MONTE CARLO TECHNIQUES FOR SOLVING TRANSPORT PROBLEMS

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INTRODUCTION

The Monte Carlo procedure is a model sampling technique. A model is established, and the behavior of sample units in this model is followed. A sufficient number of sample units are followed to obtain a statistical average or macroscopic quantities, which are the quantities of interest.

This technique was used in crude form by Fermi in connection with the building of the first atomic pile. Later, Von Neumann and Ulam developed and used the Monte Carlo procedure extensively in developing the atomic bomb. Since then this technique has gained considerable use in nuclear reactor problems (refs. 1 and 2), and we at the Lewis Research Center have been extending it to thermal radiation (refs. 3 and 4), rarefied gas flows, and plasma flow problems (ref. 5). This technique, which requires a large number of sample histories to obtain solutions with small variances, is receiving greater use because of the development of the high-speed electronic computors.

Method of Obtaining Sample Histories

The sample history is the behavior of a sample unit under the conditions of the model. The sample unit can be an actual physical quantity such as a photon in thermal radiation problems or a molecule in rarefied gas flow, or it can be some idealized nonphysical quantity such as bundle of radiation or a bundle of molecules that behave according to well defined laws. For purposes of illustration let us consider rarefied gas flow through a channel. A similar problem for ionized gas flow through a channel with a magnetic field across the channel is treated in reference 5. (The procedure applied in this sample problem would apply to other situations such as thermal radiation as well.) Our sample history will be that of a sample molecule as it passes through the channel as shown in figure 1. The sample molecule is equally likely to enter at any height x_2 between 0 and 1 for the case of a flat plate channel. To find the height at which the sample molecule enters the channel, a random number is picked between 0 and 1. This random number has an equal likelihood of being anywhere between 0 and 1 and can be generated by use of standard techniques on the high-speed computor. If a Maxwellian gas in equilibrium in the reservoir is assumed, then the distribution of speeds of the molecules entering the channel is given by

$$f_V = 2\beta^4 V^3 e^{-\beta^2 V^2} \tag{1}$$

where f_V is called the probability density distribution of V. Then $f_V\,dV$ is the fraction of all the molecules that enter the channel that have a speed in the range V to $V + dV$. This depends on the parameter $\beta = (2RT)^{-1/2}$ which is a function of the gas temperature T in the reservoir.

A velocity must now be selected for the sample molecule entering the channel from this distribution. There are several methods of picking from this distribution. One method consists of picking two random numbers R_1 and R_2 and setting R_1 equal to V. In this case every V would be equally likely. Therefore, it is necessary to reject some of the values of V so that the sample distribution will agree with f_v. This is done by using this value of V to find f_v. If f_v is less than R_2, then $R_1 = V$ is rejected (fig. 2) and a new set of random numbers is selected. If f_v is greater than R_2, then $V_1 = R_1$ is used. Thus after a large number of sample molecules are picked, the chosen velocities will satisfy the distribution given by equation (1). There are many different techniques for picking from a distribution, and these are given in the references. In a similar manner we can pick a direction from the appropriate distribution for the sample molecule entering the channel. These are given for a Maxwellian gas by $f_\theta = \theta/2\pi$ and $f_\psi = 2 \cos \psi \sin \psi$ where ψ is the cone angle and θ is the polar angle as shown in figure 1 (ref. 3). The molecule is followed until it has a collision with another gas molecule. The frequency distribution for path length to collision can be given by

$$f_l = \frac{1}{L} e^{-l/L} \tag{5}$$

where l is the path length of the sample molecule and L is the average path length of all the molecules at that location; the path length to the collision is picked from this distribution. The new molecule path must then be picked, and the molecule is followed in this manner until it leaves the channel.

