

Technical note

Generalized Treatment of Energy Accommodation in Gas-Surface Interactions for Satellite Aerodynamics Applications

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ABSTRACT

In the context of satellite aerodynamics in the Very-Low-Earth-Orbit (VLEO) regime, accurate modeling of gas-surface interactions (GSI) is crucial for determining aerodynamic forces and torques. Common models such as Sentman's assume that gas particles are reflected diffusely from a surface, which leads to the incorporation of energy accommodation into the model. This technical note discusses the limitations of existing approaches for handling energy accommodation and provides a generalized treatment thereof that is valid for any molecular speed ratio. A new general expression for the temperature ratio of reflected to impinging particles is derived, which, when used in a GSI model, does not limit it to hypothermal flows. Additionally, a simplified hypothermal approximation is presented, proven to be an asymptote of the general expression, and shown to be an improvement upon existing approximations by comparison for a realistic VLEO scenario. The results contribute to a better understanding and modeling of energy accommodation within GSI, potentially benefiting scientific investigations and operational applications of satellite aerodynamics.

1. Introduction

In the Very-Low-Earth-Orbit (VLEO) regime, the residual atmosphere is dense enough for the atmospheric drag force to represent the dominant perturbing effect acting on satellites. At the same time, the density is still low enough for the flow to be considered a free molecular flow so that the interaction of incoming particles with reflected ones is negligible. Consequently, it suffices to consider only unperturbed particles for the momentum exchange with the satellite's external surfaces to determine the aerodynamic forces and torques. To describe these gas-surface interactions (GSI), adequate models are required. Since the underlying phenomena of this interaction are very complex, advances in modeling can, for example, improve the accuracy of scientific investigations like the estimation of thermospheric density and wind from satellite data [1] or enable operational advantages such as aerodynamics-based, propellant-free attitude and orbit control of satellites [2,3].

In terms of GSI models for satellite aerodynamics, a number of approaches exists in the literature. Notable examples include those of Maxwell [4], Sentman [5], and Schaaf and Chambre [6]. The first two models explicitly assume the reflection of gas particles from the surface to be at least partially diffuse. This simplifies the treatment of the momentum exchange by fully describing it through the energy

exchange of these particles with the surface, which in turn depends on their temperature.

While Sentman, whose model is even described as the de facto standard for the computation of aerodynamic coefficients of satellites at low altitudes [7], already mentioned the relevance of a so-called energy accommodation coefficient α_E , it was Moe et al. [8] who related it to the temperature of the reflected particles and thus introduced it as an input to Sentman's model. In 2009, Koppenwallner [9] proposed a slightly different expression, which since then has been widely applied. As it will be shown in this note, however, this approximation can be used with small errors only for hypothermal flows so that a more general consideration is still pending.

This note aims to contribute to the research field by providing a more generalized treatment of energy accommodation in existing GSI models. It is valid for any molecular speed ratio and therefore does not impose an additional limitation on the usage of the encompassing GSI model to hypothermal flows. Furthermore, an approximation for hypothermal flows is derived which, unlike the one presented in Ref. [9], is shown to be an asymptote of the general expression for the temperature ratio and therefore converges to it. The contributions will help to enhance the understanding and modeling of gas-surface-interactions in VLEO and, as a consequence, scientific and operational efforts based on it could benefit in the long term.

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The note is structured as follows: in Section 2, the theoretical background of the relation between GSI models, the temperature of reflected particles and energy accommodation is discussed. Section 3 presents the derivation of a general expression for the temperature ratio of the reflected and the impinging particles, which represents the key contribution of this note. In Section 4, a simple asymptotic approximation for hyperthermal flows is derived from this general expression and subsequently compared to the existing approximation by Koppenwallner [9] in order to demonstrate the improvements.

