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Transport Calculations in Particle-Loaded Media

Gary J. Scrivner

TRANSPORT CALCULATIONS IN PARTICLE-LOADED MEDIA · SCRIVNER

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Transport Calculations in Particle-Loaded Media

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DISSERTATION

Submitted in Partial Fulfillment of the
Requirements for the Degree of
Doctor of Philosophy in Nuclear Engineering
in the Graduate School of
The University of New Mexico
Albuquerque, New Mexico
August 1970

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Transport Calculations in Particle-Loaded Media

By

Gary J. Scrivner

ABSTRACT OF DISSERTATION

Submitted in Partial Fulfillment of the
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Albuquerque, New Mexico

August 1970

Transport Calculations in Particle-Loaded Media[1]

Gary J. Scrivner, Ph.D.
Department of Nuclear Engineering
The University of New Mexico, 1970

Particle-loaded materials are sometimes used for radiation shielding. In many cases shielding calculations, performed with the assumption of a homogeneous medium having the appropriate ratio of particle-to-matrix material, are grossly inadequate. The exact distribution of particles within such materials is probabilistic in nature, and, therefore quantities, such as the transmitted flux, become random variables. To reasonably evaluate the effectiveness of this type shielding, one must obtain the expected values and corresponding standard deviations of those quantities of interest.

In this dissertation, two models of a particle-loaded shield are investigated. The first is an artificial material postulated to consist of constant-thickness slabs of infinite lateral extent, which are called "particles," randomly imbedded in a matrix material. Precise analytic results are obtained for the case in which particle and matrix are pure absorbers. The second is a more realistic model, consisting of constant-radius spheres randomly imbedded in a matrix material. A precise treatment of this model is extremely difficult; hence, the author examines two approximate schemes which are advantageous from a computational standpoint. The first approximate scheme has the characteristic that, in the limit of low volume-percent loadings, it approaches the rigorous solution. The second approximate scheme, valid when the first scheme is inadequate, provides a useful method of evaluating the behavior of highly loaded materials.

1 This work was supported by the United States Atomic Energy Commission.

Transport Calculations in Particle-Loaded Media[1]

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The University of New Mexico, 1990

Particle-loaded materials are sometimes used for radiation shielding. In many cases of practical interest, particles with the geometry of a homogeneous medium using the appropriate ratio of particle to matrix material, are already inadequate. The random distribution of particles within such materials is probabilistic in essence and, therefore, the fields, such as the transmitted flux, become random variables. To reasonably evaluate the effectiveness of this type of shielding, one must obtain the expected values and corresponding standard deviations of those quantities of interest.

In this dissertation, two models of a particle-loaded shield are investigated. The first is an analytical one-dimensional model consisting of constant-thickness slabs of infinite lateral extent, which are called "particles," randomly imbedded in a matrix material. Closed analytic results are obtained for the case in which particle and matrix are pure absorbers. The second is a more realistic model, consisting of constant-radius spherical particles imbedded in a matrix material. A Monte Carlo treatment of this model is considered. Since this model is costly to implement, the author examines two approximate methods which are advantageous from a computational standpoint. The first approximation assumes that the characteristic that, in the limit of low volume percent loadings, it approximates the rigorous solution. The second approximation method, which uses the "virtual" method in Lindquist, gives a useful result for the behavior of highly loaded materials.

[1] This work was supported in part by the United States Energy Foundation.

Again, both particles and matrix are taken to be pure absorbers. The sphere-loaded problem is investigated by employing Monte Carlo procedures to simultaneously construct transport particle histories and the structure of the medium encountered during these histories.[2]

For the pure absorption problem, it is found in both of the above models that for shields which are very thin relative to particle dimensions, the average transmission initially decreases in agreement with the homogeneous shield assumption. As the shield thickness increases, however, the average transmission can depart very quickly from the behavior one would calculate by assuming the shield to be a homogeneous mixture of particle and matrix material.

This departure asymptotically results in an exponential behavior governed by an effective constant cross section which is characteristic of the loaded shield and which is lower than the cross section associated with the homogeneous assumption. It is also observed that for the pure absorption problem, the behavior of the expected value of higher moments of the transmission is no more difficult to obtain than the first moment.

Calculational results are presented and are found to compare favorably with the limited amount of available experimental data. The extension of the developed computational techniques to transport problems which include scattering is then outlined. In the final chapter, the author discusses the implication of his results upon both experimental and additional theoretical work on transport theory in realistic particle-loaded media.

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2 The modifier "transport" is used to distinguish between transport particles, such as neutrons or photons, and the loading particles.

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CHAPTER 1 Introduction[1]

Materials used in nuclear engineering are usually classified as either homogeneous or heterogeneous. Strictly speaking, all materials are heterogeneous because of density fluctuations and the presence of impurities. Therefore, when one says a material is homogeneous, one is really assuming that, for a particular physical process, the material can be accurately modeled as being homogeneous. For transport calculations, this assumption is based on the idea that the scale of the inhomogeneities is much smaller than the transport mean free path. A more accurate model of such materials would consist of requiring the material to have properties described by constant mean values with random fluctuations about these means. Such a description is often required to investigate the detailed nature of acoustic or electromagnetic wave propagation in the atmosphere or oceans [6]. Perturbation techniques are very powerful in solving these types of problems, since the departure from the mean properties is often rather small. The interesting implication of such an analysis is that quantities such as acoustic pressure at a field point is not deterministic and one must investigate the expected values and the corresponding standard deviations of such quantities.

The great majority of materials used in nuclear engineering applications can be taken as homogeneous when one performs radiation transport calculations. Heterogeneous systems of materials can often be broken down into distinct homogeneous regions. The exceptions are those systems that are heterogeneous in an undeterministic manner. In this category are shielding materials such as Boral and some of the loaded concretes. Even

1 This work was supported by the United States Atomic Energy Commission.

for these, it is often possible to make the homogeneous approximation with respect to certain types of radiation transport. However, for Boral, it is well known that for many practical applications, the homogeneous assumption is simply not adequate [4].

The purpose of this dissertation is to investigate the shielding characteristics of undeterministic composite materials. The investigation will be restricted to homogeneous particles randomly distributed within a homogeneous matrix of different transport properties. The composite is termed undeterministic, since one usually has only bulk data on such a composite material.

Information, such as spectrum of particle sizes and shapes and the relative volume of the composite occupied by the particles, is frequently available. But for a particular sample of such a material, an exact description of the structure is not available. For different samples of such material, the shielding efficiency can differ because of the stochastic nature of the material. Hence, quantities such as transmitted flux and absorbed dose at various points within such a shield become random variables, dependent upon the statistics of the medium. The description of such shields must therefore rely on probabilistic concepts such as the expected transmission and its standard deviation. In addition, for the type materials under investigation, a perturbation approach is unsatisfactory because of either the geometric scale of the particles or the degree of difference in transport properties, or both. The material to be presented in the following chapters applies equally well to photon or neutron shielding calculations and, as a result, the term "transport particle" can be taken to imply either of these types of radiation.

In Chapter 2, a simple one-dimensional model of a stochastic shielding material is investigated. Precise analytic results are obtained for the

case in which the matrix and particle materials are pure absorbers. The results provide insight into the expected behavior of more realistic stochastic shields. Chapter 3 describes the difficulty encountered if one desires to treat the problem of uniform spherical particles distributed within a matrix filler. Chapter 4 presents an approximate technique of performing calculations in such a material which is rigorously correct only in the limit of low volume-percent loadings but which provides useful estimates for loadings up to several percent. Chapter 5 describes an alternative approximate technique, enabling one to perform calculations for highly loaded composites. In Chapter 6, the two previously developed techniques are compared with each other and with the scant amount of available experimental data. To this stage, all calculations have been based on the assumption that both matrix and particle materials are pure absorbers. In Chapter 7, the extension of the previously developed concepts to scattering problems is discussed. Finally, Chapter 8 presents a discussion of obtained results, obvious extensions of this investigation, and suggestions for continued work.

CHAPTER 2 The Slab Problem

2.1 Description of the Problem

The purpose of this chapter is to investigate a simple model problem which retains some of the salient features of radiation transport through particle-loaded media. In this model, the "particles" are taken to be slabs of infinite lateral extent and of finite thickness δ. The slabs are necessarily constrained to lie parallel to each other and to be noninterpenetrating. These slabs are randomly imbedded in a filler or matrix material such that in a gross sense the stochastic composite material is specified by the volume fractions of particle material f_p and of matrix material f_m.

The analysis is restricted to the pure absorption problem of a monoenergetic beam of radiation incident perpendicular to the faces of the slabs. With this restriction, the only transport properties of interest are Σ_m and Σ_p, the macroscopic absorption coefficients of the matrix and particle materials at the incident beam energy.

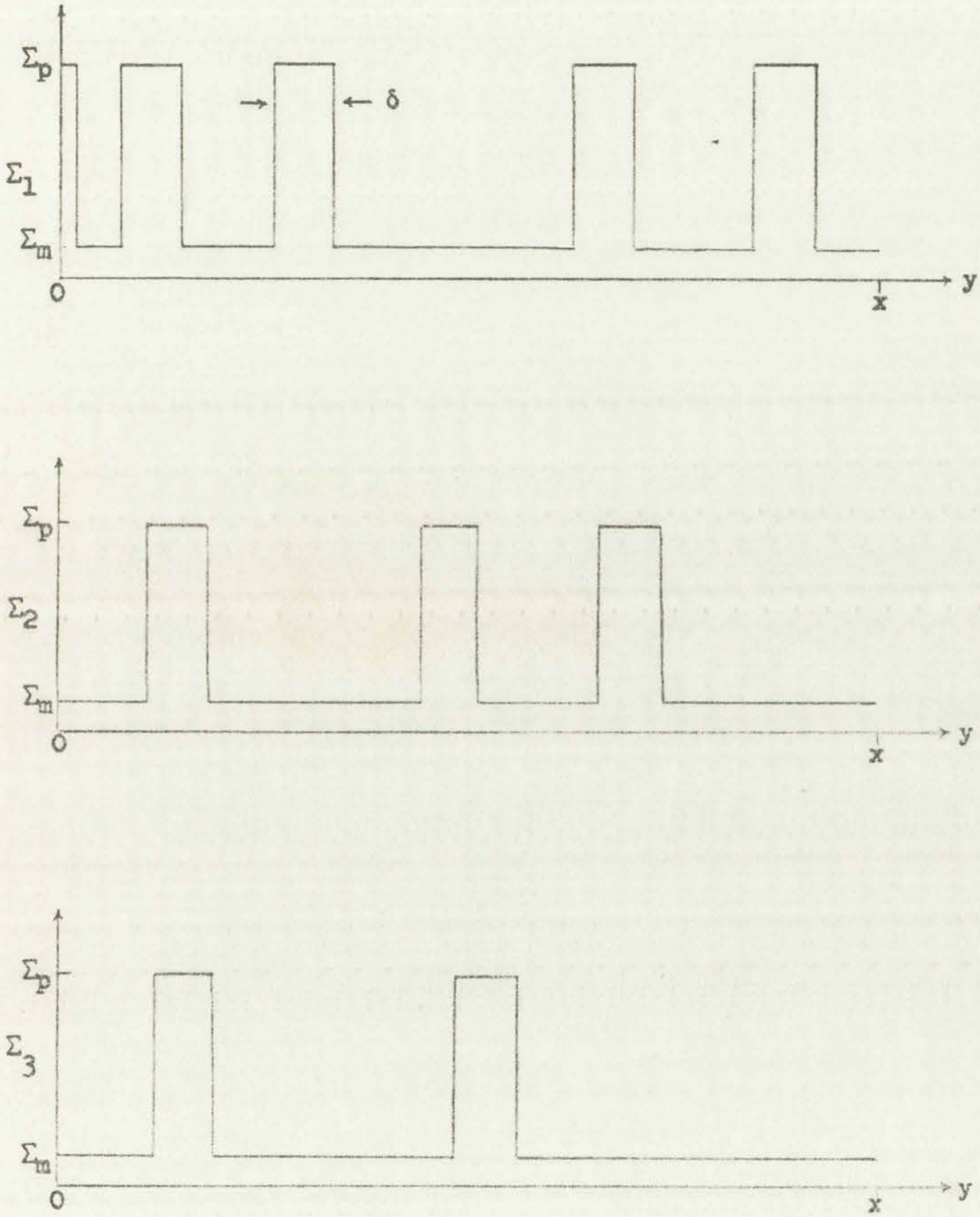
The problem is to investigate the probabilistic nature of the transmission characteristics of a thickness x of such a composite media. Figure 1 presents the variation of the macroscopic cross section Σ of the composite material for three possible samples of thickness x.

2.2 Derivation of Governing Equations

It is evident that any position $y \varepsilon [0,x]$ lies within either matrix or particle. If position y corresponds to matrix, it is meaningful to determine the probability of encountering a particle by moving to position $y + \Delta$, $\Delta > 0$. Since particles are randomly imbedded in the matrix material, this probability is $\lambda\Delta + o(\Delta)$, where λ is a constant

Figure 1

Some Sample $\Sigma(y)$ Profiles



characteristic of the loading.[1] The argument leading to this conclusion is similar to the one employed in the development of the Poisson distribution [11]. In more precise terms, one has that

$$P(\text{particle at } y + \Delta | \text{matrix at } y) = \lambda\Delta + o(\Delta) \ , \qquad (1)$$

where $P(A|B)$ is the conditional probability of event A, given the occurrence of event B.

To obtain an expression for λ in terms of the physical parameters of the media, one is led to consider the total probability of position $y + \Delta$ corresponding to particle $P(\text{particle at } y + \Delta)$. Since position y corresponds to either matrix or particle, one can employ basic probability concepts to write

$$P(\text{particle at } y + \Delta) = P(\text{particle at } y)P(\text{particle at } y + \Delta | \text{particle at } y) + P(\text{matrix at } y)P(\text{particle at } y + \Delta | \text{matrix at } y) \ . \qquad (2)$$

In order to satisfy the specified loading, it is necessary that

$$P(\text{particle at } y + \Delta) = P(\text{particle at } y) = f_p \ , \qquad (3a)$$

$$P(\text{matrix at } y) = f_m \ . \qquad (3b)$$

A simple geometric interpretation of probability yields

$$P(\text{particle at } y + \Delta | \text{particle at } y) = 1 - \frac{\Delta}{\delta} + o(\Delta) \ . \qquad (4)$$

---

1 $f(\Delta) = o(\Delta)$ if the $\lim_{\Delta \to 0} \frac{f(\Delta)}{\Delta} = 0$.

Substitution of (1), (3), and (4) into (2) yields

$$f_p = f_p\left(1 - \frac{\Delta}{\delta}\right) + f_m\lambda\Delta + o(\Delta) \ . \tag{5}$$

Solving (5) for λ in the limit as $\Delta \to 0$, one obtains

$$\lambda = \frac{f_p}{\delta f_m} \ . \tag{6}$$

Physically, λ can be interpreted as the average number of slabs per unit volume of matrix material.

At this point the analysis will focus on the determination of the average transmission of the model material. The extension to higher moments of the transmission will be discussed later in the chapter.

The function $T_m(x)$ is defined as the expected or average transmission through a shield of thickness x, given that position $y = x$ corresponds to matrix. For the present, x is taken to greater than a slab thickness δ. It is desired to formulate an expression for $T_m(x + \Delta)$ in terms of the transmission characteristics of shields of smaller thickness. If $x + \Delta$ corresponds to matrix, the probability of not encountering a particle in moving through a distance Δ to position x is $1 - \lambda\Delta + o(\Delta)$. The reduction in transmission caused by a thickness Δ of matrix is $1 - \Sigma_m\Delta + o(\Delta)$. The contribution to $T_m(x + \Delta)$ from the above event is

$$T_m(x)(1 - \lambda\Delta)(1 - \Sigma_m\Delta) + o(\Delta) \ . \tag{7}$$

The probability of encountering a particle in moving through a distance Δ to position x is $\lambda\Delta + o(\Delta)$. Since all particles are of [illegible] (7), and (8) yields

$$[illegible] \quad (9)$$

Solving (9) for λ in the limit [illegible], one obtains

$$λ = [illegible] \quad (10)$$

Physically, λ can be interpreted as the average number of atoms per unit volume of target material.

At this point the analysis will focus on the development of the average [illegible] of the [illegible]. The [illegible] higher moments of the transmission will be discussed later in the chapter.

The function $L_m(x)$ is defined as the expected or average transmission through a [illegible] thickness x, given that [illegible] particle is [illegible]. For the [illegible] is [illegible] of the [illegible] characteristics of [illegible] and [illegible], the probability of not encountering a particle in moving through a distance x [illegible] position x is [illegible]. The [illegible] by a [illegible] of [illegible]. The contribution to $L_m(x)$ from the above event is:

$$[illegible] \quad (11)$$

The probability of encountering a particle in moving through a [illegible] position x in [illegible] thickness δ, the encountered particle reduces the transmission by the factor $\exp(-\Sigma_p \delta)$ below that value corresponding to position $x - \delta$. It is then noted that position $x - \delta$ corresponds to matrix. The contribution to $T_m(x + \Delta)$ from this event is

$$\lambda\Delta \exp(-\Sigma_p \delta) T_m(x - \delta) + o(\Delta) \ . \tag{8}$$

Combining (7) and (8), one obtains

$$T_m(x + \Delta) = T_m(x)(1 - \lambda\Delta)(1 - \Sigma_m \Delta)$$

$$+ \lambda\Delta \exp(-\Sigma_p \delta) T_m(x - \delta) + o(\Delta) \ . \tag{9}$$

Performing standard algebraic manipulations and passing to the limit as $\Delta \to 0$, (9) becomes

$$\frac{dT_m(x)}{dx} = -(\Sigma_m + \lambda) T_m(x) + \lambda \exp(-\Sigma_p \delta) T_m(x - \delta) \ , \tag{10}$$

for $x > \delta$.

If $x \varepsilon [0,\delta]$, the previous analysis must be slightly modified. This is due to the fact that if the right-hand face of a particle is at position x, the reduction in transmission is $\exp(-\Sigma_p x)$ rather than $\exp(-\Sigma_p \delta)$. Hence, for this situation (10) must be modified to give

$$\frac{dT_m(x)}{dx} = -(\Sigma_m + \lambda) T_m(x) + \lambda \exp(-\Sigma_p x) T_m(o) \ , \tag{11}$$

for $x \varepsilon [0,\delta]$. Equation (10) is a differential-difference equation, with (11) specifying the required behavior over an initial interval

of width δ. To solve (11), the required initial condition is

$$T_m(0) = 1 \ . \tag{12}$$

Equations (10), (11), and (12) completely specify the behavior of $T_m(x)$ for $x > 0$. It remains to be shown how knowledge of the function $T_m(x)$ enables one to determine the average transmission T.

At any position x there are but two possibilities. Position x corresponds to either matrix or particle. As previously discussed, the probability that x corresponds to matrix is f_m. Given that x corresponds to matrix, the contribution to the average transmission is $T_m(x)$. The other possibility is that x corresponds to particle. Given that x corresponds to particle, any relative position $y \varepsilon [0,\delta]$ within the slab is equally likely. More precisely, the probability density function p(y) associated with relative particle position y is constant or

$$p(y) = \frac{1}{\delta} \tag{13}$$

for $y \varepsilon [o,\delta]$.

Again, for $x > \delta$, the attenuation associated with the particle is simply $\exp(-\Sigma_p y)$, and position $x - y$ must correspond to a matrix position. Using this information and integrating over all possible values of y, one obtains the desired expression for the average transmission

$$T(x) = f_m T_m(x) + f_p \int_0^{\delta} \exp(-\Sigma_p y) T_m(x - y) \frac{1}{\delta} \, dy \ , \tag{14}$$

for $x > \delta$.

of width [illegible]. In order [illegible]

[illegible]

Equations (10), (11), and [illegible]

$V(x)$ for $x > 0$. It [illegible]

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position. Using this information [illegible]

values of [illegible], one obtains the [illegible]

distribution

[illegible]

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For $x\epsilon[0,\delta]$, relative particle positions $y\epsilon[x,\delta]$ result in an attenuation of $\exp(-\Sigma_p x)$ rather than $\exp(-\Sigma_p y)$. To compensate for this fact (14) must be modified to read

$$T(x) = f_m T_m(x) + f_p \int_0^x \exp(-\Sigma_p y) T_m(x - y) \frac{1}{\delta} dy$$

$$+ f_p \int_x^\delta \exp(-\Sigma_p x) \frac{1}{\delta} dy , \qquad (15)$$

for $x\epsilon[0,\delta]$. Expressions (10), (11), (12), (14), and (15) completely determine the average transmission $T(x)$.

2.3 Solution Using the Laplace Transform [3]

In this section the solution for $T_m(x)$ will be obtained. The Laplace transform of $T_m(x)$, which will be denoted by $B_m(s)$, is defined as

$$B_m(s) = \int_0^\infty \exp(-sx) T_m(x)\, dx . \qquad (16)$$

To implement the approach, one multiplies (10) by $\exp(-sx)$ and integrates over $x\epsilon[\delta,\infty]$. Also, (11) is multiplied by $\exp(-sx)$ and integrated over $x\epsilon[0,\delta]$. The resulting expressions can be combined to eliminate the term $T_m(\delta)$. This procedure results in the relation

$$B_m(s) = \frac{1}{s + \Sigma_p} \frac{\left\{s + \Sigma_p + \lambda - \lambda \exp\left[-\delta(s + \Sigma_p)\right]\right\}}{\left\{s + \Sigma_m + \lambda - \lambda \exp\left[-\delta(s + \Sigma_p)\right]\right\}} . \qquad (17)$$

One can now employ the Inversion Theorem to recover $T_m(x)$. The only singularities of $B_m(s)$ occur at the zeroes of the function $F(s)$

where

$$F(s) = s + \Sigma_m + \lambda - \lambda \exp\left[-\delta(s + \Sigma_p)\right] , \qquad (18)$$

an exponential polynomial. It is now desirable to perform a change of variables by defining

$$w = \delta(s + \Sigma_m + \lambda) . \qquad (19)$$

In terms of w, (18) can be written as

$$\delta F(s) = w - \lambda\delta \exp\left[\lambda\delta - \delta(\Sigma_p - \Sigma_m)\right] \exp(-w) . \qquad (20)$$

It is further convenient to define

$$a = \lambda\delta \exp\left[\lambda\delta - \delta(\Sigma_p - \Sigma_m)\right] . \qquad (21)$$

For realistic physical parameters, a is real and positive. The zeroes of (18) can thus be determined by an investigation of the equation

$$we^w - a = 0 \qquad (22)$$

for $a > 0$.

The roots of (22) have been examined by several authors [13]. Therefore, the results will be stated here without formal proof. Expression (22) has one real root and an infinite number of complex roots occurring in conjugate pairs. All these roots are simple. Denoting a conjugate pair of roots as w_n, one writes

$$w_n = x_n \pm iy_n \qquad (23)$$

for $n \geq 1$. The one real root can be included in the above list as corresponding to $n = 0$ if one demands all roots to be simple. The real root satisfies the equation

$$x_0 \exp(x_0) = a \ . \tag{24}$$

Furthermore, it is known that

$$(2n - 1)\pi < y_n < 2n\pi \tag{25}$$

for $n \geq 1$. Finally, it is noted that the x_n's form a decreasing sequence, or

$$x_{n+1} < x_n \tag{26}$$

for $n \geq 0$. A more precise specification of the location of the roots of (22) can be obtained, but is not required for purposes of this development since the essential features are now apparent. The roots are partitioned by (25) such that an accumulation at one point in the complex w-plane is impossible. Further, the real root has the largest real part. These observations imply that the inverse of (17) is well-behaved and, for large x, $T_m(x)$ will behave exponentially with an argument determined by the location of the real root.

One can now apply the Cauchy Integral Theorem to (17) to recover the asymptotic behavior of $T_m(x)$ for large x and obtain

$$T_m(x) \simeq \frac{(\Sigma_p - \Sigma_m) \exp\left\{x\left(\frac{x_0}{\delta} - \Sigma_m - \lambda\right)\right\}}{(1 + x_0)\left(\frac{x_0}{\delta} - \Sigma_m - \lambda + \Sigma_p\right)} \tag{27}$$

as $x \to \infty$. It is convenient to define constants C_∞ and Σ_∞ such that (27) can be written

$$T_m(x) \simeq C_\infty \exp(-\Sigma_\infty x) \tag{28}$$

as $x \to \infty$, where

$$\Sigma_\infty = \lambda + \Sigma_m - \frac{x_0}{\delta} \tag{29a}$$

and

$$C_\infty = \frac{\Sigma_p - \Sigma_m}{(1 + x_0)(\Sigma_p - \Sigma_\infty)} \ . \tag{29b}$$

As one would expect on physical grounds, it can be shown that C_∞ is positive and that Σ_∞ lies somewhere between the values of the cross sections associated with matrix and particle.

