$ based on the DSMC method. In Fig. 1, which reports the upstream Mach number Ma_∞ versus α_{SC} , a comparison is performed between the results of the present work and the corresponding ones in [8] for $\tau_w = 1$ and 0.25. It is clearly seen that although the two computational approaches are completely different (the present one is deterministic, while the one in [8] is stochastic) the agreement between the results in the whole range of the sticking coefficient and for both temperature ratios is excellent with the relative error being less than 1%. Also, as shown in Fig. 1, increasing the Ma_∞ leads to higher values of α_{SC} . In addition, as τ_w is reduced, i.e., the temperature difference between the upstream gas and

surface temperatures $\Delta T = T_\infty - T_w$ is increased, for the same α_{SC} , the Ma_∞ is increased, which means that the adsorption process becomes more intense. This remark may be alternatively stated by saying that as τ_w is reduced, for the same Ma_∞ , a lower α_{SC} is needed in the specific adsorption processes. As expected the effect of ΔT is important.

3.2 Effect of partial thermal accommodation

Next, we focus to the main objective of the present work which is the investigation of the effect of α_{TAC} on the adsorption process. In Fig. 2, the magnitude of the computed far upstream velocity u_∞ is plotted as a function of α_{SC} for $\alpha_{TAC} = [1, 0.8, 0.2]$ and $\tau_w = T_w / T_\infty = [1, 0.27, 0.05]$. As seen in Fig. 2, for $\tau_w = 1$, the effect of α_{TAC} is negligible. This is well expected since when the surface and upstream temperatures are equal there is no heat transfer mechanism. However, as τ_w is reduced (the temperature difference is increased) heat transfer is enhanced and as a result the effect of α_{TAC} is also increased. In general, $|u_\infty|$ is reduced as α_{TAC} is reduced, i.e., as the gas thermal accommodation at the plate becomes less complete. This is physically justified since, in practice, a lower thermal accommodation at the surface corresponds (at some sense) to some smaller temperature difference ΔT than the imposed one. Indicatively, at fixed values of $\alpha_{SC} = 0.7$ and $\tau_w = 0.27$, when $\alpha_{TAC} = 0.8$ and 0.2 the reductions in $|u_\infty|$, compared to the ones for $\alpha_{TAC} = 1$, are 9% and 27% respectively. The corresponding reductions at $\tau_w = 0.05$ are 20% and 42%. The effect of α_{TAC} becomes more important at low and intermediate values of α_{SC} between 0.1 and 0.8. Overall, the effect of α_{TAC} is of similar importance with τ_w .

It is noted that the specific temperature ratios of 0.27 and 0.05 have been selected because, for $T_\infty = 300$ K, they correspond to $T_w = 80$ K and 15 K respectively, which are two characteristic temperatures introduced in a recent work performed within the EUROfusion programme [17] related to the design of a multistage cryopump. Of course, they are also indicative for other temperature ratios covering a wide range of temperature differences.

A more detailed insight in the adsorption flow characteristics is displayed in Figs. 3, 4, 5 and 6, where the dimensionless distributions of number density, velocity magnitude, temperature and pressure are displayed for two temperature ratios $\tau_w = [0.05, 0.27]$ and the sticking and thermal accommodation coefficients taking the typical values of $\alpha_{SC} = [0.1, 0.5, 0.9]$ and $\alpha_{TAC} = [0.2, 0.8, 1]$ respectively. In all cases the horizontal axis measures the distance L from the planar surface in mean free paths. This distance also corresponds to the thickness of the adsorption Knudsen layer where non-equilibrium transport phenomena occur. As shown in Figs. 3-6, it is influenced from both α_{SC} and τ_w . It is evident that increasing the sticking coefficient α_{SC} leads to lower values of L , which means that the far upstream conditions are recovered faster in a smaller number of mean free paths \hat{x}/λ_∞ from the adsorption surface. The effect of the temperature difference is not that clear but it has been observed that decreasing τ_w reduces the thickness L .

In Fig. 3, the number density profile $n(x)$ is plotted. The shape of $n(x)$ is qualitatively similar for $\tau_w = 0.05$ and 0.27 with the gradient dn/dx being more stiff in the former case (more rapid changes as ΔT is increased). The far upstream number density is (as it should) always equal to one. For $\alpha_{TAC} = 1$ and 0.8 , as x is reduced, for all values of α_{SC} , the number densities are monotonically increased reaching their highest values on the surface ($x=0$). In particular, for $\alpha_{SC} = 0.1$ the two profiles are very close and then for $\alpha_{SC} = 0.5$ and 0.9 there is a departure between the profiles with the number density taking lower values as the sticking coefficient is increased. This behavior remains the same for $\alpha_{TAC} = 0.2$ and $\alpha_{SC} = 0.1$. On the contrary for $\alpha_{TAC} = 0.2$ and $\alpha_{SC} = 0.5$ and 0.9 , as x is reduced, the number densities are monotonically reduced reaching their lowest values at $x=0$. Overall, increasing the sticking coefficient leads to lower values of density. For low enough values of α_{TAC} the number density is even lower than the far upstream value. This behavior in terms of the thermal accommodation is physically explained since, as pointed out above, as α_{TAC} is decreased the gas is reflected from the

surface with a temperature larger than the surface temperature and as a result the gas density is decreased.

