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Scavenging Models for Smokes

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Abstract

The smoke and obscuration computer model known as the Combined Obscuration Model for Battlefield Induced Contaminants (COMBIC) has the potential for treating the effect of precipitation scavenging as one of the model's input parameters. This report examines the impact of rainfall on the evolution of a white phosphorous (WP) smoke cloud based upon the predictions of the model. The result of the analysis indicates that the effect of precipitation scavenging is less than the error expected in COMBIC predictions. Therefore, the recommendation is not to incorporate more elaborate precipitation models in COMBIC.

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1. Introduction

The study of precipitation scavenging has an extensive history and development that began with the desire to model clouds and rain. The term "precipitation scavenging" means the removal of material present in the atmosphere by falling precipitation. When clouds form, the atmospheric water vapor is collected around a nucleation particle that floats within the cloud. As the particle moves, additional water is collected until the particle reaches sufficient size and mass to begin falling to the ground. This description and representation of the phenomenology can be traced back to the analysis of the operation of the Wilson cloud chamber (which was in use in 1903), if not earlier. Currently, the description has been extended to include many additional scientific representations including such complex phenomena as the turbulent motion of aerosols that occur within a storm cloud and the chemical interaction of the particles.

Scavenging also takes place when the precipitate from the cloud passes through aerosols nearer to the ground. Work on this phenomenology began to attract attention when a national concern about nuclear fallout was expressed. This topic received an additional analytical impetus in the 1960s and 1970s when environmental pollution began to achieve national importance. Many sophisticated models have evolved from this extensive work as well as some simple parametric representations of the phenomenology. This report addresses the question as to whether an appropriate choice for the model can be identified that can be integrated with the Combined Obscuration Model for Battlefield Induced Contaminants (COMBIC) [1]. This model predicts the growth and extent of battlefield obscurants as well as the transmission through the obscurant. Knowing the extent to which the obscurant could be reduced by precipitation scavenging could be tactically significant.

2. Scavenging

The theoretical development of many scavenging models is formulated from material balance considerations [2]. Alternate approaches to this development can be based either on energy considerations or momentum considerations. A general form of the differential equation representing the material balance for the change of the aerosol concentration is given by the following equation:

$$\frac{\partial n}{\partial t} = -\nabla \bullet (n\,\bar{v}) + w\,, \tag{1}$$

where $\bar{v}$ is the velocity of the aerosol and w is a source term. Note that all the terms in this equation can be functions of both the position, r, and time, t. In this analysis we will take the source term to be zero.

Following the analysis presented by Pruppacher and Klett [3, p. 380, eq 12-80], the scavenging coefficient, Λ, is defined by the equation

$$-\frac{1}{n}\frac{\partial n(r,t)}{\partial t} \cong \Lambda(r,t)\,, \tag{2}$$

where $n(r,t)$ is the aerosol concentration. A very simple model occurs if the scavenging coefficient does not vary with time. Then the last relationship can be integrated and written as

$$n(r,t) = n(r,0)e^{-\Lambda(r)t}. \tag{3}$$

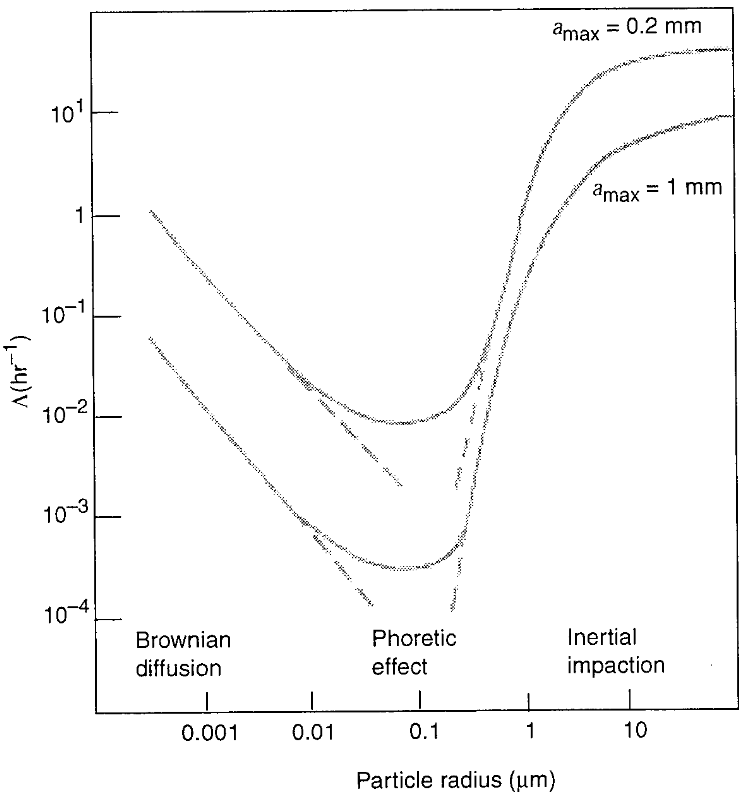
Within COMBIC, a modified form of this equation is used to model the process for removing mass by deposition on the ground or evaporation. A constant additional parameter, $\mathrm{f_d}$, is added to the equation. The purpose of this parameter is to represent a residue remaining after removing all that can possibly be scavenged. When this parameter is included, the equation takes the form

