Effects of Aerosol-Induced Heating on the Convective Boundary Layer

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(Manuscript received 22 December 1976, in revised form 29 August 1977)

ABSTRACT

A two-stream solar radiation model was combined with a mixed-layer model to study the effects of absorbing aerosols on the thermal structure of the daytime convective boundary layer. A number of simulations were conducted with the model. The results showed that the criterion used in climatic models to determine the cooling or warming effect of aerosols was not readily applicable to micrometeorological scales. It was also found that soil-interface properties were at least as important as aerosol properties in determining aerosol-induced effects. Any conclusions about aerosol effects on the PBL have to be qualified by statements about surface parameters to be meaningful.

An average of the PBL and surface temperatures ($\theta_a$) is suggested as a physically meaningful indicator of aerosol effects. The results show that aerosols increase $\theta_a$ over surfaces which are relatively wet or have high reflectances; dry, low-albedo surfaces, however, are associated with a decrease in $\theta_a$ in the presence of aerosols.

Another important conclusion of the study is that the soil-PBL system has a built-in mechanism to regulate aerosol-induced heating of the PBL and cooling of the surface. The degree of regulation is dependent on soil-PBL interface properties.

1. Introduction

In recent years, there have been a number of studies (Zdunkowski and McQuage, 1972; Bergstrom and Viskanta, 1973; Atwater, 1974; Viskanta et al., 1975; Zdunkowski et al., 1976) on the effect of gaseous and particulate pollutants on the microclimate of the urban area. The results of most of these studies indicate that gaseous pollutants, which interact primarily in the infrared spectrum, tend to heat the earth’s surface by increasing the downward thermal radiation. While there is general agreement on this result, the conclusions regarding the effects of aerosols are still the subject of considerable controversy (Ackerman et al., 1976). This lack of consensus is related to two reasons. First, radiation properties, which determine aerosol-induced effects, are poorly understood. Second, most of the studies have modeled turbulent transport via the concept of eddy diffusivity which has been shown (Deardorff, 1975) to have limited relevance to the physics of the daytime convective boundary layer. Furthermore, the availability of a multitude of eddy diffusivity models has made any general agreement between different investigators very difficult.

In this paper, we attempt to bypass the problems associated with the use of eddy diffusivities by treating the daytime PBL as a mixed layer. Current research (Deardorff and Willis, 1974; Tennekes, 1973; Carson, 1973) indicates that the dynamics of the daytime PBL indeed can be explained very well in terms of the mixed-layer (or inversion rise) concept. Then, the paper represents an attempt to study the radiative effects of aerosols by incorporating a radiative transfer model into a satisfactory PBL model.

The paper also reports results of a preliminary study to determine the role of surface parameters in partitioning the net solar energy absorbed by the earth-PBL system between the soil layer and the PBL. Previous related studies have not looked into this aspect of the local pollution problem although some global climatic studies (Mitchell, 1971) have underscored the importance of surface properties.

The model, consisting of a two-stream solar radiation model and a slab model (mixed layer) of the PBL, is admittedly less detailed than those used by other investigators (Bergstrom and Viskanta, 1973; Zdunkowski et al., 1976). However, we feel that the simple model which retains all the important physics of the problem facilitates the discovery of simple physical relationships. This type of understanding is much more difficult to obtain from a more detailed model. Also, the simplicity of the model allows the study of a number
of physical situations with almost negligible computational effort.

2. The PBL model

We assume that aerosols interact only with the solar spectrum. We will provide justification for this assumption at a later stage. Thus, from the point of view of this study, the PBL of interest is that which occurs during the daytime hours. As the convective boundary layer capped by a stable layer is a realistic representation of the daytime PBL (Carson, 1973), we use the Tennekes-Carson mixed-layer model. This choice allows us to avoid the specification of eddy diffusivities. Furthermore, the mixed-layer or inversion-rise model has gained a degree of respectability over the past few years. In the words of Tennekes (1976), "the accumulated experience of the last three years indicates that current inversion-rise models perform exceedingly well. Thus, for most practical purposes the inversion-rise problem may be regarded as solved."