In Fig. 4, the normalized velocity magnitude $|u(x)/u_\infty|$ is plotted. As expected in most cases the magnitude of the gas velocity is reduced as it approaches the adsorption surface. This speed decrease is reduced as α_{TAC} is decreased and finally for $\alpha_{TAC} = 0.2$ and $\alpha_{SC} = 0.9$ the gas moves faster as it approaches the plate. This behavior is the inverse of the one observed for the number density and it is fully justified since as shown in the Appendix the particle flux conservation law $n(x)u(x) = u_\infty$ or $n(x)u(x)/u_\infty = 1$ applies.

The dimensionless temperature profiles are displayed in Fig. 5. The gas temperature far upstream is equal to one and then in most cases, as expected, the temperature is decreased approaching to the adsorption surface. This situation is reversed only for high values of α_{SC} combined with low values of α_{TAC} . The corresponding pressure profiles are shown in Fig. 6. In all cases the variation of pressure obeys the equation of state $p(x) = n(x)\tau(x)$. As α_{SC} is decreasing, independent of α_{TAC} , the half-space pressure distribution becomes more uniform, which is well expected since the purely half-space heat transfer problem is recovered. It is also noted that the behavior of the normal pressure $p_{xx}(x)$ is similar to $p(x)$ and therefore is not displayed, while in all cases $p_{yy} = p_{zz}$ and $p_{xy} = p_{xz} = 0$.

All simulations reported above are based on the HS model. Corresponding simulations have been performed for the Maxwell interaction deducing results which are very close to the ones by the HS model. Therefore it is stated that the choice of the intermolecular potential model has negligible effect on the present adsorption flow problem. Another issue of some interest is that corresponding results have been obtained for polyatomic gases based on the Holway model [18]. It has been found that the influence of the internal degrees of freedom is small (about 10%) in this flow configuration and therefore the dimensionless results presented here may be also used in the case of polyatomic gases.

4.3 Sticking coefficients of specific gases

Closing this section is useful to provide some results in dimensional form. The dimensionless results presented in Fig. 2 are applied to plot in Fig. 7 the net molar flux in terms of the sticking coefficient for specific monatomic gases namely protium (^1H), helium (He), neon (Ne) and xenon (Xe) for reference upstream pressure and temperature $P_\infty = 0.1 \text{ Pa}$ and $T_\infty = 300 \text{ K}$ respectively and temperature ratio $T_w / T_\infty = \tau_w = 0.05$. This is easily performed as follows: For the prescribed P_∞ and T_∞ the far upstream number density N_∞ is obtained from the equation of state ($P_\infty = N_\infty k_B T_\infty$). Then, the far upstream velocity is computed as $U_\infty = v_\infty |u_\infty|$, where $v_\infty = \sqrt{2k_B T_\infty / m}$ is known for the specific gas and $|u_\infty|$ is obtained from Fig. 2. Finally, the net particle flux is computed as $J_\infty = N_\infty U_\infty$ which is divided by the Avogadro number to be converted into the net molar flux $J_\infty^{(molar)}$ shown, versus α_{SC} for $\alpha_{TAC} = [0.2, 0.8, 1]$, in Fig. 7.

It is clearly seen that as the thermal accommodation coefficient is reduced the net molar flux $J_\infty^{(molar)}$, which is equal to the adsorbed molar flux at the surface, is reduced. It is readily deduced, from the above dimensionalization, that the ratio of the net molar fluxes of two gases, for prescribed α_{SC} , α_{TAC} and τ_w , is inversely proportional to the square root of their molar masses. Thus, it is stated that under the same prescribed reference conditions and coefficients, higher adsorption molar flow rate is sustained as the gas becomes lighter. Also, the net molar flux is directly proportional to the reference pressure P_∞ . In that sense following the demonstration procedure shown here the dimensionless results of the previous subsection can be readily applied in a wide range of reference conditions and various gases for comparison with experiments and other practical purposes.

