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MONTE CARLO TREATMENT OF HEAT FLOW THROUGH A NEUTRAL GAS LAYER

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Abstract

The flow of heat through a neutral gas layer under conditions of density and temperature relevant to the cooling layer used in a reference theta-pinch reactor (RTPR) has been investigated numerically by means of a Monte Carlo technique. The necessity for corrections to the fluid model has been indicated and assessed in an example calculation presented herein.

Introduction

The use of neutral gas layers in prototype thermonuclear reactors for heat removal has been discussed by several authors.(1-4) These models make use of the multifluid MHD equations. In many applications the conditions of temperature and density are such that the small mean free path assumption implicit in the above models becomes questionable. A means to investigate the validity of this assumption as well as to correct it when necessary is to set up a model which does not make this assumption.

Monte Carlo methods have received wide usage in computational physics.(5) In particular neutron transport processes are often (though not always) calculated by this method. In neutron transport the problem is made simple by the fact that the scattering centers are the heavy nuclei which are regarded as fixed targets and the neutron-neutron interactions can be ignored. However, in the neutral gas problem the target particles and scattering centers are the same, namely the neutral gas atoms. In studying transport phenomena in an atomic gas it is possible to use a truly microscopic approach to study a small sample by following individual atomic trajectories.(6) However, this approach proves too time consuming computationally to study a large sample such as the entire neutral gas layer. Therefore, it is necessary to make a compromise and set up a computer simulation model in which each simulation particle represents a fairly large number of actual atoms and Monte Carlo (probability) procedures are used to determine the collisions and the trajectories of the simulation particles. The details of this model are described in the following section.

Monte Carlo Model

As has been indicated previously, (4) the cooling layer is fairly well divided into an ionized region in contact with the main plasma and a neutral region in contact with the wall with a partially ionized transition layer which is of small enough dimension to be ignored. The present calculation treats only the neutral portion of the cooling layer extending from the radius r_c outside which the gas is fully neutral to the wall radius r_w . The neutral gas is represented by a number N of simulation particles in the range of several thousand. Each simulation particle will represent about 10^{12} atoms depending on the dimensions of the system and the density of the gas.

The simulation particles are given initial velocities selected randomly but of magnitude weighted to correspond to the wall temperature. The radii r_c and r_w are treated as totally diffusive boundaries, i.e., the accommodation coefficient is set equal to unity. Particles which cross either of these radii from the interior region are made to reenter the interior region with a random direction, but with velocity corresponding to the transition temperature T_c (~ 1 eV) or the wall temperature T_w , respectively.

The space of the interior region is divided into cells. Local values of density, temperature, and average velocity are obtained for each cell by averaging over the particles falling within the cell. In a time step Δt a given particle undergoes a collision or does not based on a calculated probability and otherwise moves along a straight trajectory. One method of performing the collision would be to let each particle collide with other specific particles within the cell. However, the amount of bookkeeping in this procedure seems prohibitive. Instead of this, a fictitious collision partner is selected with a velocity computed on a probability which corresponds to the average temperature and density of the cell. The recoil momentum and energy of the fictitious particle is distributed equally to all the particles of the cell. This procedure was used earlier in treating plasma collision processes (7) although the probabilities were calculated differently in that case.

The scattering probability per unit time $\dot{\xi}$ between an incident particle of velocity $\vec{v}$ and a fictitious scattering partner of velocity $\vec{u}$ is given by

$$\dot{\xi} = \int \sigma v_R dn \quad (1)$$

where v_R is the relative speed given by

$$v_R^2 = v^2 + u^2 + 2uv \cos \theta \quad (2)$$

The density increment dn is given by

$$dn = 2\pi f(u) u^2 du \sin \theta d\theta \quad (3)$$

The angle θ is the supplement of the angle between $\vec{u}$ and $\vec{v}$. The fictitious distribution function $f(u)$ is given by

$$f(u) = \frac{n}{\pi^{3/2} u_o^3} \exp \left(- \frac{u^2}{u_o^2} \right) \quad (4)$$

where

$$u_o^2 = \frac{2}{3} \langle u^2 \rangle \quad (5)$$

Here n and $\langle u^2 \rangle$ are cell averages. The cross section σ is generally a function of v_R as well as of angle. However, for simplicity it is assumed to take on the hard sphere value