$$n(r,t) = n(r,0)[\mathrm{f_d} + (1-\mathrm{f_d})e^{-\Lambda(r)t}]\,. \tag{4}$$

However, within the context of this analysis, this parameter should be set to zero.

The value for the scavenging coefficient depends on the scavenging mechanism prevalent for the aerosol particle size being considered. For a small aerosol particle with a radius less than $0.1\ \mu$m, the primary capture mechanism is Brownian diffusion. For particles with a radius greater than $1.0\ \mu$m, the primary capture mechanism is inertial impaction. Particles with radius values falling between these two values (commonly called the Greenfield gap) have a number of other mechanisms that generate the scavenging. Figure 1 shows a curve of the scavenging coefficient values as a function of aerosol particle size for two different distributions of raindrop size [3, p. 395, fig. 12-10].

Figure 1. Scavenging coefficient versus aerosol particle size [3].



In this figure, the term phoretic effect refers to two phenomena called thermophoresis and diffusiophoresis. The former refers to the motion of particles arising from the nonuniform heating of particles due to temperature gradients in the suspending gas. Diffusiophoresis refers to particle motion arising from concentration gradients in a gaseous mixture. The parameter a_{max} is a value that determines the maximum raindrop size for the distribution function. This distribution function will be discussed below. Other parameters include the temperature difference between the surface of a droplet and the bulk aerosol of 3 °C, a precipitation rate of 10 mm hr^{-1}, and a drop terminal velocity given by the relationship (8000 a) cm s^{-1}, with a in cm. Note that in these curves, a particle radius of greater than $\sim 0.5\,\mu m$ or less than $\sim 0.002\,\mu m$ would be required to obtain a scavenging coefficient greater than 0.1 hr^{-1}. The value of 0.1 hr^{-1} is relatively small, since it represents only a 10-percent decrease in the particle density after 1 hr of precipitation.

3. Number Distributions

In the following analysis, I focused on white phosphorous (WP) as the obscurant and wanted to select a single value for the WP particle radius and a single value for the raindrop size. This does not represent a real situation. Each of the particles has an associated size distribution and I need to examine how well a single value represents a realistic situation.

3.1 White Phosphorous Distribution

According to the information in [4], experiments by Jennings and Gillespie in 1978 [5] have shown that the particle size spectrum is closely approximated by a lognormal distribution [4, p. 31]. This distribution is given to be [4, p. 18, eq 19]

$$n(r) = \left[\frac{N}{r\sqrt{2\pi}\,\ln(\sigma_g)}\right] \exp\left[\frac{-\,(\ln r - \ln r_g)^2}{2(\ln(\sigma_g))^2}\right] \quad , \tag{5}$$

where

σ_g = geometric mean standard deviation,
r_g = geometric mean radius in μm, and
N = aerosol particle number density (particles per cm^3).

Another equation given in the report [4, p. 19, eq 21] relates these parameters to the mass concentration C by the relationship

$$C = \frac{4}{3}\pi\rho N r_g^3 \exp\left[\frac{9}{2}(\ln\sigma_g)^2\right] \quad . \tag{6}$$

Values for these parameters are given in [4, p. 32, table 16]. Since I am interested in precipitation scavenging, the values I take here are for WP at a 90-percent relative humidity. For that case

$r_g = 0.365\ \mu$m,
σ_g = 1.450,
$\rho = 1.178$ g/cm^3, and
$C = 10^6 \mu$g/m^3.