Obtaining the Mean Properties

The mean properties are obtained by dividing the height of the channel into increments of width Δx_2 at several locations along the length of the channel (fig. 2). The amount of some quantity Q that is carried by a single molecule across Δx_2 at that axial position is given by

$$\dot{M} \int_0^\infty Q V_1 f \, dV = \rho \overline{V_1 Q} = \frac{C_L}{\Delta x_2} \left(\sum^{S^+} Q - \sum^{S^-} Q \right) \tag{6}$$

where M is the mass of a molecule and C_L is the number of molecules each sample molecule represents. The terms $\sum^{S^+} Q$ and $\sum^{S^-} Q$ are the sums of the Q contained in each sample molecule passing Δx_2 in the positive or negative axial direction, respectively. The number of these molecules is given by S. If the axial flow is desired, then $Q = 1$ and equation (6) reduces to

$$\rho \bar{V}_1 = M \int_0^\infty V_1 f \, dV = \frac{C_L}{\Delta x_2} (S^+ - S^-) \tag{7}$$

If the mass flow in the x_2 or vertical direction is desired, then $Q = V_2/V_1$ and equation (6) becomes

$$\rho\bar{V}_2 = M\int_0^\infty V_2 f\, dV = \frac{C_L}{\Delta x_2}\left(\sum^{S^+}\frac{V_2}{V_1} - \sum^{S^-}\frac{V_2}{V_1}\right) \tag{8}$$

If the density is desired, then $Q = 1/V_1$ and equation (6) reduces to

$$\rho = M\int_0^\infty f\, dV = \frac{C_L}{\Delta x_2}\left(\sum^{S^+}\frac{1}{V_1} - \sum^{S^-}\frac{1}{V_1}\right) \tag{9}$$

In this manner macroscopic flow properties in the channel can be obtained by summing these Q properties as the molecules pass the designated cross sections.

In a similar manner the shear stress or drag on the wall can be calculated. The shear stress on the wall in the x_1 direction P_{x_1,x_2} is given by

$$-P_{x_1,x_2} = \left(M\int_0^\infty V_1 V_2 f\, dV\right)_w = \frac{C_L\left(\sum^{Sq} V_1\right)}{D\,\Delta x_1}$$

That is, by summing the V_1 components of velocity of all the sample molecules hitting an elemental area Δx_1 on the wall (fig. 1) we can find the shear stress or drag at the wall at that location. If the molecules are reflected diffusely, they will not contribute to the shear stress. Some results obtained in references 5 and 6 are shown in figures 2 to 4.

Figure 3 shows the axial flow through a flat plate channel for a collisionless gas. Different channel lengths over width l were used. The solid lines are the analytical solutions (ref. 5), and the points are the Monte Carlo results (ref. 6). The cross-sectional measurements were made at the entrance $x_1 = 0$, one quarter down the channel $l/4$ and the midpoint of the channel $l/2$. The height of the channel was divided into 20 increments. The results are symmetrical around $l/2$ and also around $x_2 = 1/2$.

The densities are shown in figure 4. Again the back half of the channel is not shown because of the relation

$$\left(\frac{\rho}{\rho_L}\right)_{x_1} + \left(\frac{\rho}{\rho_L}\right)_{l-x_1} = 1$$

In figure 5 the wall shear results are presented. There is good agreement between the Monte Carlo and the analytical results.

One major drawback of this technique is the large amount of computor time required because of the fact that to obtain small variations in the average quantities a large number of trials are needed. However, various techniques have been developed that allow shorter running times to be obtained. Also, the high-speed computors are constantly being improved. This Monte Carlo procedure is relatively new and will probably be used a great deal more in the future for solving problems on widely different subjects. It has already been found very useful in solving problems that would be highly intractable using more standard procedures.

