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Coal Dust Explosibility and Particle-Size Distribution

By Robert F. Chaiken

UNITED STATES DEPARTMENT OF THE INTERIOR



BUREAU OF MINES

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**UNITED STATES DEPARTMENT OF THE INTERIOR
Bruce Babbitt, Secretary**

BUREAU OF MINES

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UNIT OF MEASURE ABBREVIATIONS USED IN THIS REPORT

cm centimeter

mg/cm³ milligram per cubic centimeter

L liter

wt % weight percent

mg/cm² milligram per square centimeter

COAL DUST EXPLOSIBILITY AND PARTICLE-SIZE DISTRIBUTION

By Robert F. Chaiken

ABSTRACT

An absorption-desorption model of particle reactivity was employed to describe the observed relationship between two apparently diverse phenomena which have been the subject of considerable study at the U.S. Bureau of Mines: (1) coal-rock dust reflectance and (2) coal-rock dust explosibility. The model accounts for heterogeneities in particle-size and material properties; however, in the present report, only particle-size distribution is considered. A mean particle-size parameter, appropriate to the explosion extinction process, is derived, and then taken as appropriate to describing optical reflectance. The derived form-to-function relationships for the two processes, when compared with experimental data, suggest that a problem exists with previously derived theory relating optical reflectance to rock dust concentration. A reexamination of that theory leads to a new theoretical expression, changed by a factor of 2, for the variation of rock dust concentration with reflectance which is in quite good agreement with experimental results. The current work offers justification for measuring and establishing rock dust requirements for specific coal dust size distribution(s) found in the mine—distributions that undoubtedly depend on the mining method and the type of coalbed.

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INTRODUCTION

It has long been understood that when dealing with the reactivity of a collection (ensemble) of solid particles, the distribution of particle sizes should be considered. This usually means determining a mean diameter for the particle ensemble, which often requires making a decision as whether the mean should be linear, area, or volume weighted. The choice is not arbitrary, but should be dictated by the mechanistic character of the particle phenomenon that is being considered, e.g., whether it is a surface reaction, volume reaction, or simply something that relates to a linear dimension. To see how particle averaging works in this approach, let us first examine the mean volume-surface radius, \bar{r}_{32} , which is defined as

$$\bar{r}_{32} = \frac{\langle r^3 \rangle}{\langle r^2 \rangle} = \frac{\int_0^{\infty} r^3 n(r) dr}{\int_0^{\infty} r^2 n(r) dr} \quad (1)$$

where $n(r)$ is the statistical number distribution of particles, a function of particle radius (r) as determined by a measuring device. The measuring device itself may implicitly add statistical weight to the particle-size distribution due to the method of measurement, e.g., Coulter Counter² measurements relate to particle volume, whereas sieve analysis relates to a particle minimal linear dimension.

The volume-surface radius is not quite the same as the mean surface radius, $\langle r^2 \rangle^{1/2}$, which is defined through the equation

$$\langle r^2 \rangle^{1/2} = \left[\frac{\int_0^{\infty} r^2 n(r) dr}{\int_0^{\infty} n(r) dr} \right]^{1/2} \quad (2)$$

In either case the mean size, while seemingly a single parameter, actually depends on the total particle ensemble whose description (i.e., size distribution) is generally

multiparametric. To illustrate this, examine a normalized lognormal number distribution of particle size, i.e.,

$$n(r) = \frac{h}{r \sqrt{\pi}} e^{-[h \ln(r/r_0)]^2} \quad (3)$$

Two parameters, r_0 , the mean particle radius, and h , the spread of the distribution (often called the variance, $1/\sigma^2$), define the lognormal distribution. The average value of r raised to any integral order, k , (i.e., the k th moment) is for this case

$$\langle r^k \rangle = \int_0^{\infty} r^k n(r) dr = r_0^k e^{(k/2h)^2} \quad (4)$$

Thus, it is seen that in general two parameters, r_0 and h , are required to define any characteristic dimension for an entire collection (or ensemble) of particles. The above discussion points out that a problem can arise when one compares experimental measurements with mathematical descriptions that model the phenomena measured. More specifically, if particle size is a factor in the model, the averaged particle size selected may not be appropriate for defining the relationship of the particle ensemble to the experiment. This is illustrated by applying equation 4 to the averaged radii depicted by equations 1 and 2:

$$\frac{\bar{r}_{32}}{\langle r^2 \rangle^{1/2}} = \exp \left[\frac{3}{4h^2} \right] \quad (5)$$

Depending on the spread of the particle-size number distribution, the two averaged radii could differ by a factor of 10 or more.

It is the purpose of this report to show how particle-size heterogeneity and the relationship of particle-size distribution to particle pyrolysis explains observed explosibility criteria of dispersed coal dust and rock dust mixtures. Rock dust or calcium carbonate (CaCO_3) is an inerting material, whose use in coal mines for the prevention of dust explosions (*1*)³ has been pioneered by the U.S. Bureau of Mines.

²Reference to specific products does not imply endorsement by the U.S. Bureau of Mines.

³Italic numbers in parentheses refer to items in the list of references preceding the appendixes at the end of this report.