The model of the study is one-dimensional in the sense that PBL variables have been horizontally averaged over the polluted region under consideration. While horizontal averaging does not eliminate the effects of horizontal inhomogeneity, we can choose our region to be large enough to make the advection terms negligible. Alternatively, the one-dimensional model could be appropriately applied to stagnation conditions under which accumulation of pollutants outweighs advection.

Fig. 1 gives a schematic representation of the potential temperature profile in the developing convective boundary layer. Velocity and potential temperature gradients are confined to the shallow superadiabatic surface layer which is typically of the order of tens of meters in depth. The turbulent layer above the surface layer is buoyancy dominated and is assumed to produce uniform profiles of potential temperature and wind. While the well-mixed assumption is satisfactory for the potential temperature, it is not clear that vertical gradients of velocity are always negligible in the mixed layer. However, there is some evidence to show that wind shear may be small even with baroclinicity (Arya and Wyngaard, 1975). The inversion layer which separates the convective boundary layer from the nonturbulent stable atmosphere above is taken to be thin enough to be represented by a first-order discontinuity in potential temperature.

We choose a right-handed system of axes such that the x axis is directed along the geostrophic wind G. The governing equations for the mixed layer have been derived elsewhere (Carson and Smith, 1974) and it is sufficient to present them here:

\[
\frac{\partial v}{\partial t} = -f(u-G)h - \nu \frac{\partial^2 v}{\partial z^2} \sin \alpha
\]

\[
\frac{\partial \theta_m}{\partial t} = \frac{\langle w' \theta' \rangle}{T_m} - \frac{\partial n}{T_m} Q_R
\]

\[
\frac{\partial C_a}{\partial t} = \langle w' C_a \rangle + (C_a - C_a)w_x; \quad C_a = C_w, C_a.
\]

In the above h is the mixed layer height, u and v are the horizontal components of the wind, w is the vertical velocity, and \(\theta_m\) is the potential temperature of the mixed layer. The thermodynamic temperature \(T_m\) has been averaged over the PBL. (In this study we will use the terms PBL and mixed layer interchangeably.) The subscript s refers to the surface and \(\theta\) to the top of the mixed layer. The radiative source term \(Q_R\) can be written as

\[
Q_R = -(F_{R_h} - F_{R_s})/\rho c_p,
\]

where \(F_{R_h}\) is the net upward radiative heat flux, \(\rho\) the air density averaged over the mixed layer and \(c_p\) the specific heat of air. In the species conservation equation (4), \(C_a\) refers to the water vapor concentration and \(C_w\) the aerosol concentration. The subscript g refers to conditions above the mixed layer.

The cross-isobar angle \(\alpha\) and the entrainment velocity \(w_e\) are given by

\[
\alpha = \tan^{-1}(u/v), \quad w_e = -\frac{\partial h}{\partial t}.
\]

Using the thermal energy equation, the inversion heat flux \(\langle w' \theta' \rangle\) can be expressed as

\[
\langle w' \theta' \rangle = -\Delta \theta w_x
\]
where $\Delta \theta$ is the temperature jump across the inversion. In this study we assume that the synoptic-scale vertical velocity $w_h$ is zero.

To complete the set of equations we need an equation for the rate of inversion rise ($\partial h/\partial t$). The required formulation for $h$ is referred to as the entrainment hypothesis, and is a counterpart of the closure hypothesis utilized in eddy diffusivity models. It needs to be mentioned that the entrainment hypothesis is less sensitive to the details of its formulation than is the "closure" hypothesis. In other words, the assumptions regarding the rate of entrainment are not terribly important insofar as estimating the mixed-layer height (Mahrt and Lenschow, 1976) is concerned. In this study we chose to use an entrainment hypothesis suggested by Zilitinkevich (1975) and Tennekes (1975). By making some "plausible" assumptions they arrive at the following equations describing the rate of inversion rise:

$$\frac{\partial h}{\partial t} = \frac{H}{\Delta \theta},$$

(8a)

$$H = -\frac{\left<\overline{w'\theta'}\right>_s}{\left<\overline{w'\theta'}\right>_a} = 0.5\left[\frac{1}{1+2.6\left<\overline{w'\theta'}\right>_a}^{1/4} \right]$$

$$\left(\frac{gh}{T_m}\right)^{1/4} \Delta \theta.$$  

(8b)

