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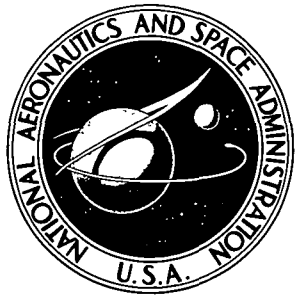

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MONTE CARLO ANALYSIS OF RAREFIED-GAS DIFFUSION INCLUDING VARIANCE REDUCTION USING THE THEORY OF MARKOV RANDOM WALKS

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16. Abstract

Molecular diffusion through a rarefied gas is analyzed by using the theory of Markov random walks. The Markov walk is simulated on the computer by using random numbers to find the new states from the appropriate transition probabilities. As the sample molecule during its random walk passes a scoring position, which is a location at which the macroscopic diffusing flow variables such as molecular flux and molecular density are desired, an appropriate payoff is scored. The payoff is a function of the sample molecule velocity. For example, in obtaining the molecular flux across a scoring position, the random walk payoff is the net number of times the scoring position has been crossed in the positive direction. Similarly, when the molecular density is required, the payoff is the sum of the inverse velocity of the sample molecule passing the scoring position. The macroscopic diffusing flow variables are then found from the expected payoff of the random walks. The confidence limit interval on the numerical results obtained for the flow variables can be reduced by increasing the number of random walks simulated or by reducing the variance of the random walk payoff. By reducing the variance, less random walks are needed for the same confidence limit interval; thus, less computer time is needed for the calculation. Biasing functions are found which change the transition probabilities such that the variance is reduced. Both a zero-variance and a minimum-variance biasing function are found. The zero-variance biasing function is approximated in the numerical calculations which were carried out to illustrate the variance reduction procedure. The resulting saving in computer running time due to the biasing procedure is shown.

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SUMMARY

Molecular diffusion through a rarefied gas is analyzed by using the theory of Markov random walks. The Markov walk is simulated on the computer by using random numbers to find the new states from the appropriate transition probabilities. As the sample molecule during its random walk passes a scoring position, which is a location at which the macroscopic diffusing flow variables such as molecular flux and molecular density are desired, an appropriate payoff is scored. The payoff is a function of the sample molecule velocity. For example, in obtaining the molecular flux across a scoring position, the random walk payoff is the net number of times the scoring position has been crossed in the positive direction. Similarly, when the molecular density is required, the payoff is the sum of the inverse velocity of the sample molecule passing the scoring position. The macroscopic diffusing flow variables are then found from the expected payoff of the random walks. The confidence limit interval on the numerical results obtained for the flow variables can be reduced by increasing the number of random walks simulated or by reducing the variance of the random walk payoff. By reducing the variance, less random walks are needed for the same confidence limit interval; thus less computer time is needed for the calculation. Biasing functions are found which change the transition probabilities such that the variance is reduced. Both a zero-variance and a minimum-variance biasing function are found. The zero-variance biasing function is approximated in the numerical calculations which were carried out to illustrate the variance reduction procedure. The resulting saving in computer running time due to the biasing procedure is shown.

INTRODUCTION

The present analysis treats the rarefied diffusion of molecules of one species, evaporated or emitted from one plate, through another nondiffusing molecular species enclosed between parallel walls (see fig. 1). The problem has been treated by straightforward analog Monte Carlo without variance reduction in reference 1. The present analysis treats the diffusing molecule as a Markov random walk, and the local macroscopic properties are found as the expected value of a random variable, the random walk payoff. By biasing the transition probabilities and changing the collision payoffs, we can retain the expected Markov walk payoff but reduce its variance so that the Monte Carlo result will have a much smaller error.

Monte Carlo methods have been extensively used in nuclear reactor radiation shielding problems, and sophisticated methods of analysis have been developed to minimize error and reduce computing time (refs. 2 and 3). These Monte Carlo techniques and methods of variance reduction would apply to any Markov random walk problem. Similar techniques to those used in the present analysis can be applied to thermal radiation and other rarefied-gas problems.

In the present analysis a zero-variance and a minimum-variance biasing function are found. These biasing functions apply only for positive event payoffs. However, by appropriately defining the scoring procedure, the event payoffs can be made positive.

The minimum-variance biasing function does not give a zero variance, as the zero-variance biasing function does, and so must give a relative minimum variance. However, in the Monte Carlo calculating procedure, when only a finite number of events can be calculated, the bias functions which would be optimum in the actual calculation have not been determined.

The zero-variance bias function is approximated so as to simplify the Monte Carlo calculations. These approximations which reduce the variance are the "next event" calculation, in which we score the probable event payoff after each event whether or not the sample molecule actually reaches the scoring position. Also used is "birth biasing," in which the expected initial or birth event payoff, which can readily be calculated, is scored for the initial event irrespective of the initial state of the molecule. Also used is "survival biasing," which prevents the sample molecule from being absorbed after only a few collisions, since then it would not contribute to the payoffs of the later collision. Survival biasing can be achieved by biasing the transition probabilities so that the sample molecule is not permitted to reach the absorbing wall. The large variation in sample molecular velocity contributes a large amount to the payoff variance; contribution can be avoided by "velocity biasing." Here we score the expected value of the event payoff averaged over all velocities due to the collision, independent of what the actual value of the velocity of the sample molecule is.

Since in survival biasing the sample history does not end, "Russian roulette" is used. When the weighting function is sufficiently small, the random walk is either ended randomly with a probability p, or the weight is increased by 1/p. Numerical results are given to illustrate the amount of variance reduction obtained by these biasing procedures.

ANALYSIS

As shown in figure 1 the Markov random walk of the diffusing molecule can be represented by the sequence of states $\{X_0, X_1, X_2, \ldots\}$. The symbol X_n denotes the state of the molecule and refers to a point in position and velocity space $\{\vec{Y}_n, \vec{V}_n\}$ taken on by the diffusing molecule immediately after the n^{th} collision. The probability corresponding to this random walk is given by

$$H(X_0, X_1, \ldots)dX_0\, dX_1 \ldots = E_0(X_0)K(X_1|X_0)K(X_2|X_1), \ldots dX_0\, dX_1 \ldots \quad (1)$$

The initial probability $E_0(X_0)dX_0$ is the probability of the molecule originating in dX_0 at X_0, where X_0 refers to the initial position and velocity of the molecule, which in this case is given by the initial position $\vec{Y}_0$ and initial velocity $\vec{V}_0$. The transition probability $K(X_{n+1}|X_n)dX_{n+1}$ is the probability of a particle that is at X_n immediately after the n^{th} collision reaching dX_{n+1} at X_{n+1} immediately after the next collision. The normalizing conditions that apply are

$$\left.\begin{aligned} \int E_0(X_0)dX_0 &= 1 \\ \int K(X_n|X_{n-1})dX_n &= 1 \end{aligned}\right\} \quad (2)$$

where the integration is over all X.

Immediately after each event, n = 0, 1, 2, . . ., where by event we mean the establishment of a value X_n, we record an "event payoff" P_n. This event payoff designates the contribution to the desired answer by the molecule immediately after the n^{th} event has occurred and the value of X_n has been established. The event payoff can be a function of the entire past history $\{X_0, X_1, \ldots, X_n\}$.

The random walk payoff for the random walk process starting from the initial n = 0 event is then given by

$$\eta_0 = \sum_{n=0}^{\infty} P_n \tag{3}$$

The expected payoff of the random walk is given by

$$\mathcal{E}(\eta_0) = \lambda = \int_{X_0} \cdots \int_{X_n} (\eta_0) H \, dX_0 \, dX_1 \cdots$$

$$= \int_{X_0} \cdots \int_{X_n} \left(\sum_{n=0}^{\infty} P_n \right) E_0(X_0) K(X_1 | X_0) \cdots dX_0 \, dX_1 \cdots \tag{4}$$

or

$$\lambda = \lambda_0 + \lambda_1 + \lambda_2 + \cdots \tag{5}$$

where λ_k is the expected event payoff

$$\lambda_k = \int \cdots \int (P_k) E_0(X_0) K(X_1 | X_0) \cdots K(X_k | X_{k-1}) dX_0 \, dX_1 \cdots dX_k \tag{6}$$

We can write the transition probability to include l events as follows

$$K^{(l)}(X_{n+l} | X_n) = \int \cdots \int K(X_{n+1} | X_n) \cdots K(X_{n+l} | X_{n+l-1}) dX_{n+1} \cdots dX_{n+l-1} \tag{7}$$