ACKNOWLEDGMENT

The author is indebted to several colleagues at the Pittsburgh Research Center for numerous illuminating discussions related to this problem: M. J. Sapko, research supervisor, for introducing the problem; H. E. Perlee,

group supervisor and J. C. Edwards, research physicist for informative discussions; and K. L. Cashdollar, research physicist, for particle-size information.

BACKGROUND

During the development of an optical reflectance meter for determining the amount of rock dust in mixtures of coal and rock dust, it was observed that an excellent correlation between the optical measurement and the mass fraction of rock dust could be obtained through the following expression (2-3):

$$\Phi \equiv \frac{I - I_c}{I_r - I_c} = \frac{f_r}{f_r + K(1 - f_r)} \quad (6)$$

Here, I is the measured reflection intensity of the dust mixture; $I_{r,c}$ is the measured reflectance of samples consisting of 100% rock dust and 100% coal dust, respectively; f_r is the mass fraction of rock dust; and K is treated as an empirical constant that is used to calibrate the meter readings for a specific coalbed. The theory used to derive equation 6 showed that K varied as the ratio of rock dust to coal dust particle sizes,

$$K(\text{theory}) = \frac{r_r \rho_r}{r_c \rho_c} \quad (7)$$

where $r_{r,c}$ and $\rho_{r,c}$ are considered surface weighted radii and densities of the rock dust and coal dust, respectively.

ABSORPTION-DESORPTION (A-D) MODEL

In the A-D model as applied to combustion, it is assumed that the rate controlling process is associated with slow mass transport within a particle via a diffusion wave (i.e., a pyrolysis front) moving along a path of "shortest distance" (λ) from a point within the particle to a point on the outer surface of the particle, or perhaps to a point in a fracture channel (or crack) through which the diffusing species is then quickly (compared with diffusion) transported to the surface. Taking the statistical number density distribution of such "shortest distances" describing an ensemble of particles to be $f(\lambda)$, then the rate of a reaction, $R(t)$, i.e., generation of pyrolysis products, due to the moving diffusion front be written as

$$R(t) = f(\lambda) (d\lambda/dt) = f(\lambda) v_\mu \quad (8)$$

However, in practice, much better correlation with experimental data is obtained when K is treated as an empirical constant whose value is determined by curve-fit of equation 6 to $\Phi(f_r)$ measurements.

Interestingly, it was also discovered in separate studies that the concentration of rock dust, which just inhibits a coal-rock dust explosion (Φ^*) appears to be relatively constant for dusts from the same type of coal independent of the particle-size distribution, e.g., $\Phi^* = 0.20 (\pm 0.03)$ for Pocahontas coal and $\Phi^* = 0.30 (\pm 0.04)$ for Pittsburgh coal (4). This implies a relationship between the K (which for the cases considered varied from about 5 to 28) and the concentration of rock dust needed to inert the coal dust (rock dust varied between 63 and 87 wt %) (1). Since variations in K for a given coal type relate to variations in particle-size distribution, it would be beneficial to be able to understand the relationship(s) between Φ^* , K , and the size distribution parameters so as to predict the explosibility of coal-rock dust mixtures. A recent absorption-desorption (A-D) model of intra-particle mass diffusion in solid particles, which is based directly on distribution theory (5), offers one possible approach to achieving this objective. The sections that follow describe this approach.

where v_μ is the velocity of the diffusion wave (related to the diffusion coefficient). In essence, reaction is the disappearance of reaction sites as they are overtaken (i.e., desorbed) by the diffusion wave. An alternative view is that reaction coincides with the appearance of a high-temperature thermal wave moving (i.e., absorbed) along paths of "shortest distance," which results in pyrolysis. The fundamental equations for describing heat conduction and mass diffusion in solids are almost identical (6-7).

It should be emphasized that λ is a *real* linear dimension in that it is measurable and relates directly to the reaction process, for every point within a particle there is at least one "shortest distance" to a surface or a crack. This can be contrasted to "particle radius" as a dimension, where except for uniformly homogeneous spheres, "particle

radius" is a *fiction*, having an effective value that usually depends on the method of measurement rather than the reaction process itself. One might expect a relationship

between λ and "particle radius;" however, it would undoubtedly depend on both the particle shape and its fracture or porosity distribution.

MODEL FOR EXPLOSIBILITY OF COAL DUST

Explosibility of a dust mixture is believed by many researchers to be associated with the generation through coal pyrolysis, of gaseous hydrocarbons that can support combustion (8). Pyrolysis of the coal will yield mostly hydrocarbon gases and pyrolysis of the rock dust will yield mostly carbon dioxide—an inerting gas. Given the above assumptions, explosibility criteria for a coal-rock dust mixture can then be defined as

$$\frac{\dot{m}_c(t)}{\dot{m}_r(t)} = \hat{m}(t) \geq \hat{m}^* \quad (\text{a constant}) \quad (9)$$

where $\dot{m}_{c,r}$ are the mass rates of gases liberated by the coal and rock dust particles, respectively, as a function of time; \hat{m} is the mass ratio of coal to rock dust pyrolysis products at time, t ; and \hat{m}^* is a certain mass ratio that must be exceeded for the pyrolysis gas mixture to be flammable. Assuming that gasification is controlled by intra-particle diffusion, then by equation 8, the ratio of the coal and rock dust rates can be expressed as

$$\hat{m} = \frac{R_c(1-f_r) M_T}{R_r f_r M_T} = \hat{R} \left[\frac{1-f_r}{f_r} \right] \quad (10)$$

where M_T is the total mass of the coal-rock dust mixture.