5. Concluding remarks

The steady one-dimensional half-space flow of a monatomic gas in the presence of an absorbing planar wall is investigated based on the direct solution of the BGK kinetic model equation. The involved flow parameters include the sticking α_{SC} and thermal

accommodation α_{TAC} coefficients, the ratio of the surface temperature over the far upstream temperature τ_w and the upstream velocity u_∞ . The problem is properly defined only when three out of the four involved parameters are given. Particular attention is given on the effect of the value of α_{TAC} on u_∞ , as well as on the half space macroscopic distribution of density, velocity, temperature and pressure, for various prescribed values of α_{SC} and τ_w . It has been found that as the thermal accommodation of the gas on the surface is reduced the adsorbing flux is also reduced or otherwise for a prescribed adsorbing flux the sticking coefficient must be increased. Furthermore, the effect of partial thermal accommodation is enlarged as the difference, between the surface temperature and the far upstream temperature, is increased. Overall, the effect of α_{TAC} is significant in all flow quantities and the type of thermal gas-surface interaction must be accordingly taken into consideration. It is hoped that the present work will support further investigation on the estimation of the sticking slip coefficients and cryopump modeling via comparison with experimental works.

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Appendix: Conservation equations

Equation (11a) is multiplied successively by 1, and c_x and the resulting equations are integrated over the molecular velocity space to yield, the following conservation equations:

$$\text{Mass: } \frac{\partial}{\partial x}(nu) = 0 \quad (\text{A1})$$

$$x\text{- momentum: } \frac{\partial}{\partial x}(p_{xx} + nu^2) = 0 \quad (\text{A2})$$

Similarly, operating on Eqs. (11a) and (11b) by $\int c_x^2(\cdot)dc_x$ and $\int(\cdot)dc_x$ respectively and following some typical manipulations the energy conservation equation is obtained:

$$\text{Energy: } \frac{\partial}{\partial x} \left[nu \left(u^2 + \frac{3\tau}{2} \right) + 2up_{xx} + q_x \right] = 0 \quad (\text{A3})$$

The above conservation equations are applied to benchmark the accuracy of the numerical scheme.

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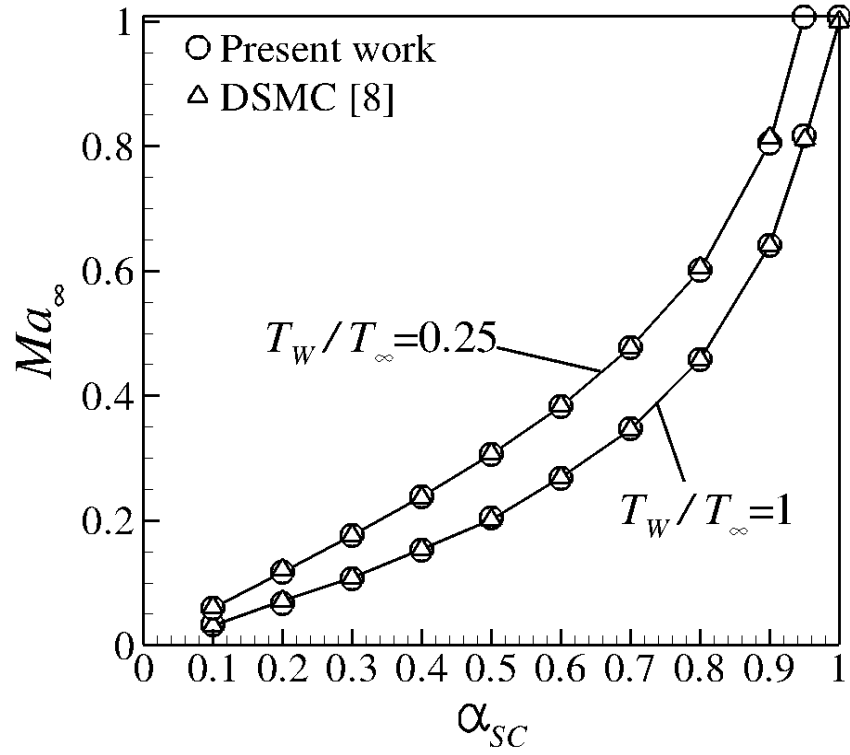


Figure 1: Upstream Mach number Ma_∞ as a function of the sticking coefficient α_{SC} for thermal accommodation coefficient $\alpha_{TAC} = 1$ and temperature ratio $\tau_w = T_w/T_\infty = [1, 0.25]$ based on the present kinetic model and the DSMC method [8].