REFERENCES

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CHANNEL MODEL

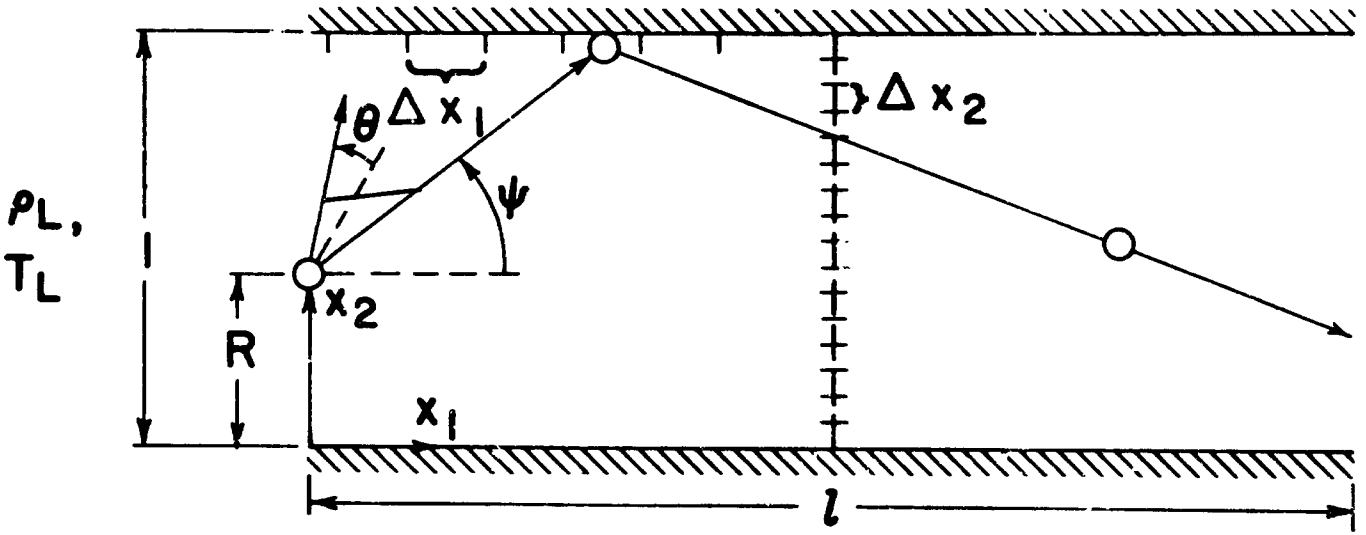