In the above expression, the mass fraction of rock dust (f_r) would actually be time dependent due to differences in the gasification rates of coal dust and rock dust. However,

when applied to the condition of explosion prevention (i.e., little or no reaction occurring), f_r should be near its initial value, which is taken to be the value referred to in equation 6. Therefore, equations 6 and 10 can be combined to eliminate f_r , yielding

$$K = \frac{1-\Phi}{\Phi (\hat{m}/\hat{R})} \quad (11)$$

Since the explosibility criteria stipulates that $\Phi = \Phi^*$ (a constant) and $\hat{m} = \hat{m}^*$ (also a constant) then

$$K/\hat{R} = A^*, \quad (\text{a constant}). \quad (12)$$

From equations 8 and 12, and for the case of dust mixtures where only the coal particle-size distribution is changed (i.e., where the rock dust and material properties are constant),

$$K = B^* f(\lambda), \quad (13)$$

where the rock dust reaction rate and the coal dust diffusion wave velocity have been incorporated, along with A^* , into the proportionality constant B^* . Equation 13 along with equation 6 represent the sought after expressions relating Φ^* , K , and $f(\lambda)$. It now remains to determine an appropriate distribution function for shortest distances for the dusts under consideration.

APPLICATION TO EXPERIMENTAL DATA

Table 1 lists material properties for two bituminous coals (Pocahontas and Pittsburgh coalbeds) whose explosibility limits have been studied extensively in the USBM 20-L dust explosion chamber (1).

Thirteen different samples (8 Pocahontas and 5 Pittsburgh) comprising a wide range of particle-size distributions were examined. The results are shown in table 2.

Also shown in table 2 are the size distribution parameters as determined by curve-fitting Coulter Counter measured diameters (coal dust and rock dust) to a lognormal distribution curve. The coefficient of determination in all

cases but two exceeds 0.8, and in most cases exceeds 0.9, which indicates that the volume of the particles making up the coal dust samples can be reasonably described by a lognormal distribution normalized to unit volume, i.e.,

$$g_v(r) = \frac{h_v}{r \sqrt{\pi}} e^{-[h_v \ln(r/r_0)]^2} \quad (14)$$

In what follows, the particle characteristic size, r , will refer to spherical radius; r_0 is the mean value of r ; the subscript v on g and h signifies the distribution is by volume.

Table 1.—Proximate analyses of sample coals, percent¹

	Coalbed	
	Pocahontas	Pittsburgh
Moisture	0.6	0.9
Ash	6.0	6.0
Volatility	17.1	36.5
Fixed carbon	76.3	56.6

¹Taken from Cashdollar and Hertzberg (7).

Table 2.—Lognormal size distribution by volume percent: regression analyses results¹

Coal sample	Median diameter, Do (micron)	Distribution spread, h _v	R square, R ²	fr at extinction ³
Pocahontas:				
A	42.51	1.26	0.965	0.63
B	42.79	.51	.924	.67
C	25.09	.58	.983	.74
D	26.70	.73	.938	.78
E	12.19	.85	.981	.83
F	15.37	.88	.526	.78
G	9.81	.79	.982	.87
H	5.22	1.89	.56	.84
Pittsburgh:				
A	36.43	.99	.960	.76
B	40.00	.83	.801	.79
C	24.88	1.04	.916	.79
D	7.02	1.74	.893	.87
E	5.66	1.79	.975	.89
Rock Dust: A	18.7	.61	.783	NAP

NAP Not applicable.

¹Based on Coulter Counter size measurements furnished by K. Cashdollar, U.S. Bureau of Mines, Pittsburgh Research Center.

²Coefficient of determination.

³Cashdollar and Hertzberg (7); Pocahontas G data by personal communication, K. Cashdollar, U.S. Bureau of Mines.

For spheres, the volume-size distribution can be easily converted to a number-size distribution by recognizing that

$$\begin{aligned}
 dv(r) &= V_T g_V(r) dr \\
 &= (4/3)\pi r^3 dn(r) \\
 &= (4/3)\pi r^3 N_T g_N(r) dr \quad (15)
 \end{aligned}$$

where $v(r)$ = volume of particles of size r in the ensemble,

V_T = total volume of particles in the ensemble,

r = particle size (radius),

$n(r)$ = number of particles of size r in the ensemble,

N_T = number of particles in the ensemble,

and $g_N(r)$ = size distribution normalized to unit number.

This yields

$$g_N(r) = \frac{3V_T}{4\pi N_T} \frac{g_V(r)}{r^3} \quad (16)$$

A lognormal size distribution by volume leads to a number distribution that is highly skewed to the smaller particle sizes. It now remains to relate particle size to the shortest distance parameter, a problem that is not readily resolved, except the simple case of particle ensembles composed of homogeneous spheres of isotropic composition—the case assumed here.