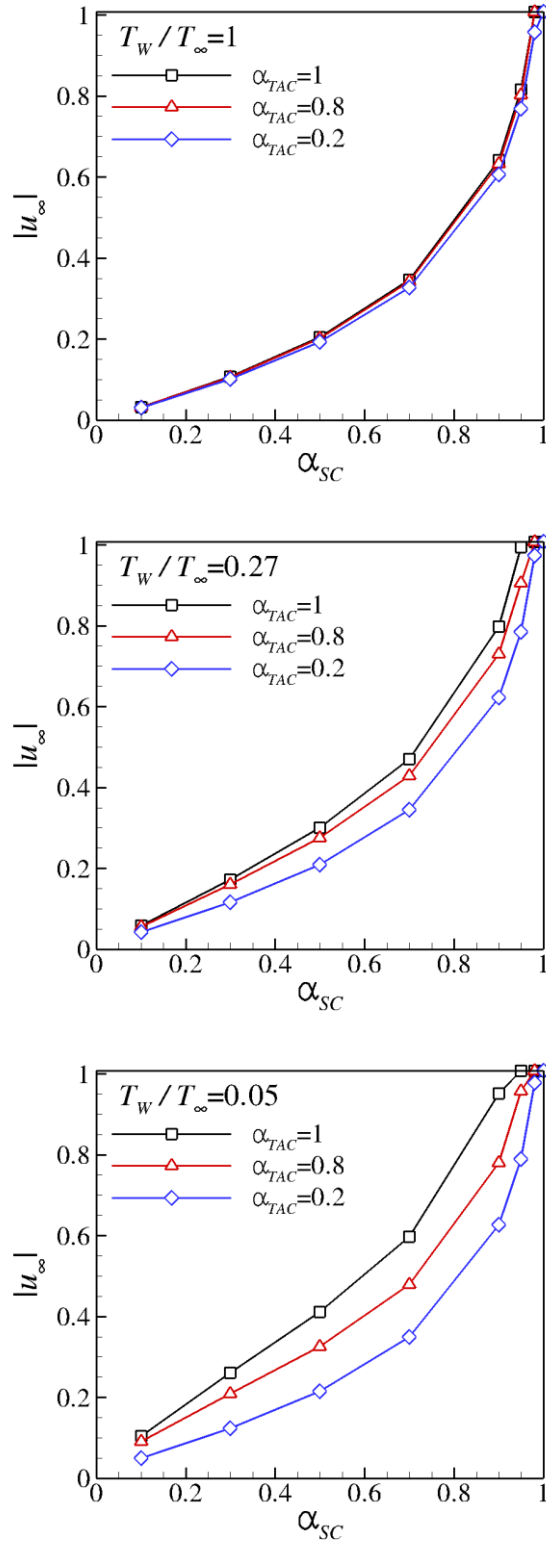


Figure 2: Upstream velocity $|u_\infty|$ as a function of the sticking coefficient α_{SC} for thermal accommodation coefficient $\alpha_{TAC} = [1, 0.8, 0.2]$ and temperature ratio $\tau_w = T_W/T_\infty = [1, 0.27, 0.05]$.

