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MINIMIZATION OF OPTICAL SCATTERING EFFECTS THROUGH USE OF OPTIMAL MONOCHROMATOR SLIT GEOMETRY

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ABSTRACT

The object of this calculation was to determine whether the effects of the scattering of resonance radiation on the data taken from an excitation cross section chamber could be minimized by adjusting the monochromator slit geometry. The study was done on a high-speed digital computer, using random numbers to pick the scattering parameters. This method is shown to give an average number of scatters per photon in agreement with previous studies of the integral equation for the scattering process. Further results of the calculation show that adjustment of the monochromator slit geometry can minimize the effect of scattering and indicate the form this geometry should take.

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SUMMARY

The object of this calculation was to determine whether the effects of scattering of resonance radiation on the output of an excitation cross section chamber could be minimized by adjusting the monochromator slit geometry. The study was done on a high-speed digital computer, using random numbers to pick the scattering parameters. This method is shown to give an average number of scatters per photon in agreement with previous studies of the integral equation for the scattering process. Further results of the calculation show that adjustment of the monochromator slit geometry can minimize the effect of scattering and indicate the form this geometry should take.

INTRODUCTION

Optical excitation chambers are generally cylindrical in shape, with an exciting beam of particles passing down the axis of the enclosure. On one side of the chamber is a lens, which focuses emitted photons on a monochromator slit. If a photon is to be focused on the slit, its line of flight must be such that, if it were projected back into the chamber, it would strike the image of the monochromator slit formed back in the chamber by the lens.

The use of such chambers to study resonance lines generally requires that the bombarded gas number density be kept low to minimize the possibility that the emitted radiation will be scattered by atoms lying outside the excitation region. Unfortunately, if the bombarded gas number density is low, decreased light output of the chamber results in increased difficulty of detection and decreased accuracy of results. Some investigators (ref. 1) have attempted to remedy the situation by the use of asymmetric geometries which minimize the distance a photon must travel through the scattering medium before leaving the chamber on the side of the lens. But such a chamber still permits some radiation to backscatter into the lens.

If all photons directly excited by the exciting beam left the chamber without being scattered, the intensity of emitted radiation would be expected to vary linearly with the bombarded gas number density. The slope of this line is proportional to the excitation cross section of the bombarded gas. However, as shown later, even at very low number densities some of the emitted radiation will be reabsorbed before leaving the chamber. Although the absorption can sometimes be neglected if the number density is kept low enough (ref. 2), it could also lead to sizable experimental error if neglected.

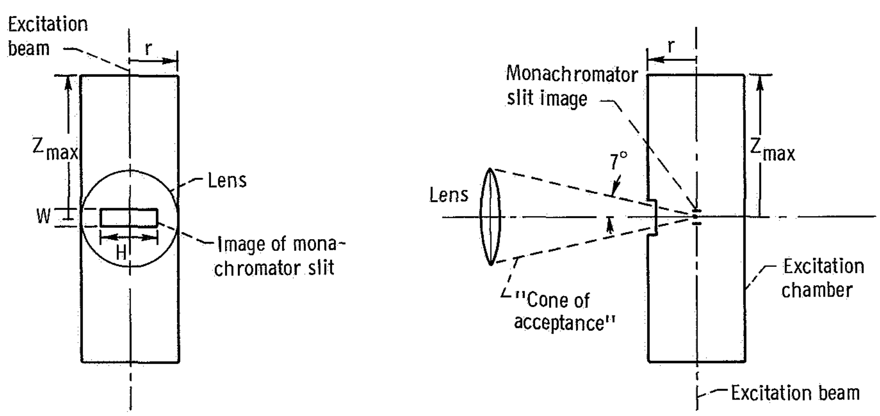
The effect of scattering is essentially to redistribute the excited atoms. Without scattering, only atoms in the direct path of the beam are excited; while for very high number densities, where each photon is likely to be scattered several times before leaving the chamber, the excited atoms essentially fill the chamber. If no quenching (i.e., nonradiative de-excitation) were present, and the detection system encompassed an angle of 4π, so that every departing photon was recorded by the detecting devices, scattering would have no effect on the total light output. However, measurements of time-dependent phenomena - such as lifetime measurements - would still be affected. Quenching effects can often be neglected, but the experimenter is always limited to measuring photons traveling in a fraction of the total solid angle; hence, his measurements will be affected by the distribution of emitting atoms in the chamber. It is the problem of the effect of scattering on measurements taken with a detector in a fraction of the total solid angle which the present calculation attempts to clarify and resolve.