Eq. (8) models the observed behavior (Carson, 1973) of the heat flux ratio $H$ fairly realistically—$H$ has small values when $h$ is small and approaches a value of 0.5 when $h$ becomes large. When, $\Delta \theta \to 0$, it can be shown that (8a) and (8b) reduce to

$$\frac{\partial h}{\partial t} = 0.19w_h, \quad w_h = \left[gh\left<\overline{w'\theta'}\right>_s / T_m\right]^{1/4}. \quad (9)$$

The attractive consequence given by (9) was one of the major reasons for the selection of (8) over the more commonly used entrainment hypothesis which takes $H$ to be a constant (Deardorff, 1972). It is easily seen that assuming $H$ to be a constant leads to serious conceptual as well as numerical problems when $\Delta \theta \to 0$.

We parameterize the surface heat flux and shear stress using one version of the bulk aerodynamic method (Deardorff, 1972). The procedure is described here for completeness. Following Deardorff's notation we write

$$\left<\overline{w'\theta'}\right>_s = C_s \theta_h (\theta_s - \theta_m),$$

(10)

where $C_s$ is the heat transfer coefficient, $\theta_s$ the surface temperature and $\theta_h$ (the surface friction velocity) is parameterized using the friction coefficient $C_u$,

$$u_h = C_u U_m,$$

(11)

where

$$U_m = (u^2 + v^2)^{1/2}.$$  

(12)

The bulk transfer coefficients $C_u$ and $C_s$ are expressed as functions of the bulk Richardson number $Ri_B$ given by

$$Ri_B = gh(\theta_m - \theta_s) / T_m U_m^2.$$  

(13)

Then, $C_u$ and $C_s$ are written as

$$C_u^{-1} = C_u^{-1} - 25 \exp(0.26x - 0.05x^2),$$

(14)

$$C_s^{-1} = C_s^{-1} + C_u^{-1} - C_u^{-1},$$

(15)

where

$$x = \log_{10}(-Ri_B) - 3.5; \quad (Ri_B < 0).$$

(16)

The neutral transfer coefficients $C_u$, and $C_s$, are given by

$$C_u = \left[\ln(0.025h/z_0)/k + 8.4\right]^{-1},$$

(17)

$$C_s = \left[0.74\ln(0.025h/z_0)/k + 7.3\right]^{-1},$$

(18)

where $z_0$ is the surface roughness length. In (17) and (18), the von Kármán constant $k$ is taken to be 0.35.

The surface temperature $\theta_s$ (at the surface the potential temperature is taken to be the same as the thermodynamic temperature) is computed from a surface energy balance (see Fig. 2):

$$R_n - \left<\overline{w'\theta'}\right>_s - L_h \left<\overline{\theta'\theta'}\right>_a - H_{si} - \sigma \theta_s^4 = 0,$$

(19)

where $R_n$ is the net incoming radiative flux (solar plus thermal) at the surface, $L_h$ the latent heat of vaporization, $H_{si}$ the heat flux into the soil and $\sigma$ the Stefan-Boltzmann constant. Assuming the equality of the bulk transfer coefficients of mass and heat we can express the surface water vapor ($C_w$) flux ($\overline{w'\theta'}$) as

$$\left<\overline{w'\theta'}\right>_s = C_{sw} (\theta_w - C_w).$$

(20)