Note that the value used for C is a representative value that was appropriate for the analysis being done in the report [4]. Since I am concerned only with the relative distribution of particle sizes, that value will be used here. However, before making the substitution, I obtain the relationship between the mass density and the number density. Substituting these values into the last relationship yields

$$C = 4.466 * 10^{-13} * N. \tag{7}$$

For the representative mass-loading value of $10^6 \mu g/m^3$, then, the particle density N is determined to be $2.24 * 10^6$ particles/cm^3.

Figure 2 shows a plot of the function for these values. Note that the particle density is not a sharp function of the particle radius. For the number density to drop by a factor of two from its peak value at 0.365 micrometers, the radius would have to be either as small as about 0.2 μm or as large as about 0.5 μm. While this particle size range lies within the inertial impaction portion of the scavenging coefficient curve, it does extend into the Greenfield gap portion of that curve.

3.2 Raindrop Distribution Function

The raindrop size distribution function used in the preceding section is given by the relationship (see the caption for figure 12- 10 in [3]),

$$n(a) = 10^{-4} \frac{R}{6} \pi a_{\max}^7 a^2 \exp(-2 \frac{a}{a_{\max}}) \ , \tag{8}$$

where a is the raindrop size in cm and R is the precipitation rate in cm s^{-1}. This relationship is also known as the Khrgian-Mazin drop-size distribution. See figure 3 for a plot of these distributions. The value used for the precipitation rate R in the curves is equal to 1/3600 cm s^{-1} = 10 mm/hr. In the PFNDAT report [4, p. 24, table 9], a rain rate of 10 mm/hr is termed a thunderstorm, 5 mm/hr is a widespread rain, and 1 mm/hr is a drizzle.

Depending on other environmental conditions such as vertical wind draft, different values can be obtained for the maximum value size. No rationale

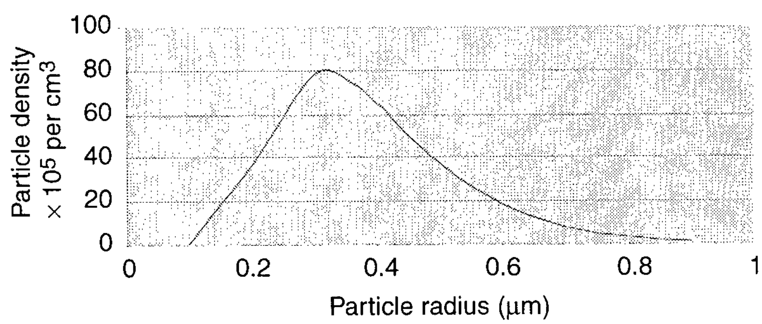


Figure 2. White phosphorous distribution.

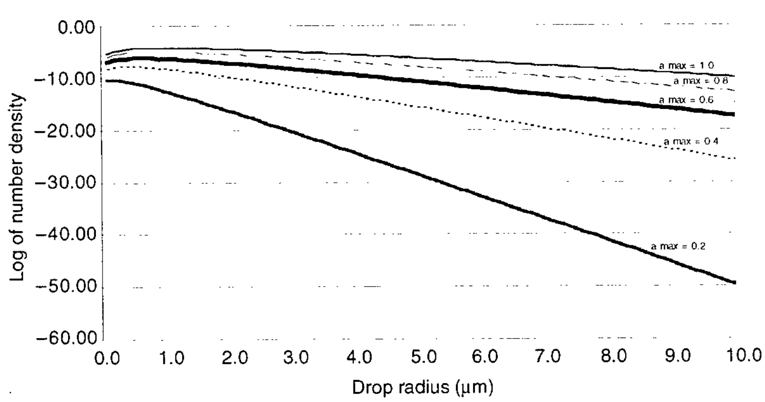


Figure 3. Raindrop distribution.

for selecting one size over another exists. This implies that we will want to consider the full dynamic range of the scavenging coefficient that is restricted only by the WP particle size. Based on the scavenging curve, the range of values for the scavenging coefficient Λ will range from about 2×10^{-4} per hr to 5×10^{-2} per hr. The impact of this range of values on the growth of a WP smoke cloud will be examined in the next section.