Expression (28) is now substituted into (14) to obtain the asymptotic behavior of the average transmission T(x). Carrying out the implied integration and, with a little algebra, one obtains

$$T(x) \simeq D_\infty \exp(-\Sigma_\infty x) \tag{30}$$

as $x \to \infty$, where

$$D_\infty = \frac{f_m}{(1 + x_0)\left(1 + \dfrac{(x_0 - \lambda\delta)}{\delta(\Sigma_p - \Sigma_m)}\right)^2} \ . \tag{31}$$

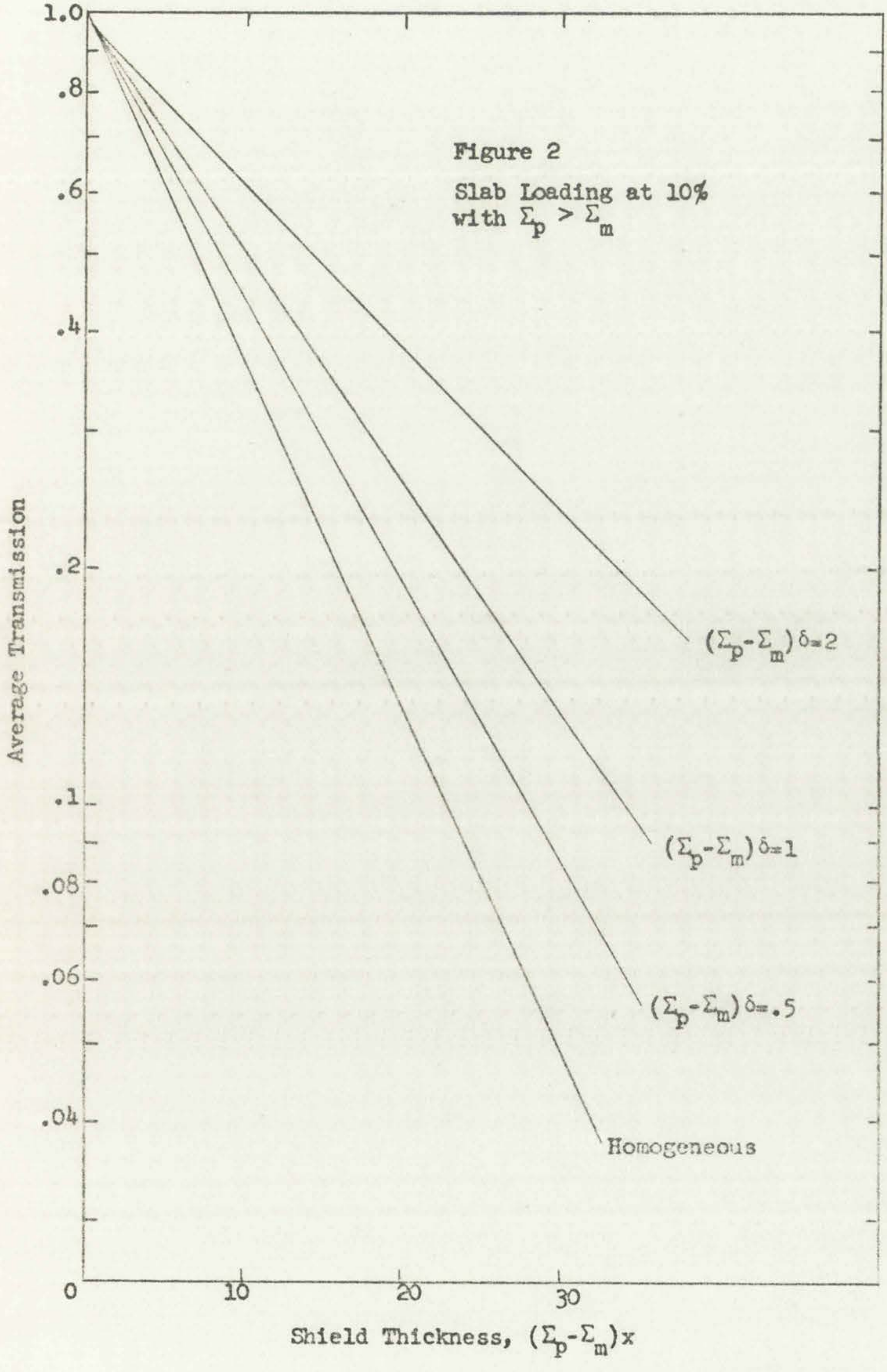
2.4 Computational Results

For practical purposes, the concentration in the preceding section was restricted to only the asymptotic solution. Equations (10), (11), (12), (14), and (15) can actually be solved numerically with less effort than is involved in obtaining the additional roots required to evaluate the "complete" analytic solution. The analytic asymptotic solution (30) can be used conveniently to check digital or analog calculational results. In practice, one can obtain an analytic expression for T(x) for $x \epsilon [0,\delta]$ by employing relations (11), (12), and (15). For practical purposes, this thin shield behavior together with the asymptotic behavior are sufficient to describe the basic attenuation properties of the model problem. The plots in this chapter were obtained in this manner.

Figures 2 through 5 present some computational results for various particle loadings and particle thicknesses. For the case that $\Sigma_p > \Sigma_m$, the matrix is taken to be transparent and the particles taken to have cross section $\Sigma_p - \Sigma_m$. Thus, the true attenuation at position x is lower by the factor $\exp(-\Sigma_m x)$. Similarly, for the case that $\Sigma_m > \Sigma_p$, the particles are taken to be transparent and the matrix to have a cross section $\Sigma_m - \Sigma_p$.

The behavior is as one would expect on physical grounds. For a fixed loading, the thinner the particles, the better the shielding efficiency for a fixed-thickness shield. In the limit that the thickness of the particles, expressed in mean free paths, becomes small, the solution corresponding to a homogeneous mix of particle and matrix material is obtained.

Based on the computational results, the most important observations are how rapidly the asymptotic solution is attained and how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0
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20
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Figure 2
Slab Loading at 10%
with $\Sigma_p > \Sigma_m$
$(\Sigma_p-\Sigma_m)\delta=2$
$(\Sigma_p-\Sigma_m)\delta=1$
$(\Sigma_p-\Sigma_m)\delta=.5$
Homogeneous
Average Transmission
Shield Thickness, $(\Sigma_p-\Sigma_m)x$

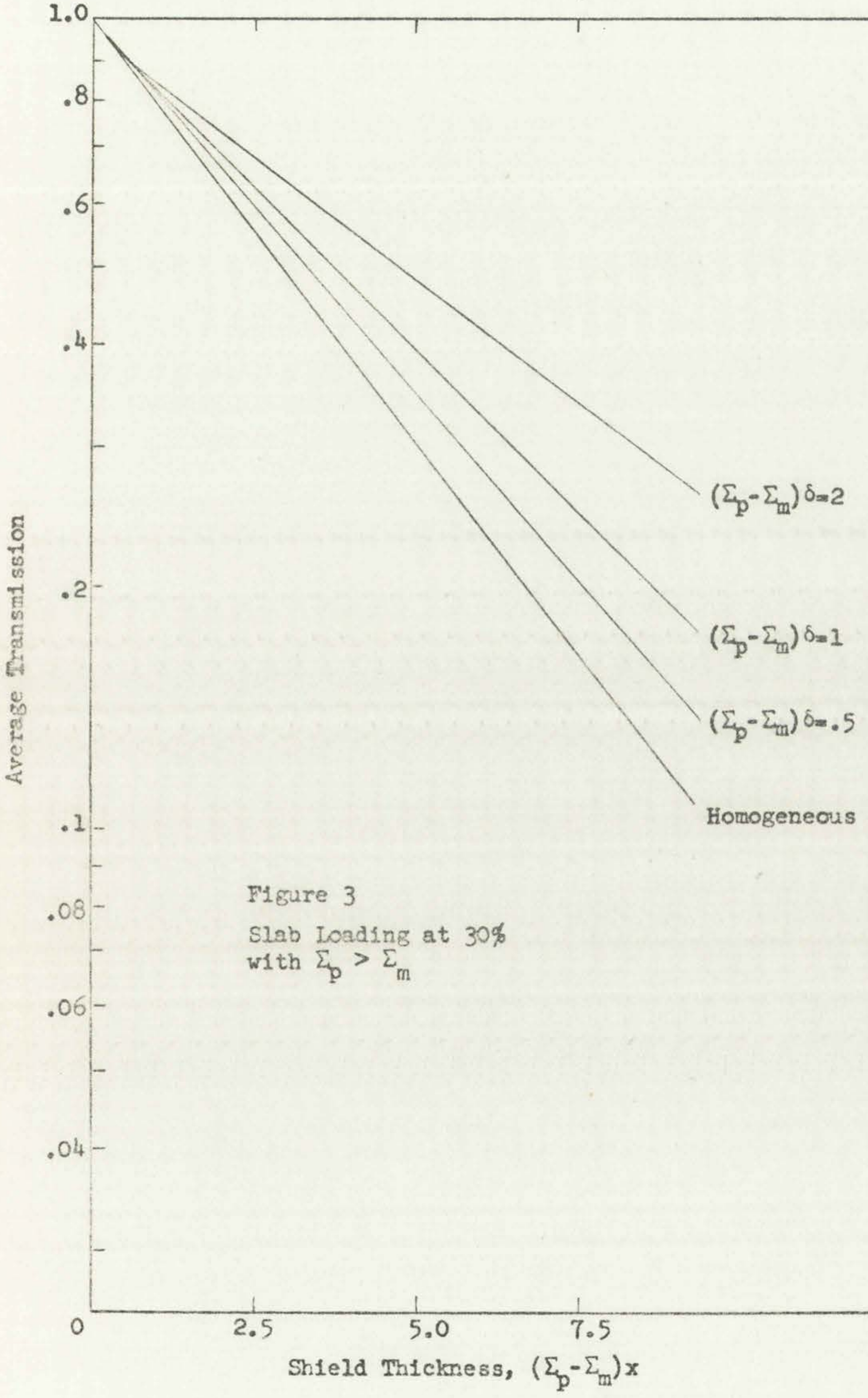

Figure 3

Slab Loading at 30%
with $\Sigma_p > \Sigma_m$

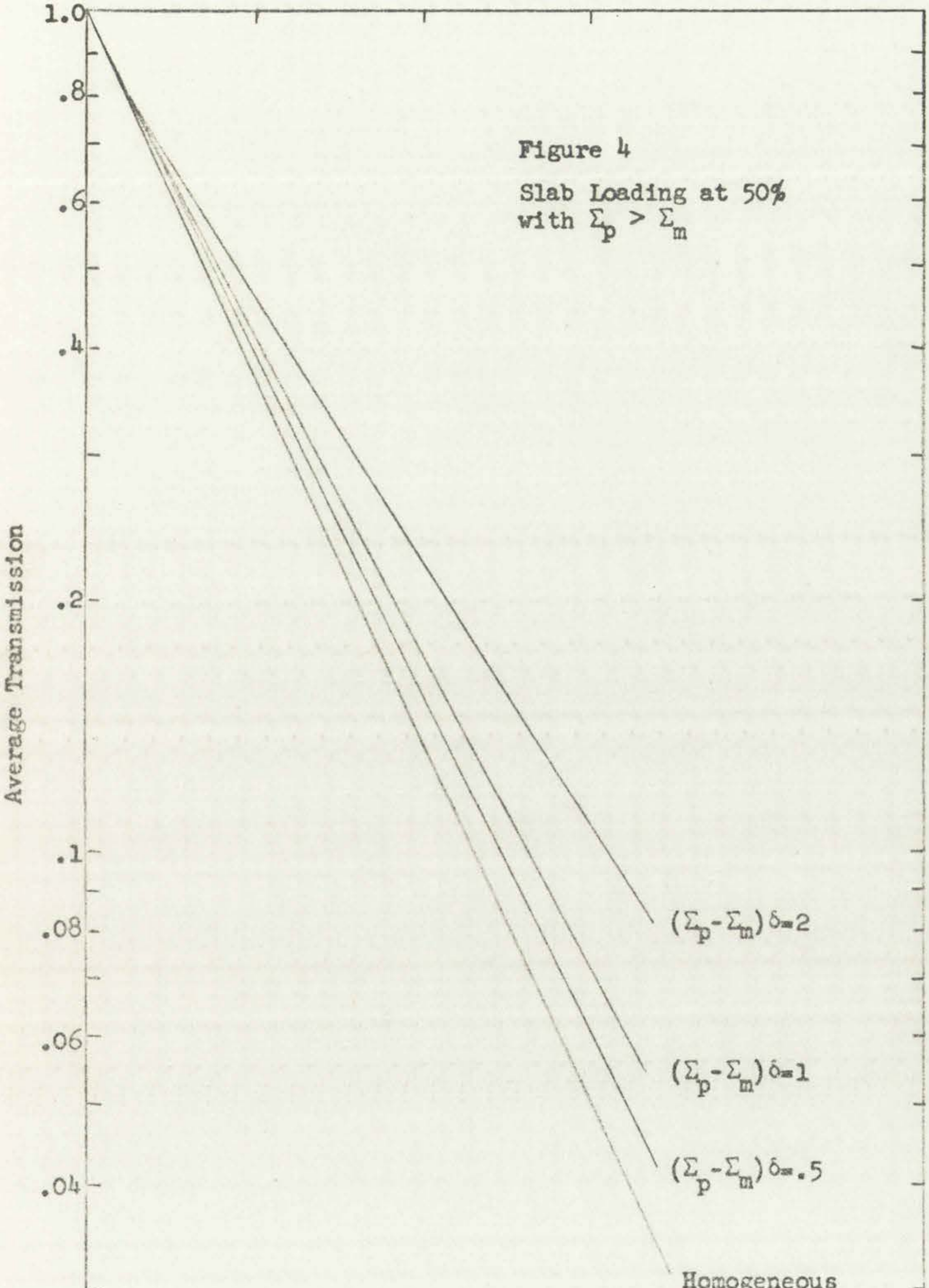

Figure 4
Slab Loading at 50% with $\Sigma_p > \Sigma_m$
1.0
.8
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.2
.1
.08
.06
.04
0
2.5
5.0
7.5
Average Transmission
Shield Thickness, $(\Sigma_p-\Sigma_m)x$
$(\Sigma_p-\Sigma_m)\delta=2$
$(\Sigma_p-\Sigma_m)\delta=1$
$(\Sigma_p-\Sigma_m)\delta=.5$
Homogeneous

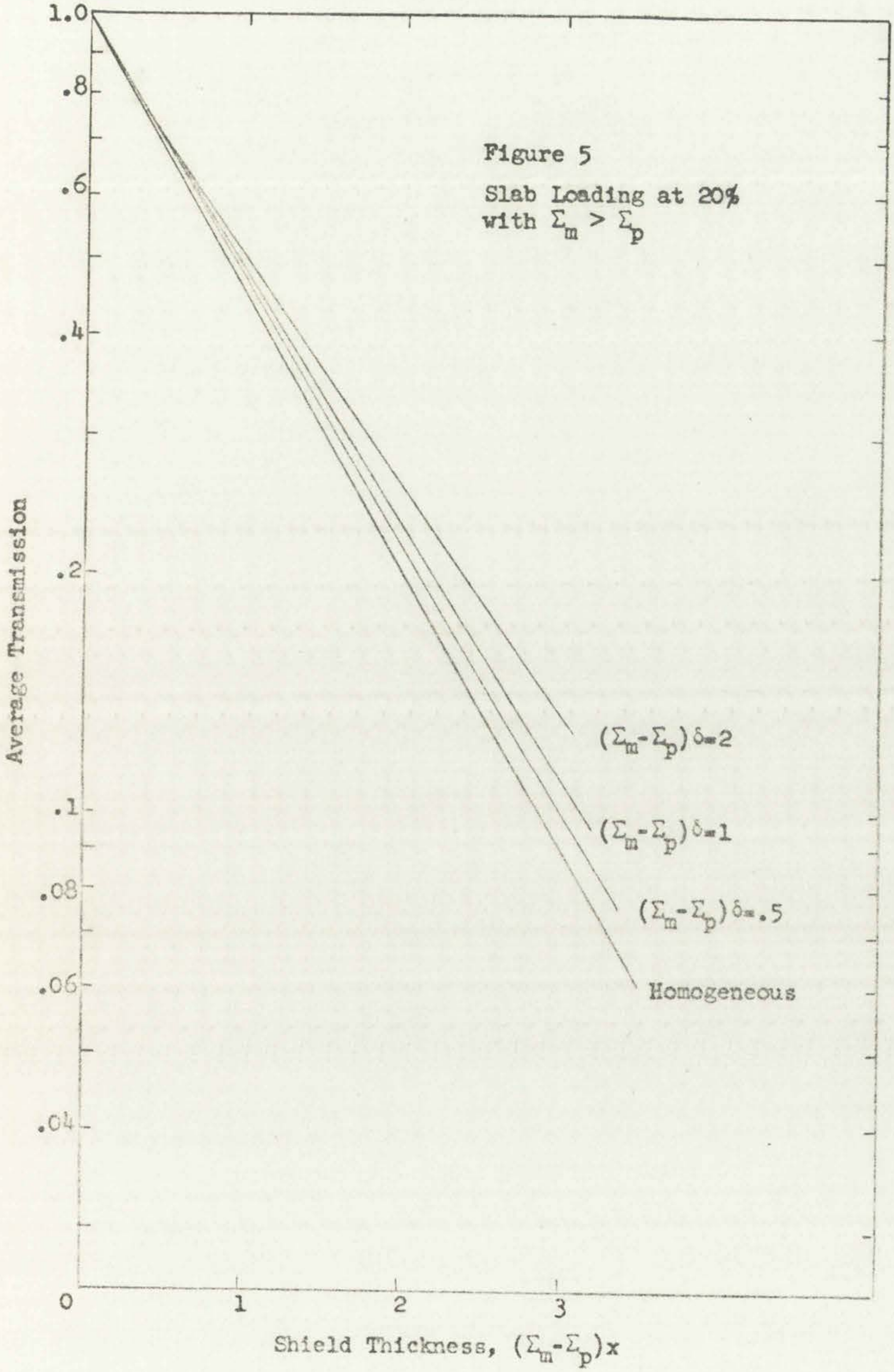

Figure 5

Slab Loading at 20% with $\Sigma_m > \Sigma_p$

severely the homogeneous mix solution can underestimate the transmission through such a composite material.

2.5 Validity of the Homogeneous Approximation

Since precise analytic results have been obtained for the slab problem, a means of estimating the error induced by treating a particle-loaded medium as homogeneous is available. In order to perform this investigation, the difference between Σ_∞ and $\bar{\Sigma} = f_m\Sigma_m + f_p\Sigma_p$ is examined as a function of particle thickness. Combining (21) and (24), one obtains

$$x_0 \exp(x_0) = \lambda\delta \exp\left(\lambda\delta - \delta(\Sigma_p - \Sigma_m)\right) . \tag{32}$$

Employing (32) and noting that $\lambda\delta = f_p/f_m$, independent of δ, one can obtain

$$\frac{x_0}{\delta} = \lambda - (\Sigma_p - \Sigma_m) \frac{\lambda\delta}{1 + \lambda\delta} + \frac{(\Sigma_p - \Sigma_m)^2 \lambda\delta}{(1 + \lambda\delta)^3} \frac{\delta}{2} + o(\delta) . \tag{33}$$

Expressions (33) and (29a) imply that

$$\Sigma_\infty = \bar{\Sigma}\left\{1 - \frac{\bar{\Sigma}\delta f_p}{2}\left(1 - \frac{\Sigma_p}{\bar{\Sigma}}\right)^2 + o(\delta)\right\} . \tag{34}$$

Equation (34) presents a convenient criterion for examining the validity of the homogeneous assumption. Expression (34) shows that the three critical factors are: (1) the thickness of the particles, $\bar{\Sigma}\delta$, (2) the relative number of particles, f_p, and (3) the degree of departure of particle cross section from the mean cross section of the medium, $1 - \frac{\Sigma p}{\bar{\Sigma}}$.

2.6 The Higher-Moment Problem

The previous treatment has concentrated on the average transmission. For engineering applications, it is also of interest to know how well the mean represents the distribution of possible values. The probability of the transmission for a specific shield exceeding twice the mean transmission, for example, could be a crucial factor in the acceptability of a particle-loaded material for a shielding application. An examination of the expected values of higher moments of the transmission can provide this type of information.

If one denotes the functional dependence of the cross section for the i^{th} sample of the model media as $\Sigma_i(y)$, $y\varepsilon[0,x]$ and the corresponding transmission as $T_i(y)$, then

$$\frac{d}{dy} T_i(y) = -\Sigma_i(y) T_i(y) \tag{35}$$

with initial condition $T_i(0) = 1$. Note that the average transmission is simply the mean value of $T_i(y)$ averaged over all possible samples of the media. In order to investigate the higher moment problem, one is led to multiply (35) by $[T_i(y)]^{n-1}$, where $n \geq 1$.

The result can be cast in the form

$$\frac{d}{dy}\Big[T_i(y)\Big]^n = -n\Sigma_i(y)\Big[T_i(y)\Big]^n , \tag{36}$$

with initial condition $\Big[T_i(0)\Big]^n = 1$. The implication is indeed fortunate. Expression (36) is identical to (35) except that the cross section variation is multiplied by the factor n. Even the initial condition at y = 0 remains unchanged. Hence the analysis presented for determination of the mean transmission is equally valid for the n^{th} moment of the transmission, provided both particle and

matrix cross sections are increased n-fold. Note that this conclusion is simply a result of the structure of equation (35) and is independent of the nature of the model problem.

2.7 Summary of Slab Problem

In this chapter, a simple model problem has been examined. The purpose was to gain some insight into the effect of particle size in a random particle-loaded medium. In the limit as $x \to 0$, it is evident that the average transmission initially decreases with $\bar{\Sigma}$. Several particle thicknesses into the medium, the average transmission approaches an asymptotic behavior and decreases exponentially with an effective cross section which has been denoted as Σ_∞. In section 2.5 an analytic result was obtained which permits one to evaluate readily the legitimacy of assuming a particle-loaded medium to be homogeneous. Although its development was based upon a simple model, equation (34) should provide a useful estimate of the departure from homogeneity for more realistic materials. Finally, in section 2.6 an important observation pertaining to the higher-moment problem was presented.

CHAPTER 3 The Complexity of the Sphere Problem

The attractive feature of the slab model of Chapter 2 was that as one exits from a particle (slab) into matrix, the probability of encountering a subsequent slab is completely specified by a constant, λ, which is completely determined by the nature of the loading. Unfortunately, the author knows of no engineering materials which have the one-dimensional loading characteristics of this model. Realistic composite materials usually have an intrinsic three-dimensional character. Slugs of steel imbedded in concrete, boron carbide spheres in aluminum, and voids distributed in foams are examples of more realistically structured composites. To examine the shielding characteristics of such materials, one must be able to treat the channeling of radiation between particles. The simplified nature of the slab model precludes this type investigation. Hence, in subsequent chapters, a more realistic model is investigated. This model consists of constant-radius spherical particles randomly imbedded in a matrix filler. Even this model would be difficult to construct physically because of the problem of achieving a truly random distribution of spheres with existing fabrication techniques. True composite materials could be expected to have pseudorandom distribution of particles related in some abstract manner to the fabrication process. Hence a truly accurate description of such materials appears to require an accumulation of experimental data specifying the variation of transport properties along a large sample of ray paths. The situation becomes even more complex if one desires to include a scattering mechanism in the transport calculations since, in this case, simple ray paths no longer suffice. Nevertheless, the spherical-particle model should provide some useful insight into the expected behavior of such materials for shielding applications.

The problem now is to formulate the construction of the sphere-loaded medium mathematically, as was accomplished for the slab problem. The inherent difficulty is that this model is closely related to the hard-sphere model of liquids and dense gases used by molecular physicists and to the random packing problem of the mathematicians. Results in these areas are quite limited, although the literature contains experimental and numerical studies [1,8]. The chief difficulty is that the medium has short-range ordering which implies that the distribution function governing the probable position of one sphere is dependent on the relative positions of many of its neighbors.

The most pertinent numerical studies are of a Monte Carlo nature. A large box of spheres is simulated on a digital computer. According to some distribution function, velocity vectors are assigned to each sphere in order to specify the initial state of the system. A many-body dynamics problem is then solved to describe the subsequent motion of the ensemble of hard spheres. After attainment of dynamic equilibrium, the state of the system at various times is used to investigate the statistical nature of such a system of particles. The most severe limitation of this approach is the number of particles which can be utilized. Ignoring this latter consideration, suppose one desired to employ the above scheme to investigate the shielding characteristics of a sphere-loaded medium. The most direct approach would be to use the above procedure to construct many samples of the pertinent shielding configuration. Each of these many samples would require a Monte Carlo transport calculation because of the complex geometry. Results of all these calculations could then be averaged to obtain estimates of the average shielding behavior of the stochastic material. It will be shown in later chapters that it is permissible to track the behavior of but one source transport particle per constructed sample,

averaging the results over many samples. If this procedure is employed, each source transport particle is traversing a random sample of the material which is completely independent of previously constructed samples. The implication is that one needs only to construct that portion of the material through which this single source particle travels. Unfortunately, the medium construction technique described above requires the establishment of a rather large volume of the medium in order to obtain these types of data.

The following two chapters present two approximate techniques of modeling a sphere-loaded stochastic shield. Each of these has the attractive feature that only the portion of material required to determine the fate of one source transport particle need be constructed. Even these approximate schemes are of sufficient complexity to demand Monte Carlo methods to carry out the construction. The basic method of attack is, then, the simultaneous construction of transport particle histories and construction of the corresponding paths through a stochastic material by means of the Monte Carlo method.

CHAPTER 4 The Random Approximation to the Sphere Problem

4.1 Introduction

As indicated in Chapter 3, the difficulty in doing transport calculations in a medium consisting of a matrix loaded with spherical particles is that the particles are not randomly positioned. As the volume fraction occupied by the particles increases, the pseudorandom nature of the loading becomes more and more pronounced. Spheres are forced into more advantageous positions by contact with their neighbors in order to achieve the increased packing density. However, for a relatively sparsely loaded material, this effect should be negligible. In this chapter, the above idea is investigated. Sphere centers will be assumed to be randomly distributed within the nonexcluded volume. The term nonexcluded volume will be used to distinguish a possible site of a sphere center from those positions within one sphere diameter of a previously established sphere center. Therefore, spheres will not be allowed to interpenetrate. Within this chapter the analysis will be restricted to the case in which all spheres have identical radius R.

4.2 Theory of Sphere Placement

The objective of this section is to develop the methods for constructing the nature of a particle-loaded material as seen by an observer moving along a ray through this material. First, the observer must be assigned a starting point. The probability that this starting point lies within matrix is simply equal to the volume fraction of matrix f_m. If the starting point does not lie in matrix, then it must lie within a spherical particle. In this case the center of sphere must lie within a spherical volume of radius R about the starting point.