For a single particle having a uniform density of points of interest, ρ_λ , the shortest distance to each point of interest is its radial distance from the particle surface. According to the A-D model, the total time derivative of the number of shortest distances, $dn_p(\lambda)/dt$, is then the single particle reaction rate $R_p(t)$ that is given by

$$\begin{aligned}
 R_p(t) &= \frac{dn_p(\lambda)}{dt} = \rho_\lambda \frac{dv_p(r,\lambda)}{dt} \\
 &= \rho_\lambda \frac{\partial v_p}{\partial \lambda} \frac{d\lambda}{dt} = 4\pi \rho_\lambda (r - \lambda)^2 v_\mu \quad (17)
 \end{aligned}$$

where the single particle volume, $v_p(r,\lambda)$ is expressed as a function of size and shortest distance. The particle size, r , is taken independent of time. Equation 17 has the implied constraint that $r \geq \lambda$. For a constant diffusion wave velocity and recognizing that $\rho_\lambda = N_T/V_T$, the rate of reaction for the entire ensemble becomes

$$R(t) = \int_{r=\lambda}^{\infty} R_p(t) g_N(r) dr = 3 v_\mu \int_{r=\lambda}^{\infty} \frac{(r-\lambda)^2}{r^3} g_V(r) dr \quad (18)$$

Assuming the maximum rate of reaction (i.e., the initial rate, equivalent to setting $\lambda = 0$) is the rate appropriate to the extinction phenomenon, we obtain from equations 4 and 18

$$R_{\max} = 3v_\mu \frac{e^{(1/4h_v^2)}}{r_0} \quad (19)$$

This same result could have been obtained more easily by recognizing from the start that the maximum rate of reaction for the single spherical particle occurs at its surface, i.e., $R_{\max} = 4\pi\rho_{\lambda}r^2v_{\mu}$. The maximum rate of reaction for the entire particle ensemble is then simply the mean of the maximum rate, i.e., $\langle R_{\max} \rangle$, which is exactly what equation 19 represents. The longer route taken to develop equation 19 serves to emphasize the reality of the "shortest distance" parameter and its role (i.e., the form-to-function relationship) in defining the reaction rate for particle ensembles that are heterogeneous in size shape, or material properties (e.g., porosity and reactant distribution)—although in the current case only size heterogeneity is considered. Also, equation 18, as derived from the A-D model has greater generality than simply assuming equation 19. One might wish to consider a reaction rate criteria different from R_{\max} in which case equation 18 would be evaluated for $\lambda \neq 0$.

Substituting equation 19 into equation 13, while combining all the material constants into a single coefficient yields

$$K = C^* \frac{e^{(1/4h_v^2)}}{r_o} \quad (20)$$

The right-hand side (RHS) argument of equation 20 is actually the mean reciprocal particle size, $\langle r^{-1} \rangle_v$, based on the lognormal volume-distribution of size (see equations 4 and 14). This is the functional size parameter that relates K to coal-rock dust explosibility, and therefore, also should relate K to coal-rock dust reflectivity. As indicated in equation 7 for $K(\text{theory})$, the coal particle-size argument (derived for mono-sized spherical particles) is indeed $1/r_c$. Hence, in evaluating the factor $K(\text{theory})$ for coal dusts having a distribution of sizes, it is reasonable to expect that $\langle r_c^{-1} \rangle_v$ should be the functional size parameter for describing the particle ensemble. By an analogous argument, the direct linear proportionality of $K(\text{theory})$ to rock dust particle size, r_r (see equation 7) would suggest the appropriate rock dust size parameter to be $\langle r_r \rangle_v$ rather than the surface weighted mean used by the previous authors (2-3).

A test of equation 20 is shown in figure 1 where the experimental values of K are plotted against the mean reciprocal diameter as determined from the curve-fitted lognormal size distributions (by volume) (see table 2). The data show a reasonable linear relationship according to

equation 20. While the curve-fitted constant coefficients, C^* , for the two coals differ by about 20%, the data scatter actually indicates little if any significant difference between them. On the basis of the observed experimental values of Φ^* (0.2 and 0.3 for Pocahontas and Pittsburgh, respectively), one might expect C^* for Pocahontas coal to be as much as 50% greater than that for Pittsburgh coal (see equation 11); however, there are material factors other than Φ^* that are included in C^* , but are not explicitly accounted for in the present discussions.

A test of the functional size parameters as found for $K(\text{theory})$ as defined by equation 7 is shown in figure 2 where $K(\text{exptl})$ is plotted against

$$\begin{aligned} K(\text{theory}) &= (2.8/1.3) \langle D_r \rangle_v \langle D_c^{-1} \rangle_v \\ &= 2.15 (D_{or}/D_{oc}) \exp[(1/2h_{vr})^2 - (1/2h_{vc})^2]. \end{aligned} \quad (21)$$

It is seen that the data points in figure 2 do indeed follow reasonably well a straight line, but the slope of that line is almost exactly one-half of what it should be to have agreement between theory and experiment.