4. Cloud Growth Modeling

The model to be used to examine the growth of a WP smoke cloud is COMBIC [1], which has two phases for computing the growth of battlefield obscurants such as dust, smoke, and clouds, and for determining atmospheric extinction along user-determined line-of-sight. The model has evolved through several versions beginning in 1982 to 1992. Source code is written in FORTRAN 77.

COMBIC can be separated into two parts. The first part computes the growth of a puff or a plume under the influence of diffusion, gravity, and external winds. A basic assumption for the computation is that the cloud is an ellipsoidal Gaussian distribution. The physical equations that describe the growth will maintain the Gaussian form of the result, although the parameters describing the shape will deform. Results of this computation are placed into an auxiliary database that is indexed based on the time since the cloud was started. If several different types of clouds are generated, each one is accorded its own descriptive growth. This database is available for further analysis and is the basis for the following discussion.

Two important points with regard to COMBIC need to be highlighted: first, an error exists in some versions of COMBIC in the way parameter initialization is performed when a nonzero scavenging coefficient is used. This problem has been corrected in the code used here. However, if a reader using the software has scavenging results that are peculiar, the code used to duplicate these results may not reflect the required correction. Second, a zero wind speed should not be used since it can cause a discontinuity in the computation for cloud growth. In part of the code, a minimum value of 0.25 m/s is required and is automatically set for the computation. An undocumented recommendation is that the lowest wind speed that should be used is 1 m/s.

Two runs were made of COMBIC. The first run assumed that no scavenging was taking place. The second run assumed that a scavenging coefficient of $2 \times 10^{-5}\ s^{-1}$ was appropriate for representing the WP distribution. All other environmental parameters were the same (wind speed = 1 m/s, relative humidity 90 percent). The results of these computations are given in table 1.

Note that the maximum mass difference between the scavenging and nonscavenging cases does not exceed 1.5 percent of the total mass produced. Similarly, the transmission measured between two points perpendicular to the windborne flow of the smoke does not show any significant differences between the two cases. The wind speed has a greater effect on the amount of time the obscurant remains within a given location, reducing the transmission. Within the accuracy of this model, scavenging effects can be ignored for determining the airborne mass and transmission of WP.

A quick check was run with the use of a scavenging coefficient that was 10 times larger and then again with the coefficient 100 times larger. Only in the latter case did significant effects begin to occur. Since those values are completely outside the range of the data considered here, the results were ignored.

Table 1. Comparison of two scavenging values.

Time (s)	Mass produced	Airborne $\Lambda = 0$	Airborne $\Lambda = .00002$	% Difference/ 100
1	189.6	189.6	189.6	0.000
10	1865.5	1865.5	1865.1	0.000
20	3663.4	3663.4	3661.9	0.000
30	5395.4	5395.4	5392.2	0.001
40	7063.5	7063.5	6995.9	0.010
50	8669.1	8669.1	8590.5	0.009
60	10214.1	10214.1	10122.8	0.009
70	11700.2	11700.2	11594.3	0.009
80	13128.9	13128.9	13011.8	0.009
90	14502.0	14502.0	14376.8	0.009
100	15821.0	15821.0	15688.2	0.008
110	17087.5	17087.5	16947.9	0.008
120	18303.1	18303.1	18157.4	0.008
130	19469.4	19469.4	19317.5	0.008
140	20587.7	20587.7	20430.0	0.008
150	21659.7	21659.7	21496.1	0.008
160	22686.8	22686.8	22517.2	0.007
170	23670.5	23670.5	23494.8	0.007
180	24612.2	24612.2	24430.3	0.007
190	25513.2	25513.2	25325.1	0.007
200	26375.1	26375.1	26180.5	0.007
210	27199.0	27199.0	26998.0	0.007
220	27986.4	27986.4	27778.7	0.007
230	28738.6	28738.6	28524.2	0.007
240	29456.9	29456.9	29235.6	0.008
250	30142.5	30142.5	29914.3	0.008
260	30796.7	30796.7	30561.4	0.008
270	31420.7	31420.7	31178.3	0.008
280	32015.7	32015.7	31766.1	0.008
290	32582.8	32582.8	32326.1	0.008
300	33123.3	33123.3	32859.3	0.008
310	33638.2	33638.2	33366.9	0.008
320	34128.8	34128.8	33850.1	0.008
330	34595.9	34595.9	34309.9	0.008
340	35040.8	35040.8	34747.3	0.008
350	35464.4	35464.4	35163.5	0.008
360	35867.8	35867.8	35559.4	0.009
370	36251.9	36251.9	35936.0	0.009
380	36617.7	36617.7	36294.4	0.009
390	36966.3	36966.3	36635.4	0.009
400	37298.4	37298.4	36960.0	0.009
410	37615.0	37615.0	37269.1	0.009
420	37917.0	37917.0	37563.5	0.009
430	38205.3	38205.3	37844.2	0.009
440	38480.6	38480.6	38111.9	0.010

Table 1. Comparison of two scavenging values (cont'd).