If we define $K^{(0)}(X | X') = \delta(X - X')$, we can obtain Green's function

$$G(X | X') = \sum_{l=0}^{\infty} K^{(l)}(X | X') \tag{8}$$

Given that an event occurs at X', $G(X | X')dX$ is the expected number of events experienced by the particle that occurs in dX near X. If we assume the event payoff is only a function of its state and not a function of its previous history, the event index of P can be dropped so that $P_n(X) = P(X)$. Then equation (4) becomes

$$\mathcal{E}(\eta) = \iint \sum_{n=0}^{\infty} P(X_n)E_0(X_0)K^{(n)}(X_n|X_0)dX_0\ dX_n$$

$$= \iint P(X)E_0(X')G(X|X')dX'\ dX \tag{9}$$

We can define the probability density for state X after n events as

$$E_n(X) = \int E_0(X')K^{(n)}(X|X')dX'$$

Letting $E(X)dX$ be the expected number of times a molecule is in state dX at X averaged over all initial states, we can write

$$E(X) = \sum_{n=0}^{\infty} E_n(X) = \int E_0(X')G(X|X')dX' = \int E_0(X') \sum_{n=0}^{\infty} K^{(n)}(X|X')dX' \tag{10}$$

We can now write the expected payoff as

$$\lambda = \int P(X)E(X)dX \tag{11}$$

From equation (10) we can write

$$E(X) = E_0(X) + \int E_0(X_0)K(X|X_0)dX_0 + \iint E_0(X_0)K(X'|X_0)K(X|X')dX'\ dX_0$$

$$+ \iint E_0(X_0)K^{(2)}(X'|X_0)K(X|X')dX'\ dX_0 + \ldots$$

$$= E_0(X) + \iint E_0(X_0)K(X|X')\left[\delta(X' - X_0) + K(X'|X_0) + K^{(2)}(X'|X_0) + \ldots\right] dX'\ dX_0$$

$$= E_0(X) + \int E(X')K(X|X')dX' \tag{12}$$

This result is the well-known Boltzmann transport equation.

Monte Carlo Process

In the Monte Carlo process, we first randomly choose an initial sample molecule position and velocity from $E_0(X_0)$. We then score $P(X_0)$. We then randomly choose a new velocity and position after collision, X_1 from $K(X_1|X_0)$. We then score $P(X_1)$. The particle history is continued in this manner until the history is completed (i. e., the molecule is incident on an absorbing wall). The random walk payoff is then given by $\eta_0 = P(X_0) + P(X_1) + \ldots$. This process is repeated for N samples to give the sample expected payoff,

$$\overline{\eta_0} = \frac{1}{N} \sum_{i=1}^{N} \eta_{0,i} \approx \mathscr{E}(\eta_0) = \lambda \tag{13}$$

This gives the desired macroscopic result. By the central limit theorem, the probability $\mathscr{P}$ that the difference between the Monte Carlo and the theoretical result is less than some error ϵ, called a confidence limit, is given by

$$\mathscr{P}\left[|\overline{\eta_0} - E(\eta_0)| < \epsilon\right] = \sqrt{\frac{2}{\pi}} \int_0^{\epsilon/\left[\sigma(\eta_0)/\sqrt{N}\right]} e^{-t^2/2}\, dt \tag{14}$$

where $\sigma^2(\eta_0)$ is the variance of the distribution of η_0. For 95 percent confidence ($\mathscr{P} = 0.95$), the confidence limit is given by

$$\epsilon = 1.96\left[\frac{\sigma(\eta_0)}{\sqrt{N}}\right] \tag{15}$$

The variance $\sigma^2(\eta_0)$ can be approximated by the sample variance $S^2(\eta_0)$, which can be obtained in the Monte Carlo calculation from

$$S^2(\eta_0) = \frac{1}{N-1} \sum_{i=1}^{N} (\eta_{0,i} - \overline{\eta}_0)^2 \tag{16}$$

We can see from equation (15) that the smaller the variance $\sigma^2(\eta_0)$, the smaller the error in the Monte Carlo calculation.

The average computer time to run a sample history α is given by $\alpha = T/N$, where T is the total computer time needed to run N sample histories. We can ratio the confidence limits for the biased process ϵ_B to that for the unbiased or analog process ϵ_A

and obtain

$$\frac{\epsilon_B}{\epsilon_A} = \frac{\sigma_B(\eta_0)}{\sigma_A(\eta_0)} \sqrt{\frac{\alpha_B T_A}{\alpha_A T_B}}$$

where the B subscript refers to the biased process and the A subscript to the unbiased or analog process.

We can compare the computing time needed to complete the random walks for the same confidence limits, $\epsilon_B = \epsilon_A$, and obtain

$$\frac{T_B}{T_A} = \frac{\alpha_B}{\alpha_A} \left[\frac{\sigma_B^2(\eta_0)}{\sigma_A^2(\eta_0)} \right]$$

Then the percent change in the computer running time for the biased case compared to the analog case for the same confidence limits can be written as

$$I = \left(\frac{T_A - T_B}{T_A} \right) \times 100 = \left[1 - \frac{\alpha_B}{\alpha_A} \frac{\sigma_B^2(\eta_0)}{\sigma_A^2(\eta_0)} \right] \times 100 \tag{17}$$

Conditional Expected Payoff

We can find the variance of the random walk payoff $\sigma^2(\eta_0)$ as follows. The probability density of a random walk from some point X_i, $\{X_i, X_{i+1}, \ldots\}$, is given by $H(X_{i+1}, X_{i+2}, \ldots | X_i)$. The payoff of this random walk is given by $\eta_i = P(X_i) + P(X_{i+1}) + \ldots$. We can then write the conditional expected payoff for a random walk starting at X_i as $W_i(X_i)$ and this is given by

$$W_i(X_i) = \mathcal{E}(\eta_i | X_i) = P(X_i) + \int P(X_{i+1}) K(X_{i+1} | X_i) dX_{i+1}$$

$$+ \int P(X_{i+2}) K^{(2)}(X_{i+2} | X_i) dX_{i+2} + \ldots$$

$$= \int \sum_{l=0}^{\infty} P(X_{i+l}) K^{(l)}(X_{i+l} | X_i) dX_{i+l} = \int P(X) G(X | X_i) dX \tag{18}$$

We can see that, for the case where the payoff is independent of the past history, the conditional expected payoff will be a function only of its state and not of the number of collisions, so that the collision index number i in $W_i(X_i)$ can be omitted. We can see that

$$W(X_{i+1}) = P(X_{i+1}) + \int P(X_{i+2})K(X_{i+2}|X_{i+1})dX_{i+2} + \int P(X_{i+3})K^{(2)}(X_{i+3}|X_{i+1})dX_{i+3} + \cdots \tag{19}$$

By multiplying equation (19) by $K(X_{i+1}|X_i)$ and integrating, we can combine the result with equation (18) and obtain

$$W(X_i) = P(X_i) + \int W(X_{i+1})K(X_{i+1}|X_i)dX_{i+1} \tag{20}$$

This can be written for the present case as

$$W(X') = P(X') + \int W(X)K(X|X')dX \tag{21}$$

A simpler method of obtaining equation (21) is to write $\eta_i = P(X_i) + \eta_{i+1}$. We then find the conditional expected value of η_i to be

$$W(X_i) = P(X_i) + \int \epsilon(\eta_{i+1}|X_{i+1})K(X_{i+1}|X_i)dX_{i+1}$$

$$= P(X_i) + \int W(X_{i+1})K(X_{i+1}|X_i)dX_{i+1} \tag{22}$$

which is identical to equation (21). We can see that the expected payoff can be obtained from the conditional expected payoff as follows

$$\lambda = \mathscr{E}(\eta_0) = \int \mathscr{E}(\eta_0|X_0)E_0(X_0)dX_0 = \int W(X_0)E_0(X_0)dX_0 \tag{23}$$

or from equation (18)

$$\lambda = \int E_0(X_0) \int P(X)G(X|X_0)dX\, dX_0$$

Conditional Expected Square Payoff

The conditional expected square payoff $Q_i(X_i)$ for a particle leaving X_i can be obtained as follows: The square of the payoff for a random walk starting at X_i can be written as

$$\eta_i^2 = \left[P(X_i) + \eta_{i+1}\right]^2$$

Then

$$Q_i(X_i) = \mathscr{E}\left(\eta_i^2 | X_i\right) = P^2(X_i) + 2P(X_i)\int \mathscr{E}(\eta_{i+1}|X_{i+1})K(X_{i+1}|X_i)dX_{i+1} + \int \mathscr{E}\left(\eta_{i+1}^2|X_{i+1}\right)K(X_{i+1}|X_i)dX_{i+1} \quad (24)$$

This can be rewritten as

$$Q_i(X_i) = P^2(X_i) + 2P(X_i)\int W(X_{i+1})K(X_{i+1}|X_i)dX_{i+1} + \int Q_{i+1}(X_{i+1})K(X_{i+1}|X_i)dX_{i+1} \quad (25)$$

Combining equation (25) with equation (22) yields

$$Q_i(X_i) = 2P(X_i)W(X_i) - P^2(X_i) + \int Q_{i+1}(X_{i+1})K(X_{i+1}|X_i)dX_{i+1} \quad (26)$$