CHAPTER 4. THE [illegible] TO THE [illegible]

4.1 Introduction

As indicated in Chapter 3, the [illegible] calculations in a medium consisting of a [illegible] with spherical particles is that, the particle [illegible] volume fraction occupied by the particles increases, the [illegible] nature of the [illegible] and more [illegible] forced into more [illegible] by [illegible] data in order to achieve the prescribed [illegible] for a relatively sparsely loaded material, [illegible] negligible. In this chapter, the above [illegible] centers will be assumed to be randomly distributed within the [illegible] excluded volume. [illegible] excluded volume will be [illegible] through a [illegible] of a [illegible] within the sphere diameter of a [illegible] Therefore, spheres will not be allowed to [illegible] object, the analysis will be restricted to the [illegible] spheres have identical radius [illegible]

4.2 [illegible] Random Placement

The objective of this section is to [illegible] governing the [illegible] of a particle-loaded [illegible] observed moving along a ray through this structure [illegible] must be assigned a starting point. The probability that this point lies within [illegible] is simply equal to the volume fraction of [illegible] matrix f_m. If the starting point does not lie [illegible] the [illegible] within a spherical [illegible]. In this case the center [illegible] must lie within a [illegible] volume of radius R about the [illegible]

Any position within this spherical volume is equally likely and, therefore, the positioning of the sphere center relative to the observer's starting point is equivalent to randomly selecting a point within a sphere of radius R. Regardless of the nature of the starting point, it is convenient to establish the origin of a Cartesian coordinate system at the point, the only requirement being that the ray through the medium will be taken to correspond to the positive x axis. The task is now to construct the nature of the medium encountered as the observer moves from the origin along the positive x axis.

The first step in the analysis is to obtain the constant probability factor for the sphere-loaded medium analogous to λ of the slab problem presented in Chapter 2. For clarity, this factor will be denoted by λ_s. One wishes to obtain the constant λ_s such that if position $(x,0,0)$ corresponds to matrix, the probability of encountering a particle by advancing to position $(x + \Delta,0,0)$ is $\lambda_s\Delta + o(\Delta)$. Following the same argument presented in section 2.2,

$$\begin{aligned} P(\text{sphere at } x + \Delta) &= P(\text{sphere at } x)P(\text{sphere at } x + \Delta|\text{sphere at } x) \\ &\quad + P(\text{matrix at } x)P(\text{sphere at } x + \Delta|\text{matrix at } x) \;. \end{aligned} \tag{37}$$

Immediately, one recognizes that

$$P(\text{sphere at } x + \Delta|\text{matrix at } x) = \lambda_s\Delta + o(\Delta) \;, \tag{38a}$$

$$P(\text{sphere at } x + \Delta) = P(\text{sphere at } x) = f_p \;, \tag{38b}$$

and

$$P(\text{matrix at } x) = f_m \;. \tag{38c}$$

any position within this spherical volume is equally likely and, therefore, the positioning of the sphere center relative to the observer's starting point is equivalent to randomly selecting a point within a sphere of radius R. Regardless of the nature of the starting point, it is convenient to establish the origin of a Cartesian coordinate system at the point, the only requirement being that the ray through the medium will be taken to correspond to the positive x axis. The task is now to construct the nature of the medium encountered as the observer moves from the origin along the positive x axis.

The first step in the analysis is to obtain the constant probability factor for the spherical-medium system analogous to λ of the sign problem presented in Chapter 2. For clarity, this factor will be denoted by λ_s. One wishes to obtain the constant λ_s such that if position $(x,0,0)$ corresponds to matrix, the probability of encountering a particle by advancing to position $(x + \Delta x,0,0)$ is $\lambda_s \Delta x + o(\Delta x)$. Following the same argument presented in section 2.2,

$$P(\text{absorb at } x + \Delta x) = P(\text{absorb in } \Delta x \mid \text{traverse to } x) \cdot P(\text{traverse to } x)$$

$$+ P(\text{absorb in } \Delta x \mid \text{absorb at } x) \cdot P(\text{absorb at } x) \qquad (37)$$

Immediately, one recognizes that

$$P(\text{absorb at } x + \Delta x \mid \text{traverse to } x) = \lambda_s \Delta x + o(\Delta x) \qquad (38a)$$

$$P(\text{absorb at } x + \Delta x \mid \text{absorb at } x) = 1 \qquad (38b)$$

and

$$P(\text{traverse to } x) = \lambda_s \qquad (38c)$$

The only remaining term in (37) is P(sphere at $x + \Delta |$ sphere at x). To obtain this conditional probability to within $o(\Delta)$, one ignores the possibility of the sphere at $x + \Delta$ being distinct from that sphere at x. With reference to figure 6, it is observed that for position (x,0,0) to lie within a particle, the center of that sphere must be contained within a spherical volume of radius R about this point. Similarly, for position $(x + \Delta,0,0)$ to lie within a particle, the center of that sphere must be contained within a spherical volume of radius R about the point $(x + \Delta,0,0)$. The desired conditional probability is simply the fraction of the volume of the sphere about (x,0,0) corresponding, in a set theory sense, to the intersection of the two spherical regions. An elementary volume integration yields the result that

$$P(\text{sphere at } x + \Delta | \text{sphere at } x) = 1 - \frac{3\Delta}{2D} + o(\Delta) \ , \tag{39}$$

where D = 2R. Employing (38) and (39), one can rewrite equation (37) as

$$f_p = f_p\left(1 - \frac{3\Delta}{2D}\right) + f_m \lambda_s \Delta + o(\Delta) \ . \tag{40}$$

Rearranging and taking the limit as $\Delta \to 0$, one obtains that

$$\lambda_s = \frac{3f_p}{2Df_m} \ . \tag{41}$$

It should be noted that the above analysis yields only the probability of encountering a sphere in moving from matrix position (x,0,0) to position $(x + \Delta,0,0)$. Given that there is such an encounter, it is now desirable to investigate that the location of the center of the encountered particle. Referring to figure 6, it is evident that the

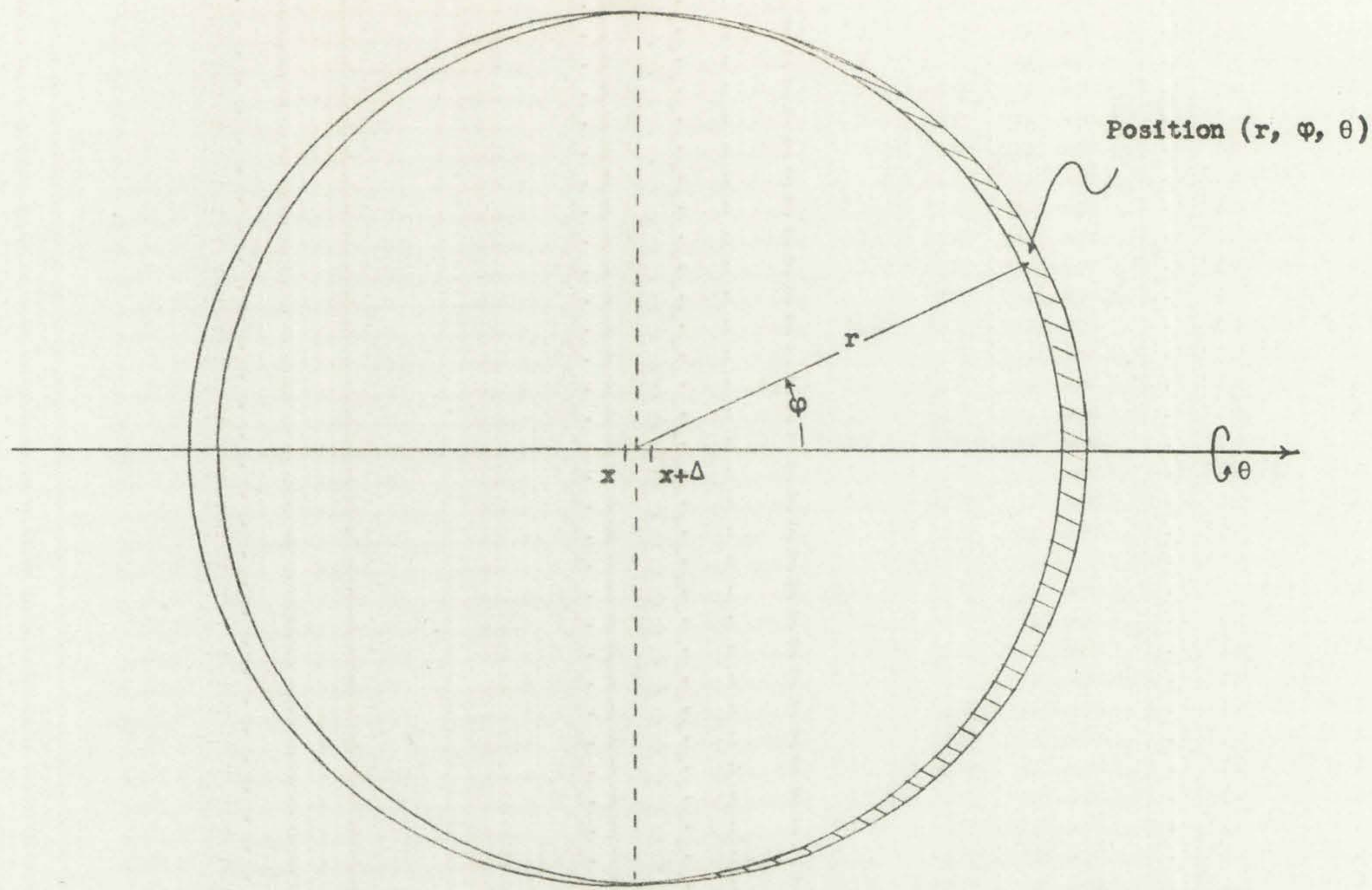

Figure 6. Intersection of Two Spheres

center of the encountered sphere must lie within the shaded volume. Relative to position $(x + \Delta/2,0,0)$, the position of such a sphere center can be described by its spherical coordinates (r,ϕ,θ), as shown in figure 6. From azimuthal symmetry, it is apparent that every value of $\theta \varepsilon [0,2\pi]$ is equally likely. Hence the probability density function $p_\theta(\theta)$ associated with the θ coordinate of the sphere center is simply

$$p_\theta(\theta) = \frac{1}{2\pi} . \tag{42}$$

The next step is to determine the density function associated with the coordinate ϕ. One notes that, by definition for $d\phi > 0$,

$$p_\phi(\phi)d\phi = P\left(\hat{\phi}\varepsilon(\phi,\phi + d\phi)\right) . \tag{43}$$

This probability can be interpreted as the fraction of the shaded volume enclosed by the coordinate surfaces represented by ϕ and $\phi + d\phi$. Performing the implied integration, one obtains

$$p_\phi(\phi) = \sin (2\phi) + o(\Delta) , \tag{44}$$

for $\phi \varepsilon (0,\pi/2)$. In the limit as $\Delta \to 0$, the shaded volume in figure 6 shrinks to a hemispherical surface upon which the center of the encountered sphere is constrained to lie. With this, the positioning of the sphere center is completely specified by the density functions associated with the θ and ϕ coordinates, namely

$$p_\theta(\theta) = \frac{1}{2\pi} \tag{45a}$$

and

$$p_\phi(\phi) = \sin (2\phi) . \tag{45b}$$

It should be noted that, so far in this section, it has been tacitly assumed that the observer is unaware of any previously established spheres which might interfere with the one encountered and then positioned. Before examining such interference effects, it is convenient to present an example of the implementation of the results obtained to this point. Assume that an observer is initially at a starting point within matrix material. He then begins to travel along the positive x-axis through the matrix until he encounters a sphere. The problem is to determine the probability that he advances a distance x without such an encounter. If one denotes this probability as P(x), then

$$P(x + \Delta) = P(x)(1 - \lambda_s\Delta) + o(\Delta) \quad . \tag{46}$$

Passing to the limit as $\Delta \to 0$, one obtains the differential equation

$$\frac{dP}{dx} = -\lambda_s P \quad . \tag{47}$$

Also, the probability of making no encounter in advancing a distance $x = 0$ is unity or $P(0) = 1$. Therefore, the solution to (47) is

$$P(x) = \exp(-\lambda_s x) \quad . \tag{48}$$

Note that equation (48) is identical to the behavior of the attenuation of a beam of radiation in a purely absorbing medium of cross section λ_s. Hence statistical samples of the distance traveled by such an observer prior to his first sphere encounter, can be constructed in a Monte Carlo fashion equivalent to sampling path lengths of a transport particle in a purely absorbing medium. Once this distance has been sampled, the placement of the encountered sphere can be completed by employing (45) in a Monte Carlo fashion.

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In order to treat the interference effects mentioned earlier, it is noted that a previously positioned sphere may preclude establishment of a new sphere center within part or all of the shaded volume in figure 6. This implies both a local reduction in the value of λ_s and a modification of the density functions in equation (45). An analytic treatment of the above effect for arbitrary interference from one or more previously established spheres would present a tedious and time-consuming task, even in light of the implied numerical treatment of the problem.

Fortunately, there is an alternate approach to the problem. This is best demonstrated by considering the transport problem of a beam of radiation in a purely absorbing material of cross section $\Sigma(x)$. Suppose $\Sigma(x)$ assumes a maximum value which will be denoted by Σ_{mx}. The differential equation governing the transmission $T(x)$ through such a material is given by

$$\frac{dT}{dx} = -\Sigma(x)T \tag{49}$$

with

$$T(0) = 1 .$$

Now, suppose one defines a parameter $\gamma(x)$ to be

$$\gamma(x) = 1 - \frac{\Sigma(x)}{\Sigma_{mx}} . \tag{50}$$

Employing (50), one can rewrite equation (49) in the form

$$\frac{dT}{dx} + \Sigma_{mx}T = \Sigma_{mx}\gamma(x)T \tag{51}$$

with T(0) = 1. The problem is now simply a matter of interpretation. One notes that $\gamma(x)\varepsilon[0,1]$. Equation (51) is equivalent to a transport problem in a medium having a constant total interaction cross section equal to Σ_{mx} but with a variable forward scattering coefficient given by $\gamma(x)$, [12]. In a Monte Carlo sense, the problem would be treated by choosing transport path lengths based upon the cross section Σ_{mx}. A random number could then be selected and, if less than $\gamma(x)$, the transport particle would be allowed to continue. If the random number was greater than $\gamma(x)$, the transport particle would experience an absorption event.

An interpretation similar to the one above can be applied to the problem of placing spheres when interference effects are present. The distance to the next sphere encounter is sampled as if no interference effects were present and hence is simply based on the constant factor λ_s. Actually, the effective λ_s may be reduced by interference corresponding to $\Sigma(x) < \Sigma_{mx}$ in the above problem. The process of selecting a random number and comparing it to $\gamma(x)$ to decide the fate of the transport particle in the previous problem has an interesting analogy in the case of sphere placement. Having chosen the point at which a sphere encounter occurs, one places the sphere by using relation (45). One then checks the validity of such a sphere placement in relation to previously established spheres. If there is no interference, then a valid sphere has been established which corresponds to an abosrption event in the transport problem. If there is interference, then the placement is not valid and the position at which the encounter would have occurred, becomes the starting point for sampling the distance to the next trial sphere encounter.

$a_i(a) = 1$. The problem is now simply a question of finding the point where V(a) [illegible] equation (26) [illegible] problem is a vector having a constant [illegible] equal to λ_{tr} and total velocity [illegible] to (18), (19). In a Monte Carlo sense, the problem [illegible] by choosing [illegible] path lengths based upon [illegible] generated. A random number could then be selected and, if less than [illegible], the transport particle would be allowed to continue. If the number was greater than [illegible], the transport particle [illegible] an absorption event.

An interpretation similar to the one above can be applied to the [illegible] of [illegible] fields are [illegible]. The [illegible] is [illegible] leakage effects were present and hence is simply [illegible] factor λ_a. Actually, the effective λ_a may be [illegible] corresponding to [illegible] λ_{tr}. In the above problem, the process of selecting a random number and comparing it to [illegible] to decide the fate of the transport particle in the previous problem may be [illegible] applied in the case of albedo placement. Having chosen [illegible] where a source [illegible] occurs, the [illegible] equation [illegible]. One then checks the validity of such a [illegible] placement in relation to previously established [illegible]. If there is no interference, then a valid albedo has been established which corresponds to an absorption event in the transport problem. If there is interference, then the placement is not valid and [illegible] which the [illegible] would have occurred, [illegible] for [illegible] the distance to the next trial albedo placement.

4.3 Implementation of Theory of Sphere Placement

In this section, three methods are presented that employ the concepts developed in the previous section to obtain the average transmission of a purely absorbing spherical particle-loaded shield. With reference to section 2.6 it should be noted that if one can obtain results for the average transmission, then one can also compute the results for the average of higher moments of the transmission.

The Direct Method

Suppose one desires to compute the average transmission of a shield of thickness x of such a particle-loaded material. Using the techniques developed in the previous section in a Monte Carlo fashion, one can construct a sample cross section profile along one ray through the medium. Let this construction be performed and the result denoted by $\Sigma_i(y)$, $y \varepsilon [0,x]$. Since the problem is restricted to pure absorption, one can compute the transmission $T_i(x)$ associated with the i^{th} sample as simply

$$T_i(x) = \exp\left(-\int_0^x \Sigma_i(y)\, dy\right) . \tag{52}$$

This procedure is then repeated for a large number I of sample paths through the medium. The average transmission T(x) is then computed as

$$T(x) \simeq \frac{\sum_{i=1}^{I} T_i(x)}{I} . \tag{53}$$

A subtle, but important, point to note is that one sample corresponds to a single ray through a shield of thickness x. Each

Implementation of [illegible]

In this section, three methods are presented that employ the results developed in the previous section to obtain the average transmission of a purely absorbing spherical particle-loaded material. With reference to section [illegible], it should be noted that if one can obtain results for the average transmission, then one can also compute the results for the averages of higher moments of the transmission.

The Direct Method

Suppose one desires to compute the average transmission of a plate of thickness x of such a particle-loaded material. Using the techniques developed in the previous section in a Monte Carlo fashion, one can construct a sample cross section profile along the ray through the medium. Let this construction be performed and the result denoted by $\Sigma_t(x)$, $x_0 \le x \le x_1$. Since the problem is restricted to pure absorption, one can compute the transmission $T_i(x)$ associated with the ith sample as simply

$$T_i(x) = \exp\left(-\int_0^x \Sigma_t(x')\,dx'\right) . \qquad (52)$$

This procedure is then repeated for a large number I of sample paths through the medium. The average transmission T(x) is then computed as

$$T(x) = \frac{\sum_{i=1}^{I} T_i(x)}{I} . \qquad (53)$$

A subtle, but important, point to note is that the sample transmittance of a single ray through a region of thickness x, with sample refers to a distinct shield so that once $T_i(x)$ has been computed for $\Sigma_i(y)$, $y\varepsilon[0,x]$, only $T_i(x)$ must be stored. In other words, each sample can be constructed independently. This is an important consideration relative to machine memory requirements.

The Double Monte Carlo Method

In the Double Monte Carlo method, one constructs a sample ray specified by $\Sigma_i(y)$, $y\varepsilon[0,x]$. Rather than computing the transmission $T_i(x)$ associated with this ray explicitly by using (52), however, one uses a Monte Carlo scheme to estimate $T_i(x)$.

Define J as the total number of source transport particles to be employed in estimating $T_i(x)$. Of the J source particles, let n_i denote the number of these source particles which penetrate a distance x into the shield along the path defined by $\Sigma_i(y)$, $y\varepsilon[0,x]$. Then $T_i(x)$ is estimated to be

$$T_i(x) \simeq \frac{n_i}{J} \; . \tag{54}$$

If the procedure is continued for I samples, the average transmission is given by

$$T(x) \simeq \frac{\sum_{i=1}^{I} T_i(x)}{I} \simeq \frac{\sum_{i=1}^{I} n_i}{IJ} \; . \tag{55}$$

Note that the product IJ is simply the total number of source transport particles. The sum $\sum_{i=1}^{I} n_i$ is the total number of particles penetrating a thickness x. The implication is that an accurate estimate of T(x) is dependent only on the product IJ. Therefore, it is

extremely convenient and acceptable to choose $J = 1$. This enables one to construct the sample of particle-loaded media and the path length of the transport particle simultaneously. Construction of the medium can often be terminated prior to position $y = x$ if the transport particle experiences an absorption event within the shield. In addition, at any position y, previously placed spheres whose centers lie to the left of position $y - D$ cannot affect the possibility of a new sphere encounter. Hence one must remember only a minimum amount of data describing the previously constructed medium along the ray.

The Perturbation Method

The Perturbation method employs the basic ideas presented in the Double Monte Carlo method in that both medium and the trajectory of the transport particle are constructed with Monte Carlo techniques. The difference is that in the previous method transport path lengths are sampled at position y based on either Σ_m or Σ_p, dependent upon whether position y corresponds to matrix or particle. In the perturbation approach, transport path lengths are sampled as if the medium were homogeneous, having a cross section equal to the larger of Σ_m and Σ_p. The pertinent concept follows immediately from the result obtained in equation (51), which pertained to an absorption problem in a medium of arbitrary cross section $\Sigma(y) \leq \Sigma_{mx}$.

Recalling (51), one can write

$$\frac{dT}{dy} + \Sigma_{mx} T = \Sigma_{mx} \gamma(y) T \ , \tag{56}$$

with $T(0) = 1$ and

$$\gamma(y) = 1 - \frac{\Sigma(y)}{\Sigma_{mx}} \ . \tag{57}$$

For present purposes, one can assume $\Sigma_p > \Sigma_m$. Then, for one sample of the particle-loaded medium characterized by $\Sigma_i(y)$, $y\varepsilon[0,x]$,

$$\Sigma_i(y) = \Sigma_p - (\Sigma_p - \Sigma_m)F_i(y) \ , \tag{58}$$

where $F_i(y) = 0$ if position y corresponds to particle and $F_i(y) = 1$ if position y corresponds to matrix. Combining (56), (57), and (58), one obtains

$$\frac{dT_i(y)}{dy} + \Sigma_p T_i = \Sigma_p \gamma_i(y) T_i \ , \tag{59}$$

with $T_i(0) = 1$ and

$$\gamma_i(y) = \frac{\Sigma_p - \Sigma_m}{\Sigma_p} F_i(y) \ . \tag{60}$$

Thus, for the problem in which the particles are better absorbers than the matrix, one again constructs path lengths of the transport particle and the sample of the medium simultaneously. However, transport path lengths are always based upon Σ_p. The position corresponding to the terminus of a path length is then compared to the medium sample. If this position corresponds to a particle, the transport particle dies in that it experiences an absorption event. If not, the position corresponds to matrix and the probability of the transport particle being scattered forward is simply $(1 - \Sigma_m/\Sigma_p)$, while the probability of an absorption event is Σ_m/Σ_p. The case in which $\Sigma_m > \Sigma_p$ can be treated by merely interchanging Σ_m and Σ_p, and conversely. The method described is termed a perturbation approach, since the contribution to $T_i(y)$ from particles having experienced j collisions corresponds to the j^{th} term of a perturbation expansion of $T_i(y)$ about

the homogeneous problem associated with the material having the larger cross section. Note that because of the physical interpretation, one is guaranteed that the perturbation scheme will converge to the desired solution.

At this point, it is convenient to compare the three techniques presented. The first has the advantage that full use can be made of each constructed sample of the medium in the sense that the associated transmission is explicitly calculated for this sample. Its chief disadvantage is the fact that one is using the knowledge of the analytic form of the solution which, for more complex problems, may not be available. The Double Monte Carlo scheme has the advantage that no such use of an analytic result is employed, and transport path lengths based upon the true medium are sampled. Its main disadvantage is that the transport calculations are strongly coupled to the constructed medium. In the context here, this means that the complete nature of the cross sectional variation along a ray must be taken into consideration in order to determine the history of a transport particle. In the perturbation scheme this is not required. The history of the transport particle is dependent only upon the nature of the constructed medium at those points at which the particle experiences collisions. Further, this method makes no use of the analytic form of the solution but only of the structure of the governing differential equation. The chief disadvantage of the perturbation approach occurs when, for example, the particle cross section is much greater than the matrix cross section and the particle loading is sparse. In this situation, the transport particle literally creeps through the medium, having an enormous number of collisions while surviving the vast majority of them. Hence, obtaining transmission

estimates for all but very thin shields $\left(x \sim \frac{1}{\Sigma_P}\right)$ can be a very time-consuming process.

4.4 Validity of the Random Assumption

This section presents an evaluation of the validity of the random placement of sphere centers. It should be noted that the validity of such an assumption is dependent only upon the volume fraction of the spheres. The size of the spheres is irrelevant, since one can always choose a distance scale based upon one sphere diameter. The procedure used to obtain an estimate of the validity of the random placement approach is straightforward. Using the results of section 4.2 one constructs many samples of rays of length x through a particle-loaded medium based on a specified loading fraction f_p. Arbitrarily, particles are taken to have a unit diameter.

Based upon these samples, one computes the fraction of the total length of constructed medium that lies within particle and defines this fraction as $\hat{f}_p$. If the construction were completely valid, one would obtain $\hat{f}_p = f_p$ in the limit of many samples. Departure from equality gives one a convenient estimate of the degree of validity of the construction technique. If such a scheme is carried out, it is found that $\hat{f}_p$ is dependent upon the sample distance x. Calculations show that, as x approaches zero, $\hat{f}_p$ approaches f_p. This is simply a result of the correct manner by which the nature of the initial point is sampled. As x increases, $\hat{f}_p$ decreases until it attains an asymptotic value characteristic of the random placement assumption. Computational results of these asymptotic values of $\hat{f}_p$ versus f_p are presented in figure 7. From the data presented in figure 7, one can estimate the percent error in f_p due to the assumption estimates for all but very thin samples (x — $\left(\frac{}{}\right)$ — [illegible] be a very thin [illegible]).

3.4 Validity of the Random Assumption

This section presents an evaluation of the validity of the random placement of sphere centers. It should be noted that the validity of such an assumption is dependent only upon the volume fraction of the spheres. The size of the spheres is irrelevant, since one can always choose a distance scale based upon the sphere diameter. The procedure used to obtain an estimate of the validity of the random placement approach is straightforward. Using the results of section 3.1 one constructs many samples of rays of length L through a particle-laden medium based on a specified loading fraction f_v, arbitrarily, particles are taken to have a unit diameter.