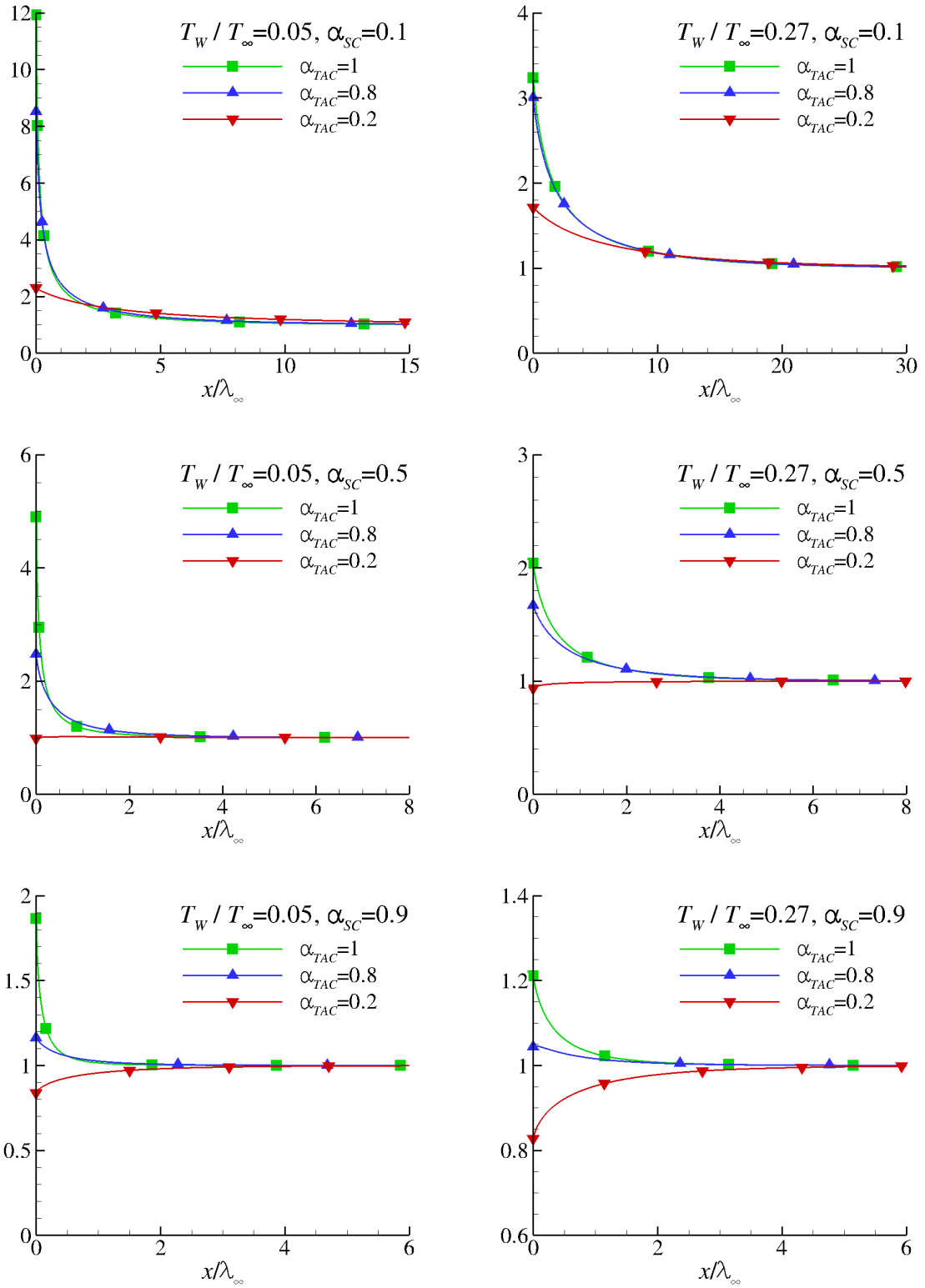


Figure 3: Dimensionless number density $n(x)$ for temperature ratios $\tau_w = T_w/T_\infty = [0.05, 0.27]$ with the sticking coefficient $\alpha_{SC} = [0.1, 0.5, 0.9]$ and the thermal accommodation coefficient $\alpha_{TAC} = [1, 0.8, 0.2]$.