Again we see that, for the case where the payoff is independent of its past history, the conditional expected square payoff will be a function only of its state and not of the number of collisions, so that the collision index number i in $Q_i(X_i)$ can be omitted. Then equation (26) can be written as

$$Q(X') = 2P(X')W(X') - P^2(X') + \int Q(X)K(X|X')dX \quad (27)$$

As in the relation between equations (19) and (21) we can write equation (27) as

$$Q(X_i) = \sum_{n=0}^{\infty} \int \left[2P(X_{i+n})W(X_{i+n}) - P^2(X_{i+n})\right] K_n(X_{i+n}|X_i)dX_{i+n} \quad (28)$$

which can also be written as

$$Q(X') = \int \left[2P(X)W(X) - P^2(X)\right] G(X|X')dX \tag{29}$$

We can now write the expected squared payoff as

$$\mathscr{E}\left(\eta_0^2\right) = \int \mathscr{E}\left(\eta_0^2|X_0\right)E_0(X_0)dX_0 = \int Q(X_0)E_0(X_0)dX_0$$

$$= \iint \left[2P(X)W(X) - P^2(X)\right] G(X|X')E_0(X')dX'\,dX \tag{30}$$

From equations (10) and (11) the variance can now be written as

$$\sigma^2(\eta_0) = \mathscr{E}\left(\eta_0^2\right) - \left[\epsilon(\eta_0)\right]^2 = \int Q(X_0)E_0(X_0)dX_0 - \lambda^2$$

$$= \int \left[2P(X)W(X) - P^2(X)\right] E(X)dX - \left[\int P(X)E(X)dX\right]^2 \tag{31}$$

Biasing the Random Walk

We wish to reduce the variance of the random walk payoff so that the error in the Monte Carlo calculation as given by equation (16) will be smaller. We can achieve this by biasing the random walk process and at the same time changing the event payoff so as to keep the expected payoff for the new process unchanged but at the same time have a reduced variance. We can bias the probabilities so that the probability density for the biased random walk is

$$H^*(X_0, X_1, X_2, \ldots) = E_0^*(X_0)K_1^*(X_1|X_0)K_2^*(X_2|X_1) \ldots \tag{32}$$

where the asterisks refer to the biased results. The subscripts on the biased transition probabilities K_n^* refer to the number of collisions since the initial event and show there is a dependency of the biased transition probability on the event number.

We can distort the event payoff for the random walk as follows:

$$\eta_0^* = P_0^* + P_1^* + P_2^* + \ldots \tag{33}$$

where

$$\left.\begin{aligned} P_0^* &= \frac{P(X_0)}{L_0(X_0)} \\ P_1^* &= \frac{P(X_1)}{L_0(X_0)L_1(X_0, X_1)} \\ P_2^* &= \frac{P(X_2)}{L_0(X_0)L_1(X_0, X_1)L_2(X_1, X_2)} \end{aligned}\right\} \tag{34}$$

and where the biasing ratios are given by

$$L_n(X_n, X_{n-1}) = \frac{K^*(X_n|X_{n-1})}{K(X_n|X_{n-1})} \qquad n \neq 0 \tag{35}$$

$$L_0(X_0) = \frac{E_0^*(X_0)}{E_0(X_0)} \qquad n = 0 \tag{36}$$

The normalizing conditions also must apply

$$\int E_0^* \, dX_0 = \int E_0(X_0)L_0 \, dX_0 = 1 \tag{37}$$

$$\int K_n^*(X_n|X_{n-1})dX_n = \int K(X_n|X_{n-1})L_n \, dX_n = 1 \qquad n = 1, 2, \ldots \tag{38}$$

These conditions are equivalent to the condition

$$\int \cdots \int E_0(X_0)L_0K(X_1|X_0)L_1 \cdots K(X_n|X_{n-1})L_n \, dX_0 \, dX_1 \cdots dX_n = 1$$

$$n = 0, 1, 2, \ldots \tag{39}$$

The biasing ratios are subject to the condition that $L_n(X_{n-1}, X_n) > 0$ and $L_0(X_0) > 0$ since the biased probabilities must be positive. We can see the equivalency between equations (38) and (39) since we can write

$$\int \cdots \int E_0^*(X_0)K_1^*(X_1|X_0) \cdots K_n^*(X_n|X_{n-1})dX_0 \, dX_1 \cdots dX_n$$

and

$$\int \cdots \int E_0^*(X_0)K_1^*(X_1|X_0) \cdots K_{n+1}^*(X_{n+1}|X_n)dX_0\, dX_1 \cdots dX_{n+1}$$

For these two equations to be true, equation (38) must be true. Then by integration of equation (39) over $X_1, X_2, \ldots$, we also prove that equation (37) must be true. Thus, equation (39) ensures that equations (37) and (38) are both satisfied.

We can see that the expected value for the biased walk payoff is given by

$$\lambda^* = \int P_0^* E_0^*\, dX_0 + \iint P_1^* E_0^* K_1^*(X_1|X_0)dX_0\, dX$$

$$+ \iiint P_2^* E_0^* K_1^*(X_1|X_0)K_2^*(X_2|X_1)dX_0\, dX_1\, dX_2 + \cdots$$

$$= \int \left(\frac{P_0}{L_0}\right)(E_0 L_0)dX_0 + \iint \left(\frac{P_1}{L_0 L_1}\right)(E_0 L_0)K(X_1|X_0)L_1\, dX_0\, dX_1 + \cdots$$

$$= \lambda \tag{40}$$

So that the expected biased walk payoff equals the unbiased value.

The expected biased walk payoff beginning at X_i is given as in equation (18) by

$$W_i^* = P_i^* + \int P_{i+1}^* K_{i+1}^*(X_{i+1}|X_i)dX_{i+1}$$

$$+ \iint P_{i+2}^* K_{i+2}^*(X_{i+2}|X_{i+1})K_{i+1}^*(X_{i+1}|X_i)dX_{i+1}\, dX_{i+2}$$

$$= \frac{P_i}{L_0 L_1 \cdots L_i} + \int \left(\frac{P_{i+1}}{t_0 \cdots t_{i+1}}\right) K(X_{i+1}|X_i)L_{i+1}\, dX_{i+1} + \cdots$$

$$= \frac{W_i(L_i)}{L_0 L_1 \cdots L_i} \tag{41}$$

Similarly to equation (24), we can write

$$Q_i^* = P_i^{*2}(X_i) + 2P_i^*(X_i) \int W_{i+1}^* K_{i+1}^*(X_{i+1}|X_i)dX_{i+1} + \int Q_{i+1}^* K_{i+1}^*(X_{i+1}|X_i)dX_{i+1} \tag{42}$$

From equations (41) and (22)

$$\left.\begin{aligned} W_i^*(X_i) &= \frac{W(X_i)}{L_0 \cdots L_i} = \frac{P_i(X_i)}{L_0 \cdots L_i} + \int \frac{W(X_{i+1})}{L_0 \cdots L_i L_{i+1}} K(X_{i+1}|X_i) L_{i+1}\, dX_{i+1} \\ \text{or} \\ W_i^*(X_i) &= P_i^*(X_i) + \int W_{i+1}^*(X_{i+1}) K_{i+1}(X_{i+1}|X_i)dX_{i+1} \end{aligned}\right\} \tag{43}$$

Then equation (42) can be written as

$$Q_i^* = \left[2P_i^*(X_i)W_i^*(X_i) - P_i^{*2}(X_i)\right] + \int Q_{i+1}^* K_{i+1}^*(X_{i+1}|X_i)dX_{i+1} \tag{44}$$

Then substituting for Q_{i+1}^* in equation (44) by letting the subscript i be $i+1$, we obtain

$$Q_i^* = \left[2P_i^*(X_i)W_i^*(X_i) - P_i^{*2}(X_i)\right] + \int \left[2P_{i+1}^*(X_{i+1})W_{i+1}^*(X_{i+1}) - P_{i+1}^{*2}(X_{i+1})\right] \times K_{i+1}^*(X_{i+1}|X_i)dX_{i+1} \tag{45}$$

Continuing this process gives

$$\begin{aligned} Q_i^* &= \left(2P_i^*W_i^* - P_i^{*2}\right) + \int \left(2P_{i+1}^*W_{i+1}^* - P_{i+1}^{*2}\right) K_{i+1}^*(X_{i+1}|X_i)dX_{i+1} \\ &\quad + \iint \left(2P_{i+2}^*W_{i+2}^* - P_{i+2}^{*2}\right) K_{i+1}^*(X_{i+1}|X_i) K^*(X_{i+2}|X_{i+1})dX_{i+1}\, dX_{i+2} + \cdots \\ &= \frac{1}{(L_0 L_1 \cdots L_i)^2} \left\{ \left(2P_i W_i - P_i^2\right) + \int \frac{\left(2P_{i+1}W_{i+1} - P_{i+1}^2\right) K(X_{i+1}|X_i)}{L_{i+1}}\, dX_{i+1} \right. \\ &\quad \left. + \iint \frac{\left(2P_{i+2}W_{i+2} - P_{i+2}^2\right)}{L_{i+1}L_{i+2}} K(X_{i+2}|X_{i+1}) K(X_{i+1}|X_i)dX_{i+1}\, dX_{i+2} + \cdots \right\} \end{aligned} \tag{46}$$

We can now write the expected square biased payoff as

$$\mathcal{E}\left(\eta_0^{*2}\right) = \int E_0^* Q_0^* \, dX_0 = \int \left(2P_0W_0 - P_0^2\right)\left(\frac{E_0}{L_0}\right) dX_0$$

$$+ \iint \left(2P_1W_1 - P_1^2\right) \frac{E_0}{L_0} \frac{K(X_1|X_0)}{L_1} \, dX_0 \, dX_1$$

$$+ \iiint \left(2P_2W_2 - P_2^2\right) \frac{E_0}{L_0} \frac{K(X_1|X_0)}{L_1} \frac{K(X_2|X_1)}{L_2} \, dX_0 \, dX_1 \, dX_2$$

$$+ \ . \ . \ . \tag{47}$$

This is the function we wish to minimize subject to conditions in equation (39).