The explanation for the factor of 2 discrepancy prompted a reexamination of the original theoretical development of Φ in terms of the mass fraction of rock dust as given by Perlee (2). The details of this reexamination are presented in the appendix to this report where it is shown that an optically thick mixture of rock dust with coal dust will reflect infrared light in a manner such that the effective mass fraction of the coal dust is exaggerated at the expense of the rock dust. This difference in reflectance of well mixed dust components relative to that of the pure components (not mixed) can account for the factor of 2 difference between $K(\text{theory})$ of equation 7 and $K(\text{exptl})$ that is depicted in figure 2. In the general case, the new expression for Φ is given by equation A-12 (in the appendix), which for the specific coal-rock dust mixtures considered here, becomes

$$\Phi = \frac{f_r}{f_r + 2 \left[\frac{\rho_r r_r}{\rho_c r_c} \right] (1 - f_r)} \quad (22)$$

with a theoretical coefficient, K , which is twice that depicted by equations 6, 7, and 21.

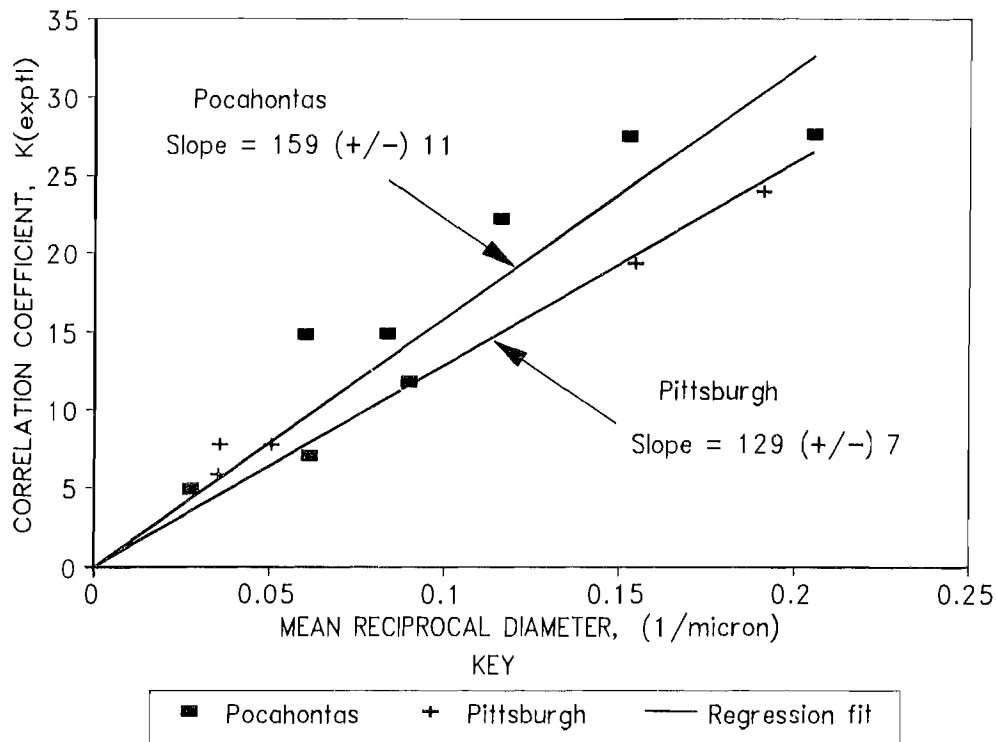


Figure 1.—Test of A-D model correlation to coal dust reflectance parameter.