2. Theoretical background

2.1. Gas temperatures in gas-surface-interaction models

A number of gas-surface-interaction models predict the forces acting on a structure in a free-molecular-flow environment based on diffuse reflection of all or at least some of the impinging gas particles from the structure's surface (e.g. Sentman [5]). This is based on the assumption that those particles lose all memory of the incident direction and can thus be modeled as being emitted from a fictitious gas in thermal equilibrium (i.e. with a Maxwellian velocity distribution). Under these assumptions, the vector of the average reflected velocity is perpendicular to the surface. Since its direction is known, the determination of this vector is simplified to finding its magnitude which can be accomplished by solely considering the average translational energy of the particles after the collision. For a gas in thermal equilibrium, this energy is related to the temperature of the gas.

This is why the temperature of the reflected particles is relevant for determining the forces that the gas exerts on the surface and consequently why its value is required as an input to the GSI model. Moe et al. [8] and Koppenwallner [9] both found solutions to this problem by deriving expressions for said temperature based on the energy accommodation coefficient α_E , which is explained in the following section.

2.2. Energy accommodation

The average energy of a particle after a collision with a surface can be determined using the energy accommodation coefficient α_E . It is defined as [10]:

$$\alpha_E = \frac{\bar{E}_i - \bar{E}_r}{\bar{E}_i - \bar{E}_w} \quad (1)$$

where \bar{E}_i and \bar{E}_r are the average energy of the impinging and reflected particles. \bar{E}_w is the average energy that particles would have if they were emitted through a surface element from a fictitious gas in thermal equilibrium with the temperature of the surface T_w .

When using this equation, it is important to carefully select the appropriate energy accommodation coefficient. Goodman [10] mentions that a distinction has to be made between equilibrium and non-equilibrium energy accommodation coefficients. The former is only defined for stationary gases in thermal equilibrium with the surface while the latter would have to be used for gases in motion. Furthermore, gas molecules generally possess internal energies, most notably due to their rotational and vibrational degrees of freedom, in addition to translational energy. According to Goodman [10], an energy accommodation coefficient could be defined for each of these terms or any combination thereof. GSI models, however, focus on momentum exchange and thus only consider the translational energy of the gas particles. As a consequence, the proper coefficient to be used for determining the forces acting on a structure in a GSI model would be a *non-equilibrium translational energy accommodation coefficient*.

Obtaining this specific coefficient through experiments is difficult. However, since the atmosphere in the VLEO regime is dominated by atomic oxygen [11], it can be modeled as a monatomic gas. As such, its particles do not possess rotational or vibrational degrees of freedom.

If this assumption also turned out to be valid during and after the collision with the surface, it would be a natural simplification to use the accommodation coefficient for the total energy instead of for the translational portion.

Goodman [10] states that, in theory, the non-equilibrium coefficient depends on the distribution of molecular energies of the incident gas in a complicated manner. In the literature, however, α_E is typically assumed to be in the range of about 0.9 to 1.0 for VLEO applications [12] indicating a relatively high degree of energy accommodation.

With this information, the approaches of Moe et al. [8] and Koppenwallner [9] for determining the temperature of the reflected particles can be reconstructed in the following section.

2.3. The temperature of the reflected particles

Under the assumption that the correct α_E is known, finding the temperature of the reflected particles is a matter of determining expressions for the energies in Eq. (1) that relate them to known inflow conditions as well as to T_r and T_w . As described in Section 2.1, diffusely reflected particles are assumed to be emitted from a fictitious gas in thermal equilibrium. Therefore, their average translational energy \bar{E}_r can be described by their temperature T_r in the same way as the term \bar{E}_w is described by the temperature of the surface T_w . Moe et al. [8] use the average translational energy of monatomic gas particles in thermal equilibrium within a given volume for both \bar{E}_r and \bar{E}_w :

$$\bar{E}_{r/w} = \frac{3}{2} k T_{r/w} \quad (2)$$

with k being the Boltzmann constant. This, however, is invalid as it is not equal to the average translational energy of the particles that are emitted through a surface element. Koppenwallner [9] therefore correctly applied:

$$\bar{E}_{r/w} = 2kT_{r/w}. \quad (3)$$

Within the GSI models, the temperature T_r appears in the form of the ratio T_r/T_i , with T_i being the temperature of the impinging gas particles. Inserting Eq. (3) into Eq. (1) and rearranging the result yields the following expression for the desired ratio:

$$\frac{T_r}{T_i} = \frac{\bar{E}_i}{2kT_i} (1 - \alpha_E) + \alpha_E \frac{T_w}{T_i}. \quad (4)$$