METHOD

In previous studies of this phenomenon, the integral equation which results from the proper description of the scattering process has been solved by approximation of certain of the functions involved (ref. 3) and by numerical methods (ref. 4). Solutions obtained in this manner are generally limited by the approximations involved in the mathematical model, the accuracy of the numerical techniques, or by the idealized geometries employed; without these simplificiations the integral equation would be unmanagable. The method used in this report was to program the equations describing a scattering event and to obtain statistical results from a large number of events. Practical geometries can then be considered, and only the statistics limit the accuracy of the results, as none of the functions involved need be approximated. The limit on accuracy may be the computing time required to get a sufficient amount of data.

In essence, the program records the path of a photon emitted from the axis of the chamber through as many scatters as are required for it to leave the chamber. The exciting beam was idealized as a line source along the axis of the cylinder. To approximate a uniform intensity line source, the axis of the cylinder was divided into as many increments as there were to be emitted photons, and then a photon was started from the midpoint of each increment. Three types of cylindrical geometries were considered: as infinite (axial) length geometry, a unit cylinder (one whose half height equalled its radius), and a cylinder whose half height was three times its radius. The infinite-length cylinder calculations were made by choosing a cylinder length which was so long that a further increase in length did not change the results. The infinite-length cylinder provided values of the average number of scatters of an emitted photon which could be compared with previous solutions of the integral equation, while the finite length geometries are of more practical interest.

The criterion for focusing by a lens was provided by accepting only those departing photons within a specified angle with respect to the line joining the center of the chamber and the center of the lens. The line of flight of each accepted photon was then projected back into the chamber to see if it fell within the image of a monochromator slit located on the cylinder's axis as shown in figure 1. Also figure 1 shows the chamber and monochromator slit criterion as constructed in the program.



(a) View from monachromator slit. (b) Side view.

Figure 1. - Geometry of lens-excitation chamber system.

The initial scattering of the photon from the axial excitation point, and each subsequent scatter, required the selection of three independent scattering parameters: two angles and a scattering distance. Each was chosen through selection of a random number. When possible, the random numbers were used directly in the calculations; in the interest of saving computer time, an indexed table of 1000 equally incremented values of each parameter was made, and the random numbers chosen called values of the parameters through the indexes. The tables were felt to be extensive enough that no significant error could have resulted from their use. It was tacitly assumed that each scattering was isotropic, and there was no correlation between successive scattering distances.

The scattering parameters were chosen in terms of a spherical polar coordinate system. The azimuthal angle and the cosine of the polar angle, whose product gives the solid angle, were each equally incremented as mentioned previously; hence, the total solid angle was divided into equal segments into which a proton could be scattered. The simplest expression for the probability that a particle will travel a distance x in an absorbing medium is

$$p(x) = e^{-K_o x}$$

where K_o, the absorption coefficient of the medium, can be thought of as the reciprocal of the mean free path of the particle in the medium. Spectral broadening and the resulting dependence of absorption coefficient on frequency changes the form of the aforementioned probability function to (ref. 3)

$$p(x) = \int W(\nu)e^{-K(\nu)x}\, d\nu \tag{1}$$

where $W(\nu)$ can be thought of as a weighting function for each frequency ν and $K(\nu)$ is the frequency-dependent absorption coefficient for the absorbing gas. The form of $W(\nu)$ generally depends on the types of broadening present. Frequent experimental interest is in the range of number densities and absorbing layer thicknesses for which Doppler broadening is predominent (ref. 2). In this case, $K(\nu)$ takes on the form

$$K(\nu) = K_o e^{-y^2} \tag{2a}$$

where

$$K_o = \sqrt{\frac{M}{2RT\pi}}\, \frac{\lambda_o^2 g_2}{3\pi g_1}\, \frac{N}{\tau} \tag{2b}$$

and

$$y = \left(\frac{\nu - \nu_o}{\nu_o}\right)\left(\frac{c}{\sqrt{\frac{2RT}{M}}}\right) \tag{2c}$$

Following a treatment by Holstein (ref. 3) $W(\nu)$ can be expressed as

$$W(\nu) = \frac{K(\nu)}{\mathscr{K}} \tag{3}$$

where

$$\mathscr{K} = \frac{\lambda_o^2 g_2}{8\pi g_1} \frac{N}{\tau}$$

and where N is the number density of the absorbing gas, M is its gram-molecular weight, R in the gas constant per mole, T is the absolute temperature, g_1 and g_2 are the statistical weights of the normal and excited states, respectively, τ is the lifetime of the line, c is the speed of light, and λ_o and ν_o are the wavelength and frequency of the center of the line, respectively. These specification give equation (1) the form

$$p(x) = \pi^{-1/2} \int_{-\infty}^{\infty} \exp - \left(y^2 - K_o x e^{-y^2}\right) dy \tag{4}$$

This equation leads to an integral equation for the scattering process, solutions of which have been experimentally verified (refs. 5 and 6).