Based upon these samples, one computes the fraction of the total length of constructed rays that lies within particle and defines this fraction as f_v'. If the construction were completely valid, one would obtain $f_v' = f_v$ in the limit of many samples. Departure from equality gives a quantitative estimate of the degree of validity of the construction procedure. If such a scheme is carried out, it is found that f_v' is dependent upon the sample distance L. Calculations show that, as L approaches zero, f_v' approaches f_v. This is simply a result of the correct manner by which the nature of the initial point is handled. As L increases, f_v' decreases until it attains an asymptotic value characteristic of the random placement assumption. Characteristic results of these asymptotic values of f_v' versus f_v are presented in Figure 17. From the data presented in Figure 17, one can estimate the percent error in f_v due to the assumption

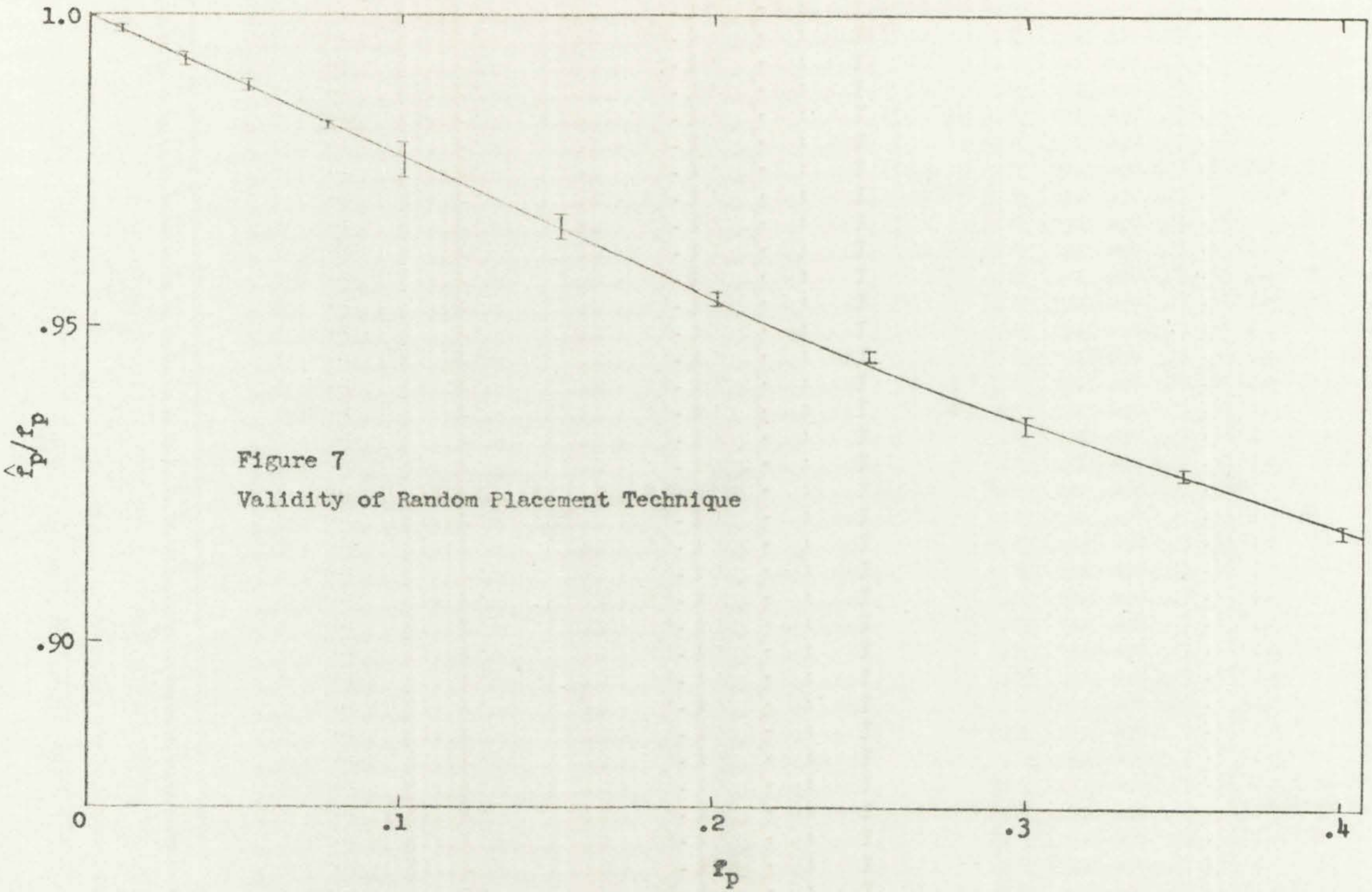


Figure 7
Validity of Random Placement Technique

of random sphere placement. A convenient rule of thumb is that

$$\% \text{ error} \equiv \frac{f_p - \hat{f}_p}{f_p} \cdot 100 \simeq +25 f_p . \tag{61}$$

Hence if one employs random sphere placement in a medium composed of 5 volume percent of spheres, the associated error in f_p will be

$$\% \text{ error} \simeq 25 (0.05) = 1.25 . \tag{62}$$

The precise effect of such errors on transmission calculations is not clear. Qualitatively, however, one can argue that such errors become more important as the difference in particle and matrix cross section increases. Also, in the case in which the particles are the more efficient absorbers, the error is such that one will overestimate the transmission, a convenient behavior from a safety standpoint. The desirability of applying this approach for various loading fractions will be discussed in Chapter 6.

4.5 Discussion of Computational Results

Figures 8 through 11 present computational results for various particle loadings and particle diameters. For the case $\Sigma_p > \Sigma_m$, the matrix is taken to be transparent and the particles taken to have cross section $\Sigma_p - \Sigma_m$. Thus the true attenuation at position x is lower than that plotted by the factor $\exp(-\Sigma_m x)$. Similarly, for the case $\Sigma_m > \Sigma_p$, the particles are taken to be transparent and the matrix to have a cross section $\Sigma_m - \Sigma_p$. The results are very similar in character to those obtained in the model slab problem.

For very thin shields, the average transmission decreases exponentially with the cross section of the homogeneous mix of particles

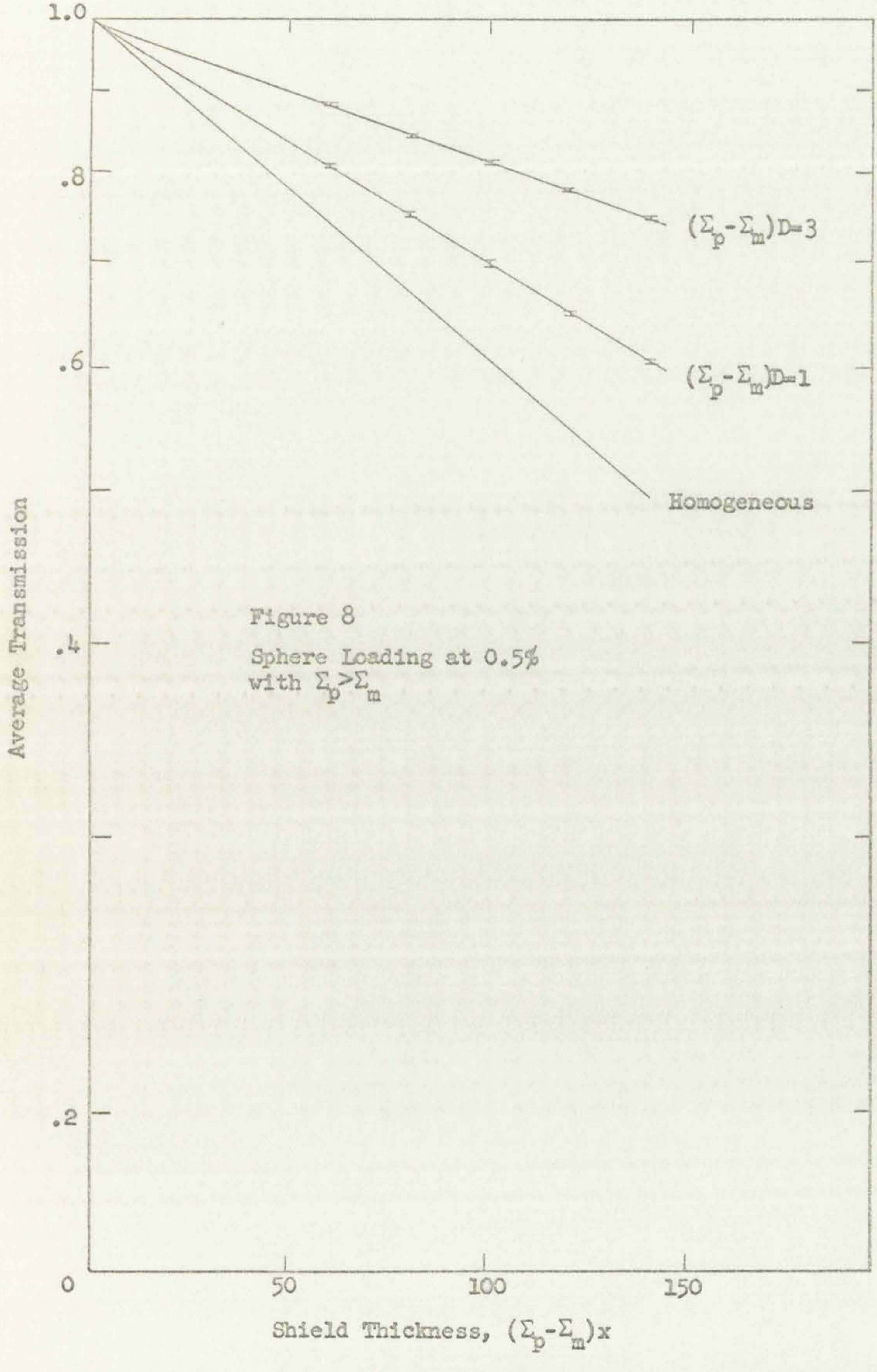


Figure 8

Sphere Loading at 0.5% with $\Sigma_p>\Sigma_m$

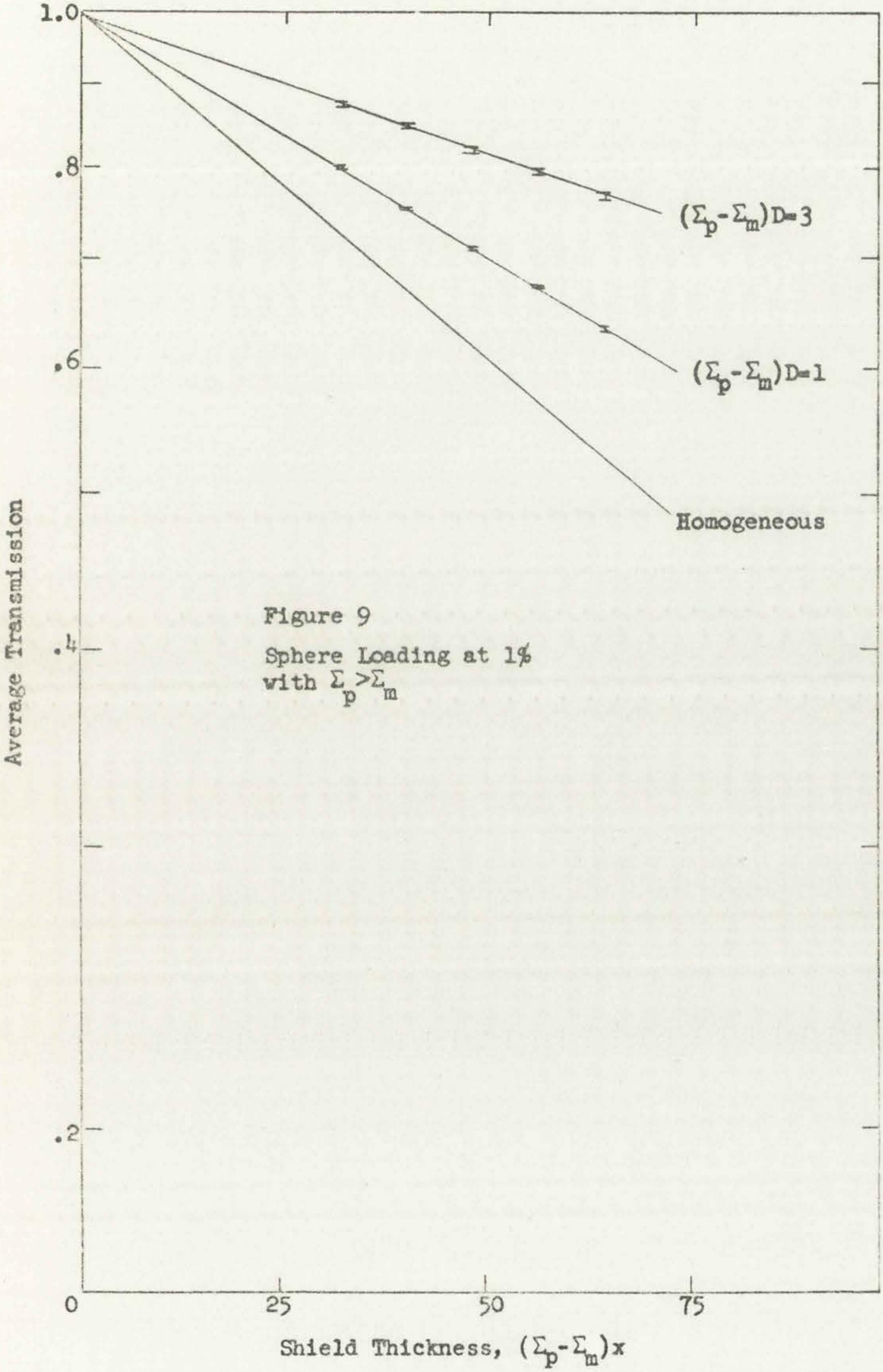
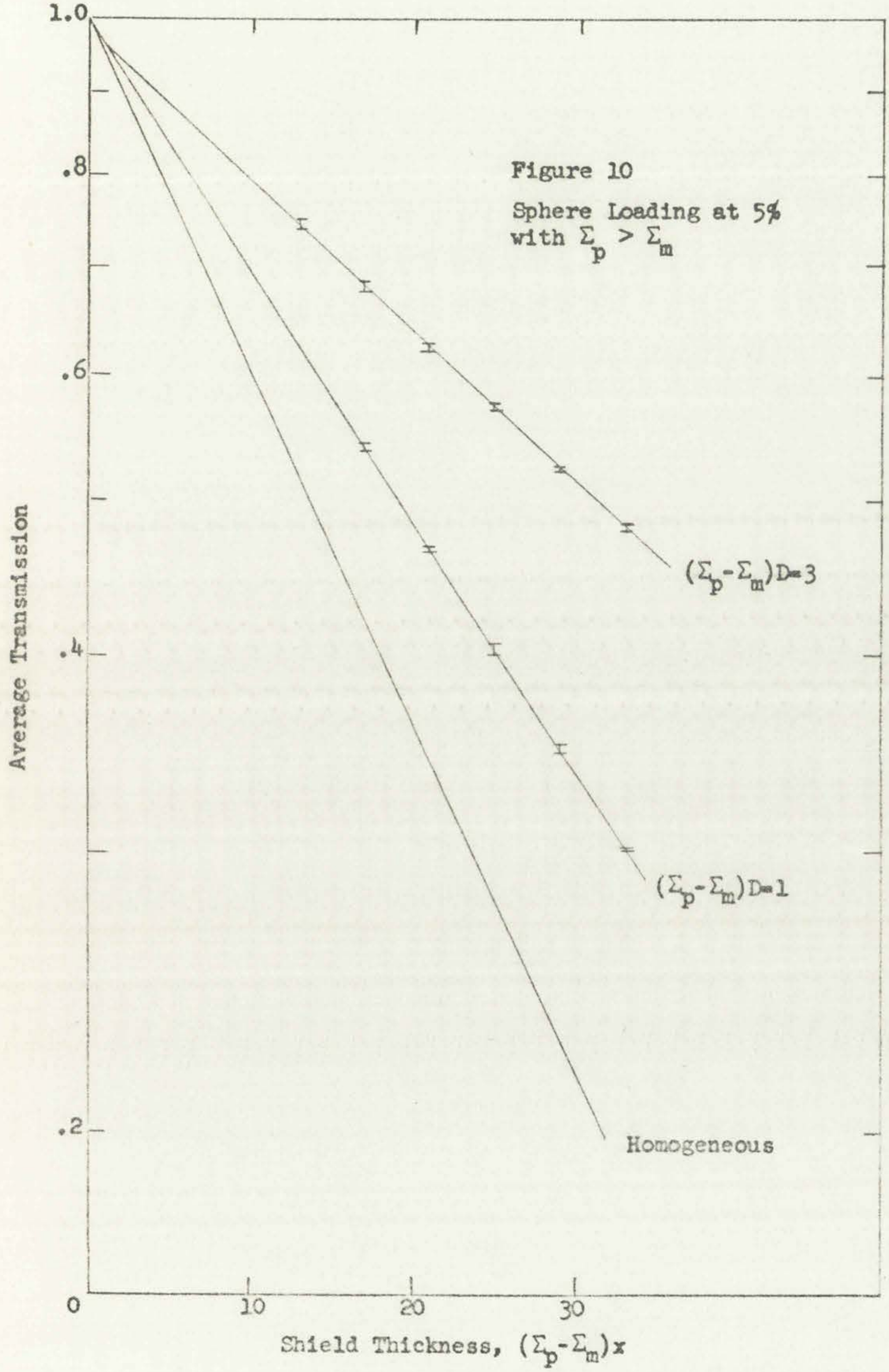


Figure 9

Sphere Loading at 1% with $\Sigma_p > \Sigma_m$


1.0
.8
.6
.4
.2
0
10
20
30
Average Transmission
Shield Thickness, $(\Sigma_p-\Sigma_m)x$
Figure 10
Sphere Loading at 5%
with $\Sigma_p > \Sigma_m$
$(\Sigma_p-\Sigma_m)D=3$
$(\Sigma_p-\Sigma_m)D=1$
Homogeneous

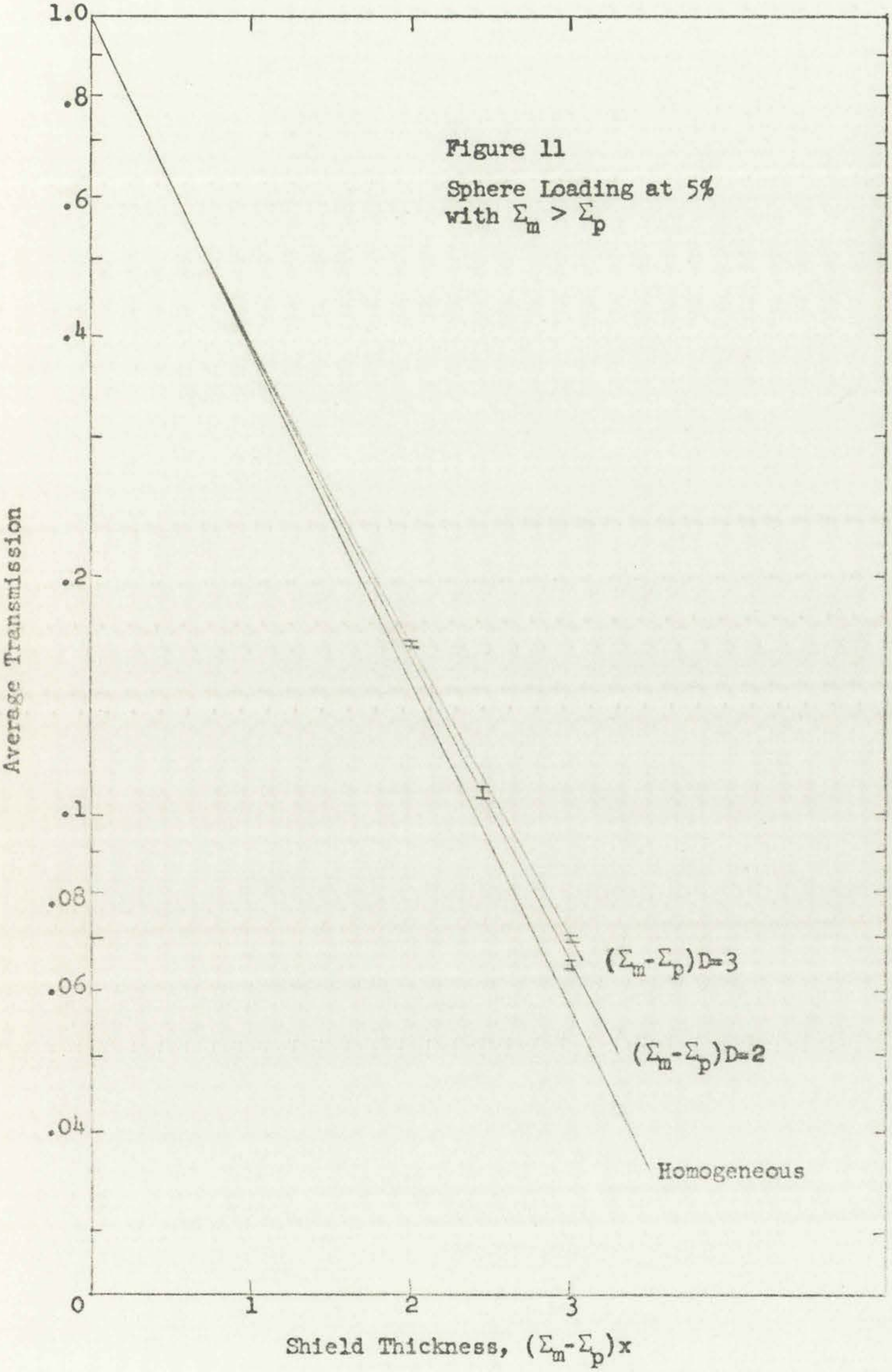


Figure 11
Sphere Loading at 5%
with $\Sigma_m > \Sigma_p$
1.0
.8
.6
.4
.2
.1
.08
.06
.04
0
1
2
3
Average Transmission
Shield Thickness, $(\Sigma_m-\Sigma_p)x$
$(\Sigma_m-\Sigma_p)D=3$
$(\Sigma_m-\Sigma_p)D=2$
Homogeneous

and matrix. For shields thicker than several particle diameters, the average transmission decreases exponentially with a cross section characteristic of the statistical nature of the material. Between these two extremes is a transition region in which the behavior begins to approach the asymptotic behavior. Again, the most important observation is how severely the solution corresponding to a homogeneous mixture underestimates the transmission. The computations presented were obtained by using the direct method presented in section 4.3. However, it has been verified that the remaining procedures give identical results.

4.6 Summary of Random Treatment

In this chapter a random approximation to the sphere problem has been investigated and evaluated. It is apparent that in the limit of low loadings an exact treatment is obtained. The computational schemes are all based upon the Monte Carlo method, and all have the advantages that the only portion of the medium to be constructed is that portion which an observer moving with a transport particle experiences. The behavior of the average transmission with shield thickness was found to behave qualitatively in the same manner as one would expect from the slab problem presented in Chapter 2. Computational time for a general problem is difficult to specify, being quite dependent upon which method in section 4.3 is employed. However, except for the perturbation technique, a reasonable description of the solution to a problem requires something like five minutes on a CDC 6600. As pointed out before, the efficiency of the perturbation technique depends strongly on the nature of the problem. For some problems this technique is competitive with the others but if the method. For example, [illegible] the various [illegible] characteristics of the [illegible] these [illegible] to [illegible] the asymptotic [illegible]. [illegible] behavior is not exactly the [illegible] [illegible]. The [illegible] were obtained by using the direct method [illegible]. However, it has been verified that the [illegible] identical results.

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CHAPTER 5 Relaxation of FCC Lattice and the Sphere Problem

5.1 Introduction

In Chapter 4, a technique of performing transport calculations in a medium consisting of a matrix loaded with spherical particles was investigated. The chief disadvantage of this technique is that as the loading increases the inherent assumptions become progressively worse. Also, with the scarce amount of available experimental data, it is difficult to evaluate the acceptability of this technique at relatively high loadings. In this chapter, a completely different approach to modeling the medium will be investigated. The only justification for this approach is that it preserves some of the character of the true problem and is computationally convenient. An evaluation of this technique is made with respect to both available data and the random placement technique. There are two lattice structures which permit maximum packing of constant radius spheres. These are known as hexagonal close packed and face-centered cubic (FCC). Because of the relative geometric simplicity of the latter, it is computationally more convenient to choose a model based upon this structure. The basic idea in this chapter is, then, to relax a rigid FCC structure of spheres in such a way that a certain degree of randomness is introduced into this artificial medium.

5.2 Theory of Relaxation

The purpose of this section is to present the technique of random relaxation of an FCC lattice and its implementation as applied to particle transport. For an FCC unit cell at maximum packing, the relation between the lattice parameter a and the sphere radius R at

CHAPTER 5. Randomized FCC Lattice and the "Pure" Problem

5.1 Introduction

In Chapter 4, a technique of performing transport calculations in a medium consisting of a matrix loaded with spherical particles was investigated. The major disadvantage of this technique is that as the loading increases the inherent assumptions become progressively worse. Also, with the scarce amount of available experimental data, it is difficult to evaluate the acceptability of this technique at relatively high loadings. In this chapter, a completely different approach to modeling the medium will be investigated. The only justification for this approach is that it preserves some of the character of the true problem and is computationally convenient. An evaluation of this technique is made with respect to both available data and the random placement technique. There are two lattice structures which permit maximum packing of constant radius spheres. These are known as hexagonal close packed and face-centered cubic (FCC). Because of the relative geometric simplicity of the latter, it is computationally more convenient to choose a model based upon this structure. The basic idea that permits this is, then, to relax a rigid FCC structure of spheres in such a way that a certain degree of randomness is introduced into this artificial medium.