Using the definitions of the molecular speed ratio s

$$s = \frac{V_i}{c_m} \quad (5)$$

where V_i is the magnitude of the average velocity of the impinging particles and c_m is the most probable thermal velocity of the impinging gas particles, which is defined as

$$c_m = \sqrt{\frac{2kT_i}{m}}, \quad (6)$$

a relation between T_i and V_i can be obtained:

$$T_i = \frac{mV_i^2}{2ks^2}. \quad (7)$$

Here, m is the mass of a gas particle. This can be used to replace the dependency of the right side of Eq. (4) on T_i by a dependency on s and V_i :

$$\frac{T_r}{T_i} = \frac{s^2}{2} \left[\frac{2\bar{E}_i}{mV_i^2} (1 - \alpha_E) + \alpha_E \frac{4kT_w}{mV_i^2} \right]. \quad (8)$$

In summary, Eq. (8) is an expression for the temperature ratio that was derived by inserting the above definitions into that of the energy accommodation coefficient in Eq. (1). The remaining task is to determine the average energy of the impinging particles \bar{E}_i and to insert it into Eq. (8).

3. Generalized temperature ratio

3.1. Average energy of impinging particles

For the average energy of the impinging particles \bar{E}_i , Moe et al. [8] as well as Koppenwallner [9] use the following relation:

$$\bar{E}_i = \frac{1}{2} m V_i^2. \quad (9)$$

This, however, represents a hyperthermal approximation that is only valid for high molecular speed ratios as will be explained in the following.

In general, the average energy of the impinging particles can be determined as the ratio of the energy flux ϵ_i and the particle flux v_i through a surface element. Both these quantities were derived by Bird [13] (Eq. 4.27¹ and 4.22) as follows:

$$\epsilon_i = \frac{m n c_m^3}{4} \left[\frac{1}{\sqrt{\pi}} (s^2 + 2) \exp(-s^2 \cos^2 \delta) + s \cos \delta \left(s^2 + \frac{5}{2} \right) (1 + \operatorname{erf}(s \cos \delta)) \right], \quad (10)$$

$$v_i = \frac{n c_m}{2} \left[\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta (1 + \operatorname{erf}(s \cos \delta)) \right]. \quad (11)$$

Here, n is the number density of the gas, δ is the angle between the average velocity vector of the impinging particles and the surface normal, and erf is the error function. As a consequence, the average energy of the impinging particles is:

$$\bar{E}_i = \frac{\epsilon_i}{v_i} \quad (12)$$

$$= \frac{m c_m^2}{2} \left[2 + s^2 + \frac{1}{2} \frac{s \cos \delta (1 + \operatorname{erf}(s \cos \delta))}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta (1 + \operatorname{erf}(s \cos \delta))} \right] \quad (13)$$

$$= k T_i \left[2 + s^2 + \frac{1}{2} \frac{s \cos \delta (1 + \operatorname{erf}(s \cos \delta))}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta (1 + \operatorname{erf}(s \cos \delta))} \right]. \quad (14)$$

For comparison with Eq. (9), Eq. (14) can also be transformed so that its explicit dependency on T_i is replaced by an explicit dependency on V_i using Eq. (7):

$$\bar{E}_i = \frac{m V_i^2}{2} \left[\frac{2}{s^2} + 1 + \frac{1}{2 s^2} \frac{s \cos \delta (1 + \operatorname{erf}(s \cos \delta))}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta (1 + \operatorname{erf}(s \cos \delta))} \right]. \quad (15)$$

This is a general expression for the average energy of particles of a gas in thermal equilibrium and with a bulk velocity V_i that collide with a surface at an angle of δ with the surface normal.