Time (s)	Mass produced	Airborne $\Lambda = 0$	Airborne $\Lambda = .00002$	% Difference/ 100
450	38743.7	38743.7	38367.4	0.010
460	38995.6	38995.6	38611.5	0.010
470	39236.8	39236.8	38844.8	0.010
480	39468.3	39468.3	39067.7	0.010
490	39690.2	39690.2	39280.7	0.010
500	39902.7	39902.7	39484.3	0.010
510	40106.2	40106.2	39678.7	0.011
520	40301.1	40301.1	39864.6	0.011
530	40487.7	40487.7	40042.1	0.011
540	40666.4	40666.4	40211.6	0.011
550	40837.5	40837.5	40373.6	0.011
560	41001.3	41001.3	40528.3	0.012
570	41158.2	41158.2	40676.0	0.012
580	41308.5	41308.5	40817.1	0.012
590	41452.4	41452.4	40951.7	0.012
600	41590.2	41590.2	41080.3	0.012
610	41722.1	41722.1	41203.0	0.012
620	41848.4	41848.4	41320.1	0.013
630	41969.4	41969.4	41431.8	0.013
640	42085.3	42085.3	41538.4	0.013
650	42196.2	42196.2	41640.1	0.013
660	42302.4	42302.4	41737.1	0.013
670	42404.2	42404.2	41829.6	0.014
680	42501.6	42501.6	41917.8	0.014
690	42594.9	42594.9	42001.8	0.014
700	42684.2	42684.2	42081.9	0.014
710	42769.7	42769.7	42158.2	0.014
720	42851.7	42851.7	42230.8	0.014
730	42930.1	42930.1	42300.1	0.015
740	43005.2	43005.2	42365.9	0.015
750	43077.1	43077.1	42435.8	0.015
760	43146.0	43146.0	42495.2	0.015
770	43212.0	43212.0	42551.6	0.015
780	43275.1	43275.1	42605.3	0.015

5. Conclusions

This simplified model predicts that the effect of scavenging on a WP smoke is minimal. While some slight changes occur both in the mass produced by the burning source and the transmission through the resulting cloud, the differences between these numbers are not great enough to warrant confidence when using results that cover long periods of time. In addition, since the assumptions about both raindrop and smoke particle size had the effect of maximizing the scavenging coefficient, the error would be on the side of a worst-case analysis, that is, the true effect of scavenging is even less than these results would indicate.

From a tactical viewpoint, when small amounts of smoke are deployed, it is better to wait for the wind to remove the smoke than depend on the scavenging by precipitation. For large amounts of smoke that are continuously deployed, scavenging is not an important factor.

I made a search to determine if any experimental data supporting the scavenging coefficient used for WP exist. None were found. The major reason for this omission is that the equipment used when WP and other militarily significant smokes were measured would not operate in a rainy environment. Measurements on WP are available for fair weather and snowy conditions.

Consider the original question of whether an appropriate choice for the scavenging model can be identified that can be combined with COMBIC. A simple model is already present within COMBIC requiring the input of only a single parameter. Until experimental data can be obtained demonstrating an error in the estimates obtained with the use of this simple approach, enhancing the representation is not necessary. Of greater importance are the effects of terrain and nonuniform wind fields on the scavenging of smokes and other obscurants.

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The smoke and obscuration computer model known as the Combined Obscuration Model for Battlefield Induced Contaminants (COMBIC) has the potential for treating the effect of precipitation scavenging as one of the model's input parameters. This report examines the impact of rainfall on the evolution of a white phosphorous (WP) smoke cloud based upon the predictions of the model. The result of the analysis indicates that the effect of precipitation scavenging is less than the error expected in COMBIC predictions. Therefore, the recommendation is not to incorporate more elaborate precipitation models in COMBIC.

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