A useful simplification is to write the biasing ratio in terms of a biasing function I_n (ref. 7) as follows:

$$L_n(X_n, X_{n-1}) = \frac{I_n(X_n)}{I_{n-1}(X_{n-1})} \tag{48}$$

The biased random walk then is

$$H^*(X_0, X_1, \ . \ . \ .) = \left[E_0^*(X_0)\right]\left[K_1^*(X_1|X_0)\right]\left[K_2^*(X_2|X_1)\right] \ . \ . \ .$$

$$= \left[E_0(X_0)I_0(X_0)\right]\left[K(X_1|X_0)\frac{I_1(X_1)}{I_0(X_0)}\right]\left[K(X_2|X_1)\frac{I_2(X_2)}{I_1(X_1)}\right] \ . \ . \ . \tag{49}$$

The normalizing conditions given by equations (37) and (38) are

$$\int E_0(X_0)I_0(X_0)dX_0 = 1 \tag{50}$$

$$\int K(X_n|X_{n-1}) \frac{I_n(X_n)}{I_{n-1}(X_{n-1})} \, dX_n = 1 \qquad n = 1, 2, 3 \tag{51}$$

Or equivalently as was shown previously

$$\int E_n(X_n)I_n(X_n)dX_n = 1 \qquad n = 0, 1, 2, \ . \ . \ . \tag{52}$$

The payoff for the biased random walk now becomes

$$\eta_0^* = P_0^* + P_1^* + \ldots = \frac{P(X_0)}{I_0(X_0)} + \frac{P(X_1)}{I_1(X_1)} + \frac{P(X_2)}{I_2(X_2)} + \ldots \tag{53}$$

Notice that the biased payoffs are now only functions of the immediate state and do not depend on past history. However, they do depend on the number of previous collisions since the biasing function I_n depends on the collision index number n.

As in equation (18) we can write the conditional expected biased payoff as

$$W_i^*(X_i) = \mathcal{E}(\eta_i^* | X_i) = P_i^*(X_i) + \int P_{i+1}^*(X_{i+1}) K_{i+1}^*(X_{i+1} | X_i) dX_{i+1}$$

$$+ \int P_{i+2}^*(X_{i+2}) K_{i+2}^{(2)}(X_{i+2} | X_i) dX_{i+2}$$

$$= \frac{P(X_i)}{I_i(X_i)} + \int \frac{P(X_{i+1})}{I_{i+1}(X_{i+1})} K(X_{i+1} | X_i) \frac{I_{i+1}(X_{i+1})}{I_i(X_i)} dX_{i+1}$$

$$+ \int \frac{P(X_{i+2})}{I_{i+2}(X_{i+2})} K^{(2)}(X_{i+2} | X_i) \frac{I_{i+2}}{I_i(X_i)} + \ldots$$

$$= \frac{W(X_i)}{I_i(X_i)} \tag{54}$$

Similarly, the conditional expected square biased payoff for the random walk leaving X_i is given by equation (46) as

$$Q_i^*(X_i) = \mathcal{E}\left(\eta_i^{*2} | X_i\right) = \frac{1}{I_i(X_i)} \int \sum_{n=0}^{\infty} \left[2P(X_{i+n}) W(X_{i+n}) - P^2(X_{i+n})\right] \frac{K^{(n)}(X_{i+n} | X_i)}{I_{i+n}(X_{i+n})} dX_{i+n} \tag{55}$$

The expected square biased payoff now becomes

$$\mathcal{E}\left(\eta_0^{*2}\right) = \int Q_0^*(X_0) E_0^*(X_0) dX_0$$

$$= \iint E_0(X_0) \sum_{n=0}^{\infty} \left\{ \left[2P(X_n)W(X_n) - P^2(X_n) \right] \frac{K^{(n)}(X_n | X_0)}{I_n(X_n)} dX_n \right\} dX_0$$

$$= \sum_{n=0}^{\infty} \int \left[2P(X_n)W(X_n) - P^2(X_n) \right] \frac{E_n(X_n)}{I_n(X_n)} dX_n \tag{56}$$

where variance for the biased process is given by

$$\sigma^2\left(\eta_0^{*2}\right) = \mathcal{E}\left(\eta_0^{*2}\right) - \mathcal{E}^2(\eta_0^*) = \mathcal{E}\left(\eta_0^{*2}\right) - \lambda^2 \tag{57}$$

Zero-Variance Bias Function

We wish to choose a biasing function that will minimize this variance. An obvious zero-variance biasing function is given by

$$I_n^\dagger(X_n) = \frac{P(X_n)}{\lambda_n} \qquad \text{if } P \geq 0 \tag{58}$$

where the dagger superscript is used to designate this particular zero-variance biasing case. We can see that $I_n^\dagger$ satisfies the normalizing conditions given by equation (52). With $I_n^\dagger$ as the zero biasing function, the event payoff after the n^{th} event is given by a constant λ_n, regardless of the state X_n of the molecule. Thus, for any random walk, irrespective of the states involved in the random walk, the individual random walk payoff is always given by

$$\eta_0^\dagger = \lambda_0 + \lambda_1 + \lambda_2 + \ldots \lambda_n + \ldots = \lambda \tag{59}$$

where there are an infinite number of terms. Since the random walk payoff is always equal to the expected random walk payoff, the variance $\sigma^2(\eta_0^\dagger)$ must be zero. This can also be seen from the previous equations by substituting $I_n^\dagger(X_n)$ from equation (58) into (56) to obtain

$$\mathscr{E}\left(\eta_0^{\dagger 2}\right) = \sum_{n=0}^{\infty} \lambda_n \int \left[2W(X_n) - P(X_n)\right] E_n(X_n) dX_n$$

$$= \sum_{n=0}^{\infty} \lambda_n \int_{X_n} \left[P(X_n) + 2 \int_{X_{n+1}} P(X_{n+1}) K(X_{n+1} | X_n) dX_{n+1} + \ldots\right] E_n(X_n) dX_n$$

Hence,

$$\mathscr{E}\left(\eta_0^{\dagger 2}\right) = \sum_{n=0}^{\infty} \lambda_n \left[\lambda_n + 2(\lambda_{n+1} + \lambda_{n+2} + \ldots)\right]$$

$$= \sum_{n=0}^{\infty} \lambda_n^2 + 2 \sum_{n=0}^{\infty} \lambda_n \sum_{i=1}^{\infty} \lambda_{n+i} = \left(\sum_{n=0}^{\infty} \lambda_n\right)^2 = \lambda^2 \tag{60}$$

and from equation (57), $\sigma^2\left(\eta_0^{\dagger 2}\right) = 0$. This result states the obvious fact that a biasing function that minimizes the variation in the event payoff to zero will reduce the variance of the Monte Carlo result to zero.

If the event payoff is negative, the zero-variance biasing function would not apply since, from equation (58), $P \geq 0$. However, it is possible to define a payoff function so that it is always positive. For instance, in the scoring of the molecular flux, the sample molecules passing in the positive direction would score a positive quantity, while the sample molecules in the negative direction would score a negative quantity. Then, since part of the payoff is negative, the zero biasing function would not apply. However, we can score the sample molecules in the positive direction and the sample molecules in the negative direction as separate positive payoffs. This would give the absolute molecular flow in the positive and negative directions, which can then be subtracted to give the net molecular flow. And the zero-variance bias function would then be applicable.

Minimum-Variance Bias Function

We can also minimize the variance by using a straightforward calculus of variations procedure as follows (see ref. 4). To minimize $\mathscr{E}\left(\eta_0^{*2}\right)$ as given by equation (58) with respect to $I_n(X_n)$ subject to the boundary condition of equation (52) and $I_n > 0$, we obtain

$$\frac{\partial}{\partial I_n(X_n)}\left\{\sum_{n=0}^{\infty}\left[2P(X_n)W(X_n) - P^2(X_n)\right]\frac{E_n(X_n)}{I_n(X_n)} + \sum_{n=0}^{\infty} D_n E_n(X_n) I_n(X_n)\right\} = 0$$

where D_n are constants to be determined. This gives

$$-\left[2P(X_n)W(X_n) - P^2(X_n)\right]\frac{E_n(X_n)}{\hat{I}_n^2(X_n)} + D_n E_n(X_n) = 0$$

This can be rewritten as

$$\hat{I}_n(X_n) D_n^{1/2} = \left[2P(X_n)W(X_n) - P^2(X_n)\right]^{1/2}$$

multiplying by $E_n(X_n)$ and integrating. Then using equation (52) to solve for D_n, we can write the minimized-variance bias function as

$$\hat{I}_n(X_n) = \frac{\left[2P(X_n)W(X_n) - P^2(X_n)\right]^{1/2}}{\int E_n(X_n)\left[2P(X_n)W(X_n) - P^2(X_n)\right]^{1/2} dX_n} \tag{61}$$

Since $\hat{I}_n > 0$ and real, then $\left[2P(X_n)W(X_n) - P^2(X_n)\right] > 0$. If all the $P(X_n) > 0$, then using equation (18) we find

$$2P(X_n)W(X_n) - P^2(X_n) = \int \sum_{l=1}^{\infty} P(X_{n+l}) K^{(l)}(X_{n+l} \mid X_n) dX_{n+l} > 0$$

as required.