It should be noted that a term like $1 - \operatorname{erf} x$ can exhibit numerical problems for large values of x which results in a loss of precision. This occurs in Eq. (15) for large values of s and when $\cos \delta < 0$. An implementation of the complementary error function ($\operatorname{erfc} x = 1 - \operatorname{erf} x$) that retains a high accuracy for large values of x exists for many programming languages. Using this function, Eq. (15) can be rewritten into a form that is more suitable for computational implementations:

$$\bar{E}_i = \frac{m V_i^2}{2} \left[\frac{2}{s^2} + 1 + \frac{1}{2 s^2} \frac{s \cos \delta \operatorname{erfc}(-s \cos \delta)}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta \operatorname{erfc}(-s \cos \delta)} \right]. \quad (16)$$

In the hyperthermal case, the average velocity V_i is much larger than the most probable thermal velocity c_m so that large values for the

molecular speed ratio s result. Investigating the limit of the average energy as s approaches infinity via Eq. (16) shows that the expression in brackets tends to one for surfaces that face the flow (i.e. $\cos \delta > 0$). Thus, the overall limit of the average energy is equal to Eq. (9) which verifies the statement that Eq. (9) represents a hyperthermal approximation.

3.2. General expression for the temperature ratio

In order to arrive at a result equivalent to Eqs. 26a and 42 of Ref. [9], Eq. (9) needs to be inserted into Eq. (8) which yields:

$$\frac{T_r}{T_i} = \frac{s^2}{2} \left[1 + \alpha_E \left(\frac{4kT_w}{mV_i^2} - 1 \right) \right]. \quad (17)$$

Since Eq. (9) was shown to be a hyperthermal approximation, the resulting expression for the temperature ratio in Eq. (17) also represents a hyperthermal approximation that is only valid as s approaches infinity.

The general expression for the temperature ratio, which is valid for any molecular speed ratio, can be obtained by inserting Eq. (16) (instead of Eq. (9)) into Eq. (8). The result represents a key contribution of this note:

$$\begin{aligned} \frac{T_r}{T_i} = \frac{s^2}{2} & \left[\alpha_E \frac{4kT_w}{mV_i^2} + (1 - \alpha_E) \left(\frac{2}{s^2} + 1 + \frac{1}{2s^2} \right. \right. \\ & \times \left. \left. \frac{s \cos \delta \operatorname{erfc}(-s \cos \delta)}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta \operatorname{erfc}(-s \cos \delta)} \right) \right] \end{aligned} \quad (18)$$

$$\begin{aligned} = \alpha_E \frac{4kT_w}{mV_i^2} s^2 + (1 - \alpha_E) & \left(1 + \frac{s^2}{2} + \frac{1}{4} \right. \\ & \times \left. \frac{s \cos \delta \operatorname{erfc}(-s \cos \delta)}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta \operatorname{erfc}(-s \cos \delta)} \right) \end{aligned} \quad (19)$$

4. Hyperthermal approximation

4.1. Derivation of an asymptotic hyperthermal approximation

The general expression for the temperature ratio presented in Eq. (19) can be used to obtain a simple hyperthermal approximation of the temperature ratio. It will be shown to represent an improvement over the approximation of Ref. [9]. In contrast to their derivation, the limit as s approaches infinity is determined directly for the general temperature ratio in Eq. (19) instead of for the average energy in Eq. (16):

$$\begin{aligned} \lim_{s \rightarrow \infty} \frac{T_r}{T_i} = \alpha_E \frac{4kT_w}{mV_i^2} & \left(\lim_{s \rightarrow \infty} \frac{s^2}{2} \right) \\ & + (1 - \alpha_E) \left[1 + \left(\lim_{s \rightarrow \infty} \frac{s^2}{2} \right) + \frac{1}{4} \right. \\ & \times \left. \left(\lim_{s \rightarrow \infty} \frac{s \cos \delta \operatorname{erfc}(-s \cos \delta)}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta \operatorname{erfc}(-s \cos \delta)} \right) \right]. \end{aligned} \quad (20)$$