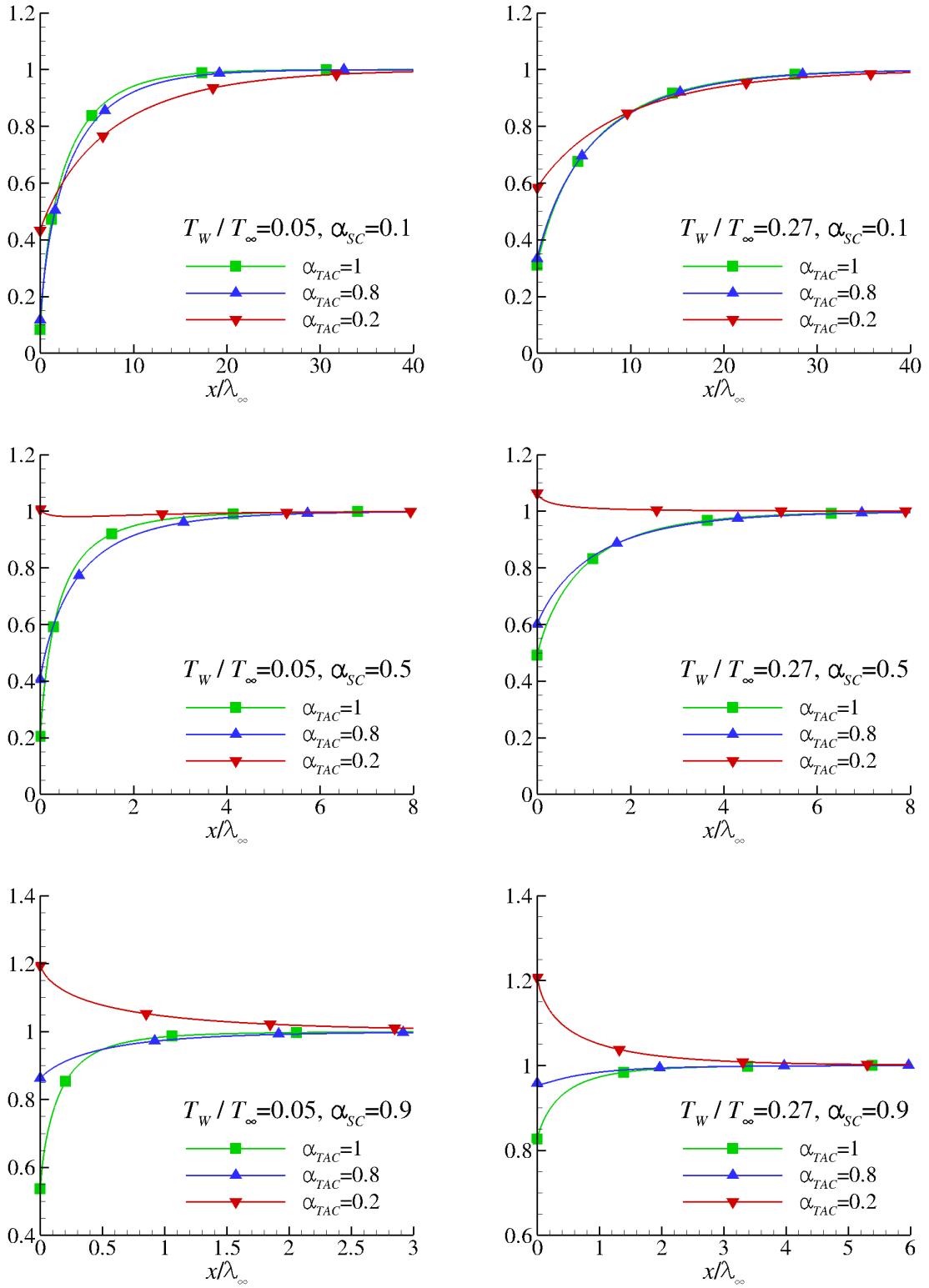


Figure 4: Normalized velocity magnitude $|u(x)/u_\infty|$ for temperature ratios $\tau_w = T_w/T_\infty = [0.05, 0.27]$ with the sticking coefficient $\alpha_{SC} = [0.1, 0.5, 0.9]$ and the thermal accommodation coefficient $\alpha_{TAC} = [1, 0.8, 0.2]$.

