TECHNICAL NOTE: AN-916 (Rev. A)
(Feb. 13, 2001)

SIGNAL LEVEL CONSIDERATIONS FOR REMOTE DIFFUSE REFLECTANCE ANALYSIS

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INTRODUCTION:

Near infrared (NIR) spectroscopy has a long history as a quality control technique for the analysis of granular scattering substances such as agricultural products. The instruments used have generally been designed to maximize collection efficiency and hence have used either internal sample compartments or optical coupling by means of large diameter fiber-optic bundles. As a result, such instruments must be located close to the sampling point. Chemical process applications present a new combination of requirements. In particular, the sample streams are often fluids containing scattering centers rather than granular solids. In addition, the process stream is often remote from the instrument, making it necessary to transmit the near-IR radiation to and from the measurement point by means of single optical fibers or economical small-diameter fiber bundles.

The present paper reviews the theoretical information needed to maximize the received signal level in the application of diffuse reflectance to remote on-line process analysis. A second paper (now in production) will consider the behavior of the diffusely reflecting systems involving the inhomogeneous mixtures common to many process applications. Both of these papers are extensions of work previously published (Ref. 1).

BASIC RADIATION TRANSFER CONSIDERATIONS:

For this discussion, we will make a few simplifying assumptions. While these may reduce the accuracy of calculated signal levels, they should not effect our overall goal, which is to provide a framework for optimizing system performance. Our primary assumptions are first that all optical elements are axially symmetric and, second, that a given signal level is constant across a specified area of illumination.

The signal level obtained in a remote diffuse reflectance installation is limited by the fact that a diffusely reflecting sample scatters light into a full hemisphere, while the fiber-optic coupled probe necessarily has a limited collecting aperture and field of view. In general, the total optical power collected by an optical probe viewing a diffuse source of radiation is equal to

$$P_c = \iint N_t \cos\theta \, d\Omega \, dA \quad \text{(Eq. 1)}$$

Here, "N_t" is the radiance of the target. Radiance is defined as the power radiated by the source, in a specific direction, per unit area and solid angle (Ref. 2). For an ideal diffuse (Lambertian) radiator, N is independent of angle, and we can write

$$P_c = \int \cos\theta \, d\Omega \int N_t \, dA =$$

$$\pi \sin^2\alpha_c \int N_t \, dA \quad \text{(Eq. 2)}$$

Where α_c is the half angle field of view of the collecting optics, centered on the normal to the target surface. (See Figure 1.) Using our assumption that the radiance is spatially uniform across the area being viewed, we perform the integral in Equation 2 and write

$$P_c = \pi \sin^2\alpha_c \, N_t A_c$$

Where A_c = viewed area

(Eq. 3)

Note that most diffusely reflecting samples will approximate a Lambertian radiator for illumination within typically 40^o of normal incidence (Ref.3).

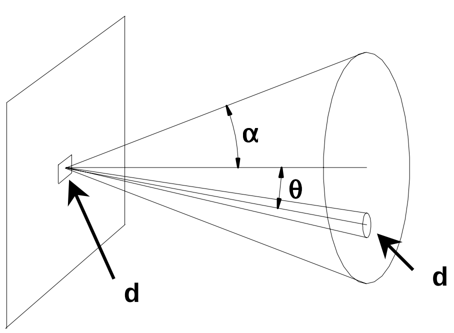

Figure 1. Signal Collection Geometry

GEOMETRIC THROUGHPUT CONSIDERATIONS

Radiation transfer calculations can often be simplified by introducing the concept of "Throughput" (Ref. 4). The "Throughput" of any circular aperture in an optical system is given by:

$$\tau_a = \pi A_a \sin^2\alpha_a \quad \text{(Eq. 4)}$$

where A_a is the area of the aperture, and α_a is the maximum divergence angle of radiation passing through the aperture. (See Figure 2.) Using this definition, we can now rewrite Equation 3 as

$$P_c = \tau_c N_t \quad \text{(Eq. 5)}$$

Where τ_c is the throughput of the collection optics.

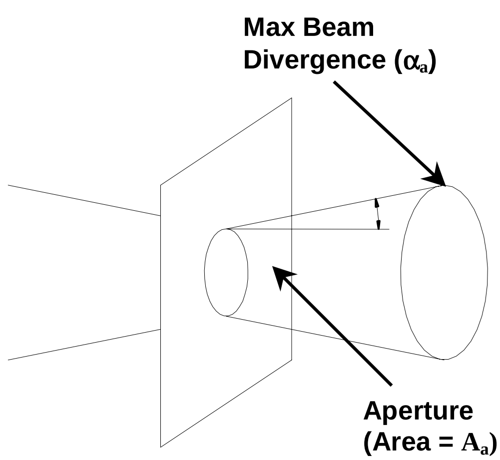

Figure 2: Throughput Definitions

Throughput is often confused with transmission. However, throughput is strictly a geometric quantity whereas transmission is concerned with the various losses of a system caused by such factors as absorption and reflection. Much of the value of "throughput" is embodied in the **Conservation of Throughput Principle**. This states that the throughput of an optical system can be no greater than the lowest throughput of any aperture in the system. Thus, once we have determined the minimum (or "limiting") throughput of a system, we can use to estimate performance under various conditions.