5.2 Theory of Randomization

The purpose of this section is to present the technique of random relaxation of an FCC lattice and its implementation as applied to particle transport. For an FCC unit cell at maximum packing, the relation between the lattice parameter a and the sphere radius R is maximum packing [10] is given by

$$a = 4R/\sqrt{2} \ . \tag{63}$$

For this configuration, the volume fraction of the unit cell occupied by sphere material is roughly 0.74. The first step in the relaxation process is to expand the dimensions of the unit cell to a value $\hat{a}$, which results in a volume fraction of sphere material corresponding to f_p of the loaded material. The desired value of $\hat{a}$ satisfies the relation

$$\hat{a} = \left(\frac{16\pi}{3f_p}\right)^{1/3} R \ . \tag{64}$$

The next step is to allow the sphere centers to drift about these rigid lattice sites. The governing criterion for this process is that any one sphere is restricted to lie within an assigned volume about its rigid lattice site, and thereby the mechanism for relaxation precludes the interpenetration of two neighboring spheres. Therefore, to maximize the degree of relaxation, one concludes that the spheres are restricted to lie within an artificial spherical volume about their respective lattice sites, having radius $\hat{R}$ given by

$$\hat{R} = \sqrt{2}\ \hat{a}/4 \ . \tag{65}$$

Radius $\hat{R}$ corresponds to the radius of that sphere which would result in maximum packing of the unit cell having lattice parameter $\hat{a}$. If the sphere of radius R is to remain within a spherical volume of radius $\hat{R}$, it follows that the sphere center is contained to lie within a third spherical volume of radius $R^* = \hat{R} - R$. Basically, the above concepts fully describe the FCC relaxation scheme.

The procedure for constructing a ray through this pseudorandom medium is now straightforward. First, a starting point must be selected. Since every point within the medium corresponds to a point within a unit cell, this simply amounts to randomly selecting a point within a unit cell. If this point does not lie with a radius $\hat{R}$ of the lattice sites, the point must lie within matrix. If the point does lie within a radius $\hat{R}$ of a lattice site, the sphere corresponding to that site is placed by randomly selecting the coordinates of its center from within a region of radius R* about the lattice site. Whether the starting point lies within particle or matrix is thereby determined. Once the starting point has been selected, the direction of the ray in relation to the lattice structure must be decided. This amounts to randomly selecting a point on the surface of a unit sphere and hence the random selection of a unit vector relative to the lattice. As one then progresses along the ray from the initial point, the medium is completely specified until one enters a subsequent region of radius $\hat{R}$ about a new lattice site. This occurrence requires an additional sphere placement. The procedure is continued in similar fashion along the entire required ray length.

5.3 Implementation of this Theory

Although it is completely feasible to construct entire rays using the model described in section 5.2, actual calculations employing this model have been restricted to the perturbation approach. For this approach only the nature of the medium at the location of transport particle interactions must be determined. Since interactions always occur with a unit cell, the coding of this approach is simple. Because of the nature of the model, as a ray exits from a spherical region of

radius $\hat{R}$ about a lattice site, there is no mechanism to return to this region, and hence memory of the placement of the corresponding sphere is no longer required. If one desires to employ this model on a production basis, the author recommends that the effort be taken to implement the Double Monte Carlo Method referred to in section 4.3. This recommendation is based on the inefficiency of the perturbation approach for a large class of interesting problems as previously discussed in section 4.3.

5.4 Validity of the FCC Relaxation Technique

Evaluation of the accuracy of this technique must rely completely upon the extent of agreement with experimental data. It is recognized that a rather crude model of a complex physical problem has been presented. The model does duplicate the required loading fraction and enables one to perform calculations for any attainable packing density. Again, in the case in which the particles are better absorbers than the matrix, one will obtain an upper bound on the transmission by using this model. The argument leading to this conclusion is based on the fact that the structure of this model is much greater than the truly random structure, and hence the probability of obtaining matrix paths through this model medium will be greater.

5.5 Discussion of Computational Results

Figures 12 through 15 present computational results for various particle loadings and particle thickness. Results are presented in the same manner as those described in section 4.5. Again, it is noted that the results are qualitatively identical to those obtained both for the slab problem and for the random sphere placement problem. For thin shields, the average transmission decreases exponentially

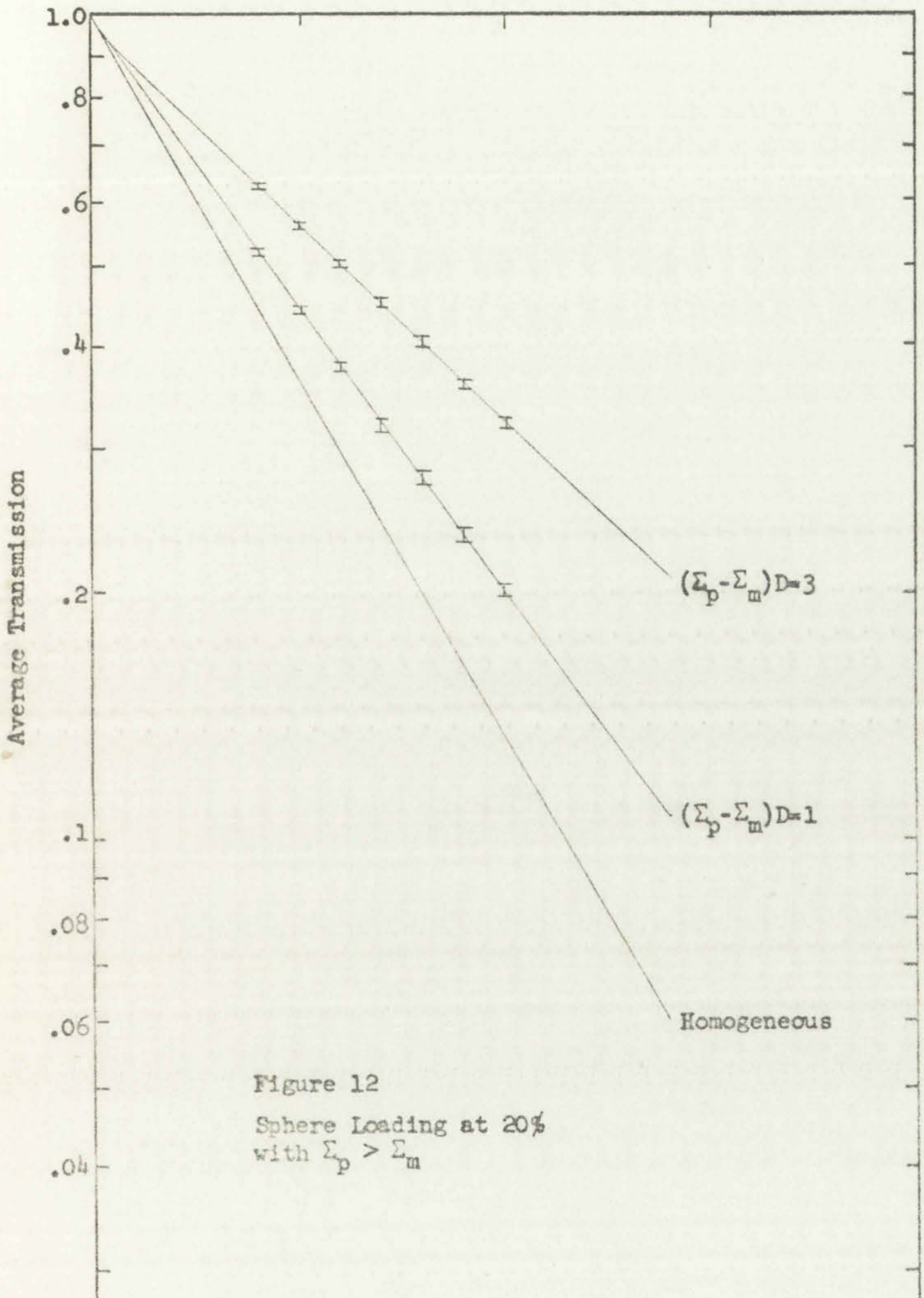


Figure 12

Sphere Loading at 20%
with $\Sigma_p > \Sigma_m$

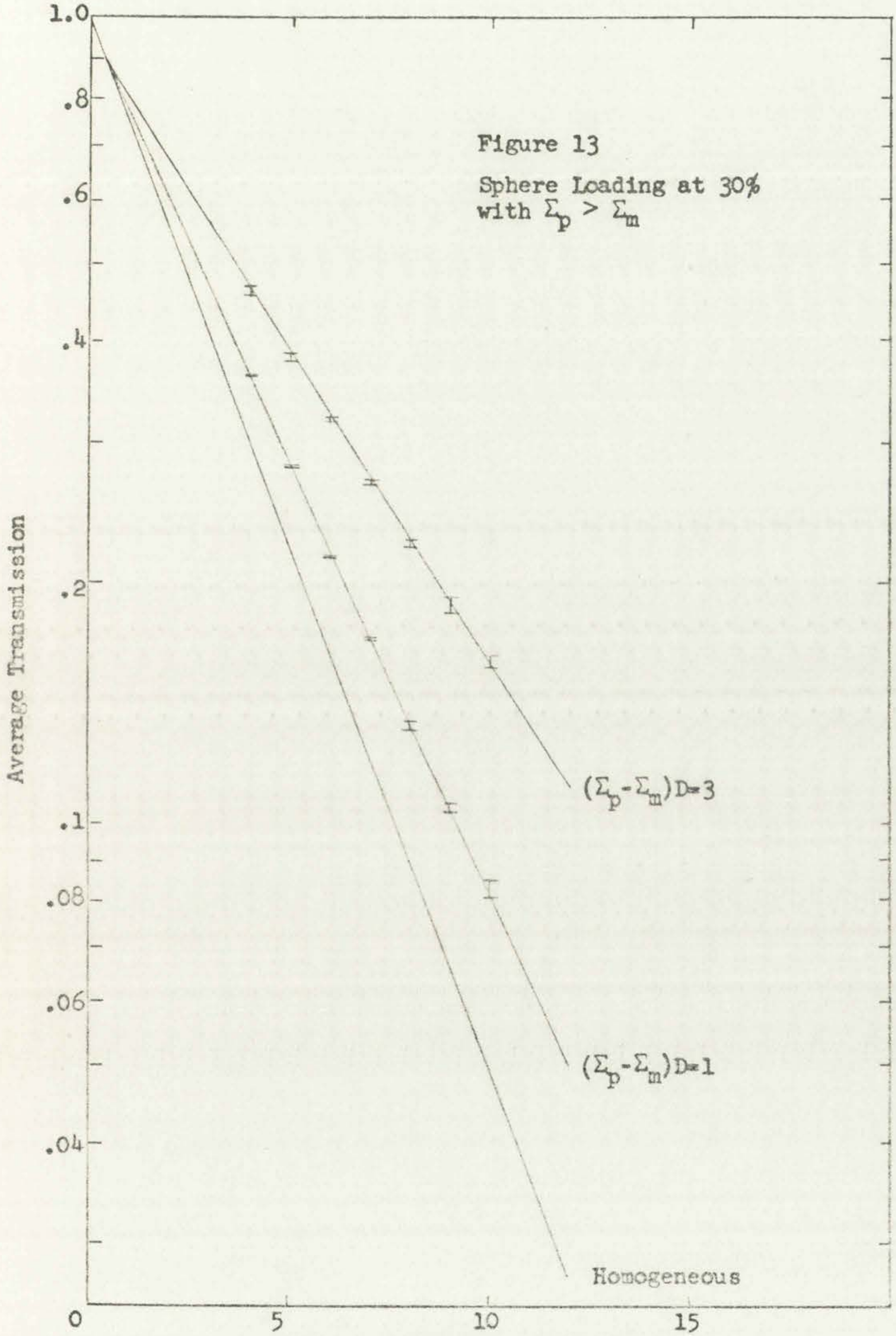


Figure 13
Sphere Loading at 30%
with $\Sigma_p > \Sigma_m$
1.0
.8
.6
.4
.2
.1
.08
.06
.04
0
5
10
15
Average Transmission
Shield Thickness, $(\Sigma_p-\Sigma_m)x$
$(\Sigma_p-\Sigma_m)D=3$
$(\Sigma_p-\Sigma_m)D=1$
Homogeneous

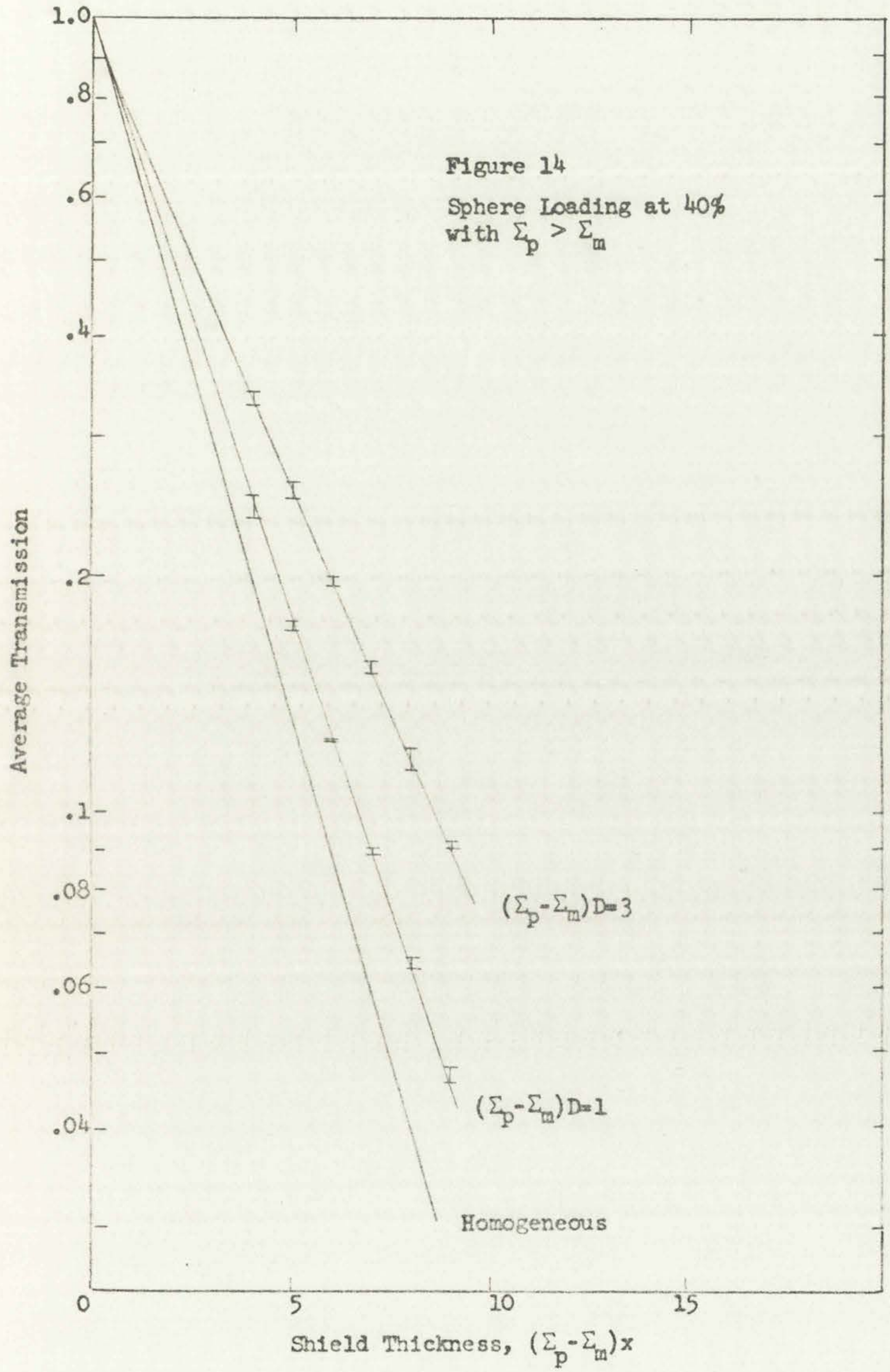


Figure 14
Sphere Loading at 40%
with $\Sigma_p > \Sigma_m$
1.0
.8
.6
.4
.2
.1
.08
.06
.04
Average Transmission
$(\Sigma_p-\Sigma_m)D=3$
$(\Sigma_p-\Sigma_m)D=1$
Homogeneous
0
5
10
15
Shield Thickness, $(\Sigma_p-\Sigma_m)x$

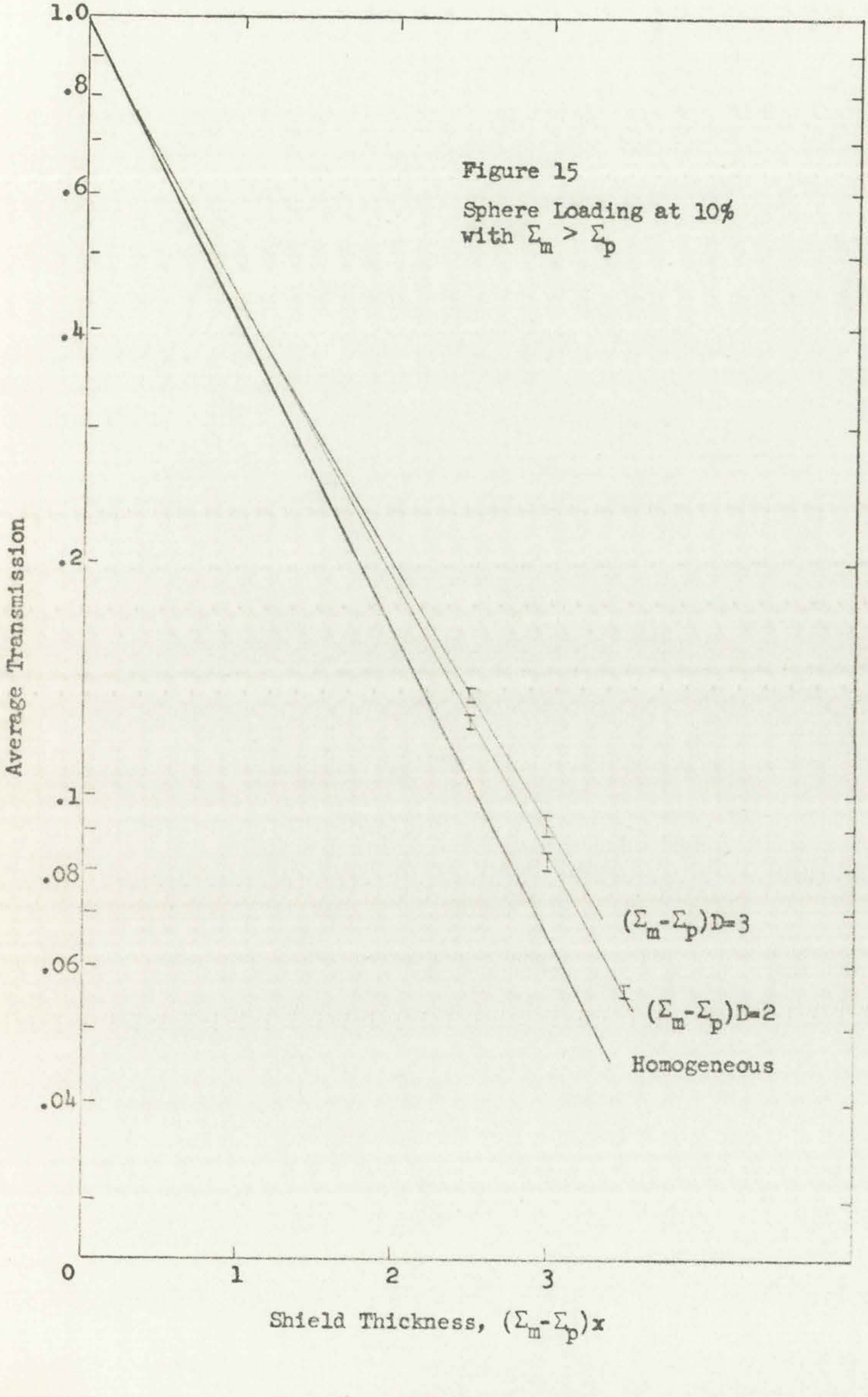


Figure 15

Sphere Loading at 10% with $\Sigma_m > \Sigma_p$

with the cross section corresponding to a homogeneous mix of particles and matrix. A transition region follows in which the transmission begins to take on an asymptotic behavior. Several particle diameters into the shield, the average transmission is seen to acquire an asymptotic behavior decreasing exponentially with a cross section characteristic of the statistical nature of the medium. At high particle loadings, the difference between the statistical treatment and the homogeneous assumption is dramatic.

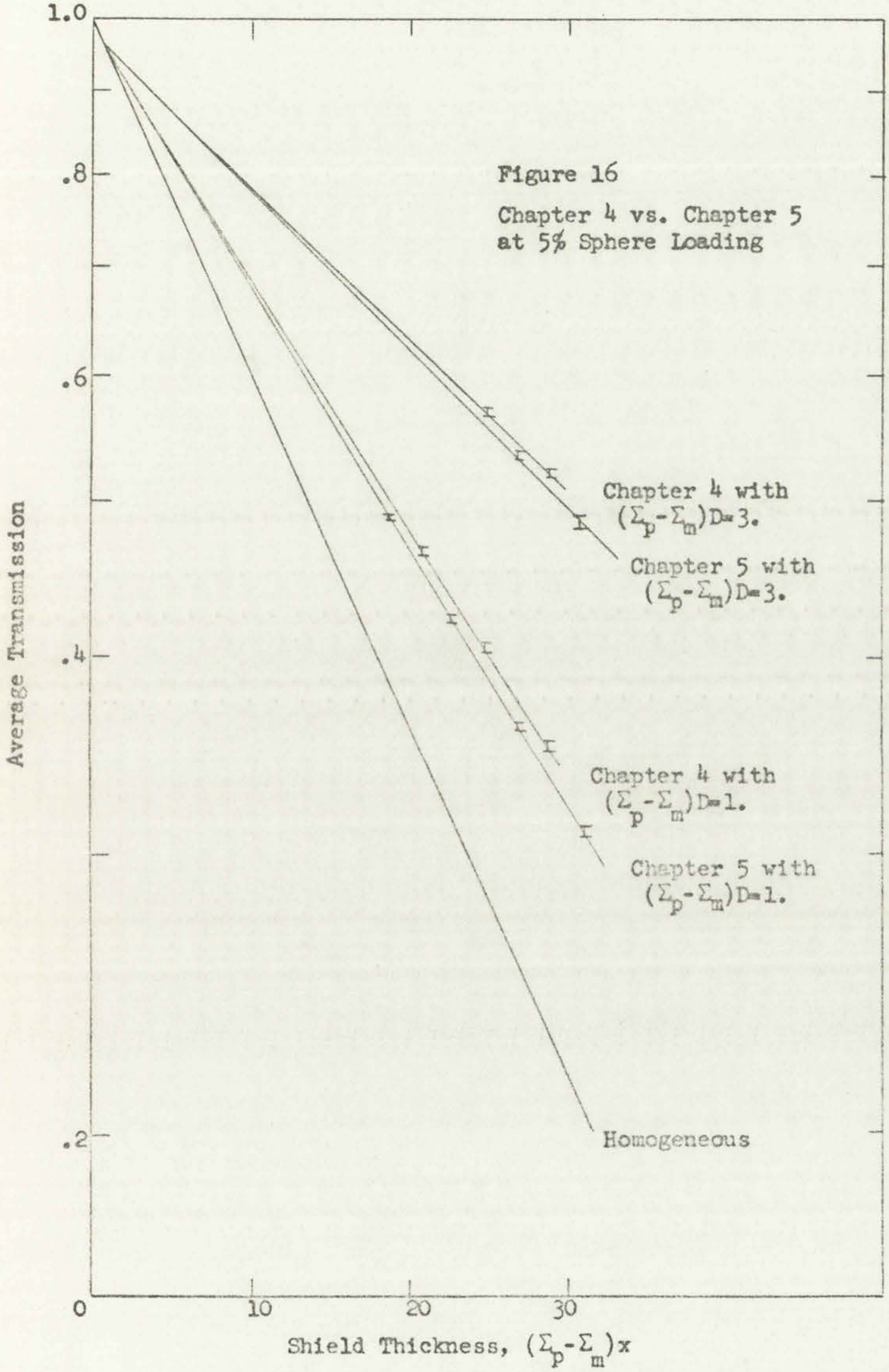
5.6 Summary of FCC Relaxation Technique

In this chapter, an approximate model has been developed for performing transport calculations in a particle-loaded medium. The model permits calculations for any degree of loading and yields calculational results that are reasonable, at least in a qualitative sense. An evaluation of required computer time in comparison with the random-placement technique is unfair, since the perturbation approach alone has been employed for these types of calculations. However, the author feels that implementation of the Double Monte Carlo Method would result in run times consistent with those discussed in section 4.7.

CHAPTER 6 Comparison of Theoretical and Experimental Results

In the preceding two chapters, two methods of performing transport calculations in a sphere-loaded medium, have been presented. The analysis in both chapters was restricted to the case in which both particles and matrix are pure absorbers. It was also argued that, in the case in which the particles are more efficient absorbers than the matrix, both methods yield upper bounds on the transmission. It should be noted that, as the packing approaches maximum, the structure of the medium will closely correspond to the FCC structure if the method of Chapter 5 is employed. The fact that maximum packing can also be attained with a hexagonal close-packed structure casts some doubt on whether the FCC relaxation method provides a rigorous upper bound at very high loadings. Perhaps this point needs further investigation, but it will be shown that for the limited experimental data, the FCC method does appear to provide an upper bound.