Regarding the last limit term in brackets, a distinction has to be made between the cases where $\cos \delta$ is positive and where it is negative. The first case is more relevant for aerodynamics since $\cos \delta > 0$ means that the surface is facing the flow. It is also easier to find an asymptote for this case since the last term will tend to one as s approaches infinity, eliminating the dependency on the angle δ :

$$\lim_{s \rightarrow \infty} \frac{T_r}{T_i} = \left[1 + \alpha_E \left(\frac{4kT_w}{mV_i^2} - 1 \right) \right] \left(\lim_{s \rightarrow \infty} \frac{s^2}{2} \right) + \frac{5}{4} (1 - \alpha_E). \quad (21)$$

¹ Eq. 4.27 of Ref. [13] erroneously features an exponent of 2 for c_m . This note uses the correct exponent of 3.

According to this, the following equation is an asymptote for the temperature ratio as the molecular speed ratio tends to infinity and thus can serve as a hyperthermal approximation for flow-facing surfaces:

$$\frac{T_r}{T_i} \approx \frac{s^2}{2} \left[1 + \alpha_E \left(\frac{4kT_w}{mV_i^2} - 1 \right) \right] + \frac{5}{4} (1 - \alpha_E). \quad (22)$$

While both approximations (Eq. (22) and the result of Ref. [9] in Eq. (17)) share the general solution's property of tending to infinity with growing s , a comparison shows a constant offset of $5(1 - \alpha_E)/4$ between them. Therefore, Eq. (17) cannot be an asymptote for the general solution of the temperature ratio.

Finding an approximation like Eq. (22) for the rear-facing surfaces ($\cos \delta < 0$) is more difficult since the last term in brackets does not simply tend to a constant value now. For completeness' sake, an asymptotic approximation shall also be mentioned for this case while its derivation is omitted:

$$\frac{T_r}{T_i} \approx \frac{s^2}{2} \left[1 - \cos^2 \delta + \alpha_E \left(\frac{4kT_w}{mV_i^2} - (1 - \cos^2 \delta) \right) \right] + \frac{1}{2} (1 - \alpha_E). \quad (23)$$

A proof that this equation is an asymptote of the general solution is given in the Appendix. As can be seen, the approximation for these surfaces still depends on the angle δ unlike the one for the flow-facing surfaces. Since the hyperthermal approximation of Sentman's model disregards the rear-facing surfaces altogether, the approximation in Eq. (23) is irrelevant for the calculation of aerodynamic forces in practice.

4.2. Asymptoticity of hyperthermal approximations

The dependency on T_i and V_i of neither the average energy nor the temperature ratio is completely contained within the molecular speed ratio s . Even though s was introduced in both Eqs. (16) and (19), they still explicitly depend on V_i . Using Eq. (7), the dependency on V_i can be replaced by a dependency on T_i . While this has no effect on the validity of the general equations, it might affect the hyperthermal approximations because in one case V_i and in the other case T_i is kept constant while s approaches infinity. This is shown in Fig. 1 where multiple curves of constant s are plotted in a T_i - V_i -plane. From a given point (marked by a blue cross), the limit as s approaches infinity can be evaluated by moving along two different paths: 1.) a path on which V_i is kept constant and 2.) a path on which T_i is kept constant. For quantities that depend on T_i and V_i in this manner, there may be asymptotes for one of these directions that cannot simply be transformed using Eq. (7) and expected to be an asymptote for the other direction. If, for example, an asymptote was found for the direction where V_i is kept constant, its expression will depend on this value of V_i . Using Eq. (7) to transform this expression into one that explicitly depends on T_i may not necessarily yield an asymptote for the other direction.