Figure 1

SAMPLING TECHNIQUE

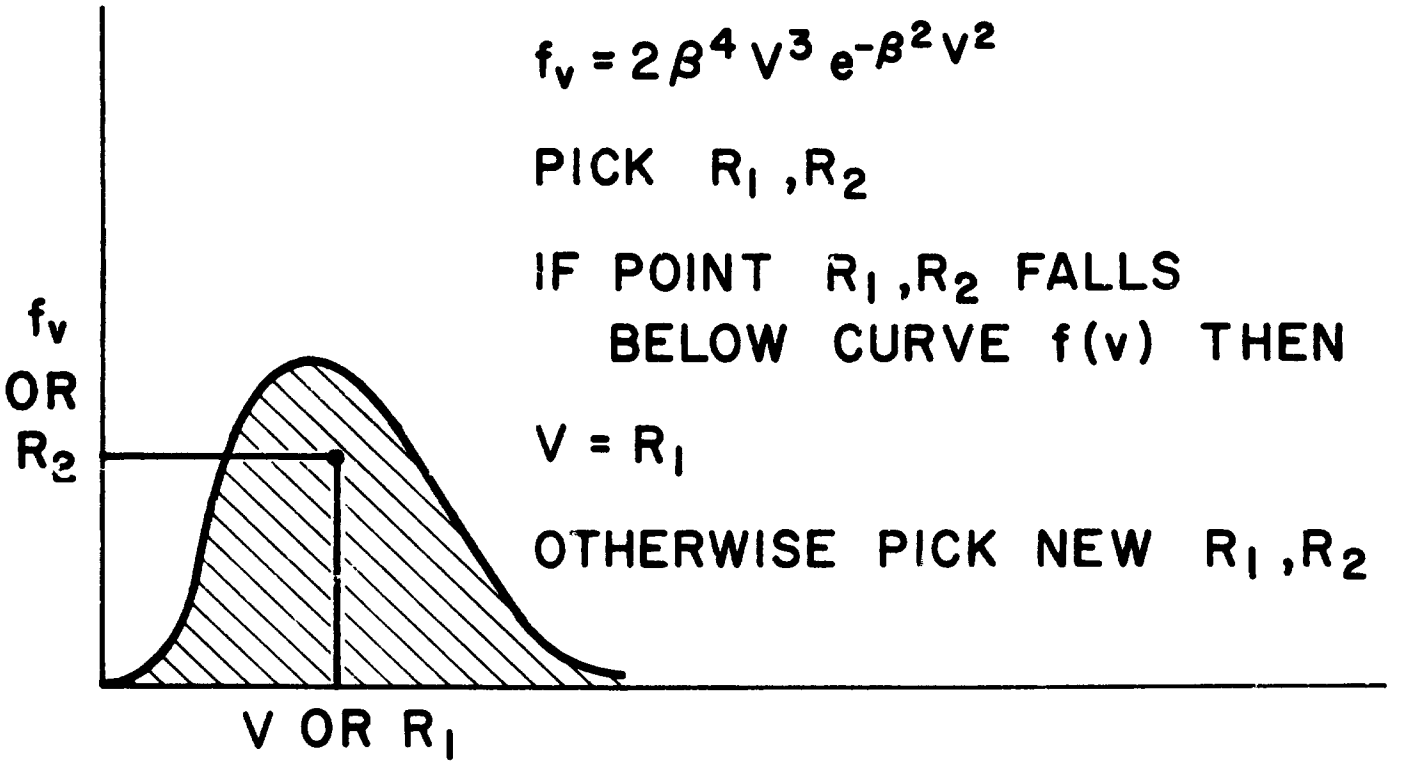

Figure 2

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AXIAL