Substitution of $\hat{I}_n(X_n)$ into equation (56) gives for the minimized expected squared bias payoff

$$\mathscr{E}\left(\hat{\eta}_0^{*2}\right) = \sum_{n=0}^{\infty}\left\{\int\left[2P(Y)W(Y) - P^2(Y)\right]^{1/2} E_n(Y) dY\right\}^2$$

We can show that $\mathscr{E}\left(\hat{\eta}_0^{*2}\right)$ is less than $\mathscr{E}\left(\eta_0^2\right)$ as follows: Consider the inequality

$$\int \left\{ \left[2P(Y)W(Y) - P^2(Y) \right]^{1/2} - \int \left[2P(X)W(X) - P^2(X) \right]^{1/2} E_n(X)dX \right\}^2 E_n(Y)dY \geq 0$$

Then we can show that

$$\sum_{n=0}^{\infty} \int \left[2P(Y)W(Y) - P^2(Y) \right] E_n(Y)dY - \sum_{n=0}^{\infty} \left\{ \int \left[2P(Y)W(Y) - P^2(Y) \right]^{1/2} E_n(Y)dY \right\}^2 \geq 0$$

This can be written as

$$\epsilon\left(\eta_0^2\right) \geq \epsilon\left(\hat{\eta}_0^{*2}\right)$$

This equation shows the Monte Carlo error would be larger for the unbiased as compared to the minimized-variance bias case. Since from equation (27)

$$2P(X_n)W(X_n) - P^2(X_n) = Q(X_n) - \int Q(X_{n+1})K(X_{n+1}|X_n)dX_n$$

The result for the minimized-variance bias function equation (61) implies that the probability distributions should be increased at those values of X_n that contribute most to the variance.

The minimized-variance bias function $\hat{I}_n$ is not the same as the zero-variance bias function $I_n^\dagger$ and so must be a relative minimum because it does not give a zero variance as $I_n^\dagger$ does. This is true for the case where the Monte Carlo calculation is carried out with bias functions exactly as given and where an infinite number of terms are evaluated. In the actual calculation, since the bias functions are approximated and only a finite number of transitions are evaluated, it is not known which bias function is preferable.

Molecular Diffusion Numerical Results

We wish to apply the results of the random walk theory to the specific problem of rarefied-gas diffusion where the diffusing molecule is considered to be undergoing a Markov random walk. The diffusion molecule originates at the emitting plane surface with the initial probability distribution given by $E_0(X_0)$. Because the geometry is one dimensional (see fig. 1) where the direction from the emitting plate to the parallel absorbing wall is along the Z-axis, we need only be concerned with the Z-component of the

molecular position. Inasmuch as in this report we will be finding only the molecular flux and molecular density at various positions across the gap, we also need consider only the Z-component of velocity. The position of the molecule is designated by the dimensionless coordinate z, which represents the distance that the molecule is from the emitting plate divided by the mean free path λ_c. Similarly, the symbol v is employed to represent the velocity, where v equals the Z-component of velocity V divided by the thermal velocity c. Thus, the state of the molecule is given by the ordered pair $\{z, v\}$. If we assume thermal equilibrium for the molecules leaving the emitting wall, $z_0 = 0$, the initial distribution of the state of the molecule is given by (see appendix A, eq. (A2))

$$E_0(z_0, v_0) = \left[2v_0 \exp\left(-v_0^2\right)\right]\delta(z_0) \tag{62}$$

The transition probability density can be written as

$$K(z_{n+1}, v_{n+1} | z_n, v_n) = T(z_{n+1} | z_n, v_n)C(v_{n+1} | z_{n+1}, v_n) \tag{63}$$

The transport distribution $T(z_{n+1} | z_n, v_n)$ is the probability of having a collision in dz_{n+1} at z_{n+1} after leaving z_n. The collision distribution $C(v_{n+1} | z_{n+1}, v_n)$ is the probability that a molecule with velocity v_n after undergoing a collision at z_{n+1} will have a velocity after collision in dv_{n+1} at v_{n+1}. However, once the molecule is incident on a wall either at $z = 0$ or $z = l$ (where l is the inverse Knudsen number, i. e., the distance between the plates divided by the mean free path L/λ_c), the molecule history is ended. The molecule is then assumed to remain at the wall with zero velocity so that the transition kernel is then given by

$$K(z_{n+1}, v_{n+1} | z_n, v_n) = \delta(z_{n+1} - z_n)\delta(v_{n+1}) \qquad \text{for } z_n = 0 \text{ or } l;\ n > 0 \tag{64}$$

where δ refers to the usual Dirac delta function.

As shown in appendix A (eq. (A10)), the transport probability for the case of Maxwellian-type collisions, where the collision rate Θ is a constant, can be written as

$$T(z_{n+1} | z_n, v_n)dz_{n+1} = \frac{1}{|v_n|} \exp\left(\frac{-|z_{n+1} - z_n|}{|v_n|}\right) dz_{n+1} \tag{65}$$

In the present case, the molecules are assumed to emerge from the collision with a Maxwellian distribution. Thus, the collision probability is not a function of the previous velocity and position and can be written as (see appendix A, eq. (A17))

$$C(v)dv = \frac{1}{\sqrt{\pi}} \exp(-v^2)dv \tag{66}$$

(Other types of collisions, either classical or quantum mechanical can be used.)

We are interested in determining the macroscopic flow quantities: the molecular flux and molecular density of the diffusing species at various positions z_s across the gap between the walls. These positions z_s are called scoring positions and are illustrated in figure 1. Thus, $z_s = (0.1)l$ corresponds to a scoring position at 1/10 of the distance across the gap from the emitting surface.

Scoring Payoff

Each sample molecule that crosses the scoring position contributes, to the measurement of some macroscopic flow quantity of interest, and amount given by an appropriate scoring function π. This scoring function will, in general, be a function of the dimensionless velocity of the molecule as it crosses the scoring position. Since the number of molecules per unit time crossing the scoring position in the steady-state case μ_s is directly proportional to the rate at which the molecules leave the emitting plate, μ_{0+}, the net flux of π crossing the scoring position can be expressed as

$$\frac{\mu_s^{(\pi)}}{\mu_{0+}} = \frac{\nu_s \mathscr{E}_s\left[v\pi(v)\right]}{\nu_{0+}\mathscr{E}_{0+}(v)} \approx \overline{\sum_i \pi_i(v)} \tag{67}$$

The $\overline{\sum_i \pi_i(v)}$ is obtained by scoring the value of π for each sample molecule passing the scoring position and then averaging this result over N samples. The ν_s is the local molecular density at the scoring position s, while $\mathscr{E}_s\left[v\pi(v)\right]$ is the value of $v\pi(v)$ averaged over the local molecular velocity distribution of the molecules at the scoring position s and is therefore equal to $\mu_s^{(\pi)}$, the net mass flux of π transported across the scoring position. Similarly, ν_{0+} is the molecular density of the molecules being emitted from the surface, while $\mathscr{E}_{0+}(v)$ is the value of v averaged over the molecular velocity distribution of the molecules at the surface leaving the emitting walls per unit time and therefore equals μ_{0+}, the mass flux emitted from the wall.

When the molecular flux μ at the scoring position is desired, the appropriate scoring payoff is

$$\pi_\mu = \pm 1 \qquad \text{when} \quad v \gtrless 0 \tag{68}$$

Then equation (67) becomes

$$\frac{\mu_s^{(\pi_\mu)}}{\mu_{0+}} = \frac{\nu_s \mathscr{E}_s(v)}{\mu_{0+}} = \frac{\mu_s}{\mu_{0+}} \approx \overline{\sum_i \pi_{\mu,i}} \tag{69}$$

When the desired macroscopic quantity is the molecular density ν at the scoring position, the appropriate scoring payoff is

$$\pi_\nu = \frac{1}{|v|_s} \tag{70}$$

For this case, equation (67) becomes

$$\frac{\mu_s^{(\pi_\nu)}}{\mu_{0+}} = \frac{\nu_s \mathscr{E}_s(1)}{\mu_{0+}} = \frac{\nu_s}{\mu_{0+}} \approx \left(\overline{\sum_i \pi_{\nu,i}}\right)_s \tag{71}$$

Analog Calculation

For the first example the "analog" Monte Carlo method is used. First, the sample molecule birth velocity v_0 is randomly picked using equation (A4). Then similarly a point z_1 of first collision is obtained from equation (A12). If the sample molecule in going from z_0 to z_1 passes z_s, the appropriate scoring payoff $\pi(v_0)$ is scored as the zero event payoff P_0. If the sample molecule does not pass z_s, $P_0 = 0$. Then a new velocity v_1 after first collision is found from equation (A21), and a position of second collision z_2 is found as before. Again if z_s is passed by the sample molecule in going from z_1 to z_2, then $P_1 = \pi(v_1)$; if not, $P_1 = 0$. The process is continued in this manner until the molecule is incident on either wall where the random walk terminates. The sum of all the event payoffs for this random walk then gives η_0. The random walk process is repeated until N independent samples are obtained yielding the average value $\bar{\eta}_0$, which is an unbiased and consistent estimate of the expected value of the random walk payoff λ.