$$\sigma = 4\pi a^2 \quad (6)$$

where a is the atomic radius. Carrying out the integration indicated in (1) yields

$$\dot{\xi} = \frac{4\sigma n u_o}{3\sqrt{\pi}} A \left(\frac{v}{u_o} \right) \quad (7)$$

where

$$A(x) = x^2 I_1(x) + 3x I_2(x) + 3I_3(x) + \frac{1}{x} I_4(x) \quad (8)$$

$$I_1(x) = \frac{1}{2} e^{-x^2} \quad (9)$$

$$I_2(x) = \frac{\sqrt{\pi}}{4} \text{Erf}(x) - \frac{x}{2} e^{-x^2} \quad (10)$$

$$I_3(x) = I_1(x) + \frac{x^2}{2} e^{-x^2} \quad (11)$$

$$I_4(x) = \frac{3}{2} I_2(x) - \frac{x^3}{2} e^{-x^2} \quad (12)$$

Through expression (7) the total probability of a collision in a time step Δt is computed for a given particle.

Once it is known that a collision is to take place, the speed u of the colliding partner is obtained from

$$u = u_o a^{-1} \left(\frac{v}{u_o}, R \right) \quad (13)$$

where R is a random number

$$0 < R < 1 \quad (14)$$

and $a^{-1}(\alpha, R)$ is the inverse at constant α of the function

$$a(\alpha, w) = \frac{\tilde{a}(\alpha, w)}{A(\alpha)} \quad (15)$$

where

$$\tilde{a}(\alpha, w) = \begin{cases} 3wI_2(w) + \frac{I_4(w)}{w}, & w \leq \alpha \\ I_2(\alpha) + \frac{I_4(\alpha)}{\alpha} + 3[I_3(\alpha) - I_3(w)] + \alpha^2 I_1(\alpha) - w^2 I_1(w), & w \geq \alpha \end{cases} \quad (16)$$

The value of the scattering angle θ is given in terms of its cosine, y selected by

$$y = b^{-1}\left(\frac{v}{u_0}, \frac{u}{u_0}, R\right) \quad (17)$$

where R is a random number in the same range but independent of the one used in (13).

b^{-1} is the inverse at constant α and w of the function

$$b(\alpha, w, y) = \frac{1}{3\alpha w I(\alpha, w)} \left[(\alpha^2 + w^2 + 2\alpha w y)^{3/2} - |\alpha - w|^3 \right] \quad (18)$$

where

$$I(\alpha, w) = \begin{cases} \frac{2}{3\alpha} (3\alpha^2 + w^2), & \alpha \leq w \\ \frac{2}{3w} (3w^2 + \alpha^2), & \alpha \geq w \end{cases} \quad (19)$$

The polar scattering angle χ and azimuthal scattering angle ϕ are given in terms of two further independent random numbers by

$$\chi = \cos^{-1} (1 - 2R) \quad (20)$$

$$\phi = 2\pi R \quad (21)$$

Thus, by means of four random numbers and equations (13), (17), (20), and (21), the scattering geometry is completely determined. The scattering is implemented numerically by a sequence of coordinate rotation on the incident particle.

Results and Discussion

The example cases were run with 2000 simulation particles. Initial average densities of 10^{16} , 10^{17} and 10^{18} cm^{-3} were used. It required between 30 minutes and one hour of CDC-7600 computer time to reach the steady state heat flow condition. Figure 1 shows a plot of the temperature profile as computed from classical theory (4, 8) (solid curve) along with the cell temperatures from the Monte Carlo calculation (individual points) for a gas density of 10^{16} cm^{-3} . The overall heat flow rate in the Monte Carlo calculation turned out to be about a factor of 20 smaller than predicted by classical theory. The precipitous drop of the temperature in the region of high temperature (and low relative density) is characteristic of the breakdown of the short mean free path approximation. In fact, it is this portion of the gas which limits the flow rate most strongly. The implications are that the initial cooling layer density will have to be increased in order to extract the heat at the rate projected in the RTPR. Higher initial density cases were run and it was found that 10^{18} cm^{-3} was required to give a heat removal rate about equal to the RTPR value, namely 137 w/cm^2 . Although these higher densities are more difficult to handle in terms of pumping, they serve to additional protection to the wall against fast charge exchange neutrals.

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FIG. 1
The classical temperature profile (smooth curve) has been plotted along with isolated cell temperatures from the Monte Carlo calculation.