Following a suggestion made by Myrup (1969) the
surface water vapor concentration $C_{wv}$ is expressed as
\[ C_{wv} = MC_{wv(\theta_i)}, \tag{21} \]
where $C_{wv}$ is the saturation water vapor concentration at saturated conditions and $M$ represents the fraction of the urban area covered by water. The soil heat flux $H_{st}$ is given by
\[ H_{st} = \left. k_{st} \frac{\partial T_{st}}{\partial z} \right|_{z=0}, \tag{22} \]
where $k_{st}$ is the soil heat conductivity and $T_{st}$ the soil temperature. The diffusion equation governing the variation of soil temperature is
\[ \frac{\partial T_{st}}{\partial t} = \alpha_{st} \frac{\partial^2 T_{st}}{\partial z^2}, \tag{23a} \]
where $\alpha_{st}$ is the soil heat diffusivity ($=k_{st}/\rho_{soil}c_{soil}$; the subscript $st$ refers to soil). The boundary conditions for the solution of (23a) are
\[ T_{st=\theta_{st}(t)}, \quad z=0; \quad T_{st=T_D}, \quad z=-D, \tag{23b} \]
where $D$ is the effective penetration depth of the temperature wave imposed at the soil surface.

3. The solar radiation model

As radiative transfer was just one of the several physical processes modeled in this investigation, it was necessary to use a radiation model which would be simple and at the same time yield relatively accurate estimates of the solar fluxes. An examination of the available methods to compute solar fluxes showed that the two-stream method met the requirement of computational convenience without introducing unacceptable idealizations such as neglect of multiple scattering. As the name implies, the method approximates the angular distribution of intensity by two intensities, one of which characterizes the radiation field in the forward direction and the other in the backward direction. Also, the phase function is parameterized by introducing the forward and backward scattering factors which are the fractions of the radiative flux scattered in the forward and backward directions. The two-stream method has been used by Sagan and Pollack (1967) to study scattering in Venustian clouds and by Rasool and Schneider (1971) to study the effect of aerosols on global climate. More recently, Wang and Domoto (1974) have adapted the method to treat nongray gaseous absorption with multiple scattering in the planetary atmosphere.

In the solar spectrum ($0.3 \mu m < \lambda < 4 \mu m$) emission of radiation can be neglected, and the radiative transfer equation for a plane-parallel atmosphere reduces to
\[ \frac{dI}{d\tau} = -I + \frac{\omega}{2} \int_{-1}^{+1} \rho(\mu' \rightarrow \mu)I(\tau, \mu')d\mu', \tag{24} \]
where $I$ denotes the intensity, $\tau$ the optical depth, $\mu$ the cosine of the zenith angle, $\rho(\mu' \rightarrow \mu)$ the averaged phase function and $\omega$ the single-scattering albedo. For reasons of convenience the dependence of the radiation parameters on the frequency $\nu$ and vertical coordinate $z$ has been dropped.

The boundary conditions for (24) can be written as
\[ I(0, \mu) = 2 \int_{0}^{\tau_{0}} f_0(-\mu' \rightarrow \mu)I(0, -\mu')d\mu', \quad \mu > 0, \tag{25} \]
and
\[ I(\tau_0, \mu) = S \delta[\mu - (\mu_0)] + I_D, \quad \mu < 0, \tag{26} \]
where $f_0(-\mu' \rightarrow \mu)$ is the mean bidirectional reflectance of the earth’s surface, $\tau_0$ the optical thickness of the model layer, $S$ the direct beam component (at zenith angle $\cos^{-1} \mu_0$) of the solar radiation at the top of the model layer and $I_D$ the intensity of the diffuse component. Eq. (25) states that the intensity of the radiation traveling in the $+\mu$ direction (upward) at the earth’s surface is the sum of the contributions from the beams of radiation reflected at the surface. Eq. (26) specifies the direct (collimated) and diffuse solar fluxes at the top of the model layer.

