Heat Transfer in Very Low Pressure Stagnation Flow CVD Reactors

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Heat transfer from the hot susceptor to the flowing gas in a stagnation flow very low pressure CVD reactor (see figure 1) is investigated using the Direct Simulation Monte Carlo (DSMC) method (1). Results for the heat flux are given as a function of the Péclet (Pe) and Knudsen (Kn) numbers.

INTRODUCTION

Stagnation flow configurations are frequently used in Chemical Vapor Deposition in order to obtain uniform films on large surface areas. For sufficiently high pressures, the continuum regime equations that describe heat and mass transfer in this geometry are well known, and for simplified one-dimensional problems, analytical solutions exist for mass (2,3) and heat transfer (3) to the susceptor as a funcion of Pe. To obtain more accurate results, including e.g. non-constant gas properties and multi-component effects, a computational package (e.g. SPIN (4)) can be used.

However, many CVD processes, and especially plasma (enhanched) CVD processes, are run at very low pressures of 0.1 - 10 Pa. For these low pressures the continuum equations are no longer valid, and other techniques must be used to obtain solutions of heat and mass transfer. This regime, which is called the rarefied regime, is defined using the Knudsen (Kn) number as:

$$Kn = \frac{\lambda}{D} > 0.01 \qquad (1)$$

In this equation, λ is the mean free path of the gas molecules, and D is a characteristic length scale of the flow. Conventional CFD solvers, which are based on the continuum Navier Stokes equations, will not be able to solve the flow accurately for this Kn range. The physical background of this breakdown of the continuum equations stems from the decreased importance of gas phase inter-molecular collisions compared to collisions of gas molecules with solid walls. For small Kn, inter-molecular collisions dominate due to the relatively small mean free path and the gas can be considered a continuum. For larger Kn, the wall collisions start to dominate and the particulate nature of the gas has to be taken into account. One of the simulation methods capable of capturing the particulate nature of a gas is the Direct Simulation Monte Carlo (DSMC) method (1). This method performs simulations of the flow by calculating molecular movements and collisions using molecular models.

RESULTS

One of the results of the DSMC calculations can be seen in figure 2. In this figure, the heat flux at the center of the susceptor is shown as a function of Pe and Kn. It can be seen clearly that the heat flux drops significantly with increasing Kn. This was expected because it is known that the thermal conductivity of a

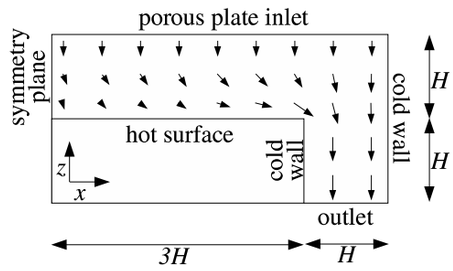

Figure 1

The stagnation flow geometry used for the simulations. H is 5.0 cm.

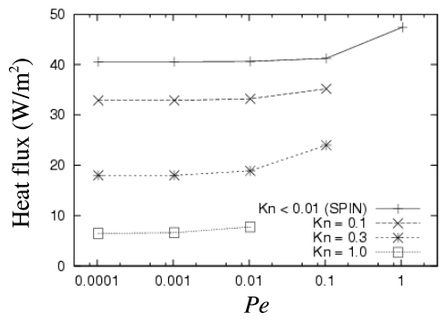

Figure 2

Results for the heat flux at $x = 0$ as a function of Pe for the DSMC simulations ($Kn = 0.1 - 1.0$) and the SPIN calculations ($Kn < 0.01$).

gas decreases for increasing Kn in the rarefied regime. Other results that will be shown in the presentation are the variations of the heat transfer across the susceptor for varying Kn and the temperature jump that was found at the hot susceptor surface and at the cold porous inlet.

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