This problem does not occur for the approximation derived in this note (Eq. (22)). It is an asymptote for the direction where V_i is kept constant and can be transformed into an asymptote for the direction where T_i is kept constant using Eq. (7).

4.3. Assessment of the approximation accuracy

To assess the accuracy of the available approximations, their relative error R can be considered. It shall be defined as:

$$R = \left| \frac{\tau - \tau_{\text{appr}}}{\tau} \right|. \quad (24)$$

Here, τ represents the temperature ratio as given by the general Eq. (19) while τ_{appr} is the temperature ratio as given by one of the approximations (Eqs. (17), (22), or (23)).

In Fig. 2, the relative error of all these approximations is plotted for increasing molecular speed ratios. Since the general solution as well as the approximation for rear-facing surfaces depend on δ , the relative

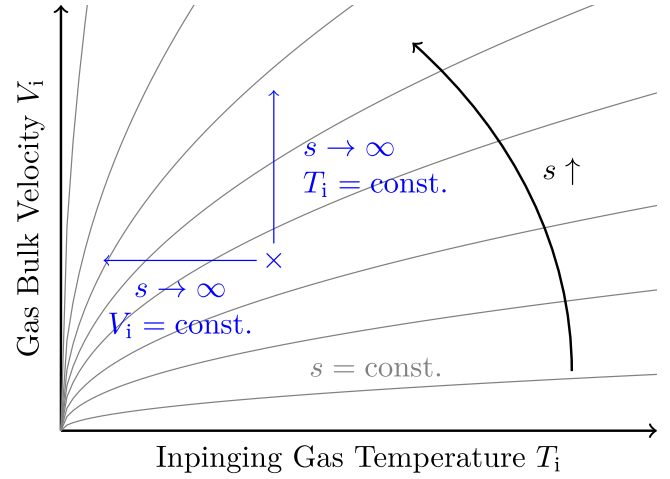


Fig. 1. Different hyperthermal approximations.

Table 1
Parameters used for the assessment of the approximations.

Parameter	Value
T_w	300 K
V_i	7.8 km s ⁻¹
α_E	0.95
m	$2.72 \cdot 10^{-26}$ kg

error is evaluated for four different values (two for flow-facing and another two for rear-facing surfaces). For the remaining parameters, a plausible set of values is chosen that could be encountered in a VLEO satellite mission. These are listed in Table 1.

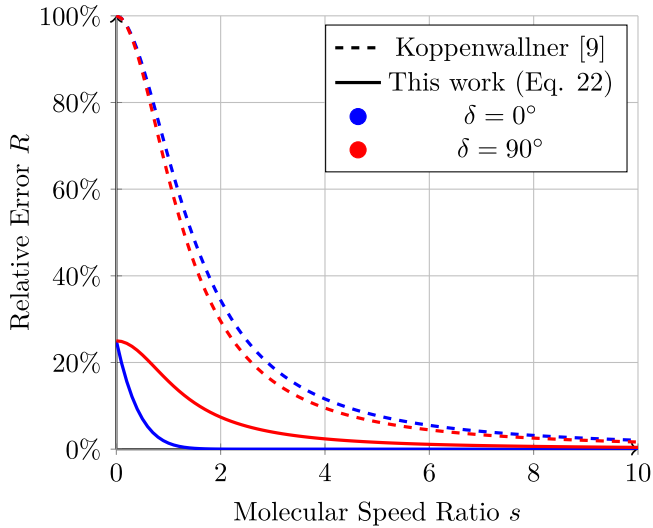
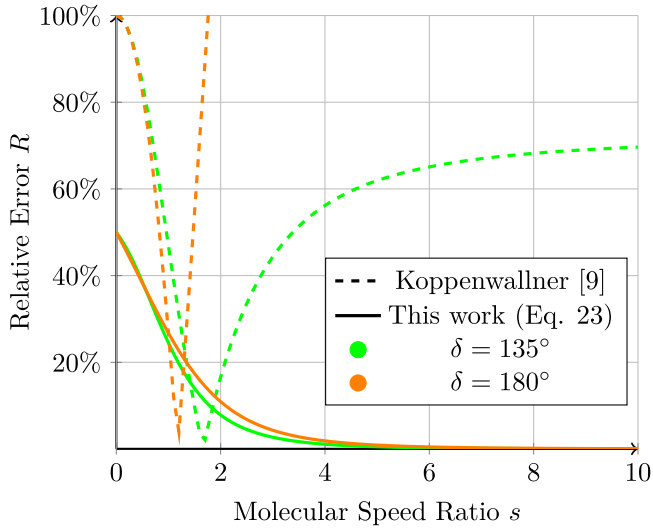
Regarding the flow-facing surfaces, it is clearly visible that the relative error of the new approximation Eq. (22) derived in this note (labeled “This work”) has a significantly smaller value for $s = 0$ compared to that of Ref. [9] and converges much quicker to zero. Specifically for the scenario where $\delta = 0^\circ$ (i.e. incoming flow is perpendicular to the surface), it has decreased below 1.4% for $s \geq 1$. The approximation in Ref. [9] (labeled “Koppenwallner”), on the other hand, shows a relative error of more than 67% at $s = 1$ which does not decrease below 2% until $s = 10$.

