Heat conduction from spherical nano-particles

F. Liu∗, K. J. Daun, G. J. Smallwood, and D. R. Snelling
National Research Council of Canada, Ottawa, Canada

This study describes the physics of conduction heat transfer from nano-sized spherical particles and interpolation techniques used to calculate heat transfer in the transition regime. The accuracy of these techniques is evaluated by comparing their results with those obtained by direct Monte Carlo simulation.

Introduction
An accurate model of conduction heat transfer from a small sphere immersed in a gas and an understanding of the underlying physics are essential when analyzing data from time-resolved laser-induced incandescence experiments. This work summarizes recent reviews [1, 2] of this problem.

The governing physics is specified by the Knudsen number, Kn = λMFP/a. If Kn is very large, heat transfer occurs in the free-molecular regime. In this regime molecules travel between the particle and the equilibrium gas without colliding, and the heat transfer rate is given by

\[
q_{\text{FMR}}(Kn) = \alpha_T \pi a^2 P_g \frac{\bar{c}}{2} \left( T_p - T_g \right),
\]

where \(\alpha_T\) is the thermal accommodation coefficient, \(\bar{c}\) is a characteristic molecular speed, and \(\gamma^*\) is the temperature-averaged adiabatic gas constant. The heat transfer rate increases with increasing molecular number density and is thus proportional to \(P_g\) and \(Kn^{-1}\).

If Kn is very small heat transfer occurs in the continuum regime,

\[
q_c = 4 \pi a \bar{k}_c \left( T_p - T_g \right),
\]

where \(\bar{k}_c\) is the temperature-averaged thermal conductivity. In this regime \(q_c\) is independent of pressure and Kn since increasing \(P_g\) increases the molecular number density but decreases the distance between intermolecular collisions.

If Kn is neither small nor large conduction occurs in the transition regime. The physics of this regime is dominated by a collisionless layer surrounding the particle that causes a temperature jump at the gas-surface interface. Since the Boltzmann equation is analytically intractable in this regime, heat transfer is instead estimated using schemes that interpolate between \(q_{\text{FMR}}\) and \(q_c\).

Transition-Regime Interpolation Schemes
Transition-regime interpolation schemes are categorized as being either simple-interpolative, diffusion-approximation, or boundary-sphere methods. The most popular simple-interpolative technique is by McCoy and Cha [3], who defined an overall collision frequency as the sum of intermolecular and molecule-wall collision frequencies. Substituting this into the Chapman-Enskog approximation for \(k_c\) results in

\[
\frac{q_{\text{trans}}(Kn)}{q_c} = \frac{1}{1 + GKn},
\]

where G is a geometry-specific parameter.

Diffusion-approximation (DA) techniques estimate \(q_{\text{trans}}\) using Eq. (2) but adjust \(T_p\) to account for the temperature-jump specified by the slip parameter \(\xi\). After rearranging, it can be shown that

\[
\frac{q_{\text{trans}}(Kn)}{q_c} = \frac{1}{1 + \frac{\xi}{Kn}},
\]

where \(\xi\) is given by Loyalka [4].

Boundary-sphere (BS) methods work by finding the unknown temperature at the interface of the collisionless layer and the continuum gas, \(T_\delta\), by solving \(q_{\text{FMR}}(T_p, T_\delta) = q_c(T_\delta, T_g)\). Although this is traditionally done analytically, a numerical technique [2] has recently been proposed that accounts for temperature-dependent gas properties.

Figure 1 shows solutions obtained using the interpolation schemes and by direct Monte Carlo simulation. Note that temperature-dependent gas properties must be considered when analyzing LII data, and the Loyalka DA model only applies to monatomic gases. The BS method of [2] is the most accurate scheme for analyzing LII data.