By invoking the conservation of throughput principle, we can now replace Equation 5 by

$$P_c = \tau_L N_t \qquad \text{(Eq. 6)}$$

where τ_L is the limiting throughput of the system. In the case where the limiting throughput is determined by the collection optics we have $\tau_L = \tau_c$.

To obtain an expression for the radiance, N_t, we can take advantage of the fact that the total reflected power is scattered into 180°. For a Lambertian reflector, we can thus write

$$P_t = \tau_\pi N_t, \quad \text{where } \tau_\pi = \pi A_I, \qquad \text{(Eq. 7)}$$

Here, P_t is the total reflected power, i.e. the incident power, P_I, times the reflectance of the target (assumed to be constant), A_I is the illuminated area and τ_π can be thought of as the "Lambertian equivalent throughput".

Thus, if $A_c \leq A_I$,

$$P_c = (\tau_L/\tau_\pi)P_t = (\tau_L/\pi A_I)P_t. \qquad \text{(Eq. 8)}$$

By a similar development, we can show that, if $A_c \geq A_I$, Equation 8 will still be valid if we change A_I to A_c. We thus can generalize this equation to

$$P_c = (\tau_L/\pi A_e)P_t, \qquad \text{(Eq. 9)}$$

Where A_e is the greater of A_I or A_c.

APPLICATION TO A FIBER-OPTIC COUPLED PROBE

For most fiber-optic coupled systems, the fiber cable will present the limiting throughput, i.e. $\tau_L = \tau_{fr}$ and

$$P_c = (\tau_{fr}/\pi A_e)P_t, \qquad \text{(Eq. 10)}$$

where $\tau_{fr} = \pi A_{fr}\sin^2\alpha_{fr}$, and A_{fr} is the optical area of the fiber.

Fiber throughput can be expressed in terms of the numeric aperture $(NA)_{fr}$ of the fiber. This is defined as

$$(NA)_{fr} = \sin \alpha_{fr}. \qquad \text{(Eq. 11)}$$

Thus

$$\tau_{fr} = \pi A_{fr}(NA)_{fr}^{\,2}. \qquad \text{(Eq. 12)}$$

Substituting Equation 12 into Equation 10 yields a simple expression for the collected power in terms of known quantities, i.e:

$$P_c = (A_{fr}/A_e)\,(NA)_{fr}^{\,2}P_t. \qquad \text{(Eq. 13)}$$

where,

A_{fr} = optical area of the receiving fiber or fiber bundle

A_e = the larger of the illuminated or viewed area

$(NA)_{fr}$ = numeric aperture of the fiber

P_t = total power scattered by the Lambertian target.

So far we have only considered the geometrical aspects of signal collection. We now generalize Equations 9 and 13 to take into consideration the various losses in the system.

$$P_r = d_r R_t T_r (\tau_{L}/\pi A_e) P_I \quad \text{(Eq. 14)}$$

$$P_r = d_r R_t T_r (A_{fr}/A_e)(NA)_{fr}{}^2 P_I. \quad \text{(Eq. 15)}$$

Here,

P_r = received power at the detector

P_I = incident power at the target

d_r = core packing density of the receiving fiber bundle

R_t = target reflectance

T_r = overall receiving system transmission on axis

τ_L = the limiting throughput of the system.

TARGET ILLUMINATION

To estimate the power transmitted from the source of radiation to the surface of the target, we can again invoke the conservation of throughput principle. The considerations are similar to those considered above. Assuming that the source is larger than the field of view of the collecting optics, the total power collected will be given by

$$P_s = \tau_s N_s \quad \text{(Eq. 16)}$$

Where τ_s is the throughput of the source collecting optics and N_s is source radiance.

Just as in the case of the receiving system, the transmitted power will be dependent on the limiting throughput of the system. If the transmission system employs fiber optics, its throughput will generally be the determining factor. In this case τ_s will be replaced by τ_{ft} the throughput of the transmitting fiber bundle. The total power delivered to the target will then be

$$P_I = d_t T_t \tau_{Lt} N_s \quad \text{(Eq. 17)}$$

Where,

d_t = core packing density of the transmitting fiber bundle

T_t = overall transmitting system transmission on axis

τ_{Lt} = the limiting through put of the transmitting system

N_s = source radiance

or,

$$P_I = \pi d_t T_t A_{ft} (NA)_{ft}{}^2 N_s \quad \text{(Eq. 18)}$$

where,

A_{ft} = optical area of the transmitting fiber or fiber bundle

$(NA)_{ft}$ = numerical aperture of the transmitting fiber.