The detailed derivation of the two-stream equations can be found elsewhere (Wang and Domoto, 1974) and need not be repeated here in detail. The general principle of the derivation can be explained as follows. The scattering phase function is expanded into a series of Legendre polynomials and the two-stream equations are obtained by substituting the expanded phase function into (24), multiplying the resulting equation by $d\mu$ and $\mu d\mu$, and integrating over $\mu$ from $+1$ to $-1$ to obtain
\[ \frac{1}{\sqrt{3}} \frac{dI^+}{d\tau} = (f_0-1)I^++b_0I^- \]
\[ \quad + \frac{1}{\sqrt{3}} b_0S[1-\sqrt{3}(1-2b_0)\mu_0]e^{-(\tau_0-1)/\mu_0}, \tag{27} \]
\[ \frac{1}{\sqrt{3}} \frac{dI^-}{d\tau} = (f_0-1)I^-+b_0I^+ \]
\[ \quad + \frac{1}{\sqrt{3}} b_0S[1+\sqrt{3}(1-2b_0)\mu_0]e^{-(\tau_0+1)/\mu_0}, \tag{28} \]
where $I^+$ and $I^-$ are defined by
\[ \int_{-1}^{+1} \tilde{I}(\tau, \mu) d\mu = (I^+-I^-)/\sqrt{3}. \tag{29} \]
\[ \tilde{I}(\tau, \mu) = I(\tau, \mu) - S \delta[\mu - (\mu_0)]e^{-(\tau_0-1)/\mu_0}. \tag{30} \]
It is noted from (30) that $\tilde{I}(\tau, \mu)$ represents the diffuse component of radiation. Also, we see from (29) that $I^+$ denotes the intensity of radiation traveling in the $\mu = 1/\sqrt{3}$ direction, and $I^-$, that of the radiation in the $\mu = -1/\sqrt{3}$ direction. The choice of $\mu = 1/\sqrt{3}, -1/\sqrt{3}$ is based on the two-point Gaussian quadrature formula.
The backscattering factor \( b \) and the forwards-scattering factor \( f \) are defined by the equations
\[
2b = 1 - \int_{-1}^{1} \int_{-1}^{1} \rho(\mu,\mu') \mu d\mu d\mu',
\]
(31)
\[
f = 1 - b.
\]
(32)
Physically, \( b \) represents the fraction of energy scattered in the backward direction.

Assuming that the Earth's surface reflects diffusely, the boundary conditions (25) and (26) can be expressed in terms of \( I^+ \) and \( I^- \) as
\[
I^+(0) = r_s(I^-(0) + \sqrt{3} \mu \rho \sigma e^{-\tau_0(0)/\mu}),
\]
(33)
\[
I^-(0) = I_d.
\]
(34)
Even with the simplifications afforded by the two-stream approximation it is not possible to obtain closed-form analytic solutions of (27) and (28) for an inhomogeneous atmosphere. However, the equations can be numerically solved by dividing the model layer into a number of \( j \) sublayers depending on the degree of accuracy required. The aerosol parameters \( \omega_j, f_j \) can then be appropriately defined for each sublayer. The definitions will be discussed in a later section. Then, analytic solutions of (27) and (28) for each of the \( N \) layers can be readily written as
\[
I^+_j(\tau) = \alpha_1 j \rho e^{\alpha_1 \tau} + \alpha_2 j \rho e^{-\alpha_1 \tau} + C_j \rho e^{\alpha_2 \tau},
\]
(35)
\[
I^-_j(\tau) = \beta_1 j \rho e^{\beta_1 \tau} + \beta_2 j \rho e^{-\beta_1 \tau} + C_j \rho e^{\beta_2 \tau},
\]
(36)
\[
C_j = [S_j (1/\mu_0 + a_j) - S_j b_j]/D_j,
\]
(37)
\[
C_j = [-S_j (1/\mu_0 - a_j) - S_j b_j]/D_j,
\]
(38)
\[
a_j = \sqrt{3} (f_j \omega - 1);
\]
(39)
\[
d_j = \sqrt{3} \beta_j \omega_j,
\]
(40)
\[
S_j = \sqrt{3} \mu \rho \sigma [1 + \sqrt{3} (1 - 2b_j) \mu \rho e^{-\tau_0(0)/\mu}/2],
\]
(41)
\[
S_j = \sqrt{3} \mu \rho \sigma [1 + \sqrt{3} (1 - 2b_j) \mu \rho e^{-\tau_0(0)/\mu}/2],
\]
(42)
\[
\alpha_j = (a_j^2 - d_j^2)^{1/2},
\]
(43)
\[
\alpha_j = (a_j^2 + d_j^2)^{1/2},
\]
(44)
where \( j = 1, \ldots, N \). The \( 2N \) constants \( \beta_j \) and \( \alpha_j \) are determined by applying boundary conditions (33) and (34) and by requiring that \( I^+(\tau) \) and \( I^-(\tau) \) are continuous, i.e.,
\[
I^+_j(\tau_j) = I^+_{j+1}(\tau_j),
\]
(45)
\[
I^-_j(\tau_j) = I^-_{j+1}(\tau_j),
\]
(46)
Then \( F_{BS} \) the total solar flux can be calculated from
\[
F_{BS}(\tau_0) = \int_{\nu_1}^{\nu_2} \left[ 2\pi I^+(\tau_0) - I^-(\tau_0) \right] d\nu,
\]
(47)
where \( I \) is the precipitable water vapor (cm), \( A \) the band absorptance and the subscript \( i \) refers to each of the six bands. The expressions given by (47) were obtained by fitting power curves to data presented by McDonald (1960).