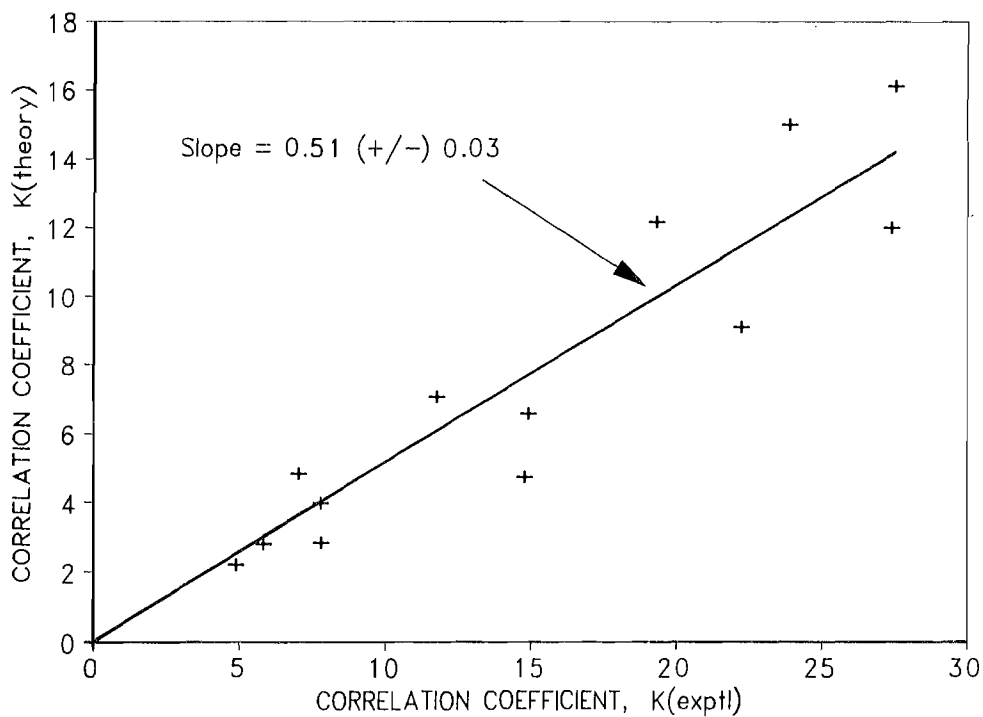


Figure 2.—Test functional size parameter for K(theory).

SUMMARY

Mechanistic considerations of particle reactivity in coal-rock dust mixtures were employed to describe the observed relationship between two apparently diverse phenomena, namely (1) coal-rock dust reflectance and (2) coal-rock dust explosibility. An absorption-desorption model of intra-particle mass transport, which makes use of distribution theory, was used to describe the rate of the dust particle devolatilization reaction during combustion. The model explicitly accounts for heterogeneities in the particles making up the dust mixtures being tested—such heterogeneities being differences in size, shape, and/or material properties. In the current case, only size difference was treated—the coal dust being taken as spheres having isotropic material properties. An averaged particle-size parameter appropriate to explosion extinction was derived from the model. This same size parameter (i.e., the reciprocal of particle size) should be identical to that which relates the particle-size distribution to the reflectance phenomena.

The above findings, while consistent with limited available experimental data, also pointed out an apparent factor of 2 discrepancy between the theoretical and

experimental coefficients relating the rock dust mass fraction to reflectance intensity, i.e., $K(\text{theory})$ and $K(\text{exptl})$. This led to a reexamination of the theory of optical reflectance as applied to a dust mixture where one component of the mixture is semi-transparent and the other semi-opaque (9-10). For the coal-rock dust mixtures described in this report, these considerations (see appendix) lead to a factor of 2 increase in the value of $K(\text{theory})$, thereby bringing theory and experiment into agreement.

The findings in this study follow in part from the use of a lognormal size distribution (by volume) to describe the coal dust samples. While this particle distribution does represent a good fit to the coal dusts studied, other size distributions should be evaluated to see if they would lead to different results.

The derived relationships between those particle-size parameters associated with reflectance and those associated with explosibility offer an opportunity to establish rock dust requirements for specific coal dust size distribution(s) found in the mine—distributions that undoubtedly depend on the mining method and the type of coalbed.

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APPENDIX A.—REFLECTANCE FROM COAL-ROCK DUST PILE

The optical reflectance parameter, Φ , as defined previously by Perlee (2)¹ compares in a relative way the reflection intensity of an optically thick pile of coal-rock dust (well mixed) with the reflection from piles of pure rock dust and pure coal dust, i.e.,

$$\Phi = \frac{I - I'_c}{I'_r - I'_c} = \frac{I_r + I_c - I'_c}{I'_r - I'_c} \quad (\text{A-1})$$

where $I_{r,c}$ are the respective rock and coal dust contributions to the overall reflection, I , from the mixture; the primed quantities referring to the pure infinitely thick dust layer.

When reflection occurs solely from the top layer of the dust pile (i.e., the illuminated surface), or if the transmission of the incident light through the pile were the same for both components of the mixture, the contribution of each component to the overall reflection intensity would be in proportion to their respective particle areas in the mixture, e.g.,

$$\Phi = \frac{\epsilon_r I_o P + \epsilon_c I_o (1-P) - \epsilon_c I_o}{\epsilon_r I_o - \epsilon_c I_o} = P \quad (\text{A-2})$$

where P is the fractional area of rock dust in the dust pile (equal to that in a given layer of dust); and $\epsilon_{r,c} I_o$ are the reflected intensities from optically thick piles of pure rock dust and pure coal dust, respectively.

Converting the area ratios to mass ratios is accomplished through the expression

$$\begin{aligned} \text{AREA OF PARTICLES} &= \frac{(4/3)\pi r^3 \rho n}{(4/3)\rho r} \\ &= \frac{f M_T}{(4/3)\rho r} \end{aligned} \quad (\text{A-3})$$

where f is the mass fraction of one component of the dust layer; M_T is the total mass; and n is the number of component particles.

This leads directly to equation 6 which is repeated here, i.e.,

$$\Phi_p = P = \frac{f_r}{f_r + K(1-f_r)} \quad (\text{A-4})$$

with $K = (\rho r)_r / (\rho r)_c$ being the K_p (theory) described in equation 7; the subscript p is employed here to distinguish these quantities from the ones that are developed in what follows.