Combining Equations 15 and 18 gives an overall expression for the signal obtained in a diffuse reflectance system employing optical fibers for both transmission and reception:

$$P_r = \pi d_r d_t R_t T_r\, T_t\, (A_{fr} A_{ft}/A_e)(NA)_{fr}^{2}(NA)_{ft}^{2} N_s.$$

(Eq. 19)

THEORETICAL MAXIMUM SIGNAL FOR AN OPTIMUM PROBE DESIGN

As a specific example, we will consider an idealized probe system employing a bifurcated fiber bundle with equal numbers of randomized illuminating and receiving fibers. For a typical bundle, we can expect (NA) = 0.22 and a packing density for all fibers of d = 0.55. Thus, for the bifurcated case, we have $d_r = 0.275$. In addition, we will assume the ideal case in which $R_t = T_r = 1$. Substituting these values in Equation 15 yields

$$P_r = 0.0133\, (A_{fr}/A_e) P_I$$

(Eq. 20)

Where, again

P_r = received power
P_I = incident power at the target.

Using the same set of assumptions for the transmitting portion of the system, we have

$$P_I = 0.0418\, A_{ft} N_s.$$

(Eq. 21)

And finally, since $A_{fr} = A_{ft} = A_f$,

$$P_r = 5.56\text{x}10^{-4} (A_f^{2}/A_e) N_{s.}$$

(Eq. 22)

This example illustrates two important points:

First, the total signal power available is proportional to the area of the receiving fiber times the area of the transmitting fiber. This is a consequence of the fact that the diffuse reflectance process destroys the spatial coherence of the signal. Thus, the target must be considered as a new Lambertian source having a total power determined by the signal transmitted from the original source.

Second, the available power is inversely proportional to the effective area of the target (i.e the greater of the illuminated or viewed areas).

CONCLUSIONS AND IMPLICATIONS FOR SYSTEM DESIGN

This paper has provided a simple framework for estimating the signal levels to be expected in the design of fiber-optic coupled diffuse reflectance sampling systems. It illustrates the fact that the performance obtained is ultimately limited by the area and numeric aperture of the fiber cables used for both illumination and detection. In addition, there is an inherent trade-off between signal level and illuminated area.

In practice, the problem of limited fiber throughput is mitigated to a certain extent by the extremely high sensitivities of the InGaAs detectors now available for us in the near-IR spectral region. However, for many applications, there is marked trade-off between cost and performance. This is particularly true when long fiber runs are required or when granularity of the samples necessitates a large illuminated area.

From Equations 15 and 18, it is clear that for a given illuminated and view area, the signal level in the ideal case can only be increased by increasing the areas of the receiving and/or transmitting fibers or by increasing the source power. However, for many spectroscopic analyzers, other limitations will soon come into play even if the economics allows an increase in fiber area. For example, rapid scanning systems such as FTIR spectrometers require high speed detectors, which are generally not available in large areas. In addition, the throughput of the spectrometer optics can be a significant limitation.

One possibility for increasing performance is to include both of the elements with inherently limited throughput (i.e. the spectrometer optical system and detector subsystem) in the same leg of the analysis system. This enables the signal level in the illuminating portion of the system to be increased by maximizing fiber-optic throughput and possibly source intensity. In the extreme case, the source can be located close to the measurement point. In this case it may be practical and economical to use a large fiber bundle or to eliminate the transmitting fibers completely. However, for many process applications this would require an intrinsically safe, and hence expensive, source subsystem.

Despite the limitations of remote fiber-optic coupled diffuse reflectance analysis, there are many situations in the benefits greatly outweigh the difficulties. This field is still at an early stage of implementation. However, it offers promise for a number of different areas of application, and there is yet much that can be done to match performance to the needs of the various requirements.

REFERENCES:

1. W. M. Doyle, Remote Diffuse Reflectance Analysis for Process Applications, in: *Proceedings of the Conference on Spectroscopy in Process and Quality Control*, East Brunswick NJ, June 7-8, 1999.

2. W. L. Wolf, (Ed.), *Handbook of Military Infrared Technology*, Office of Naval Research, Washington DC. 1965, p. 22.

3. Gustav Kortuem, *Reflectance Spectroscopy*, Springer-Verlag, Berlin, p. 33.

4. W. L. Wolf and G. J. Zissis (Eds.), *The Infrared Handbook*, prepared by the Environmental Research Institute of Michigan for the Office of Naval Research. Washington DC. 1978, p. 20-8.