MASS-FLOW PROFILE

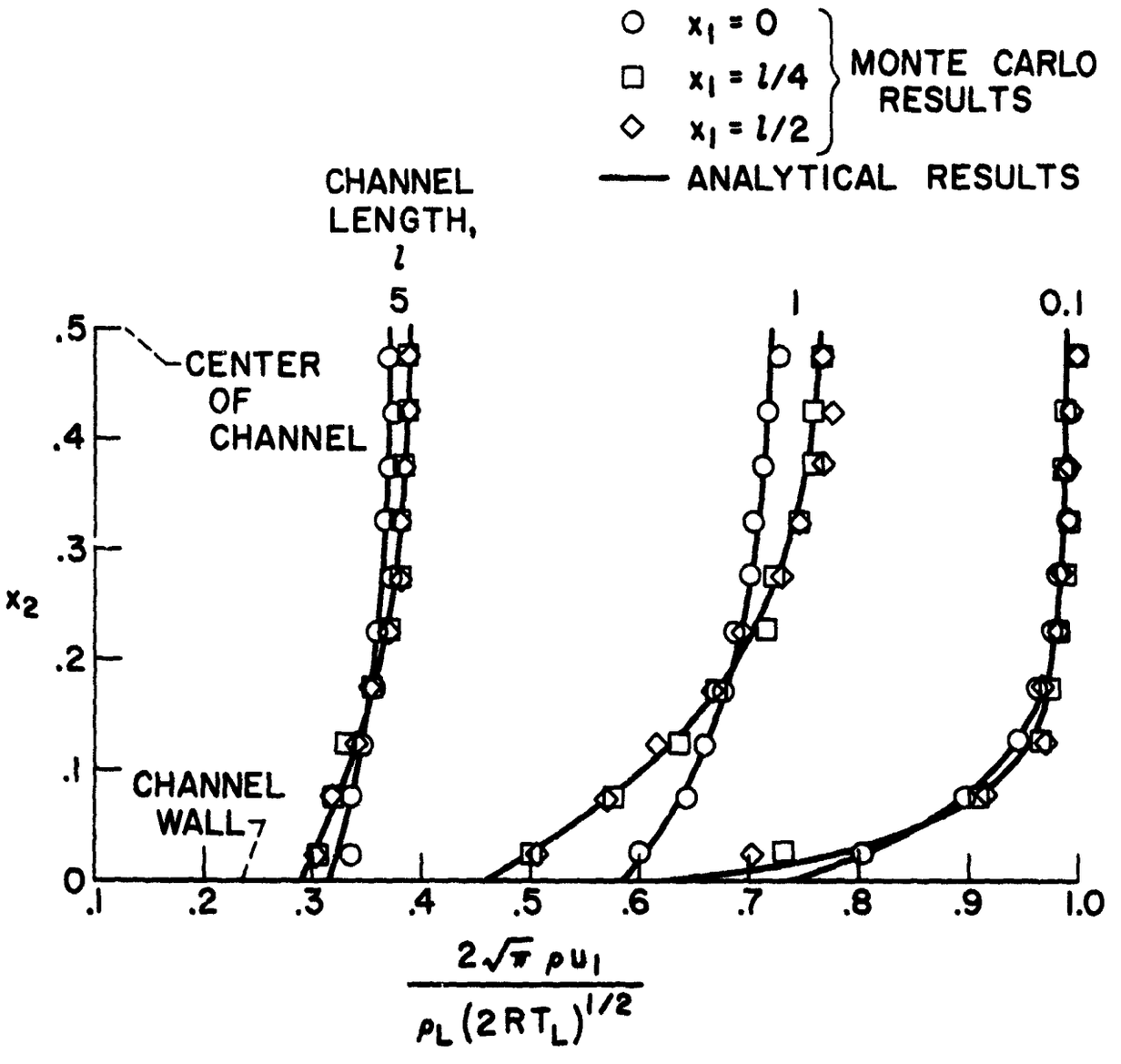

Figure 3

DENSITY DISTRIBUTION IN CHANNEL