The water vapor optical thickness for the \( i \)th band is defined in a manner similar to Braslav and Dave (1973), i.e.,

\[
\Delta \tau_{ij} = \mu_0 \ln \left[ \frac{[1 - A_i(l_j + \mu_j)]}{[1 - A_i(l_j, \mu_j)]} \right],
\]

where the subscript \( j \) refers to the atmospheric layer for which \( \Delta \tau \) is defined and \( l_j \) is the water vapor thickness measured from the top of the atmosphere.

Then, using the optical thicknesses discussed in the previous paragraphs average radiation parameters for the \( j \)th layer can be defined as

\[
\begin{align*}
\omega_j &= (\omega_0 \Delta \tau_{aj} + \Delta \tau_{aj})/ (\Delta \tau_{aj} + \Delta \tau_{aj} + \Delta \tau_{aj}), \\
\beta_j &= (\beta_0 \omega_0 \Delta \tau_{aj} + 0.5 \Delta \tau_{aj}) / (\omega_0 \Delta \tau_{aj} + \Delta \tau_{aj}), \\
\Delta \tau_{aj} &= \Delta \tau_{aj} + \Delta \tau_{aj} + \Delta \tau_{aj},
\end{align*}
\]

where \( \Delta \tau_{aj} \) is the optical thickness due to Rayleigh (subscript \( r \) ) scattering.

5. Thermal fluxes

As the major emphasis of the study was on the interaction of aerosols with solar radiation, it was felt that an accurate computation of thermal fluxes was not warranted. Treating the mixed layer as a single layer the flux divergence (cooling rate) of thermal radiation can be written as

\[
\frac{\partial F_{RT}}{\partial z} = [1 - T_w(l_m)](2\sigma T_m^4 - \sigma \theta_s^4 - F_{Th}),
\]

where \( T_w(l_m) \) is the infrared transmittance of \( l_m \) centimeters of water vapor in the PBL, \( T_m \) the average temperature of the mixed layer, \( F_{Th} \) the downward thermal flux at \( z = h \), and the subscript \( T \) refers to the thermal spectrum. The transmittance \( T_w(l_m) \) is computed from a formula suggested by Kondratyev (1969), i.e.,

\[
T_w(l_m) = \sum_{j=1}^{4} \exp(-k_j l_m)/4,
\]

where \( k_1 = 0.10 \text{ cm}^{-1}, k_2 = 4.96 \text{ cm}^{-1}, k_3 = 19.6 \text{ cm}^{-1} \) and \( k_4 = 114.0 \text{ cm}^{-1} \).