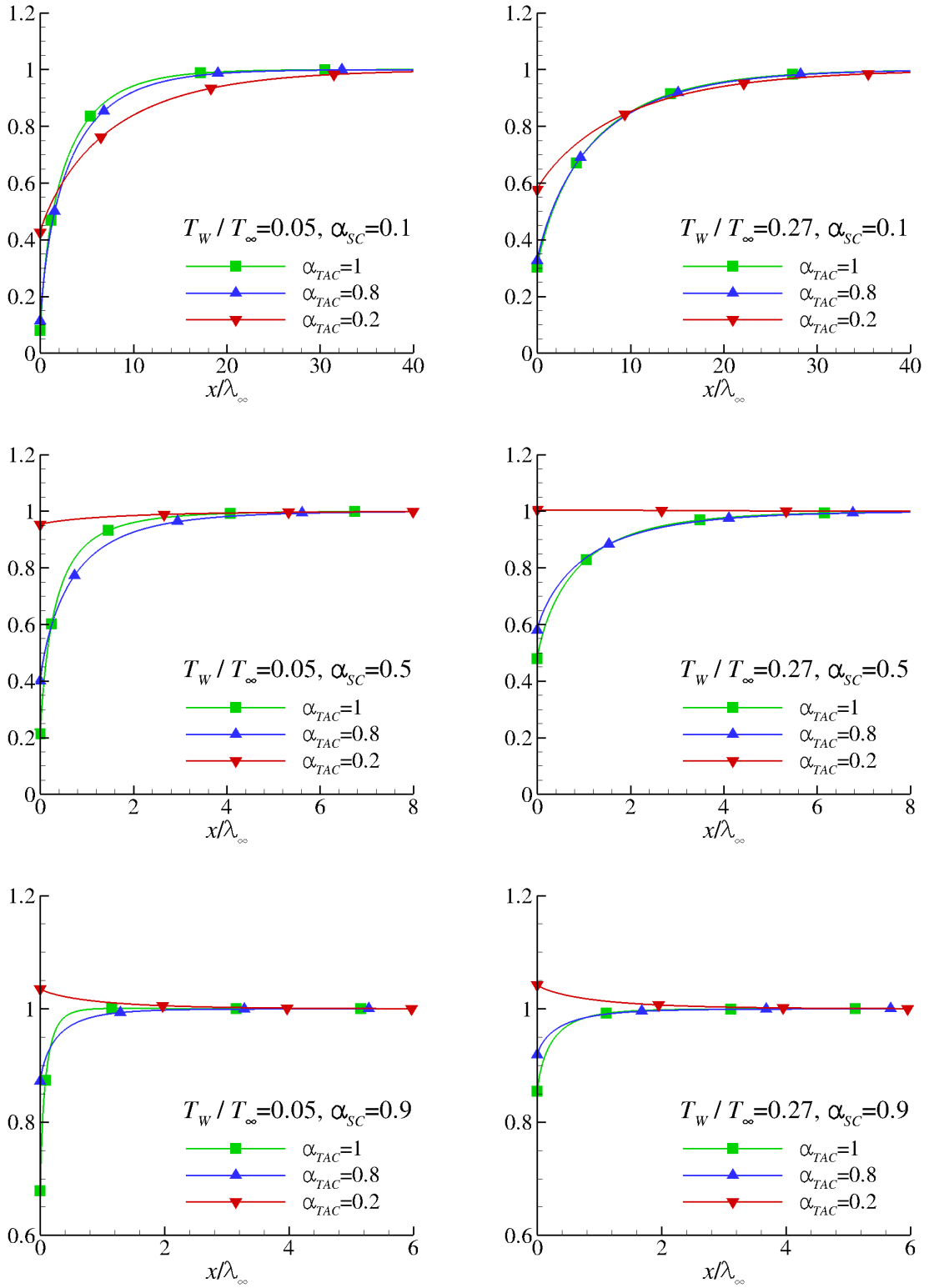


Figure 5: Dimensionless temperature $\tau(x)$ for temperature ratios $\tau_w = T_w/T_\infty = [0.05, 0.27]$ with the sticking coefficient $\alpha_{sc} = [0.1, 0.5, 0.9]$ and the thermal accommodation coefficient $\alpha_{TAC} = [1, 0.8, 0.2]$.