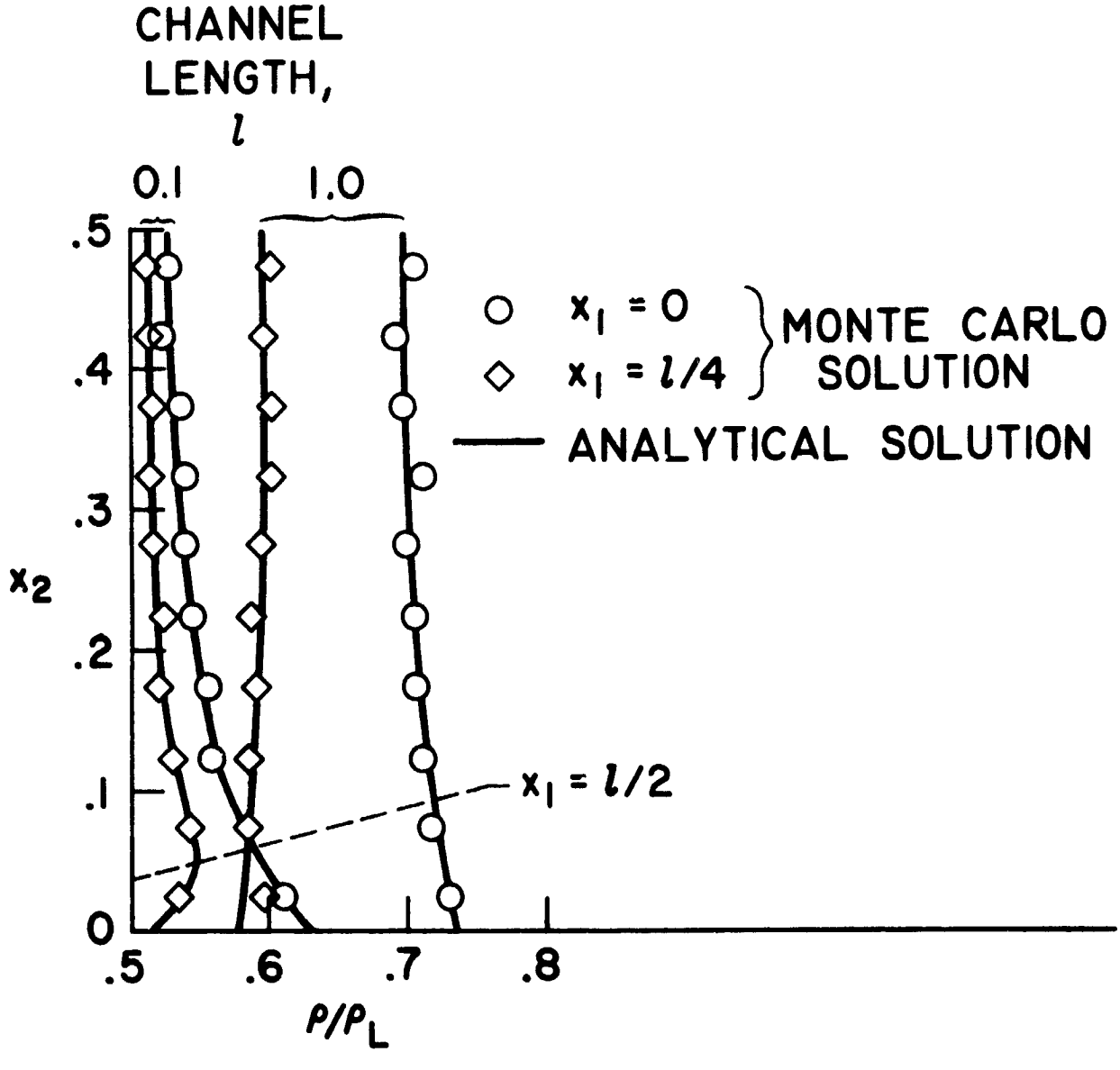

Figure 4

WALL SHEAR DISTRIBUTION

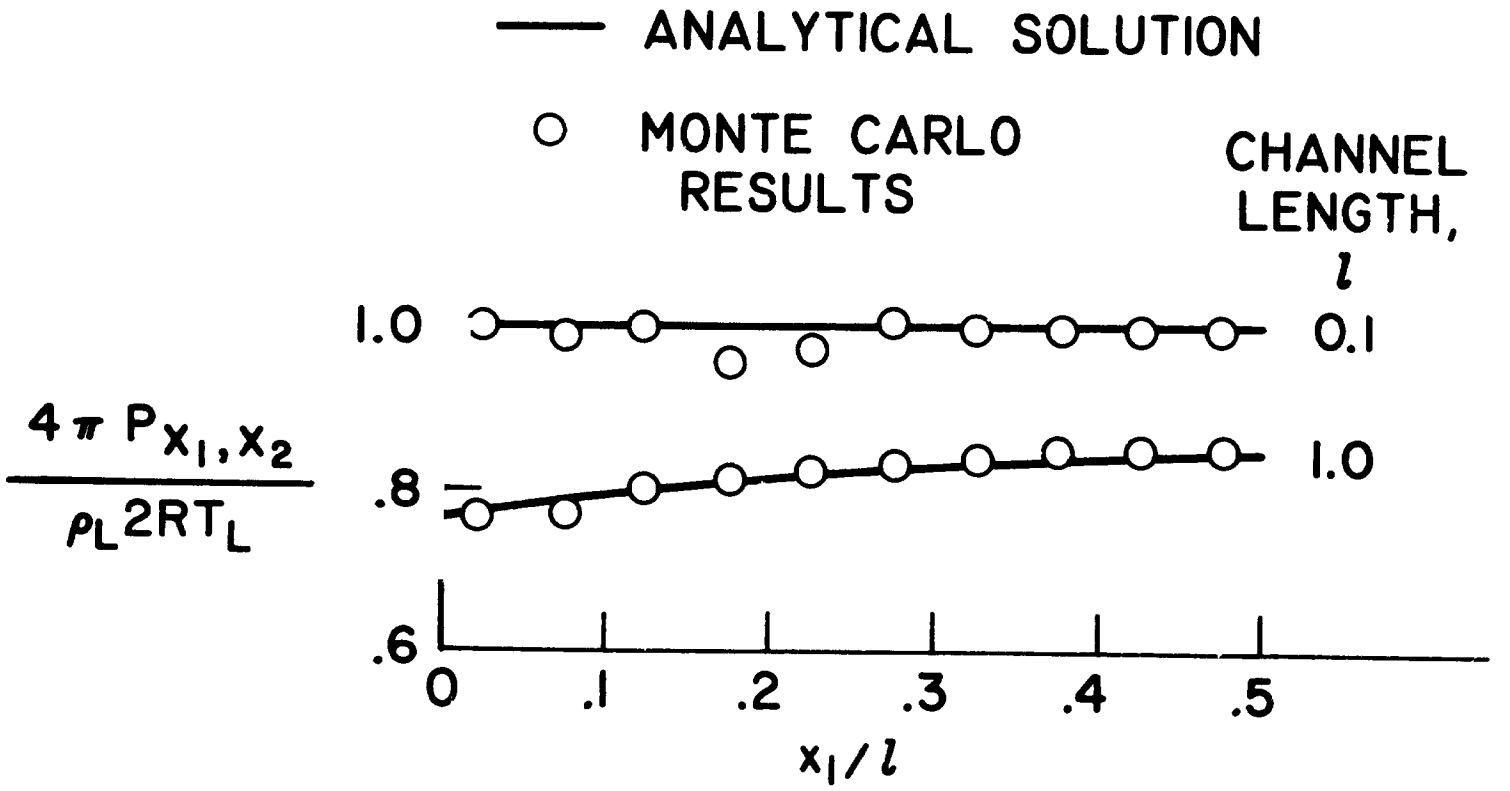

Figure 5