A problem in applying equation A-4 arises when one of the components of the dust mixture is somewhat transparent (e.g., rock dust) and the other component somewhat opaque (e.g., coal dust). Coal particles in layers at some depth under the rock dust will then contribute to the overall reflection while rock dust particles in layers under the coal dust will not. Relative to the reflection intensity from single component dust piles, the reflecting area of coal dust particles in a mixture of coal and rock dust will be enhanced while the reflecting area of the rock dust particles will be decreased. This is the situation that is considered here, which accounts for the factor of 2 discrepancy between K (theory) and K (exptl) as depicted in figure 2.

From the theoretical treatment of reflectance from layers of coal and rock dust given Sapko (9), the reflection intensity as a function of depth into a dust pile situated atop a totally absorbing substrate can be expressed as

$$I = \alpha I_o \int_0^X e^{-2Bx} dx = \frac{\alpha I_o}{2B} (1 - e^{-2BX}) \quad (\text{A-5})$$

where α is the reflectance per unit thickness of the dust, B is a Bouguer-Beer-Lambert transmission coefficient for the dust, and X is the depth into the pile. Constructing the pile in layers of thickness, D , the particle diameter, enables X to be expressed as several layers, $k = X/D$. The contribution of reflectance from any given layer, ΔI_k , is then

$$\Delta I_k = I_k - I_{k-1} = \frac{\alpha I_o}{2B} (1 - e^{-2BD}) e^{-2BD(k-1)}. \quad (\text{A-6})$$

The total reflectance is the sum of all the layers, N , i.e.,

$$I(N) = \sum_{k=1}^N \Delta I_k = \frac{\alpha I_o}{2B} (1-b) \left[\frac{b^N - 1}{b - 1} \right] \quad (\text{A-7})$$

where $b = \exp(-2BD)$. For many layers, $I(N=\infty) = \alpha I_o / 2B = \epsilon I_o$, the reflection intensity from an optically thick pile of dust of one component.

For a two component mixture of dust particles such as rock dust that is semi-transparent, and coal dust, which is semi-opaque, contributions to the reflection intensity will be from all particles in which light is not blocked by the appearance of opaque coal dust in an overlying layer.

¹Italic numbers in parentheses refer to items in the list of references preceding the appendixes at the end of this report.

Thus coal dust under rock dust will contribute, but rock dust under coal dust will not.

Since P , the area fraction of rock dust particles in a dust pile, is also the effective probability of light falling on a rock dust particle in any given layer of a well-mixed dust pile, the probability that light will not be blocked by a coal particle to a depth of k layers is given by P^k . Likewise the probability of a coal dust particle lying below $k-1$ rock dust particles is $P^{k-1}(1-P)$. From equation A-7, the rock dust reflectance becomes (where ΔI_k is replaced by $P^k \Delta I_k$).

$$I_r(N=\infty) = \epsilon_r I_o P \left[\frac{1-b_r}{1-Pb_r} \right] \quad (A-8)$$

where subscript r is used to delineate the rock dust characteristics. The contribution from coal dust particles in the first layer is given by

$$I_c(N=1) = \epsilon_c I_o (1-b_c)(1-P) \approx \epsilon_c I_o (1-P) \quad (A-9)$$

and from those lying under a continuous string of $k-1$ rock dust particles, it is

$$I_c(N \geq 2) = \frac{\alpha_c I_o}{2B_r} (1-b_r)(1-P) \sum_{k=2}^{\infty} (Pb_r)^{k-1}. \quad (A-10)$$

Adding equations A-9 and A-10 together, one gets the total contribution from the coal namely,

$$\frac{I_c}{I_o} = \epsilon_c (1-P) + \epsilon_r \left[\frac{\alpha_c}{\alpha_r} \right] \left[\frac{(1-b_r)(1-P)(Pb_r)}{1-Pb_r} \right]. \quad (A-11)$$

After some manipulation, and noting that $I'_r - I'_c = (\epsilon_r - \epsilon_c)I_o$, equations A-1, A-8, and A-11 yield

$$\Phi = P \left\{ \frac{\left[\frac{1-b_r}{1-Pb_r} \right] \left[1 + (\alpha_c/\alpha_r)(1-P)b_r \right] - (\epsilon_c/\epsilon_r)}{1 - (\epsilon_c/\epsilon_r)} \right\}. \quad (A-12)$$

This expression for Φ when compared with equation A-4 indicates the theoretical correlation constant will indeed be different from that represented by K_p . To preview the difference, consider the conditions where the alpha and epsilon ratios in equation A-12 are much less than unity so that

$$\Phi \approx P \left[\frac{1-b_r}{1-Pb_r} \right]. \quad (A-13)$$

A value of b_r equal to 0.5 then leads to $\Phi = P/(2-P)$, and from equation A-4 for P ,

$$\Phi = \frac{f_r}{f_r + 2 \left(\frac{r_r \rho_r}{r_c \rho_c} \right) (1-f_r)}. \quad (A-14)$$

Under these conditions, the appropriate K (theory) is actually a factor of 2 greater than that predicted by equation 22 (or equation A-4 for Φ_p), and within experimental scatter, leads to good agreement with the K (exptl) (see figure 2).