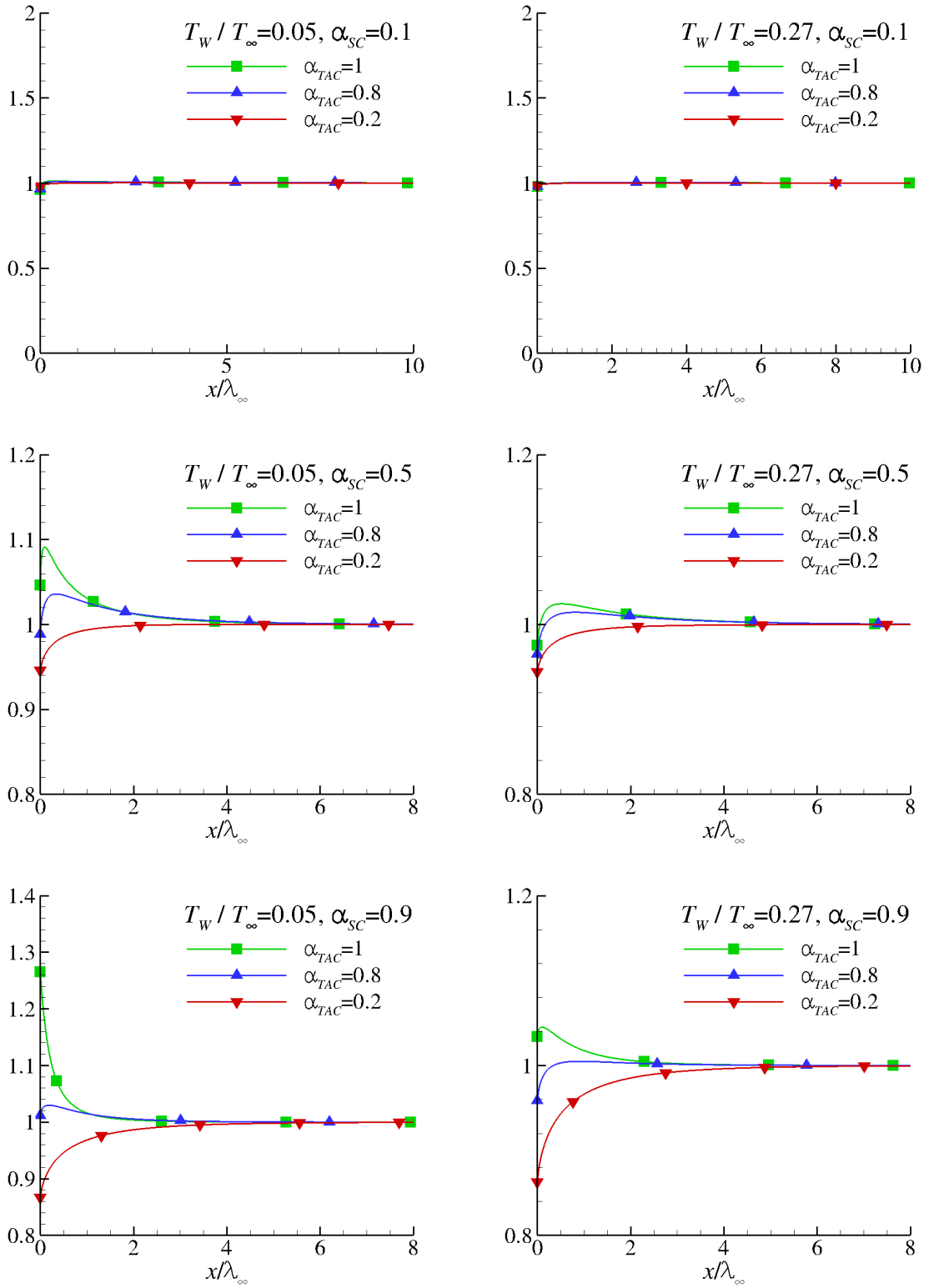


Figure 6: Dimensionless pressure $p(x)$ for temperature ratios $\tau_w = T_w/T_\infty = [0.05, 0.27]$ with the sticking coefficient $\alpha_{SC} = [0.1, 0.5, 0.9]$ and the thermal accommodation coefficient $\alpha_{TAC} = [1, 0.8, 0.2]$.

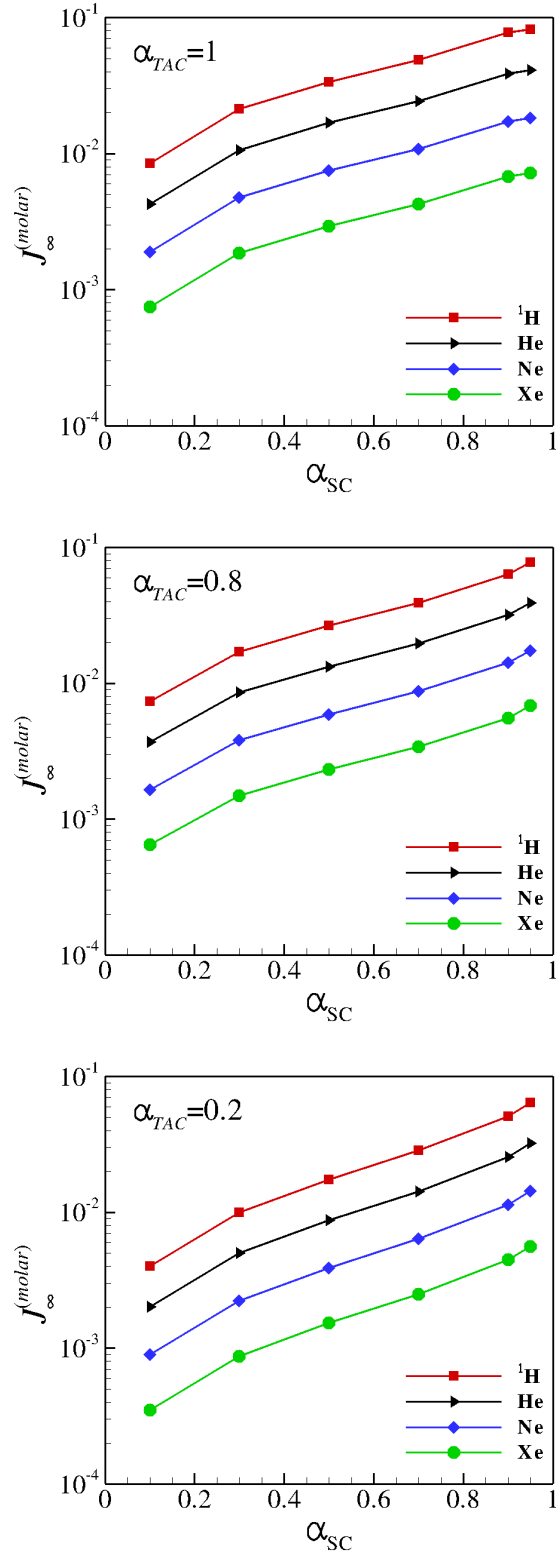


Figure 7: Net molar flux $J_\infty^{(molar)}$ of various gases as a function of the sticking coefficient α_{SC} for thermal accommodation coefficient $\alpha_{TAC} = [1, 0.8, 0.2]$ with $P_\infty = 0.1 \text{ Pa}$, $T_\infty = 300 \text{ K}$ and $\tau_w = 0.05$.