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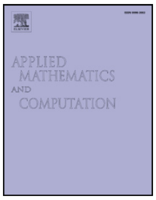

Estimating heat transfer coefficients for solid–gas interfaces using the Landau–Teller model

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ABSTRACT

In this work, a new approach to estimate heat transfer coefficients for solid–gas interfaces is proposed. The new formulation takes into account that the photon transfer process between solid walls and gases is not instantaneous, but involves electronic transitions, even when low frequency radiation is exchanged. The delay required to electron cloud transitions, called relaxation time, which plays a crucial role in the heat transfer process, is evaluated using the Landau–Teller model.

1. Introduction

The empirical correlations between the non-dimensional groups Nusselt, Reynolds and Prandtl furnish reasonable estimations to the heat transfer coefficients for several realistic scenarios. Nevertheless, for some problems involving convection heat transfer between low-density fluids and solid interfaces, these values becomes unreliable. It occurs because the contributions of two molecular effects to the heat transfer coefficient are not taken into account in these empirical correlations: the Brownian motion and the molecular relaxation time, associated to electronic transitions.

The Brownian motion of the molecules in gaseous phase is often more intense than the own coherent flux which defines the main flow. For instance, at room temperatures, the mean velocity of N_2 and O_2 molecules in “stagnated” air are typically about 20 m/s. Hence, for gas flows, the classical advection terms in convective heat transfer can no longer be considered as the main mechanism responsible to remove the molecules from the wall after exchanging heat by conduction. It becomes necessary to take into account the contribution of the Brownian “fluctuations” to the convective heat transfer.

Moreover, it is widely recognized that the underlying mechanism behind thermal conduction is based on photon absorption, scattering and emission [1]. This idea has been propagated due to the good estimates for molecular properties obtained via quantum models, which treats heat transfer and electromagnetism in the same foot. In short, these molecular models

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shows that thermal and electric conductivity are closely related to photon scattering cross sections, which depends on the wave functions and the corresponding energy levels of a given compound. Thus, the thermal inertia of a given material can be fully justified by the delay associated with electronic transitions, even when dealing with a crystal lattice. It must be taken in mind that the vibration and rotational degrees of freedom of solids are ultimately related to small electronic transitions suffered by the whole cluster of atoms, which defines a bound state.

The time elapsed between photon absorption and emission is usually ignored in most calculations involving heat transfer from surfaces to gases. The immediate consequence of neglecting this delay is to expect that the heat transfer coefficient being approximately proportional to the average velocity of the gas flow, which removes heat from a surface.

Although this idea being intuitively appealing due to its simplicity, it produces poor estimations for heat transfer coefficients. For instance, the convection coefficient for air flowing toward a flat plate with an average speed about 2 m/s ranges from 10 to 14 W/m^2 K. When the speed is increased to 10 m/s, h is about 30 W/m^2 K, while a further increase to 35 m/s produces $h \sim 72$ W/m^2 K. The origin of this nearly asymptotic behavior is discussed as follows.

2. Heat exchange as a photon transfer process

When a molecule collides with a wall, a bound state with the atoms belonging to the solid phase is temporarily produced, because the electronic clouds suffer a rearranging, such as in chemical reaction processes. After the collision, the molecule returns to the gaseous phase with a different electron cloud configuration. This process can be regarded as photon transference, although radiation scattering also occurs during the interaction. In the particular case when photon exchange process occurs in a solid medium, it is interpreted as a purely conductive phenomenon, but the basic transfer mechanism being essentially analogous. Therefore, the time required to transfer thermal energy along any material medium is given not only by the period elapsed to propagate photons between adjacent atoms. There is another delay, demanded to rearrange the electronic cloud between successive emissions, which constitutes precisely the major contribution to the corresponding total time required to carry out the transfer process. It occurs that, after interacting with incident photons, each molecular orbital suffer energy transitions and decays in a certain time interval, emitting photons to its neighbors. This process is called relaxation. In most cases, the time required to propagate the photons from one atom to another is negligible when compared to the relaxing time. Since the distance between atoms in a typical lattice is about 1–2 Å, the resulting time scale for photon transfer (at the speed of light) between two adjacent atoms in a lattice is usually about 2.10^{-10} m/3.10^{8} m/s–10^{-18} s, while the time required to undergo a typical transition sequence ranges from 10^{-9} to 10^{-5} s.

The relaxation process defines a time scale for the interaction between molecules at the interface. The time residence of a molecule in a region near the wall is usually a fraction of the typical time required to perform all the transitions necessary to establish thermal equilibrium. Hence, for high velocity flows, the molecules emerge from the collision with an energy corresponding to a temperature, which is slightly higher than the one before the interaction.

This is the reason why the heat transfer coefficient does not grow linearly with the speed of the incoming molecules. If the component of the velocity vector normal to the surface increases, the amount of thermal energy removed from the boundary would no longer be defined by the classical expression $q = h\,A\,(T_w - T_o)$, but by $q = h\,A\,(T_w - T_r)$, where T_r stands for a reference temperature used instead of T_o, the numerical value at large distances of the wall. Since the molecules leave the interface with $T = T_r$, there is no reason to believe that the temperature representing the molecules which really interact with the boundary should be given by T_o. Although such a nonlocal assumption being obviously unreasonable, it becomes more convenient to preserve the original form of the expression defining q, and then calculate h from classical expressions. It is important to remember that the global thermal coefficient U is defined as a function of heat transfer coefficients and wall conductivities. Thus, for practical purposes, calculating h instead of redefining q is indeed a more suitable engineering procedure.

In order to calculate the residence time of a given molecule near the wall, it becomes necessary to delimitate a region into which the interaction between the atoms belonging to solid and gas phases really occurs. The typical distance between two interacting molecules in a gas–solid interface is approximately the length of a van der Waals bond (2.5–4 Å). Thus, it is possible to define an “interaction region” in which the molecules effectively exchange photons. More specifically, these photons are transferred when a bound state is supposed to be produced between molecules belonging to the wall surface and the gas phase. In this work, the following preliminary assumption about the interaction region is adopted: when the molecule enters a region whose distance from the wall is less than 5 Å, it is considered that the photon transfer process begins.

As mentioned earlier, the residence time inside such a small region is often not enough to perform the number of energy transitions typically required to establish thermal equilibrium between the gas molecules and the atoms that compounds the wall. This time interval (and so the energy state of the molecule after the collision) is determined by the projection of the velocity vector over the direction perpendicular to the wall. Hence, it seems reasonable to expect that the amount of energy removed by the gas flow grows less that linearly with the incoming velocity. As will be showed later, a simply collision model can be employed to obtain suitable estimates for the residence time. This time interval is the upper limit to the total period available for transitions, so the number of energy gaps transposed depends upon this bound.