It is of interest to compare calculated average transmission profiles for identical problems using the methods of Chapter 4 and Chapter 5. Figures 16 and 17 provide such a comparison. Perhaps the most interesting point to note is that the curves corresponding to the random-placement technique never lie below the curve resulting from the FCC relaxation approach. This is surprising since, in the limit of low loading fraction, the random-placement technique should provide the correct solution. There is no such guarantee on the FCC technique. To the calculational accuracy the author has been able to achieve, however, the two techniques do appear to give identical results for loadings of 1% and below. At 5% particle loading, the two techniques yield distinctly different results. The figures provide a useful guide for deciding when the random placement technique becomes


1.0
.8
.6
.4
.2
0
10
20
30
Average Transmission
Shield Thickness, $(\Sigma_p - \Sigma_m)x$
Figure 16
Chapter 4 vs. Chapter 5
at 5% Sphere Loading
Chapter 4 with
$(\Sigma_p - \Sigma_m)D = 3.$
Chapter 5 with
$(\Sigma_p - \Sigma_m)D = 3.$
Chapter 4 with
$(\Sigma_p - \Sigma_m)D = 1.$
Chapter 5 with
$(\Sigma_p - \Sigma_m)D = 1.$
Homogeneous

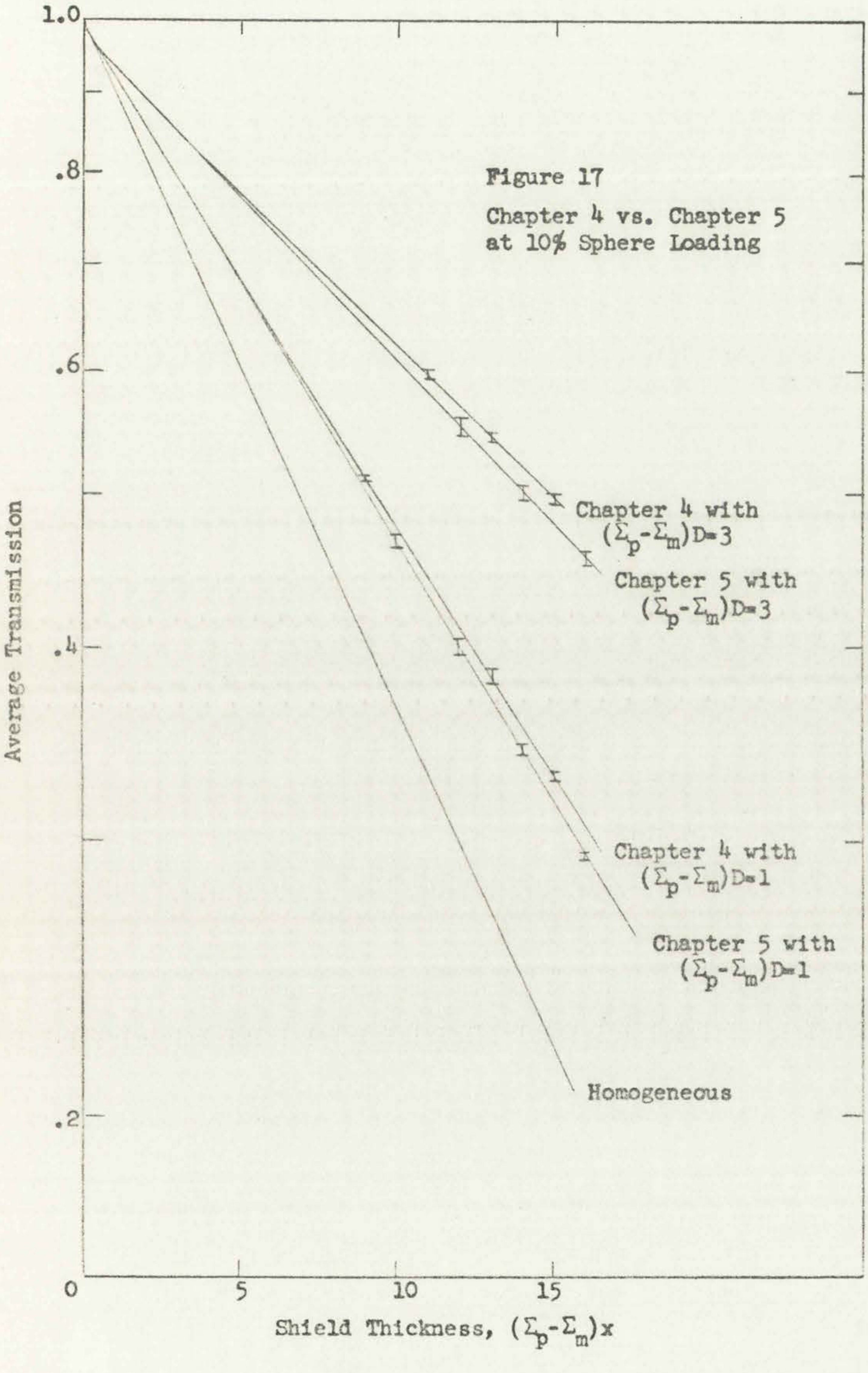


Figure 17

Chapter 4 vs. Chapter 5 at 10% Sphere Loading

unacceptable for a specific problem. It should be mentioned that since the FCC relaxation method has only been coded for use with the perturbation scheme, it is less efficient computationally than the other method.

The problem of radiation transport in a particle-loaded medium has received previous attention in the investigations of Burrus [4], Cantwell [5], Anderson and Dunbar [2], and MacCallum [7]. Cantwell basically constructs a three-dimensional sample of the medium by randomly placing spheres in a cubical box. Edge effects are treated by requiring the cubical box to periodically repeat itself in all directions. In principle, if the dimensions of the box are taken large enough, such a scheme should provide the most precise treatment of the problem. The difficulty with this approach is that the required computation time becomes excessive, especially at higher loading fractions. However, this treatment does have the advantage over the other three previous investigations in that scattering can be treated. The works of Burrus, Anderson and Dunbar, and MacCallum are basically similar. Each artificially stratifies the medium into a number of statistically independent sublayers, with the difference being the chosen sublayer thickness. MacCallum corrects some errors in the previous paper of Anderson and Dunbar, which eliminates the need for a computer solution and results in an analytic expression describing the behavior of the average transmission in a particle-loaded medium. The analytic expressions obtained by MacCallum and by Burrus are almost identical in structure. Anderson and Dunbar reported some experimental transmission studies for spherical particle-loaded slabs irradiated with a monoenergetic beam. The nature of the experiment enables one to neglect scattering and to assume pure absorption. For the purposes of this investigation, MacCallum's presentation of the pertinent information concerning these experiments is presented in Table 1. In this table are also found unacceptable for a specific problem. It should be mentioned that the two-dimensional method has only been coded for use with the [illegible] scheme, it is less efficient [illegible] only when the other [illegible].

The problem of radiation transport in a particle [illegible] has received previous attention in the investigations of [illegible] [1], [illegible] [3], Anderson and Dunbar [4], and Macmillan [5]. [illegible] constructs a three-dimensional sample of the medium by randomly placing spheres in a cubical box. Edge effects are treated by requiring the cubical box to periodically repeat itself in all directions. In principle, if the dimensions of the box are taken large enough, this method should provide the most precise treatment of the problem. The difficulty with this approach is that the required computation time [illegible] especially at higher loading fractions. However, this treatment has the advantage over the other three previous investigations [illegible] ing can be treated. The works of [illegible], Anderson and Dunbar, and Macmillan are basically similar. Each artificially splits the medium into a number of statistically independent sublayers, with the thickness being the chosen sublayer thickness. Macmillan corrects some errors in the previous paper of Anderson and Dunbar, which allows him to find a complete solution and results in an analytic expression for the behavior of the average transmission in a particle-loaded medium. The analytic expressions obtained by Macmillan and by [illegible] are almost identical in structure. Anderson and Dunbar reported some experimental transmission studies for spherical particle-loaded glass [illegible] with a monoenergetic beam. The effect of the significant [illegible] of scattering and to assume pure absorption. For the purpose of comparison, [illegible] Macmillan's presentation of the pertinent data from these experiments is presented in Table I. In this table the [illegible]

TABLE 1

Theory Versus Experiment

Experiment	1	2	3	4	5
Σ_m (cm^{-1})	1.38	1.38	5.5	5.5	8.78
Σ_p (cm^{-1})	827	899	130	130	203
f_p	0.052	0.042	0.108	0.108	0.108
D (cm)	0.0317	0.0406	0.004	0.004	0.004
x (cm)	0.375	0.375	0.0635	0.127	0.0635
T (Experimental)	0.14±?	0.28±?	0.34±?	0.11±?	0.20±?
T (MacCallum)	0.228	0.326	0.338	0.115	0.201
T (Burrus)	0.231	0.328	0.340	0.117	0.203
T (Chapter 4)	0.224	0.310	0.339	0.117	0.201
T (Chapter 5)	0.204	0.301	0.33	0.111	0.193

computational results derived from the methods of Chapters 4 and 5, in addition to the results of the analytic expressions of Burrus and MacCallum. Figures 18 through 21 present the corresponding predicted dependence of the average transmission versus depth into the experimental slabs. As in previous figures, the attenuation attributable to the matrix has been factored out.

The agreement between theory and experiment is striking for the last three experiments. The results for the second experiment are probably acceptable. In the first experiment, however, one would expect better agreement. Structurally, the first experiment does not differ that much from the second, and the loading fraction is relatively low. The consistency of agreement among the theoretical results is striking in all cases and perhaps the first experimental value should be questioned. Much more experimental data would be desirable, especially at higher loadings, where the FCC relaxation method predicts a much lower transmission than the other theoretical treatments.

The author also desires to point out the possibility of extending the applicability of the random-placement method to somewhat higher particle loading by increasing the corresponding λ_s factor above the value computed from equation (41). The idea is to use a value of λ_s which will guarantee the proper particle volume fraction in an average sense along constructed rays but which will result in errors in the placement of particles. It should be recognized that this would result in an empirical scheme, which, again, would require experimental evaluation of its range of applicability.

The agreement among the various theoretical approaches is excellent. This is basically due to the rather thin slabs and weak loadings involved in the experiments. In figures 22 and 23, the method of Chapter 5 is compared with the predictions of Burrus and MacCallum at higher loading

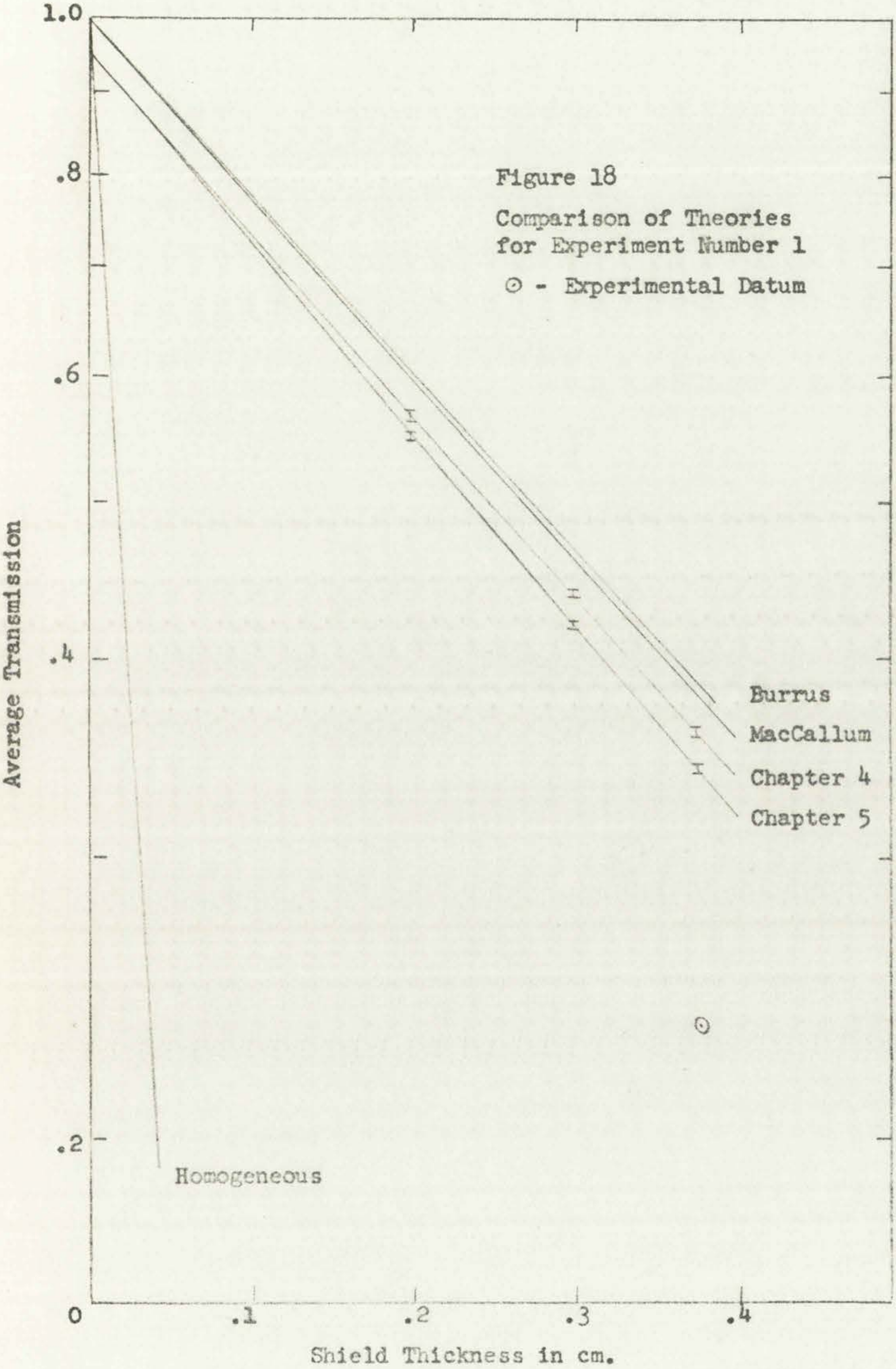


Figure 18
Comparison of Theories
for Experiment Number 1
⊙ - Experimental Datum
1.0
.8
.6
.4
.2
0
.1
.2
.3
.4
Average Transmission
Shield Thickness in cm.
Burrus
MacCallum
Chapter 4
Chapter 5
Homogeneous

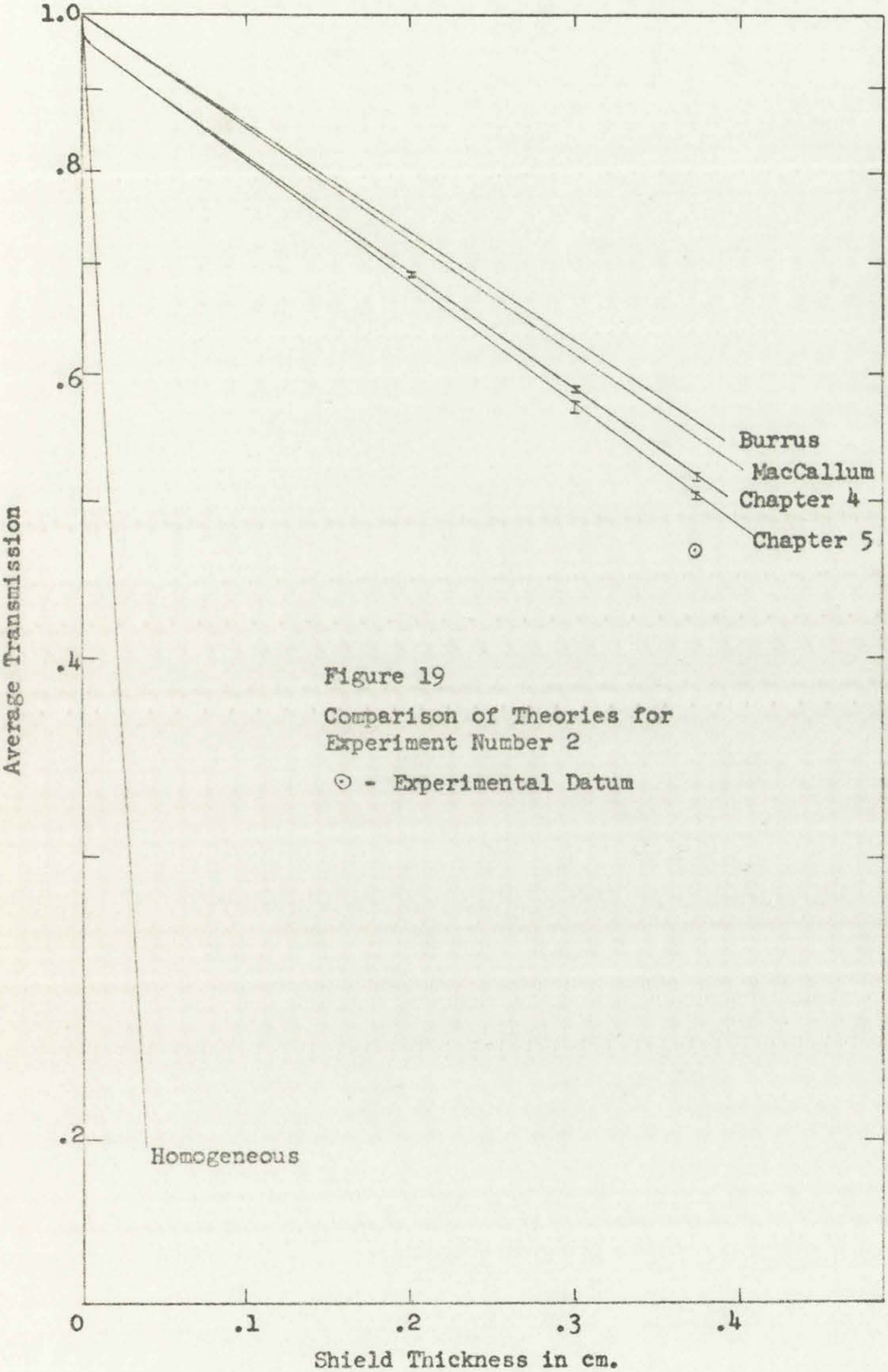
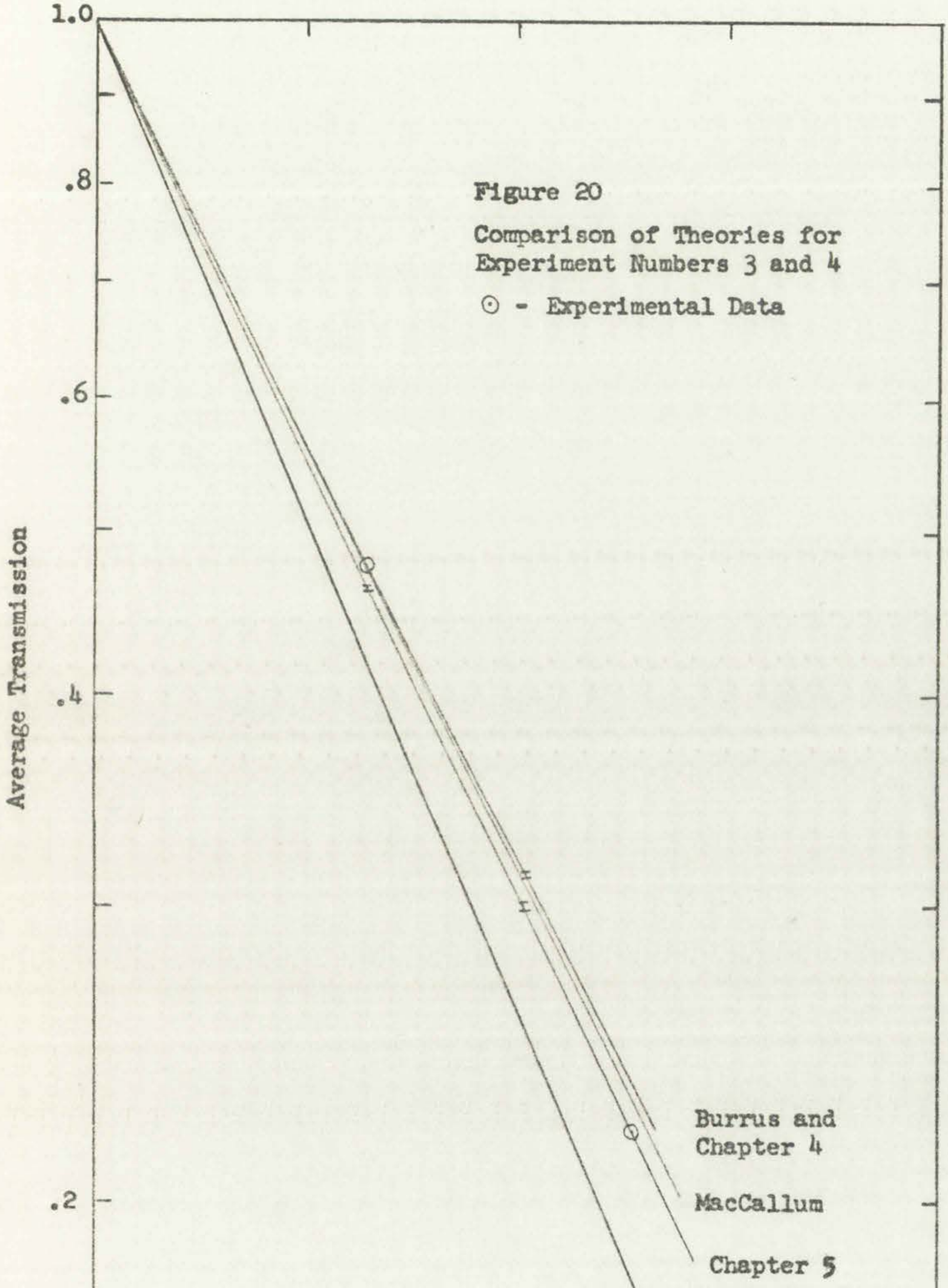


Figure 19

Comparison of Theories for Experiment Number 2



1.0
.8
.6
.4
.2
0
.05
.10
.15
Average Transmission
Shield Thickness in cm.
Figure 20
Comparison of Theories for Experiment Numbers 3 and 4
⊙ - Experimental Data
Burrus and Chapter 4
MacCallum
Chapter 5
Homogeneous