In figure 2 the molecular flux across the gap per unit molecular flux leaving the surface is plotted as a function of inverse Knudsen number l.

In figure 3 is shown the molecular density at the various scoring positions across the gap per unit molecular density of the molecular flux entering the gap from the emitter. These results are shown for a different inverse Knudsen number l.

In table I the value of the normalized molecular density ν_s/ν_{0+} at the scoring position adjacent to the absorbing wall $z_s = l$ is given for the analog calculation. Also given is the sample standard deviation $S(\eta_0)$ obtained by use of equation (21). And in addition, the average running time per sample α is shown.

Next-Event Calculation

In this calculation we take the first step to reduce the variance. As shown previously, if the variance can be decreased for each event payoff P_n, the variance of the random walk payoff η_0 would also be reduced. In the analog calculation, we registered a nonzero event payoff only if a sample molecule actually crossed the scoring position. In the present case, called the "next event" calculation, we register a nonzero event payoff at each molecular collision within the gap whether or not the sample molecule actually crosses the scoring position. We can achieve this as follows: We can write the n^{th} expected event payoff as

$$\lambda_n = \iint \pi(v_n) E_0(X_0) K^{(n)}(X_n | X_0) \tau(z_s, X_n) dX_0 \, dX_n \tag{72}$$

where the term $\tau(z_s, X_n)$ is the scoring probability, that is, the probability that a molecule in state X_n will reach the scoring position z_s without incurring a molecular collision. Therefore, immediately after each collision we can score the event payoff

$$P(X_n) = \pi(v_n)\tau(z_s, X_n) \tag{73}$$

and obtain an unbiased estimate of λ_n. The scoring probability as shown in appendix A (eq. (A13)) is given by

$$\tau(z_s, X_n) = \exp\left(\frac{-|z_n - z_s|}{|v_n|}\right) \tag{74}$$

The results of using the next-event calculation to find the normalized molecular density at the scoring position adjacent to the absorbing wall is shown in table I and can be compared to the results for the analog calculation. The next-event calculations generally resulted in a decrease in variance with some increase in running time. This did not result in a net saving in computing time as shown by the tabulated values of I, which is the percent decrease (+) or increase (-) in computing time for the biased case compared to the analog case for the same confidence limits (eq. (17)). The negative values

of I indicate an increase in computing time is necessary to obtain the same confidence limits in the biased case as in the unbiased case. Careful design of the computer program, which can reduce computing time per sample, would be very effective in reducing total computer time needed since large numbers of samples are calculated.

Birth Biasing

It is possible to use the zero biasing function given in the analysis by equation (58) for the initial event,

$$I_0^\dagger = \frac{P(X_0)}{\lambda_0} \tag{75}$$

because we can evaluate numerically the equation

$$\lambda_0 = \int E_0(X_0)P(X_0)dX_0 \tag{76}$$

For this case, the initial or "birth" payoff would be given by $P_0^\dagger = P_0/I_0^\dagger = \lambda_0$; thus, we can take λ_0 as our initial payoff irrespective of the initial state X_0 found for the sample molecule.

The results for the case where we treat the initial event by the birth bias and use the next-event calculation for all subsequent events are shown in table I. For the same conditions used in the previous examples in table I, it can be seen from the table that there is a decrease in variance for the smaller values of l. There is also a decrease in running time. This generally resulted in a savings in computer time, as shown by the positive values of I in table I.

Survival Biasing

The variance in the random walk payoff of the molecule η_0 is in part caused by the variation in the number of payoffs that are scored before the walk terminates. That is, if a sample molecule is incident on one of the walls when the number of previous scorings is small, it would be expected that the random walk payoff η_0 for this molecule would be small compared to a sample molecule that had a very large number of previous scorings. Hence, if we reduce the variation in the number of collisions, we could expect to reduce the variation in η_0. One method of accomplishing the aforesaid purpose is to bias the transition probability so that the sample molecule is not permitted

to reach an absorbing wall. We can write the survival transport distribution $T^{(s)}$ for the molecules so that the next collision occurs before the molecule is incident on the absorbing surface as

$$T^{(s)}(z_n|X_{n-1}) = \frac{T(z_n|X_{n-1})}{\overline{T}^{(s)}(X_{n-1})} \qquad \text{for } z_n < \mathscr{L} \tag{77}$$

where $\mathscr{L}$ is either 0 or l depending on whether the sample molecule velocity v_{n-1} is less than or greater than 0.

The normalizing factor $\overline{T}^{(s)}$ is given by

$$\overline{T}^{(s)}(X_{n-1}) = \int_{z_n=z_{n-1}}^{\mathscr{L}} T(z_n|X_{n-1})dz_n \tag{78}$$

These results are shown in appendix A (eq. (A15)).

Since the event payoff $P(X_n)$ is zero for all $z \geq \mathscr{L}$, we can write the expected value for the n^{th} event payoff as

$$\lambda_n = \int \cdots \int \left[P(X_n)\overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1) \cdots \overline{T}^{(s)}(X_{n-1})\right]$$

$$\times E_0(X_0)T^{(s)}(z_1|X_0)C(v_1)T^{(s)}(z_2|X_1)C(v_2) \cdots T^{(s)}(z_n|X_{n-1})C(v_n)\Big]dX_0 \cdots \tag{79}$$

The Monte Carlo procedure for the survival biasing case now consists of picking the new position X_n by using the survival-biased transport probability $T^{(s)}(z_n|X_{n-1})$ and scoring the survival-biased payoff

$$P_n^{(s)} = P(X_n)\overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1) \cdots \overline{T}^{(s)}(X_{n-1}) \tag{80}$$

Velocity Biasing

Much of the event payoff variance is caused by the large variations in velocity of the scoring sample molecules. In the zero biasing analysis we wished to minimize the variation in the event payoff. We can do this by defining a biased collision distribution

$$C^{(c)}(v_n|z_n) = C(v_n)I^{(c)}(v_n, z_n) \tag{81}$$

where $I^{(c)}(X_n)$ is the collision bias function and is subject to the condition

$$\int C(v_n)I^{(c)}(v_n, z_n)dv_n = 1 \tag{82}$$

The biased random walk distribution is now given by

$$H^{(c)} = E_0(X_0)K^{(s)}(X_0|X_1)K^{(s)}(X_2|X_1) \cdots T^{(s)}(z_n|X_{n-1})C(v_n)I^{(c)}(X_n) \tag{83}$$

and the biased random walk payoff is now

$$P_n^{(c)} = \frac{P(X_n)}{I^{(c)}(X_n)} \overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1) \cdots \overline{T}^{(s)}(X_{n-1}) \tag{84}$$

The variance of the event payoff $\sigma^2(P_n)$ is given by

$$E\left(P_n^2\right) = \sigma^2(P_n) - \lambda_n^2 = \int \left[P_n^{(c)}\right]^2 H^{(c)}\, dX_0 \cdots dX_n \tag{85}$$

We can minimize equation (85) with respect to $I^{(c)}(X_n)$ by using the calculus of variations to obtain

$$\int \cdots \int \left\{ - \frac{P^2(X_n)}{\hat{I}^{(c)^2}(X_n)} \left[\overline{T}^{(s)}(z_1) \cdots \overline{T}^{(s)}(z_{n-1})\right]\left[E_0(X_0) \cdots C(v_n)\right] \right.$$

$$\left. + D^2\left[E_0(X_0) \cdots C(v_n)\right] \right\} dX_0 \cdots dX_{n-1} = 0 \tag{86}$$

where D^2 is the Lagrange multiplier. This result can be rewritten as

$$DI^{(c)}(X_n) = P(X_n)\overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1) \cdots \overline{T}^{(s)}(X_{n-1}) \tag{87}$$

which can be solved for D by using equation (82) to give

$$I^{(c)}(X_n) = \frac{P(X_n)}{\overline{CP}(z_n)} \tag{88}$$

where

$$\overline{CP}(z_n) = \int C(v_n)P(X_n)dv_n$$

Then the velocity-biased n^{th} event payoff becomes

$$P_n^{(c)} = \overline{PC}(z_n)\overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1) \ldots \overline{T}^{(s)}(X_{n-1}) \tag{89}$$