For rear-facing surfaces, the relative error of the respective approximation of Eq. (23) starts with a higher value but still converges to zero while that of Ref. [9] converges to a nonzero value.

5. Conclusion and outlook

This technical note points out the significant role that the temperature of reflected particles plays in force calculations with existing GSI models. The current state-of-the-art derivations of said temperature via energy accommodation are reconstructed, and their limitations are highlighted. As the main innovative contribution of this note, an alternative derivation of the average energy of impinging particles is used to develop a generalized expression of the temperature ratio of impinging and reflected particles. It is shown to be valid for any molecular speed ratio and therefore does not additionally limit GSI models but retains their general validity even in hypothermal flows. Furthermore, a simplified approximation of the temperature ratio for hyperthermal flows is derived which is shown to asymptotically converge to the previously mentioned general expression.

The results of this note are believed to enhance the understanding of incorporating energy accommodation into GSI models with (partially) diffuse reflection. If the general expression for the temperature ratio (Eq. (19)) derived in this note is used in such a model, its general

(a) Flow-facing surfaces (i.e. $\delta \leq 90^\circ$).(b) Rear-facing surfaces (i.e. $\delta > 90^\circ$).**Fig. 2.** Relative error of approximations for increasing molecular speed ratios.

validity for any value of s is retained. If the other assumptions of a GSI model allow for it, using the novel general expression would extend the usability of those models to suborbital flights with hypothermal flows for which no accurate treatment of the energy accommodation exists in the literature. In hyperthermal regimes, an approximation of the temperature ratio for very high molecular speed ratios might suffice. Here, the application of the one derived in this note (Eq. (22)) does not add any impractical complexity, as it only differs from the result in Ref. [9] by a constant offset. Unlike the latter, the new expression of this note was shown to be an asymptote of the general expression and therefore converges to it with increasing s , yielding a lower relative error.

The aerodynamic forces caused by particles interacting with a surface can be split into two parts: the impingement and the reflection. The temperature ratio that this note is concerned with is only needed in the calculation of the second part. However, since the particles' velocity after the collision with the wall is generally much smaller than before (which is of the order of the satellite's orbital velocity), reflection plays a minor role in the overall force computation in practice. Thus, the correction of the temperature ratio presented within this note is

not expected to completely invalidate results achieved with existing temperature ratio expressions.

It remains to be shown how much of a difference the usage of the general expression for the temperature ratio or the new approximation will make in the simulation of existing GSI models. Moreover, further investigation is required to determine to which extent the results of this note can impact practical applications, such as improving the computation of thermospheric density data from satellite dynamics.