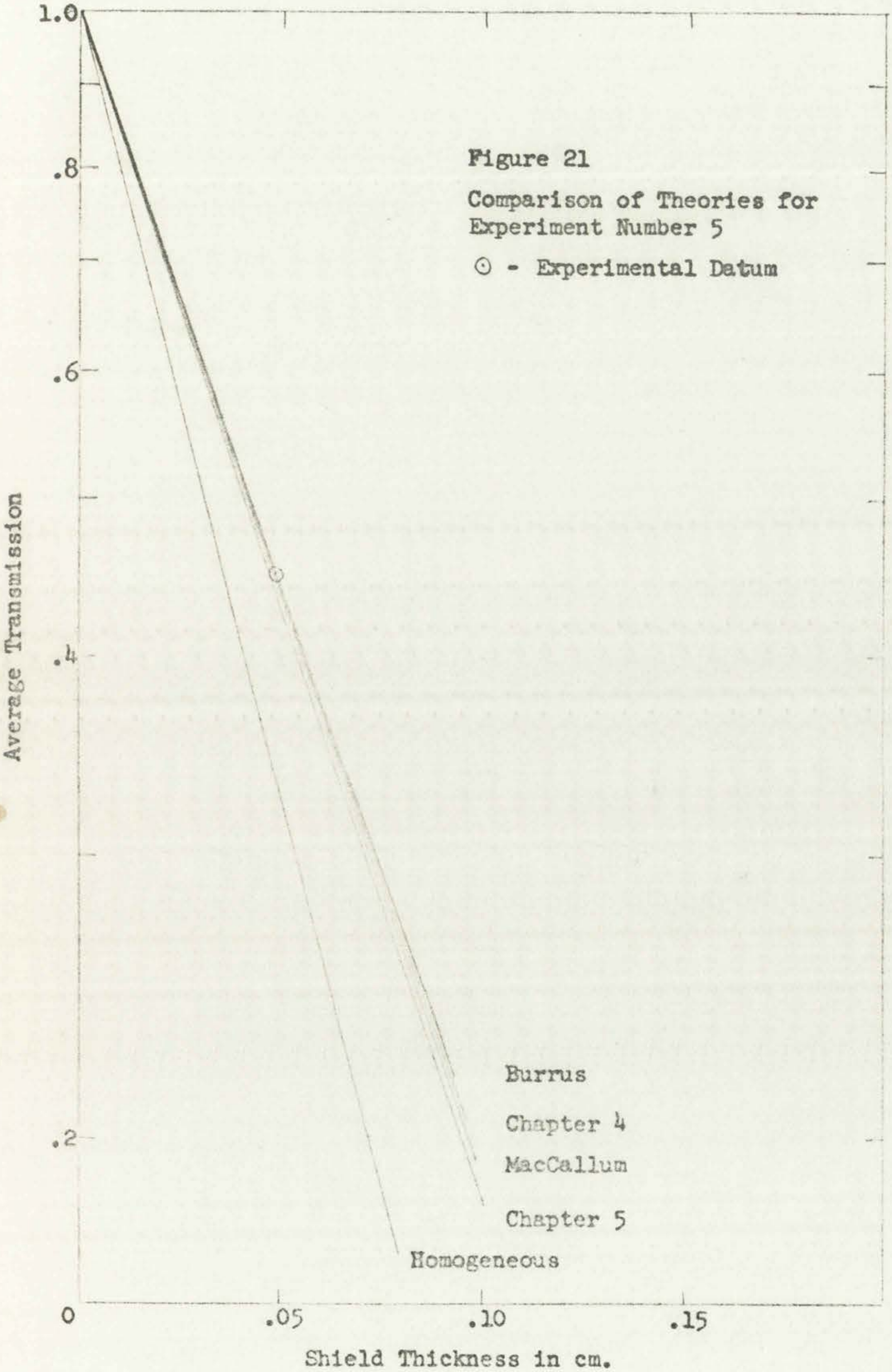


Figure 21

Comparison of Theories for Experiment Number 5

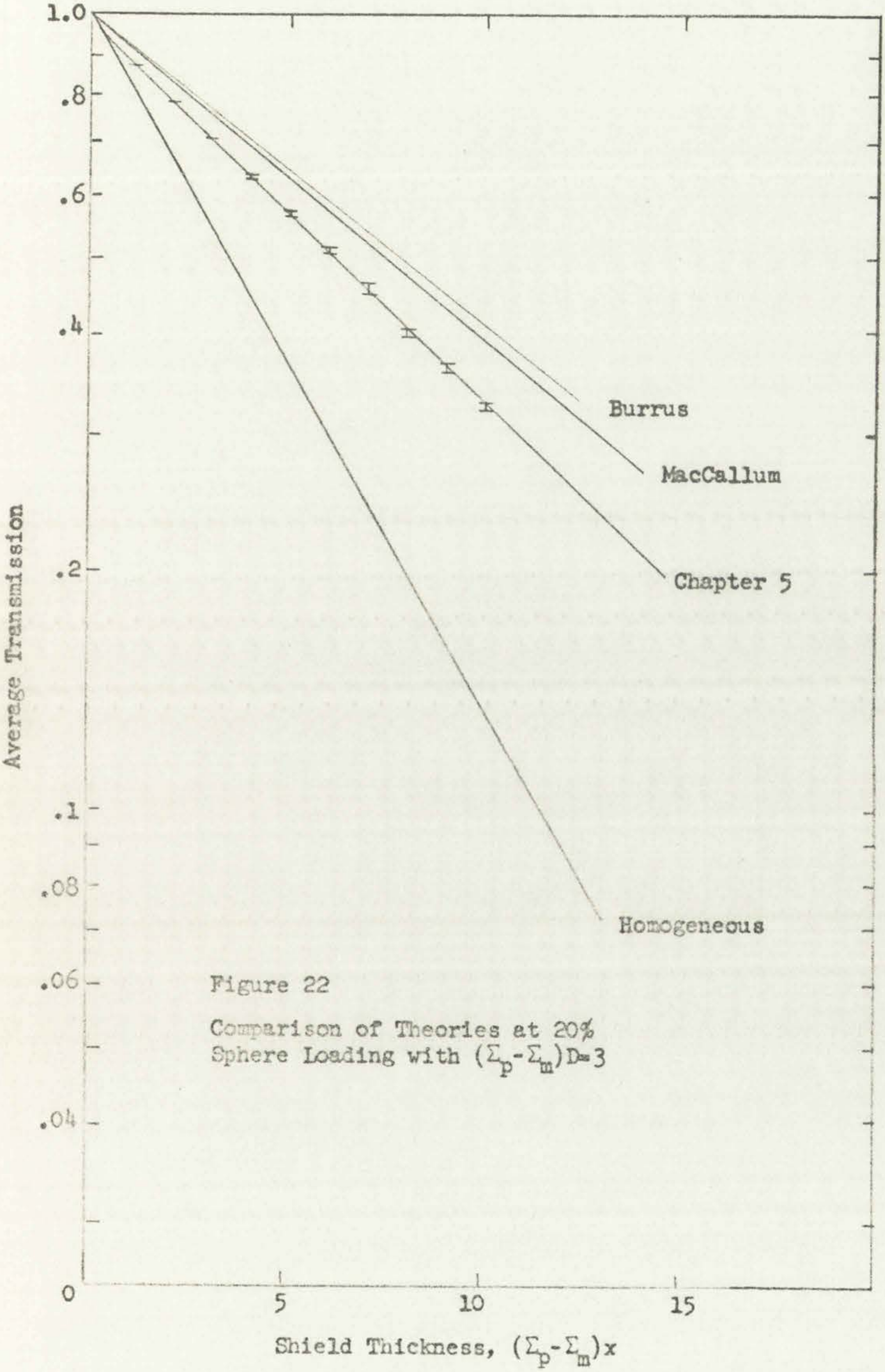


Figure 22

Comparison of Theories at 20% Sphere Loading with $(\Sigma_p-\Sigma_m)D=3$

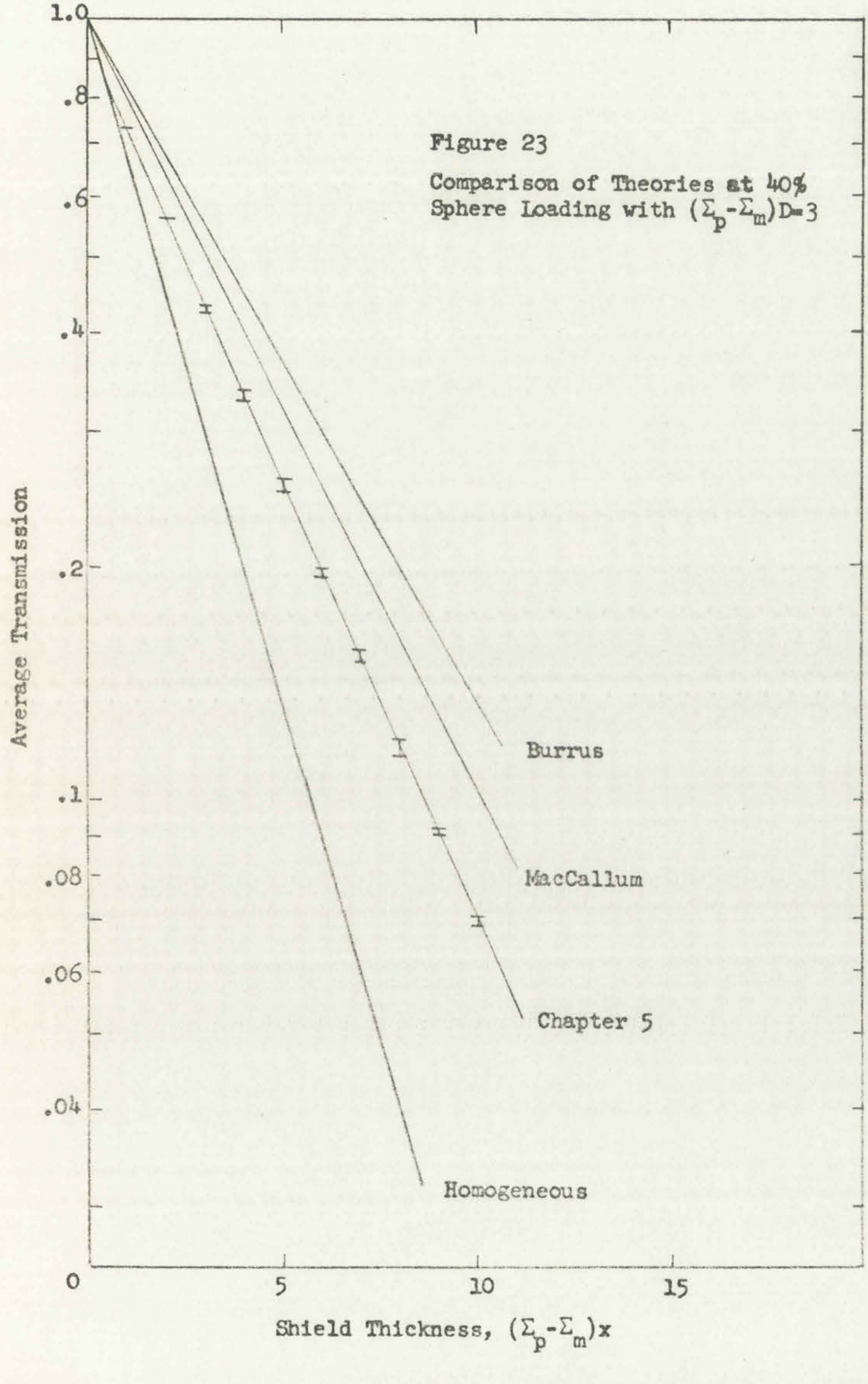


Figure 23
Comparison of Theories at 40% Sphere Loading with $(\Sigma_p-\Sigma_m)D=3$
1.0
.8
.6
.4
.2
.1
.08
.06
.04
0
5
10
15
Average Transmission
Shield Thickness, $(\Sigma_p-\Sigma_m)x$
Burrus
MacCallum
Chapter 5
Homogeneous

fractions. In these problems, the FCC relaxation method predicts considerably lower values for the average transmission and a more reasonable thin shield behavior. Since this method should provide an upper bound for the case in which $\Sigma_p > \Sigma_m$, it should provide results closer to the truth. In addition, the methods of Chapters 4 and 5 are easily extended to more complex problems, while the methods developed by previous investigators are not. Some of the more complex problems for which the methods of this work can be applied are described in the remaining chapters.

therefore, at these positions, the SPS [illegible] nearly [illegible] [illegible] reasonably large values for the average [illegible] this should [illegible]. Since that [illegible] should [illegible] for the case in which $I_p > I_a$, it should provide [illegible] truth. In addition, the methods of Chapters 4 and 5 are easily extended to more complex problems, while the methods developed by previous investigators are not. Some of the more complex problems for which the methods of this work can be applied are described in the following chapters.

CHAPTER 7 The Scattering Problem

7.1 Introduction

In the previous chapters, the author has restricted the analysis to the case for which particles and matrix are pure absorbers. Two methods of constructing the sphere-loaded medium have been presented. Both methods have the advantage that only the region of the material encountered along the ray traversed by a single transport particle must be constructed. As noted in Chapter 6, others have investigated the pure absorption problem, but only the work of Cantwell provides a workable scheme for investigating the effect of scattering caused by matrix, particle, or both. The purpose of this chapter is to extend the ideas of Chapters 4 and 5 in order to treat this complication. Based upon the exact nature of the random-placement technique in the limit of low particle loadings and the efficiency of the random lattice relaxation technique at high loadings, these techniques should provide a much more efficient method of treating the scattering problem than the one previously available. In general, the introduction of scattering requires one to remember much more of the previously constructed medium, since there is now a mechanism by which a source transport particle can return to previously traversed positions. In practice, it is very unlikely that a transport particle at a specific position will escape a spherical volume which is centered about that position and which has a radius equal to several effective absorption mean-free paths relative to the loaded medium. This suggests that meaningful calculations can be performed with a rather limited memory of previously constructed media.

CHAPTER 7 [illegible]

7.1 Introduction

In the previous chapters, the [illegible] to the case for which particles and [illegible] both [illegible]. Two methods of constructing the [illegible]. Both methods have the advantage that only [illegible] encountered along the two waves and [illegible] must be constructed. As noted in Chapter [illegible] the pure [illegible] problem, but [illegible] a workable scheme for investigating [illegible] by matrix, particle, or both. The [illegible] and the ideas of Chapters 4 and 5 [illegible] tion. Based upon the exact nature of the [illegible] in the limit of low particle loadings [illegible] lattice relaxation technique of [illegible] provide a much more efficient method [illegible] ing than the one [illegible] of scattering [illegible] constructed [illegible] tremendous potential [illegible] practice, it is very unlikely that a [illegible] position will escape a [illegible] positive [illegible] mean-free path relative to the [illegible] meaningful calculations can be [illegible] of providing [illegible]

7.2 Construction of the Medium

The main difficulty introduced by scattering is that a transport particle no longer is restricted to move along a single ray. A scattering event results in the establishment of a new ray path. This presents no difficulty to either of the previously developed construction schemes. The only requirement is that the nature of the medium constructed along this new ray path must not contradict the nature of the previous ray path. It also holds, by an argument identical to that presented in section 4.3, that one can restrict himself to the behavior of one source Monte Carlo particle per constructed sample.

7.3 Implementation of Theory

From the discussion in the previous section, it is observed that except for the added memory requirement, one can proceed in the tracking of a single particle while simultaneously constructing the traversed medium. The Double Monte Carlo scheme is, therefore, equally applicable to the scattering problem. It is not immediately obvious, however, that the perturbation approach can be extended to the scattering problem. The perturbation approach depends to a certain extent on the structure of the governing differential equation describing the pure absorption problem. This structure is immediately modified by the introduction of scattering. With this in mind, one can write the transport equation, including scattering and a source, as

$$\vec{\Omega} \cdot \nabla\phi(\vec{r},\vec{\Omega},E) + \Sigma_t(\vec{r},E)\phi(\vec{r},\vec{\Omega},E) = S(\vec{r},\vec{\Omega},E)$$

$$+ \iint dE'd\Omega'\Sigma_s(\vec{r},E' \to E,\vec{\Omega}' \to \vec{\Omega})\phi(\vec{r},\vec{\Omega}',E') \ . \qquad (66)$$

It is convenient to represent the total interaction cross section at energy E for particle and matrix by $\Sigma_t^p(E)$ and $\Sigma_t^m(E)$, respectively. Similarly, the scattering cross sections are represented by $\Sigma_s^p(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$ and $\Sigma_s^m(E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$. In addition, one can define

$$\Sigma_t^H(E) = \text{Max}\left\{\Sigma_t^p(E),\ \Sigma_t^m(E)\right\} , \tag{67a}$$

$$\Sigma_t^L(E) = \text{Min}\left\{\Sigma_t^p(E),\ \Sigma_t^m(E)\right\} , \tag{67b}$$

$$\Sigma_s^H(E' \rightarrow E,\ \vec{\Omega}' \rightarrow \vec{\Omega}) = \text{Max}\left\{\Sigma_s^p(E' \rightarrow E,\ \vec{\Omega}' \rightarrow \vec{\Omega}),\ \Sigma_s^m(E' \rightarrow E,\ \vec{\Omega}' \rightarrow \vec{\Omega})\right\} , \tag{67c}$$

$$\Sigma_s^L(E' \rightarrow E,\ \vec{\Omega}' \rightarrow \vec{\Omega}) = \text{Min}\left\{\Sigma_s^p(E' \rightarrow E,\ \vec{\Omega}' \rightarrow \vec{\Omega}),\ \Sigma_s^m(E' \rightarrow E,\ \vec{\Omega}' \rightarrow \vec{\Omega})\right\} , \tag{67d}$$

$$F(\vec{r},E) = \begin{cases} 1 & \text{if} \quad \Sigma_t(\vec{r},E) = \Sigma_t^L(E) \\ 0 & \text{if} \quad \Sigma_t(\vec{r},E) = \Sigma_t^H(E) , \end{cases} \tag{67e}$$

$$F_s(\vec{r},E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) = \begin{cases} 1 & \text{if} \quad \Sigma_s(\vec{r},E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s^H(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) \\ 0 & \text{if} \quad \Sigma_s(\vec{r},E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s^L(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) . \end{cases} \tag{67f}$$

Finally, one is led to define

$$\gamma(\vec{r},E) = \frac{\left(\Sigma_t^H(E) - \Sigma_t^L(E)\right)}{\Sigma_t^H(E)} F(\vec{r},E) \tag{68a}$$

and

$$\gamma_s(\vec{r},E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) = \Sigma_s^L(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) + \Big(\Sigma_s^H(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) - \Sigma_s^L(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega})\Big) F_s(\vec{r},E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega}) . \tag{68b}$$

Employing relations (67) and (68), one can rewrite (66) to read

$$\vec{\Omega} \cdot \nabla\phi(\vec{r},\vec{\Omega},E) + \Sigma_t^H(E)\phi(\vec{r},\vec{\Omega},E) = S(\vec{r},E,\vec{\Omega})$$

$$+ \gamma(\vec{r},E)\Sigma_t^H(E)\phi(\vec{r},\vec{\Omega},E)$$

$$+ \iint dE'd\Omega'\Sigma_s^L(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega})\phi(\vec{r},\vec{\Omega}',E')$$

$$+ \iint dr'd\Omega'\gamma_s(r,E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega})\phi(\vec{r},\vec{\Omega}',E') \ . \qquad (69)$$

Equation (69) can be interpreted to imply that the transport particles are moving in a homogeneous medium having a total interaction cross section $\Sigma_t^H(E)$ and a scattering kernel represented by $\Sigma_s^L(E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega})$. In addition, there are two other possible scattering mechanisms governed by the factors $\gamma(\vec{r},E)$ and $\gamma_s(\vec{r},E' \rightarrow E,\vec{\Omega}' \rightarrow \vec{\Omega})$ which are dependent upon whether the interaction position lies within particle or matrix. It should be noted that the term involving $\gamma(\vec{r},E)$ in equation (69) results in either absorption or straight-ahead scatter with no change in transport particle energy.

One concludes that the perturbation approach is indeed applicable to the scattering problem. Therefore, both the Double Monte Carlo and the perturbation techniques developed in previous chapters extend quite naturally to the scattering problem. As mentioned before, the only real difficulty is the additional memory requirements. How much memory is required would be a very interesting numerical study. Perhaps it should be pointed out that one can treat first-order scattering of those particles scattered in the forward direction without any real increase in memory requirements above that required in earlier

chapters. Such scattered particles retain their motion away from previously constructed media.

For the more general problem, the nature of the constructed medium along a specific ray could be stored, together with the initial point on the ray, the direction cosines of the ray, and the length of the ray. The vector description of the ray could be stored in core memory while the constructed media data could be stored on tape or disc. A simple geometric calculation, based upon the location and velocity vector of a transport particle coupled with the vector description of a previously established ray, could then be performed in order to establish whether or not the precise nature of the medium along this prior ray could have any interference effects in the region presently being constructed. If so, the required information could then be buffered into core.

7.4 The Higher-Moment Problem

The ideas described in the previous sections apply only to the expected values of quantities such as total flux, right-going flux, and absorbed dose. If scattering is included, there seems to be no convenient way of obtaining the expected value of the higher moments of such quantities. Basically, the transformation employed to associate the higher-moment problem with a first-moment problem in the case of pure absorption was dependent on the structure of the governing differential equation. The introduction of scattering modifies this structure sufficiently to preclude this type of transformation.

However, a reasonably accurate calculation of the expected values of quantities of interest is usually more important than accurate calculations of their respective standard deviations. In many

applications, one could estimate standard deviations by computing the first and second moments of the noninteracted transmitted flux.

CHAPTER 8 Results and Conclusions

The transmission of radiation through a purely absorbing particle-loaded medium has been investigated. This investigation was initiated with the analysis of an artificial slab problem. Because of the simplicity of this model, precise analytic results were obtained. It was found that in the limit of thin shields, the expected value of the transmission corresponds to that calculated when the assumption is made that the material is a homogeneous mixture of particle and matrix material. As the shield thickness increases, this is no longer true, and the expected value of the transmission rather quickly attains an asymptotic behavior, decreasing exponentially with an effective cross section characteristic of the exact nature of the loading. This effective cross section deviates progressively further from the homogeneous cross section as the slab thickness is increased.

The investigation was then extended to the more realistic model of constant-radius spheres imbedded in a matrix filler. Two approximate methods were then developed for constructing the nature of such a composite material. The combination of these two methods enables one to perform calculations at any loading fraction with reasonable expenditures of computing time. Because of the complexity of the models, the transmission was investigated with the use of Monte Carlo techniques. The resulting calculations predicted a behavior qualitatively identical to that predicted by the slab model. One expects that the behavior carries over to materials having variable particle size and nonspherical shape. The implication is, that for pure absorption problems, realistic materials can be experimentally analyzed by determination of the effective cross section from studies on relatively thick shields, coupled with experiments on thin shields to

describe the initial behavior of transmission versus depth. The scattering problem was also discussed and the applicability of prior results described. A thorough evaluation of these ideas demands much more experimental data for comparison with predicted results.

It should be noted that the random-placement ideas extend quite nicely to nonspherical particles and different size particles, at least at loadings low enough that the random assumption is approximately valid. The main difficulty is that nonspherical particles would require establishment and memory of the orientation of a particle as it is placed.

It should be noted that the results for the higher moment problem have been of an extremely specialized nature. In fact, the only result obtained is for a monoenergetic beam impinging on a purely absorbing particle-loaded medium. Here, it was observed that the expected value of higher moments of the transmission are no more difficult to attain than the first moment. Just how important the monoenergetic restriction is perhaps best pointed out in an example. Suppose the same problem is considered except that the beam is now composed of a continuum of energies. In this case the intensity of the beam within an energy interval dE centered at E is I(E)dE. Assume that, for one ray sample through a particle-loaded medium, the functional dependence of the transmission with energy E and position x is given by $T_i(E,x)$. The total transmission is then

$$T_i(x) = \int_{\text{all } E} I(E) T_i(E,x)\, dE \,. \tag{70}$$

Since I(E) is not stochastic, if one averages over all possible configurations of the medium, one obtains

$$T(x) = \int_{\text{all } E} I(E) T(E,x)\, dE \,, \tag{71}$$

where T without the subscript i represents the expected value of the transmission. Since T(E,x) is the expected transmission at x resulting from a monoenergetic beam of energy E, it can be computed by the methods previously outlined. However, if one desires the expected value of the second moment of the total transmission, one finds that

$$\mathscr{E}\left(T_i^2(x)\right) = \int_{\text{all } E} \int_{\text{all } E'} I(E)I(E')\mathscr{E}\left(T_i(E,x)T_i(E',x)\right) dE' \, dE \ , \quad (72)$$

where $\mathscr{E}$ represents the expected value operator. Hence, to evaluate (72), one must obtain the autocorrelation function of the transmission with respect to energy. This is not difficult since one can employ previously developed concepts by noting that

$$\frac{d}{dx}\left(T_i(E,x)T_i(E',x)\right) = -\left(\Sigma_i(E,x) + \Sigma_i(E',x)\right)\left(T_i(E,x)T_i(E',x)\right) \ , \quad (73)$$

with initial condition $\left(T_i(E,0)T_i(E',0)\right) = 1.$

If one takes the beam to be monoenergetic and desires the expected value of the first and second moment of the transmission averaged over a finite area surface perpendicular to the incident radiation, one encounters basically the same difficulties: namely, one must obtain the autocorrelation function of transmission with respect to the separation between two parallel rays. It should be noted that a finite area detection system results in the above type averaging. For this problem, a transformation similar to (73) can be performed, but now the cross section term is dependent upon the nature of two adjacent rays rather than of two energies. Both models for constructing the sphere-loaded medium permit the simultaneous construction of two adjacent rays and, therefore, such calculations can be performed.

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$$\mathcal{E}\left(T_i^2(x)\right) = \int_{\text{all } E} \int_{\text{all } E'} \mathcal{E}\left(T_i(E,x)\,T_i(E',x)\right) dE'\, dE \quad (73)$$

where $\mathcal{E}$ represents the expected value operator. Hence, to evaluate (72), one must obtain the autocorrelation function of the transmission with respect to energy. This is not difficult since one can employ previously developed concepts by noting that

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with initial condition $\left(T_i(E,0)\,T_i(E',0)\right) = 1$.

If one takes the beam to be monoenergetic and desires the expected value of the first and second moments of the transmission averaged over a finite size surface perpendicular to the incident radiation, one encounters basically the same difficulties. Namely, one must obtain the autocorrelation function of transmission with respect to the separation between two parallel rays. It should be noted that a finite area detection system results in the above type averaging. For this problem, a transformation similar to (73) can be performed, but now the cross section term is dependent upon the nature of two adjacent rays rather than of two energies. Both models for representing the nonhomogeneous medium permit the evaluation [illegible] of the adjacent rays and, therefore, such calculations can be performed.

As one considers more complex problems, including scattering with respect to both energy and direction, one must investigate simultaneous correlation of position, direction, and energy. Simple transformations such as (73) can no longer be obtained, and the author has been unable to devise any reasonable scheme of performing these types of investigations. As pointed out by MacCallum, Tshebysheff's Lemma [9] becomes useful for these types of problems. This lemma implies that if x is a positive stochastic variable with $\mathscr{E}(x) = \sigma^2$, then the probability P of the inequality $x \geq v$, has the following upper bound:

$$P \leq \frac{\sigma^2}{v} , \tag{74}$$

for $v \geq \sigma^2$. Since, in a particle-loaded medium, quantities such as particle density, activation, and flux become positive stochastic variables, this lemma can provide useful upper bounds based upon only expected values.

It is desirable to evaluate this research with respect to the previous investigations. For the pure absorption problem at particle loadings below 5 volume-percent, the methods of all previous investigators and the methods of this research appear to provide an accurate description of the shielding characteristics of particle-loaded materials. This agreement leads one to conclude that the analytic solutions of Burrus and MacCallum are perhaps much more accurate than has previously been realized. However, for more complex problems, such as the treatment of scattering, only the methods of this research and the method of Cantwell are appropriate. Of these methods, the random-placement method of Chapter 4 should be, by far, the most efficient, both in terms of required computation time and in terms of computer coding simplicity. At higher loadings

for the pure absorption problem, the FCC relaxation method should predict an expected transmission much closer to reality than either Burrus or MacCallum. Any statement of the accuracy of this model must await additional experimental data. Cantwell's method extends to higher loadings, but the cost in computer time soon becomes prohibitive. If the FCC relaxation method is found to predict reasonably accurate shielding characteristics for the pure absorption problem, then this method can be extended to the treatment of scattering problems with a reasonable degree of confidence. Another important result of this research is its implication on future experimental work in the area of particle-loaded shields. A complete description of the absorption characteristics of a particle-loaded shield requires the determination of both an asymptotic cross section and a thin shield behavior.

APPENDIX

Program EXØS employs the Double Monte Carlo method and the random sphere placement assumption described in Chapter 4. In the early stages of the author's investigation, it was desirable to obtain a rather independent check of the analytic results of Chapter 1. Therefore, EXØS also has the capability of performing the Double Monte Carlo calculations for the slab problem described in Chapter 2. Program RANLAT employs the perturbation method and the random lattice relaxation technique described in Chapter 5. The combination of these codes presents both approximate methods for constructing the sphere-loaded medium and both computational schemes for performing the transport calculations. Both codes have the capability of computing the expected value of the transmission and of higher moments of the transmission at various desired depths within a slab of particle-loaded material. Fortran listings are included but the reader is cautioned that little effort was spent on maximizing the efficiency of these codes. If extensive calculations are contemplated, the author feels that a careful "cleaning up" of the codes, especially by a professional programmer, should be able to provide a worthwhile decrease in run time.

Two other features of these codes should be noted. First, if the particle cross section is higher than that of the matrix, the values calculated are based on a transparent matrix containing particles of cross section equal to $\Sigma_p - \Sigma_m$. If the matrix cross section is higher, the calculations are based on transparent particles imbedded in a matrix of cross section $\Sigma_m - \Sigma_p$. Second, the user must specify the number of batches of source particles to be employed and the number of source particles per batch. This enables the codes to compute expected values and unbiased estimates of the standard deviation based upon batch-to-batch results.