While the random walk needed for scoring is given by

$$H^{(c)} = E_0(X_0)T^{(s)}(z_1|X_0)C(v_1) \ldots T^{(s)}(z_n|X_{n-1}) \tag{90}$$

We can now proceed to use the technique of survival and velocity biasing in evaluating λ_1. Of course, λ_1 can be evaluated by numerical integration and this value used for all first-event payoffs, as in the birth case, regardless of the state X_1. However, this numerical integration would be difficult and instead we proceed as follows: We wish to evaluate the biased payoff previously derived in equation (89) as

$$P_1^{(c)} = \overline{T}^{(s)}(X_0)\overline{CP}(z_1) \tag{91}$$

The biased random walk is thus given by equation (90) as

$$H^{(c)} = E_0(X_0)T^{(s)}(z_1|X_0) \tag{92}$$

To evaluate $P_1^{(c)}$, we randomly choose v_0 from $E_0(X_0)$ as shown in appendix A (eq. (A3)). This allows us to evaluate $\overline{T}^{(s)}(X_0)$. Then z_1 is found by randomly picking $T^{(s)}(z_1|X_0)$ as given in appendix A (eq. (A16)). With v_0 and z_1 evaluated, the first-event payoff $P_1^{(c)}$ is scored. We can continue and evaluate $P(X_2), P(X_3), \ldots$ with an unbiased procedure so that the random walk is then given by

$$H^{(c)} = E_0(X_0)T^{(s)}(z_1|X_0)C(v_1)K(X_2|X_1) \ldots \tag{93}$$

Then for the correct n^{th} payoff we have

$$P_n^{(c)} = P(X_n)\overline{T}^{(s)}(X_0) \qquad n > 1 \tag{94}$$

The result for the birth bias and first-term bias with the remaining walk unbiased is shown in table I under the "+1 Term bias." The results show a significant decrease in sample variance, except for the largest value of l, although there is a corresponding increase in computer running time. The net savings in computer time was mixed, improving some of the cases only.

The biasing can be continued to the second collision, which would have the payoff

$$P_2^{(c)} = \overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1)\overline{CP}(z_2) \tag{95}$$

The biased random walk is now given by

$$H^{(c)} = E_0(X_0)T^{(s)}(z_1 | X_0)C(v_1)T^{(s)}(z_2 | X_1) \tag{96}$$

To evaluate $P_2^{(c)}$ we have previously obtained values of X_0, z_1, and $\overline{T}^{(s)}(v_0)$ used in finding $P_1^{(c)}$. We then randomly pick v_1 from $C(v_1)$ and evaluate $\overline{T}^{(s)}(X_1)$. Then z_2 is found by randomly picking from $T^{(s)}(z_2 | X_1)$ as shown in appendix A (eq. (A15)). We can then evaluate the biased second-event payoff $P_2^{(c)}$. We can continue in either a biased or unbiased manner in this fashion. The result for biasing to the third collision $P^{(c)}(X_0) + P^{(c)}(X_1) + P^{(c)}(X_2) + P^{(c)}(X_3)$ while the remaining collisions are unbiased $\overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1)\overline{T}^{(s)}(X_2)\left[P(X_4) + P(X_5) + \ldots\right]$ are shown in table I labeled "+3 Term bias." Now significant reduction in variance is seen even for l of 50 in this case. There was a net savings in computer time for all values of l.

Russian Roulette

Finally we can bias continuously; however, in this case, the random walk does not end because the transport probability biasing does not allow the molecules to be incident on the walls. In this case, Russian roulette was used to end the random walks. The sample histories were followed until the weighting $\overline{T}^{(s)}(X_0)\overline{T}^{(s)}(X_1) \ldots \overline{T}^{(s)}(X_{n-1})$ was less than 0.001. Then if a randomly picked number uniform between zero and unity was greater than 0.1, the history was ended. If less, the sample weight was multiplied by 10 and the process continued. These results are given in table I under "Russian roulette." This resulted in decreasing the variance but increasing the computer time

such that the net saving in time was not greatly improved over the three-term bias case. However, no effort was made to optimize the values used, 0.001 or 0.1. Further effort in this direction could significantly improve the Russian roulette procedure.

CONCLUSIONS

Molecular diffusion through a rarefied gas was analyzed by the theory of Markov random walks. The results indicate variance reduction techniques can be successfully used in Monte Carlo analyses of rarefied-gas problems. This can be important in cases where "analog" Monte Carlo analysis of unbiased random walks gives such large variances that unreasonably large amounts of computer time are needed to obtain acceptable confidence limits on the results.

In the present analysis, both a zero-variance and a minimum-variance biasing function are found. These biasing functions, however, apply only for positive event payoffs. However, by appropriately defining the scoring, the event payoffs can be made positive.

The minimum-variance biasing function does not give a zero variance, as the zero-variance biasing function does, and so must give a relative minimum variance. However, in the Monte Carlo calculation procedure when only a finite number of events can be calculated and the bias functions are approximated, which of the biasing functions is optimum has not been determined.

The present results can be applied to any Markov process such as thermal radiation, where instead of following molecules through various molecular collisions we can follow photons through the random walks and apply these same variance reduction techniques.

The "Russian roulette" procedure did not significantly increase the running time saved. The reason may be that the parameters used in the Russian roulette procedures were not optimized.

Since the Monte Carlo procedure is a continuous sampling process, further improvement can be obtained in computer time saving by introducing a learning process into the program so that the bias function would be changed as additional samples are obtained.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, June 22, 1973,
502-28.

APPENDIX A

BIRTH DISTRIBUTION

Assume that the molecules leaving the emitting surface at $z = 0$ are in thermal equilibrium with the emitting surface and that the z-component of velocity v in dv is divided by the total molecular flux leaving the surface μ_{0+} given by

$$\mu_{0+} = \frac{\nu_{0+}}{\sqrt{\pi}} \tag{A1}$$

Then the flux of molecules leaving the emitting surface at $z = 0$ gives the initial z-component of velocity distribution of the molecules leaving the surface (ref. 3) as

$$E_0(v) = 2v \exp(-v^2) \tag{A2}$$

In the Monte Carlo calculation we can randomly choose a v_0 from this distribution by using

$$\int_0^{v_{z0}} 2v_z \exp\left(-v_z^2\right) dv_z = 1 - R = R \tag{A3}$$

where R is a random number generated on the computer from a uniform distribution between zero and unity. Equation (A3) can be rewritten as

$$v_0 = (-\ln R)^{1/2} \tag{A4}$$

Path Length to Collision

The distance a molecule travels between collisions can be found as follows: The probability of a molecule having a collision in time dt is given by

$$-\frac{dN}{N} = +\Theta \, dt \tag{A5}$$

where Θ is the collision rate. The probability of not having a collision during time t is given by N/N_0, which can be obtained by integration of equation (A5) to give

$$\frac{N}{N_0} = \exp(-\Theta t) \tag{A6}$$

Then the probability for having a collision in dt after having no collision in time t_c is given by

$$\frac{N}{N_0} \times \frac{dN}{N} = \left[\exp(-\Theta t_c)\right](-\Theta)dt \tag{A7}$$

The distance between collisions is then given by

$$\Delta = |V| t_c = \frac{|V|}{\Theta} (t_c \Theta) \tag{A8}$$

In reference 3 for a Maxwellian-type collision the collision rate Θ is shown to be a constant. Then if we define a mean free path $\lambda_c = C/\Theta$ and normalize so that $\delta = \Delta/\lambda_c$ we obtain for the distance between collisions

$$\delta = \frac{\Delta}{\lambda_c} = \frac{|V|}{C} (t_c \Theta) = |v|(t_c \Theta) \tag{A9}$$

Combining equations (A7) and (A9) gives the probability of having a collision to be

$$T(z_{n+1} | z_n v_n) = \left[\exp\left(- \frac{\delta_n}{|v_n|}\right)\right] \frac{d\delta_n}{|v_n|} \tag{A10}$$

where

$$\delta_n = |z_{n+1} - z_n|$$

We can randomly pick from this distribution by using

$$R = \int_0^{\delta_n} T(\delta | v_z) d\delta \tag{A11}$$

This can be integrated to give

$$\delta_n = - |v_z| \ln R \tag{A12}$$

The scoring probability, which is the probability of reaching a scoring position z_s from some point z without having an intervening collision, is given by the probability of having a first collision at $\delta > \delta_s = |z_s - z|$. This is given by

$$\tau(\delta_s|v_z) = \int_{\delta=\delta_s}^{\infty} T(\delta|v)d\delta = e^{-\delta_s/|v|} \tag{A13}$$

In some biasing cases we wish to pick from a transport distribution containing distances to collision which are limited to values smaller than those which would cause the molecules to be absorbed at the walls:

$$\delta < \delta_{\mathscr{L}} \qquad \text{where} \qquad \delta_{\mathscr{L}} = \begin{cases} |\ell - z| & \text{for } v > 0 \\ |z| & \text{for } v < 0 \end{cases} \tag{A14}$$