CRediT authorship contribution statement

Friedrich Tuttas: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization. **Constantin Traub:** Writing – review & editing. **Marcel Pfeiffer:** Writing – review & editing. **Walter Fichter:** Writing – review & editing, Supervision, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix. Proof of the asymptoticity of the hyperthermal approximation for rear-facing surfaces

In order to prove that the approximation for rear-facing surfaces is an asymptote of the general expression of the temperature ratio, the difference of the two expressions must be shown to converge to zero. If τ denotes the general expression of Eq. (19) and τ_{appr} the approximation of Eq. (23), their difference can be rewritten as: (see Eqs. (A.1) and (A.2) in Box I).

When $\cos \delta < 0$, both the numerator and the denominator of the term in brackets tend to zero as s approaches infinity. L'Hôpital's rule can be applied to determine the limit of this term. Repeated application of this rule leads to the following four terms (labeled L_1 through L_4), the last of which allows for a direct evaluation of the limit:

$$L_1 = \frac{\frac{6}{\sqrt{\pi}} s \cos^2 \delta \exp(-s^2 \cos^2 \delta) + 3(1 + 2s^2 \cos^2 \delta) \cos \delta \operatorname{erfc}(-s \cos \delta)}{\cos \delta \operatorname{erfc}(-s \cos \delta)}, \quad (\text{A.3})$$

$$L_2 = \frac{\frac{12}{\sqrt{\pi}} \cos^2 \delta \exp(-s^2 \cos^2 \delta) + 12s \cos^3 \delta \operatorname{erfc}(-s \cos \delta)}{\frac{2}{\sqrt{\pi}} \cos^2 \delta \exp(-s^2 \cos^2 \delta)}, \quad (\text{A.4})$$

$$L_3 = \frac{12 \cos^3 \delta \operatorname{erfc}(-s \cos \delta)}{-\frac{4}{\sqrt{\pi}} s \cos^4 \delta \exp(-s^2 \cos^2 \delta)}, \quad (\text{A.5})$$

$$L_4 = \frac{\frac{24}{\sqrt{\pi}} \cos^4 \delta \exp(-s^2 \cos^2 \delta)}{\frac{4}{\sqrt{\pi}} \cos^4 \delta (2s^2 \cos^2 \delta - 1) \exp(-s^2 \cos^2 \delta)} \quad (\text{A.6})$$

$$= \frac{6}{2s^2 \cos^2 \delta - 1}. \quad (\text{A.7})$$

The limit of L_4 as s approaches infinity is equal to zero. Therefore, the difference of the general expression and the approximation for rear-facing surfaces also tends to zero, which proves the asymptoticity of the approximation in Eq. (23).

$$\tau - \tau_{\text{appr}} = \alpha_E \frac{2kT_w}{mV_i^2} s^2 + (1 - \alpha_E) \left(1 + \frac{s^2}{2} + \frac{1}{4} \frac{s \cos \delta \operatorname{erfc}(-s \cos \delta)}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta \operatorname{erfc}(-s \cos \delta)} \right) - \frac{s^2}{2} \left[1 - \cos^2 \delta + \alpha_E \left(\frac{4kT_w}{mV_i^2} - (1 - \cos^2 \delta) \right) \right] - \frac{1}{2} (1 - \alpha_E) \quad (\text{A.1})$$

$$= \frac{1}{4} (1 - \alpha_E) \left[\frac{\frac{2}{\sqrt{\pi}} (1 + s^2 \cos^2 \delta) \exp(-s^2 \cos^2 \delta) + (3 + 2s^2 \cos^2 \delta) s \cos \delta \operatorname{erfc}(-s \cos \delta)}{\frac{1}{\sqrt{\pi}} \exp(-s^2 \cos^2 \delta) + s \cos \delta \operatorname{erfc}(-s \cos \delta)} \right]. \quad (\text{A.2})$$

Box I.

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