Before proceeding, it is worth noting the K_o retains its interpretation as the reciprocal of the average path length, in the sense that it now represents an average weighted with respect to frequency as well as averaged over all distances. While making use of equation (2b) it is interesting to note the range of number densities necessary to attain average path lengths of the order of typical chamber dimensions. For the $6^2\ S_{1/2}$-$6^2\ P_{3/2}$ line of cesium (λ_o = 8521 Å), a value of K_o of 1 centimeter^{-1} (average path length of 1 cm) requires a number density of 2.57×10^{10} per cubic centimeter or a pressure of 9.9×10^{-7} torr.

The probability function p(x) in equation (4) with K_o set equal to unity was divided into 1000 equal intervals, and the value of x which produced the midpoint of each interval was calculated. Thus an indexed table was built up which corresponded to equally probable distances a photon could travel. Before being used the table was multiplied by a chosen average path length ($1/K_0$), and hence the number density of the bombarded gas was reintroduced as an adjustable parameter. Again it was felt the table was of sufficient length so that, although only discrete scattering distances were possible, this contributed no significant error to the calculation.

RESULTS

Figure 2 shows the agreement of the results of the program for the average number of scatters a photon undergoes before leaving the chamber with a theoretical curve derived by Holstein (ref. 7) through solution of the integral equation for the scattering process. The dimensionless parameter K_0r is the ratio the chamber radius r to the average path length $1/K_0$, and for a fixed value of r is directly proportional to the

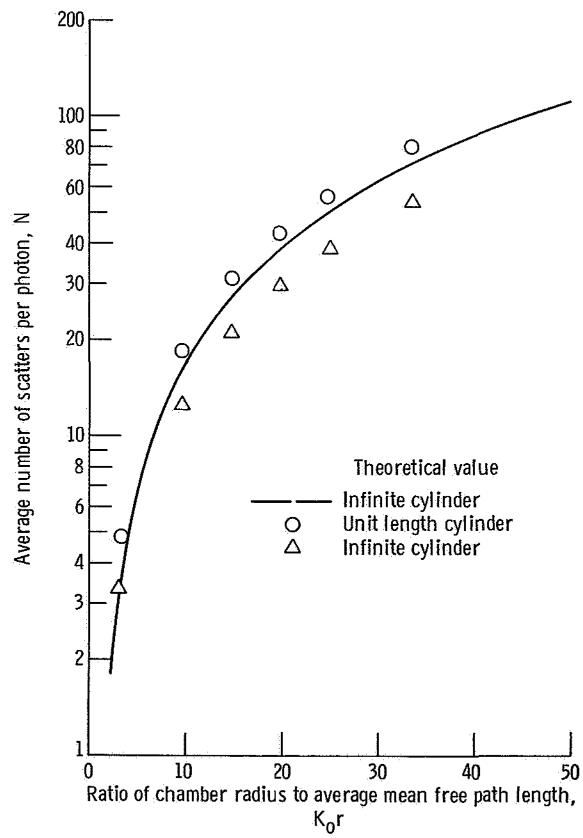


Figure 2. - Average number of scatters per photon N plotted against ratio of chamber radius to average mean free path length K_0r.

number density of the bombarded gas. The theoretical curve is for an infinite cylinder. Plotted with it are values the program produced for the infinite and unit cylinder geometries. It is interesting to note that the results of these two cases do not differ by a great deal.