SUMMARY

Program CSSS employs the Double Monte Carlo method and the random sphere placement scheme as described in Chapter 4. In the early stages of the author's investigation, it was desirable to obtain a rather independent check of the analytic results of Chapter 3. Therefore, CSSS also has the capability of performing the Double Monte Carlo calculations for the slab problems described in Chapter 2. Program ADRAT employs the perturbation method and the random lattice relaxation technique described in Chapter 5. The combination of these codes presents both approximate methods for constructing the sphere-loaded medium and both computational schemes for performing the transport calculations. Both codes have the capability of computing the expected value of the transmission and of higher moments of the transmission at various desired depths within a slab of particle loaded material. Fortran listings are included but the reader is cautioned that little effort was spent on optimizing the efficiency of these codes. If extensive calculations are contemplated, the author feels that a careful "cleaning up" of the codes, especially by a professional programmer, should be able to provide a worthwhile decrease in run time.

Two other features of these codes should be noted. First, if the particle cross section is higher than that of the matrix, the values calculated are based on a transparent matrix containing particles of cross section equal to $\Sigma_p - \Sigma_m$. If the matrix cross section is higher, the calculations are based on transparent particles imbedded in a matrix of cross section $\Sigma_m - \Sigma_p$. Second, the user must specify the number of matrices of sphere particles to be employed and the number of source particles per batch. This enables the codes to compute expected values and unbiased estimates of the standard deviation from batch-to-batch results.

TABLE 2

Program EXØS Input Format

Card No.	Variable	Format
1	CSM,CSP,EP,D,NPØS,NSØR,KBAT,	4E10.3, 3I10,
	NTYP, NMØM	2I5
2	(WØRD(I), I = 1, 10)	10A8
3	(XB(I), I = 1, NPØS	(8E10.3)

TABLE 3

Definitions of Variables for EXØS Input

Item No.	Variable Name	Identification
1	CSM	Macroscopic cross section of matrix material (cm^{-1})
2	CSP	Macroscopic cross section of particle material (cm^{-1})
3	FP	Volume fraction of particle material
4	D	Diameter of particles (cm) for spheres, thickness of particle (cm) for slabs
5	NPØS	The number of distinct positions at which the expected value of a moment of the transmission is desired. NPØS must be less than 101
6	NSØR	Number of source particles per batch
7	KBAT	Number of batches to be run for this problem
8	NTYP	Slab or sphere option switch = 0 Sphere option desired ≠ 0 Slab option desired
9	NMØM	Moment of transmission to be calculated. Note that NMØM = 1 corresponds to simply the expected value of the transmission
10	WØRD	Arbitrary alphanumeric identification of problem
11	XB	Depths (cm) at which calculations are desired. These must be arranged in ascending order

TABLE 4

Program RANLAT Input Format

Card No.	Variable	Format
1	CSM,CSP,FP,D,NPØS,NSØR,KBAT,	4E10.3, 3I10,
	NMØM	5X, I5
2	(WØRD(I), I = 1, 10)	10A8
3	(XB(I), I = 1, NPØS)	(8E10.3)

TABLE 5

Definitions of Variables for RANLET Input

Item No.	Variable Name	Identification
1	CSM	Macroscopic cross section of matrix material (cm^{-1})
2	CSP	Macroscopic cross section of particle material (cm^{-1})
3	FP	Volume fraction of particle material
4	D	Diameter of particles (cm)
5	NPØS	The number of distinct positions at which the expected value of a moment of the transmission is desired. NPØS must be less than 101
6	NSØR	Number of source particles per batch
7	KBAT	Number of batches to be run for this problem
8	NMØM	Moment of transmission to be calculated. Note that NMØM = 1 corresponds to simply the expected value of the transmission
9	WØRD	Arbitrary alphanumeric identification of problem
10	XB	Depths (cm) at which calculations are desired. These must be arranged in ascending order

Both EXØS and RANLAT are written for the CDC 6600 computer under the Scope 3.2.0 Operating System.

```
      PROGRAM EXOS(INPUT,OUTPUT,TAPE60=INPUT)
      DIMENSION XB(100),ANS(100),NSP(100),NSP2(100),
     1NSMX(100),WORD(10),ABAR(100),ASIG(100)
    1 READ 2,CSM,CSP,FP,D,NPOS,NSOR,KBAT,NTYP,NMOM
    2 FORMAT(4E10.3,3I10,2I5)
      IF(EOF,60)1000,3
    3 IF(NMOM.EQ.0)NMOM=1
      IF(KBAT.EQ.0)KBAT=1
      READ 4,(WORD(I),I=1,10)
      READ 5,(XB(I),I=1,NPOS)
    4 FORMAT(10A8)
    5 FORMAT(8E10.3)
      PRINT 6
    6 FORMAT(*1*/* EXPONENTIAL ATTENUATION USING ORDERS OF*
     1X*PARTICLES*)
      PRINT 7,(WORD(I),I=1,10)
    7 FORMAT(X10A8)
      PRINT 8,NMOM,NSOR,CSM
    8 FORMAT(/* STATISTICAL MOMENT=*I3,/* NO. SOURCE*
     1X*PARTICLES=*I10,/* MATRIX CROSS SECTION(1./CM.)=*E10.3)
      IF(NTYP.NE.0)GO TO 10
      PRINT 9,CSP,FP,D
    9 FORMAT(* SPHERE CROSS SECTION(1./CM.)=*E10.3,/* SPHERE*
     1X*VOLUME FRACTION=*E10.3,/* SPHERE DIAMETER(CM.)=*E10.3)
      GO TO 12
   10 PRINT 11,CSP,FP,D
   11 FORMAT(* SLAB CROSS SECTION(1./CM.)=*E10.3,/* SLAB VO*
     1*LUME FRACTION=*E10.3/* SLAB WIDTH(CM.)=*E10.3)
   12 XMOM=NMOM
      CSM=CSM*XMOM
      CSP=CSP*XMOM
      IF(CSP.GT.CSM) GO TO 13
      CSR=CSP
      SIG=CSM-CSP
      WP=0.
      GO TO 14
   13 CSR=CSM
      SIG=CSP-CSM
      WP=1.
   14 PRINT 16,CSR,SIG
   16 FORMAT(* BASE CROSS SECTION(1./CM.)=*E10.3,/* DELTA C*
     1*ROSS SECTION(1./CM.)=*E10.3)
      DO 600 I=1,NPOS
      ABAR(I)=0.
  600 ASIG(I)=0.
      LINE=11
      DO 999 J=1,KBAT
      DO 15 I=1,NPOS
      ANS(I)=0.
      NSP(I)=0
      NSP2(I)=0
   15 NSMX(I)=0
      DO 21 I=1,NSOR
```

```
      X=0.
      K=0
      W=1.
      INT=0
      XF=XB(NPOS)
      N=0
   17 XS=XB(K+1)
      IF(X.LT.XS)GO TO 18
      K=K+1
      ANS(K)=ANS(K)+1.
      NSP(K)=NSP(K)+N
      NSP2(K)=NSP2(K)+N*N
      MAX=NSMX(K)
      IF(N.GT.MAX)NSMX(K)=N
      IF(K.EQ.NPOS) GO TO 21
      GO TO 17
   18 IF(W.EQ.0.) GO TO 21
      XT=XF
      IF(WP.EQ.1.) GO TO 19
      R=RANF(0.)
      XT=X-ALOG(R)/SIG
   19 CALL PROBE(X,XL,XR,D,FP,NTYP,INT)
      IF(XT.GT.XL)GO TO 20
      X=XT
      W=0.
      N=N+1
      GO TO 17
   20 N=N+1
      X=XR
      IF(WP.EQ.0.) GO TO 17
      R=RANF(0.)
      XT=XL-ALOG(R)/SIG
      IF(XT.GT.XR) GO TO 17
      X=XT
      W=0.
      GO TO 17
   21 CONTINUE
      XTOT=NSOP
      LINE=LINE+3
      IF(LINE.LT.60) GO TO 555
      LINE=3
      PRINT 556
  556 FORMAT(*1*)
  555 CONTINUE
      PRINT 601,J
  601 FORMAT(/* BATCH=*I3,/3X*X(CM.)*8X*PHI*8X*NBAR*8X*NSIG*
     18X*NMAX*)
      DO 22 I=1,NPOS
      PHI=ANS(I)/XTOT
      ABAR(I)=ABAR(I)+PHI
      ASIG(I)=ASIG(I)+PHI*PHI
      X=XB(I)
      MAX=NSMX(I)
```

```
      CB=NSP(I)/ANS(I)
      SCB=ANS(I)*NSP2(I)-NSP(I)*NSP(I)
      SCB=SCB/ANS(I)/(ANS(I)-1.)
      SCB=SQRT(SCB)
      LINE=LINE+1
      IF(LINE.LT.60) GO TO 557
      LINE=1
      PRINT 556
  557 CONTINUE
   22 PRINT 23,X,PHI,CB,SCB,MAX
   23 FORMAT(4E12.4,I12)
  999 CONTINUE
      IF(KBAT.EQ.1) GO TO 1
      XBAT=KBAT
      LINE=LINE+3
      IF(LINE.LT.60) GO TO 558
      LINE=3
      PRINT 556
  558 CONTINUE
      PRINT 700
  700 FORMAT(/* BATCH STATISTICS*/3X*X(CM.)*8X*PHI*8X*1SIG*)
      DO 701 I=1,NPOS
      PHI=ABAR(I)/XBAT
      SPH=(ASIG(I)-XBAT*PHI*PHI)/(XBAT-1.)
      SPH=SQRT(SPH)
      X=XP(I)
      LINE=LINE+1
      IF(LINE.LT.60) GO TO 559
      LINE=1
      PRINT 556
  559 CONTINUE
  701 PRINT 702,X,PHI,SPH
  702 FORMAT(3E12.4)
      GO TO 1
 1000 CONTINUE
      END
      SUBROUTINE SPEAR(XL,XR,XP,YP,ZP,D)
      R=RANF(0.)
      RC=D*SQRT(R)
      XP=XL+RC/2.
      XR=XL+RC
      R=RANF(0.)
      TH=6.283185307*R
      RHO=.5*SQRT(D*D-RC*RC)
      YP=RHO*COS(TH)
      ZP=RHO*SIN(TH)
      RETURN
      END
      SUBROUTINE PROBE(X,XL,XR,D,FP,NTYP,INT)
      DIMENSION XM(10),YM(10),ZM(10)
      IF(NTYP.EQ.0) GO TO 3
      IF(INT.GT.0) GO TO 2
      INT=1
```

```
      XLAM=FP/D/(1.-FP)
      R=RANF(0.)
      IF(R.GT.FP) GO TO 1
      R=RANF(0.)
      XR=X+R*D
      XL=XR-D
      IF(XL.LT.0.)XL=0.
      GO TO 100
    1 R=RANF(0.)
      XL=X-ALOG(R)/XLAM
      XR=XL+D
      GO TO 100
    2 R=RANF(0.)
      XL=X-ALOG(R)/XLAM
      XR=XL+D
      GO TO 100
    3 IF(INT.GT.0) GO TO 5
      INT=1
      XLAM=1.5*FP/D/(1.-FP)
      MEM=1
      R=RANF(0.)
      IF(R.LE.FP) GO TO 4
      R=RANF(0.)
      XL=X-ALOG(R)/XLAM
      CALL SPEAR(XL,XR,XM(1),YM(1),ZM(1),D)
      GO TO 100
    4 R=RANF(0.)
      TH=6.283185307*R
      R=RANF(0.)
      XMU=2.*R-1.
      R=RANF(0.)
      RHO=.5*D*R**.3333333333
      YM(1)=RHO*SQRT(1.-XMU**2)
      XM(1)=YM(1)*COS(TH)+X
      YM(1)=YM(1)*SIN(TH)
      ZM(1)=RHO*XMU
      RHO=YM(1)**2+ZM(1)**2
      RHO=D*D/4.-RHO
      RHO=SQRT(RHO)
      XR=XM(1)+RHO
      XL=XM(1)-RHO
      IF(XL.LT.0.)XL=0.
      GO TO 100
    5 KEM=MEM
      DO 6 I=1,KEM
      SEP=X-XM(I)-D
      IF(SEP.GE.0.)MEM=MEM-1
    6 CONTINUE
      DO 7 I=1,MEM
      KM=MEM+2-I
      XM(KM)=XM(KM-1)
      YM(KM)=YM(KM-1)
    7 ZM(KM)=ZM(KM-1)
```

```
      MEM=MEM+1
      XL=X
    8 R=RANF(0.)
      XL=XL-ALOG(R)/XLAM
      CALL SPEAR(XL,XR,XM(1),YM(1),ZM(1),D)
      LV=0
      DO 9 I=2,MEM
      SEP=XM(1)-XM(I)
      IF(SEP.GE.D) GO TO 9
      SEP=(XM(1)-XM(I))**2+(YM(1)-YM(I))**2+(ZM(1)-ZM(I))**2
     1 -D*D
      IF(SEP.LT.0.)LV=1
    9 CONTINUE
      IF(LV.EQ.1)GO TO 8
      MEM=MIN0(2,MEM)
  100 CONTINUE
      RETURN
      END
```

```
      PROGRAM RANLAT(INPUT,OUTPUT,TAPE60=INPUT)
      DIMENSION XB(100),ANS(100),WORD(10),ABAR(100),ASIG(100)
    1 READ 2,CSM,CSP,FP,D,NPOS,NSOR,KBAT,NMOM
    2 FORMAT(4E10.3,3I10,5X,I5)
      IF(EOF,60) 1000,3
    3 IF(NMOM.EQ.0)NMOM=1
      IF(KBAT.EQ.0)KBAT=1
      READ 4,(WORD(I),I=1,10)
      READ 5,(XB(I),I=1,NPOS)
    4 FORMAT(10A8)
    5 FORMAT(8E10.3)
      PRINT 6
    6 FORMAT(*1*/* EXPONENTIAL ATTENUATION IN A RANDOM FCC*
     1X*LATTICE*)
      PRINT 7,(WORD(I),I=1,10)
    7 FORMAT(X10A8)
      PRINT 8,NMOM,NSOR,CSM
    8 FORMAT(/* STATISTICAL MOMENT=*I3,/* NO. SOURCE PARTIC*
     1*LES=*I10,/* MATRIX CROSS SECTION(1./CM.)=*E10.3)
      PRINT 9,CSP,FP,D
    9 FORMAT(* SPHERE CROSS SECTION(1./CM.)=*E10.3,/* SPHERE*
     1X*VOLUME FRACTION=*E10.3,/* SPHERE DIAMETER(CM.)=*E10.3)
   12 XMOM=NMOM
      CSM=CSM*XMOM
      CSP=CSP*XMOM
      IF(CSP.GT.CSM) GO TO 13
      CSR=CSP
      SIG=CSM-CSP
      WP=1.
      WM=0.
      GO TO 14
   13 CSR=CSM
      SIG=CSP-CSM
      WP=0.
      WM=1.
   14 PRINT 16,CSR,SIG
   16 FORMAT(* BASE CROSS SECTION(1./CM.)=*E10.3,/* DELTA C*
     1*ROSS SECTION(1./CM.)=*E10.3)
      DO 600 I=1,NPOS
      ABAR(I)=0.
  600 ASIG(I)=0.
      LINE=11
      DO 999 J=1,KBAT
      DO 15  I=1,NPOS
   15 ANS(I)=0.
      DO 20  I=1,NSOR
      K=0
      INT=0
      W=1.
      X=0.
   17 R=RANF(0.)
      X=X-ALOG(R)/SIG
      CALL LACE(X,FP,TYP,D,INT)
```

```
 18 XS=XB(K+1)
    IF(X.LT.XS) GO TO 19
    K=K+1
    ANS(K)=ANS(K)+W
    IF(K.EQ.NPOS) GO TO 20
    GO TO 18
 19 W=WP*TYP+WM*(1.-TYP)
    IF(W.NE.0.) GO TO 17
 20 CONTINUE
    XTOT=NSOR
    LINE=LINE+3
    IF(LINE.LT.60) GO TO 555
    LINE=3
    PRINT 556
556 FORMAT(*1*)
555 CONTINUE
    PRINT 601,J
601 FORMAT(/* BATCH=*I3,/3X*X(CM.)*8X*PHI*)
    DO 21 I=1,NPOS
    PHI=ANS(I)/XTOT
    ABAR(I)=ABAR(I)+PHI
    ASIG(I)=ASIG(I)+PHI*PHI
    X=XB(I)
    LINE=LINE+1
    IF(LINE.LT.60) GO TO 557
    LINE=1
    PRINT 556
557 CONTINUE
 21 PRINT 22,X,PHI
 22 FORMAT(2E12.4)
999 CONTINUE
    IF(KBAT.EQ.1) GO TO 1
    XBAT=KBAT
    LINE=LINE+3
    IF(LINE.LT.60) GO TO 558
    LINE=3
    PRINT 556
558 CONTINUE
    PRINT 700
700 FORMAT(/* BATCH STATISTICS*/3X*X(CM.)*8X*PHI*8X*1SIG*)
    DO 701 I=1,NPOS
    PHI=ABAR(I)/XBAT
    SPH=(ASIG(I)-XBAT*PHI*PHI)/(XBAT-1.)
    SPH=SQRT(SPH)
    X=XB(I)
    LINE=LINE+1
    IF(LINE.LT.60) GO TO 559
    LINE=1
    PRINT 556
559 CONTINUE
701 PRINT 702,X,PHI,SPH
702 FORMAT(3E12.4)
    GO TO 1
```

```
 1000 CONTINUE
      END
      SUBROUTINE LACE(S,FP,TYP,D,INT)
      DIMENSION XC(4,8),YC(4,8),ZC(4,8),XM(2),YM(2),ZM(2)
      IF(INT.EQ.1) GO TO 1
      INT=1
      MEM=0
      A=6.283185307/3./FP
      A=D*A**.3333333333
      RI=A*SQRT(2.)/4.
      RW=RI-D/2.
      A2=A/2.
      R=RANF(0.)
      XO=R*A
      R=RANF(0.)
      YO=R*A
      R=RANF(0.)
      ZO=R*A
      R=RANF(0.)
      WZ=2.*R-1.
      R=RANF(0.)
      TH=6.283185307*R
      WY=SQRT(1.-WZ*WZ)
      WX=WY*SIN(TH)
      WY=WY*COS(TH)
      XC(1,1)=0.
      YC(1,1)=0.
      ZC(1,1)=0.
      XC(2,1)=A2
      YC(2,1)=A2
      ZC(2,1)=0.
      XC(3,1)=A2
      YC(3,1)=0.
      ZC(3,1)=A2
      XC(4,1)=0.
      YC(4,1)=A2
      ZC(4,1)=A2
      XC(1,2)=0.
      YC(1,2)=A
      ZC(1,2)=0.
      XC(2,2)=A2
      YC(2,2)=A2
      ZC(2,2)=0.
      XC(3,2)=A2
      YC(3,2)=A
      ZC(3,2)=A2
      XC(4,2)=0.
      YC(4,2)=A2
      ZC(4,2)=A2
      XC(1,3)=0.
      YC(1,3)=0.
      ZC(1,3)=A
      XC(2,3)=A2
```

```
YC(2,3)=A2
ZC(2,3)=A
XC(3,3)=A2
YC(3,3)=0.
ZC(3,3)=A2
XC(4,3)=0.
YC(4,3)=A2
ZC(4,3)=A2
XC(1,4)=0.
YC(1,4)=A
ZC(1,4)=A
XC(2,4)=A2
YC(2,4)=A2
ZC(2,4)=A
XC(3,4)=A2
YC(3,4)=A
ZC(3,4)=A2
XC(4,4)=0.
YC(4,4)=A2
ZC(4,4)=A2
XC(1,5)=A
YC(1,5)=0.
ZC(1,5)=0.
XC(2,5)=A2
YC(2,5)=A2
ZC(2,5)=0.
XC(3,5)=A
YC(3,5)=A2
ZC(3,5)=A2
XC(4,5)=A2
YC(4,5)=0.
ZC(4,5)=A2
XC(1,6)=A
YC(1,6)=A
ZC(1,6)=0.
XC(2,6)=A2
YC(2,6)=A2
ZC(2,6)=0.
XC(3,6)=A
YC(3,6)=A2
ZC(3,6)=A2
XC(4,6)=A2
YC(4,6)=A
ZC(4,6)=A2
XC(1,7)=A
YC(1,7)=0.
ZC(1,7)=A
XC(2,7)=A2
YC(2,7)=A2
ZC(2,7)=A
XC(3,7)=A
YC(3,7)=A2
ZC(3,7)=A2
```

```
      XC(4,7)=A2
      YC(4,7)=0.
      ZC(4,7)=A2
      XC(1,8)=A
      YC(1,8)=A
      ZC(1,8)=A
      XC(2,8)=A2
      YC(2,8)=A2
      ZC(2,8)=A
      XC(3,8)=A
      YC(3,8)=A2
      ZC(3,8)=A2
      XC(4,8)=A2
      YC(4,8)=A
      ZC(4,8)=A2
    1 X=XO+S*WX
      Y=YO+S*WY
      Z=ZO+S*WZ
      IF(MEM.EQ.0) GO TO 2
      SEP=(X-XM(1))**2 +(Y-YM(1))**2+(Z-ZM(1))**2-RI*RI
      IF(SEP.GT.0.) GO TO 2
      SEP=(X-XM(2))**2+(Y-YM(2))**2 +(Z-ZM(2))**2-D*D/4.
      TYP=0.
      IF(SEP.GT.0.) GO TO 100
      TYP=1.
      GO TO 100
    2 NX=ABS(X)/A
      XR=NX
      XR=XR*A
      IF(X.LT.0.) XR=-A-XR
      NY=ABS(Y)/A
      YR=NY
      YR=YR*A
      IF(Y.LT.0.) YR=-A-YR
      NZ=ABS(Z)/A
      ZR=NZ
      ZR=ZR*A
      IF(Z.LT.0.) ZR=-A-ZR
      X=X-XR
      Y=Y-YR
      Z=Z-ZR
      IF(X.GT.A2)   GO TO 6
      IF(Y.GT.A2)   GO TO 4
      IF(Z.GT.A2)   GO TO 3
      NOC=1
      GO TO 10
    3 NOC=3
      GO TO 10
    4 IF(Z.GT.A2) GO TO 5
      NOC=2
      GO TO 10
    5 NOC=4
      GO TO 10
```

```
  6 IF(Y.GT.A2) GO TO 8
    IF(Z.GT.A2) GO TO 7
    NOC=5
    GO TO 10
  7 NOC=7
    GO TO 10
  8 IF(Z.GT.A2) GO TO 9
    NOC=6
    GO TO 10
  9 NOC=8
 10 K=0
 11 K=K+1
    SEP=(X-XC(K,NOC))**2+(Y-YC(K,NOC))**2+(Z-ZC(K,NOC))**2
   1-RI*RI
    IF(SEP.GT.0.) GO TO 13
    MEM=1
    XM(1)=XR+XC(K,NOC)
    YM(1)=YR+YC(K,NOC)
    ZM(1)=ZR+ZC(K,NOC)
    R=RANF(0.)
    TH=6.283185307*R
    R=RANF(0.)
    XMU=2.*R-1.
    R=RANF(0.)
    RHO=RW*R**.3333333333
    ZM(2)=RHO*XMU+ZC(K,NOC)
    YM(2)=RHO*SQRT(1.-XMU*XMU)
    XM(2)=YM(2)*COS(TH)+XC(K,NOC)
    YM(2)=YM(2)*SIN(TH)+YC(K,NOC)
    SEP=(X-XM(2))**2+(Y-YM(2))**2+(Z-ZM(2))**2-D*D/4.
    TYP=0.
    IF(SEP.GT.0.) GO TO 12
    TYP=1.
 12 XM(2)=XM(2)+XR
    YM(2)=YM(2)+YR
    ZM(2)=ZM(2)+ZR
    GO TO 100
 13 IF(K.NE.4) GO TO 11
    MEM=0
    TYP=0.
100 CONTINUE
    RETURN
    END
```

References

1. Alder, B. J., and Wainwright, T. E., "Studies in Molecular Dynamics," J. Chem. Phys., 31, No. 2, August 1959.

2. Anderson, P. D., and Dunbar, G. R., Title Classified, Sandia Corporation Report, April 1966.

3. Bellman, R., and Cooke, K. L., Differential-Difference Equations, Academic Press, 1963.

4. Burrus, W. R., "How Channeling between Chunks Raises Neutron Transmission through Boral," Nucleonics, 16, No. 1, January 1958.

5. Cantwell, R. M., M0322 and M0332 - Fortran Programs for Calculating Neutron Absorption in Spheres Distributed Randomly, Bettis Atomic Power Laboratory, WAPD-TM-352, October 1962.

6. Chernov, L. A., Wave Propagation in a Random Medium, McGraw-Hill, 1960.

7. MacCallum, C. J., Title Classified, Sandia Corporation Report, July 1967.

8. Soloman, H., "Random Packing Density," Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability, 3, University of California Press, 1967.

9. Uspensky, J. V., Introduction to Mathematical Probability, McGraw-Hill, 1937.

10. Van Vlack, L. H., Elements of Material Science, Addison-Wesley, 1964.

11. Wadsworth, G. P., and Bryan, J. G., Introduction to Probability and Random Variables, McGraw-Hill, 1960.

12. Wing, G. M., An Introduction to Transport Theory, John Wiley and Sons, 1962.

13. Wright, E. M., "Solution of the Equation $ze^z = a$," Bull. Amer. Math. Soc., 65, 1959.

CURRICULUM VITAE

The author was born on March 22, 1942 in Hamilton, Ohio. Remaining in Hamilton, he obtained his primary and secondary education at St. Ann Grade School and Hamilton Catholic High School. He received his B.S. in Engineering Science from the University of Notre Dame in June 1964. The same month, he accepted a position on the technical staff at Sandia Laboratories in Albuquerque, New Mexico. Through the various continued education programs of this employer, the author was able to continue his education at the University of New Mexico. In June 1966, he was awarded an M.S. degree by the Mechanical Engineering Department. He then began his doctoral studies in the Nuclear Engineering Department in January 1967.

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