For this case the transport probability is given by

$$T^{(s)}(\delta|v)d\delta = \frac{\exp\left[-\left(\frac{\delta}{|v|}\right)\left(\frac{d\delta}{|v|}\right)\right]}{\int_0^{\delta_{\mathscr{L}}} \exp\left(-\frac{\delta}{|v|}\frac{d\delta}{|v|}\right)} = \frac{\exp\left[-\left(\frac{\delta}{|v|}\right)\frac{d\delta}{|v|}\right]}{1 - \exp\left(\frac{-\delta_{\mathscr{L}}}{|v_z|}\right)} = \frac{T(\delta|v)}{\overline{T}^{(s)}} \tag{A15}$$

We can randomly pick from this distribution by using

$$\delta = -|v|\ln\left\{1 - R\left[1 - \exp\left(\frac{-\delta_{\mathscr{L}}}{|v|}\right)\right]\right\} \tag{A16}$$

Sample Velocity After Collision

The molecules coming out of collision are assumed to be in Maxwellian equilibrium. We can thus write for the distribution of molecules coming out of collision the Maxwellian v-component of velocity as

$$C(v)dv = \frac{1}{\sqrt{\pi}} e^{-v^2} dv \tag{A17}$$

To randomly sample from this distribution we can write

$$f(v, X) = \frac{1}{\sqrt{\pi}} e^{-v^2} \frac{2e^{-X^2}}{\sqrt{\pi}} dv\, dX = 2e^{-\rho^2} \rho\, d\rho \frac{d\theta}{\pi} d\rho\, d\theta \tag{A18}$$

with

$$\left.\begin{aligned} v &= \rho \cos\theta \qquad 0 \le \rho \le \infty \\ X &= \rho \sin\theta \qquad 0 \le \theta \le \pi \end{aligned}\right\} \tag{A19}$$

We can then find

$$\left.\begin{aligned} \rho &= (-\ln R_1)^{1/2} \\ \theta &= R_2 \pi \end{aligned}\right\} \tag{A20}$$

so that

$$v = (-\ln R_1)^{1/2} \cos(\pi R_2) \tag{A21}$$

APPENDIX B

SYMBOLS

$C(V_{n+1} \mid Z_{n+1}, V_n)$	collision distribution
$C^{(c)}(V_n \mid Z_n)$	biased collision distribution
c	thermal velocity
D	constant
E(X)	distribution at X
$E_n(X)$	distribution at X after n events
$E_0(X)$	initial or birth distribution
$\mathscr{E}( )$	expected value
$\mathscr{E}_s( )$	expected value based on local molecular distribution
$G(X \mid Y)$	Green's function
$H(X_0, X_1, \ldots)$	random walk distribution
I	percent running time (saved +, lost -)
$I^{(c)}$	collision bias function
I_n	bias function for n events
$I_n^{\dagger}$	zero-variance bias function
$\hat{I}_n$	minimized-variance bias function
$K(Y \mid X)$	transition distribution
$K^{(l)}(Y \mid X)$	transition distribution for l events
$\mathscr{L}$	limiting value
L	distance across gap
L_n	biasing ratio
l	inverse Knudsen number, L/λ_c
P	event payoff
Q(X)	conditional expected square payoff for a random walk leaving X
R	random number picked from a uniform distribution between zero and unity
S^2	sample variance

$T(Z_n \mid X_{n-1})$	transport distribution
$T^{(s)}(Z_n \mid X_{n-1})$	survival transport distribution
$\overline{T}^{(s)}(X_{n-1})$	normalizing factor
V	point in velocity space (Z-component of velocity)
v	dimensionless velocity in z-direction, V/c
W(X)	conditional expected payoff for a random walk leaving X
X_n	point in position and velocity space immediately after n^{th} event
Y	point in position space
Z	coordinate across gap
z	dimensionless distance across gap, Z/λ_c
α	average running time per sample
Δ	distance between collisions
δ	dimensionless distance between collisions
ϵ	confidence limit
η_0	random walk payoff
Θ	collision rate
λ	expected payoff for random walk
λ_c	mean free path
λ_k	expected value of k^{th} event payoff
λ_μ, λ_n	expected molecular flux and density payoff
μ	molecular flux
$\mu_s^{(\pi)}$	molecular flux of π at scoring position s
μ_{0+}	molecular flux emitted at plate
ν_s	molecular density at scoring position
π	scoring function
σ^2	variance
τ	scoring probability

Subscripts:

c	thermal velocity

n	event index
s	scoring position
z	position in channel
μ	molecular flux
ν	molecular density
0	evaluated at z = 0
+, -	positive and negative z-direction

Superscripts:

(s), (c)	survival biasing, velocity biasing
μ	molecular flux
ν	molecular density
†	zero-variance case
^	minimum-variance case
*	biased case
‾	sample average

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TABLE I. - NUMERICAL RESULTS - 10 000 SAMPLES

Monte Carlo method	Density ratio, ν/ν_{0+}	Standard deviation, $S(\eta_0)$	Average running time per sample, α, min	Percent change in running time (saved +, lost -), I
$l = L/\lambda_c = 0.1$				
Analog	0.848	0.923	0.13×10^{-4}	0
Next event	.844	.867	.15	-1.8
Birth bias	.845	.741	.12	+40.5
+1 Term bias	.850	.1568	.42	+90.6
+3 Term bias	.855	.116	.64	+92.2
Russian roulette	.854	.115	.61	+92.7
$l = L/\lambda_c = 1$				
Analog	0.4914	0.7494	0.31×10^{-4}	0
Next event	.4881	.7188	.35	-3.8
Birth bias	.4881	.7185	.32	+5.1
+1 Term bias	.4958	.5728	.59	-11.2
+3 Term bias	.487	.336	.95	+38.4
Russian roulette	.491	.259	2.33	+10.2
$l = L/\lambda_c = 10$				
Analog	0.1202	0.578	2.14×10^{-4}	0
Next event	.11965	.527	2.33	+9.49
Birth bias	.11965	.527	2.31	+10.2
+1 Term bias	.1171	.463	2.48	+25.6
+3 Term bias	.1195	.402	3.22	+27.2
Russian roulette	.1172	.244	13.97	-16.3
$l = L/\lambda_c = 50$				
Analog	0.0261	0.224	10.78×10^{-4}	0
Next event	.0263	.238	11.61	-21.6
Birth bias	.0263	.238	11.60	-21.5
+1 Term bias	.0263	.2759	11.34	-59.6
+3 Term bias	.0246	.183	14.17	+12.27
Russian roulette	.0245	.168	39.50	-106.1

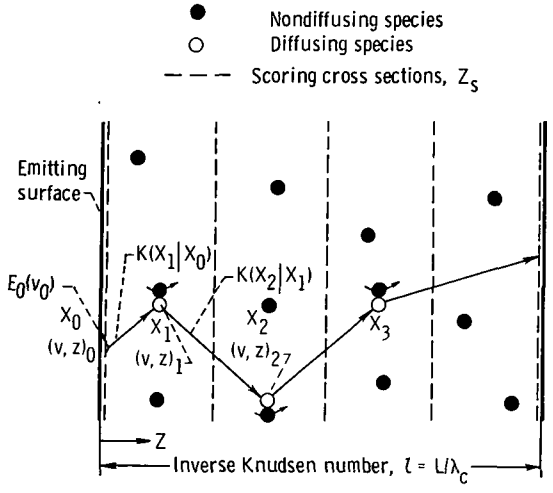

Figure 1. - Analytical model.

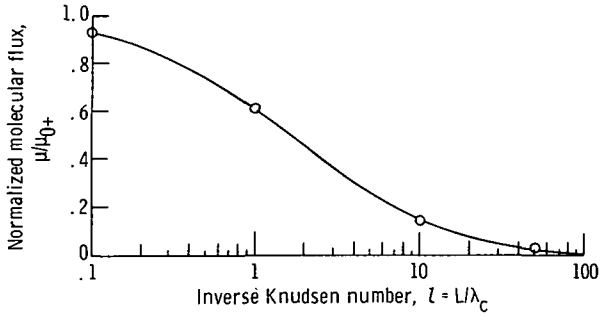

Figure 2. - Molecular flux across gap per unit molecular flux as function of inverse Knudsen number - analog calculation for 10 000 samples.

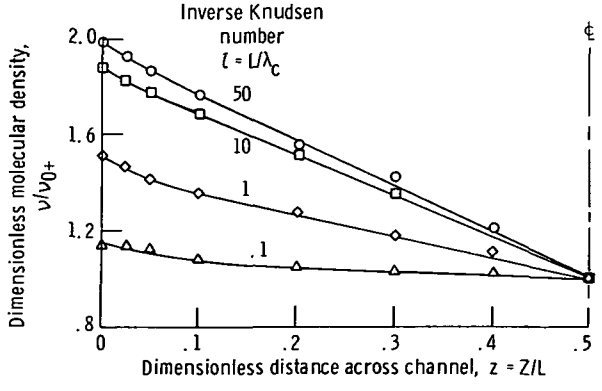

Figure 3. - Molecular density at various scoring positions across gap per unit molecular density entering gap from emitter - analog calculation for 10 000 samples.

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