### Table 1. Surface parameters and initial conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \epsilon )</td>
<td>1.0</td>
</tr>
<tr>
<td>( k_0 )</td>
<td>1.0 W m(^{-1}) C(^{-1})</td>
</tr>
<tr>
<td>( \alpha_0 )</td>
<td>1.0 \times 10^{-4} m(^2) s(^{-1})</td>
</tr>
<tr>
<td>( D )</td>
<td>0.5 m, ( z_0 = 0.1 \text{ m} )</td>
</tr>
<tr>
<td>( (\omega/C_0) )</td>
<td>5 \mu g m(^{-2}) s(^{-1})</td>
</tr>
</tbody>
</table>

The rest of the parameters are shown in Table 2.

\[
\omega = \gamma = 0.05 \text{ K km}^{-1}, \quad \Delta \theta = 0.25^\circ \text{C}, \quad \theta_a = 287 \text{ K} \\
T_D = 290 \text{ K}, \quad h = 200 \text{ m}
\]

### Table 2. Summary of simulations.

<table>
<thead>
<tr>
<th>Case I</th>
<th>( M = 0.2 ), ( r_a = 0.2 ), ( G = 4.0 \text{ m s}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) ( \omega_a = 0.8 ), ( \beta_a = 5.0 \times 10^{-4} \text{ m}^2 \mu g^{-1} ), ( b_a = 0.15 ), no aerosol participation (NP)</td>
<td></td>
</tr>
<tr>
<td>(2) ( \omega_a = 0.8 ), ( \beta_a = 5.0 \times 10^{-4} \text{ m}^2 \mu g^{-1} ), ( b_a = 0.15 ), aerosol participation (P)</td>
<td></td>
</tr>
</tbody>
</table>

| Case II         | \( M = 0.4 \), \( r_a = 0.2 \), \( G = 4.0 \text{ m s}^{-1} \) |

| Case III        | \( M = 0.2 \), \( r_a = 0.4 \), \( G = 4.0 \text{ m s}^{-1} \) |

The thermal flux \( F_{Th} \) at the top of the PBL is specified. The downward thermal flux at the air-soil interface can be written as

\[
F_{Ts} = F_{Th} T_w(l_m) + \alpha T_m^4[-1 - T_w(l_m)].
\]

6. Model simulations

The surface parameters and initial conditions used in the simulations are presented in Table 1. It is noted that the soil properties are representative of urban areas (Myrup, 1969), and the solar declination of 11° typifies summer conditions. The initial conditions were chosen so that they were reasonably compatible with each other in the sense that there was no rapid readjustment at the beginning of the simulations. The aerosol and water vapor concentrations above the inversion were fixed at nominal values of 10^{-3} \mu g m^{-3} and 10^{-3} g m^{-3}, respectively, to ensure that radiative cooling or heating was negligible above the inversion. We also notice that the water vapor concentration is small enough so that there is no necessity to formulate the problem in terms of the virtual potential temperature. The soil temperatures were initialized with the temperature \( T_D \). The time step was fixed after a number of simulations showed that a reduction of the time step did not affect the results to an appreciable extent.

Before going into the simulations in detail, it is necessary to discuss briefly the computation of boundary radiative fluxes. The downward thermal flux \( F_{Th} \)
was fixed at 250 W m\(^{-2}\) using computations involving the atmosphere above the model layer at 3 km. The direct and diffuse solar fluxes at the top of the model layer are computed at each time step using empirical methods described by Paily et al. (1974). Implicit in this method of specification of the solar fluxes at the boundary is the assumption that second-order effects in the downward Rayleigh intensities due to differences between the surface reflection and the polluted layer reflection can be neglected.