Support for the above considerations comes from the experimental reflection studies carried out at the U.S. Bureau of Mines on layers of rock dust and layers of coal dust (9). First, are measurements of reflection from rock dust on a thick coal dust substrate at different rock dust loading densities up to 10 mg/cm². From these data, an experimental value for b is obtained. In the notation of the current report, Sapko (9) reports that²

$$2B_r DN = (0.24 \pm 0.04) \sigma_r \quad (A-15)$$

where the surface loading density of the rock dust, σ_r is given in milligram per square centimeter. The thickness of a single layer of rock dust is represented by the particle diameter of the rock dust used in the experiments, $D = 0.001$ cm, and $N=1$. This leads to a value of $\sigma_r = \rho_r D = 2.7$ mg/cm², and a best value for b ,

$$b = e^{-2B_r D} = 0.52 \quad (A-16)$$

which is quite consistent with the discussions leading to equation A-14.

Additional support for equation A-14 comes from the data on reflection from coal dust layers on a thick rock dust substrate. Here, it is found that

$$2B_c DN = (0.96 \pm 0.14) \sigma_c, \quad (A-17)$$

²Readers are advised that the paper by Sapko (9) contains an error where the expressions for rock dust reflectivity and coal dust reflectivity have been apparently switched (equations 5 and 6; equations 10 and 11).

which is equivalent to

$$2 B_c = 0.96 \rho_c \quad (\text{A-18})$$

where the volume density is given in milligram per cubic centimeter. Noting that $\epsilon_{c,r} = \alpha_{c,r}/2B_{c,r}$, the numerical values of $B_{c,r}$ as obtained from the reflection measurements lead to

$$\frac{\epsilon_c}{\epsilon_r} = \frac{324 \alpha_c}{624 \alpha_r} = 0.52 \left[\frac{\alpha_c}{\alpha_r} \right]. \quad (\text{A-19})$$

Equation A-12 for Φ can now be evaluated numerically for different values of P and the alpha ratio, and the results compared with the value of Φ obtained from equation A-13 with $b_r = 0.52$. Over a wide range of values, ($0.1 \leq P \leq 1$) and ($0.001 \leq \alpha_c/\alpha_r \leq 1$), the two Φ 's are the same within 2%. The apparent insensitivity of Φ , as calculated from equation A-12, to changes in the value of the alpha

ratio lends some additional support for equation A-13 and for setting $K(\text{theory})$ equal to $2K_p$.

It is interesting that the relatively simple one-dimensional theory of reflection by Sapko (9) still appears applicable to so complex a phenomena as reflection from a multicomponent dust pile. Factors such as nonisotropic photon scattering within the pile, multiple three-dimensional reflections, particle-packing arrangement, and varying surface effects (e.g., water absorption) are known to influence reflectivity (10), yet they are not explicitly accounted for in this treatment. One might presume that their role in reflectivity has been accounted for by the empirical determination of the transmission and reflectance coefficients (see equations A-15 and A-17), and hence, the simple geometrical approach of assuming opaque and non-opaque areas is appropriate. However, as in the case of many modeling studies, the adequacy of one model to fit experimental data does not exclude the possibility that another model may be more appropriate; particularly when all possible factors have not been considered.

APPENDIX B.—SYMBOLS USED IN THIS REPORT

Upper Case

A^*, B^*, C^*	= proportionality constants set by extinction criteria
B	= light transmission coefficient for a dust pile
D	= particle diameter
I, I'	= measured reflection intensity of optically thick dust pile (two component mixture, single component) - (see equation A-1)
K or K_p	= a geometric coefficient relating rock dust mass fraction to reflectance area (see equations 7, 20, and A-4)
M_T	= total mass of dust mixture
N	= total number of layers in a dust pile
N_T	= total number of particles
P	= probability factor (geometric area)
R or $R(t)$	= rate of reaction (particle pyrolysis)
\hat{R}	= ratio of rates of reaction (coal dust to rock dust)
V_T	= total volume of particles

Lower Case

b	= light transmittance (see equations A-6 and A-7)
f_r	= mass fraction of rock dust
$f(\lambda)$	= number density distribution of λ , a "shortest distance"
$g_N(r)$	= number density distribution of s , a particle size
$g_V(r)$	= volume density distribution of r , a particle size
h	= spread parameter for density distribution (related to standard deviation, σ)
\dot{m}	= rate of mass gasification
\hat{m}	= ratio of mass gasification rates (coal dust to rock dust)

Lower Case—Continued

$n(r)$	= number of particles of size, r
r	= particle radius
$\langle r^k \rangle$	= mean of r^k , i.e., the k th moment of a size distribution
t	= time
v_μ	= diffusion wave velocity
$v(r)$	= volume of particles of size, r

Greek Symbols

α	= reflectance per unit thickness of dust
ϵ	= reflectance for an optically thick pile of dust consisting of a single component
Φ	= relative reflection intensity (see equations 6 and A-1)
λ	= a "shortest distance" parameter (see equation 8)
ρ	= density of mass
ρ_λ	= density of points of interest within a particle - generally the sites of reactant material (see equation 17)

Subscripts

c	= refers to coal dust
N	= refers to number
o	= statistical mean value (when referred to particle size); incident condition (when referred to light)
p	= refers to single particle
r	= refers to rock dust
v	= refers to volume