The photon acceptance ratio is defined as the ratio of the fraction of photons accepted by the lens-slit criterion with scattering present to the fraction that would be accepted if no scattering were present. Figure 3 shows the photon acceptance ratio for a unit cylinder excitation chamber. The abscissa of these plots is the previously mentioned dimensionless parameter $K_0 r$. An optimal slit geometry should have the ratio of accepted photons near one for a wide range of values of $K_0 r$. The slit dimensions W and H are expressed as fractions of the radius of the chamber. Hence, a slit with H = 2.0 is a slit whose radial dimension spans the chamber. Figure 3 illustrates the effects of slit alinement on the number of photons accepted. Also shown in figure 3 is the estimated statistical fluctuation introduced by the computational method. It can be seen that, as the mean path gets smaller (pressure increases), the number of photons accepted by the slit alined parallel to the excitation beam decreases. For example, in the cesium case mentioned, values of average path length of the order of 1 centimeter required pressure of the order of 10^{-6} torr. This pressure can be increased to 10^{-4} torr without the adverse effects of scattering by alining the slit long dimension perpendicular to the excitation beam.

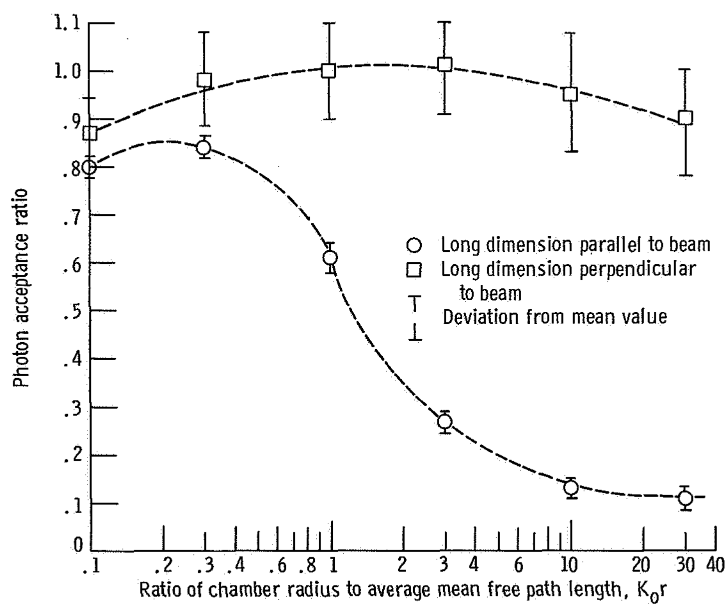


Figure 3. - Ratio of scattered to unscattered accepted photons for rectangular slit with W = 0.1 and H = 2.0 as a function of scattering parameter for two slit orientations. Excitation chamber is cylinder with height equal to diameter.

This figure indicates that slits whose greatest dimension is alined perpendicular to the path of the exciting beam are less affected by scattering than slits whose greatest dimension is alined parallel to the exciting beam. This is true since more photons are scattered out of than into the acceptance region in the latter case because it is the smaller fraction of the chamber volume.

Calculations were made to determine the effect of W, H, and Z_{max} (chamber length) on the number of photons scattered. Qualitative trends are all that can be deduced from the calculations without using a large amount of calculating machine time. This large amount is unwarranted because the applicability of the result is still limited by assumptions (e.g., the assumption regarding the line broadening mechanism.) However, based on other calculations made by the author, it is possible to deduce the following:

(1) The ratio of accepted photons is more sensitive to changes in the radial dimension of the slit than in the axial dimension for a fixed slit alinement. The ratio increases with increasing radial dimension,

(2) The dependence of the ratio of accepted photons upon K_0r at increasing Z_{max} shows the same qualitative trends as shown in figure 3.

(3) The estimated error in the results starting with a fixed number of photons increases as the axial dimension gets smaller. The reduced number of accepted photons is responsible.

Each case in figure 3 was run for two independent trials with completely different sets of random numbers. This not only improved the statistics, but provided a means of estimating the accuracy of the results. In the case of the unit length cylinder, the two different corresponding values showed a percentage difference from their respective means of a maximum of 10 percent and an average of a few percent. A similar calculation with a longer cylinder ($Z_{max} = 3$) did not provide quite as good statistics, with a maximum percentage difference from the mean of 30 percent and an average percentage difference of about 5 percent. The reason for the decreased accuracy in the latter case is that the same number of emitting photons are now spread out over three times the emitting distance that was used in the unit cylinder and this results in fewer photons being accepted by the test, and a corresponding decrease in the accuracy of the statistics.

CONCLUSIONS

Results indicate that a proper choice of slit alinement allows the experimenter to increase his pressure by several orders of magnitude over the pressure that provides a mean free path comparable to the chamber size without significant distortion of the intensity of emitted radiation due to scattering.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, August 9, 1968,
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