A summary of the simulations performed in this study is presented in Table 2. The major thrust of this paper was to study the thermal effects of aerosols; we have not attempted to look into the details of aerosol-induced modification of the wind field. It is only necessary to present sample results which show the behavior of the winds during the simulations. Fig. 3 illustrates the variation of the parameters describing the wind field during the 12 h of simulation. The top figure shows the damped inertial oscillation of the horizontal velocity in the mixed layer. We note that the velocity becomes super-geostrophic around 1500 hours. In the lower figure we see that the surface shear velocity \(u_\ast\) increases rapidly after sunrise, varies very little for about 9 h and then drops rapidly around 1500 h. This behavior is very similar to that observed by Clarke et al. (1971) in the Wangara experiment. The cross-isobar angle \(\alpha\) increases from 0\(^\circ\) to a maximum of about 10\(^\circ\) at 1200 hours before decreasing. As the cross-isobar angle is computed using winds which represent averages over the mixed layer, we expect its variation to be less than that typically observed. It is instructive to note that the modeled variation of \(u_\ast\) suggests that it might be possible to specify a constant \(u_\ast\) if thermal effects are of primary importance.

7. Radiative effects

Fig. 4 illustrates the effect of aerosol participation on the absorbed solar flux at the surface and the effective albedo of the earth-mixed-layer system which is defined by

\[
R = \frac{\uparrow F_s(h)}{\downarrow F_s(h)},
\]

(55)

where \(\uparrow F_s(h)\) and \(\downarrow F_s(h)\) are the upward and downward solar fluxes at the top of mixed layer. Thus the fraction \(1 - R\) would represent the fractional solar energy absorbed by the earth-mixed-layer system. Also, the sign of \(r_s - R\) would determine whether the aerosols have a warming or cooling effect on the system (Coakley and Chylek, 1975; Russell and Grams, 1975). We note that for a radiatively nonparticipating (NP) boundary layer, Rayleigh scattering increases the effective albedo \(R\) over that of the surface (\(r_s=0.2\)). It is evident that the effects of absorption of solar energy by the relatively small amount of water vapor in the PBL are not significant. Also, as the mixed layer grows the accompanying increase in the molecular scattering optical thickness increases \(R\). For simulation P (participating aerosols), aerosol absorption effects are dramatically evident in the substantial reduction of \(R\) below the surface albedo during the hours of 0800 to 1600. At noon \(R\) becomes as low as 0.15 which is about 25% less than the surface albedo. We note that about 70% of the total solar energy available during the day is incident on the earth-PBL system during the hours \(R\) is depressed below 0.2. This clearly shows that in the presence of slightly absorbing aerosols, the earth-PBL system absorbs more solar energy than it would if no aerosols were present. It should be mentioned that the two-stream approximation is least accurate (Liou, 1973) at small zenith angles (around noon). However, as the zenith angle varies during the course of the simulation the integrated heating effect on the earth-mixed-layer system does not reflect the error at small zenith angles to the same extent (3–10%).

It is instructive to test whether the aerosols used in the simulation do indeed give rise to heating by the criterion derived by investigators (Chylek and Coakley, 1974; Russell and Grams, 1975) for use in simple climatic models. It can be shown that

\[
\text{sign}(r_s - R) = \text{sign}[(1 - \omega)/\omega b - (1 - r_s)^2/2r_s].
\]

(56a)
Then the conditions which determines whether an aerosol layer will heat or cool the earth-PBL system are given by

\[
(1 - \omega_b) / \omega_b - (1 - r_f) / 2r_f \begin{cases} 
= 0, & \text{no change} \\
> 0, & \text{heating} \\
< 0, & \text{cooling}. 
\end{cases} \tag{56b}
\]

Using the parameters in Table 3 we see from (56b) that aerosols caused heating in the case considered. We might note that the derivation of (56) assumes diffuse radiation at the top of the mixed layer and in a sense the condition would determine the aerosol effect integrated over the simulation period.

We see from Fig. 4 that aerosol extinction reduces the surface solar flux by about 15% (100 W m\(^{-2}\)) around noon and by as much as 50% at large zenith angles. This reduction which is associated with aerosol concentrations of \(~80\ \mu g\ m^{-3}\) (see Table 3) is well within the range of values measured in polluted urban areas (Randerson, 1970; Stair, 1966). We note that the maximum heating rate of the PBL is around 10 K day\(^{-1}\), a value which is comparable to heating rates computed by Try (1972) for model urban atmospheres. It is worthwhile to point out that on the basis of a number of aircraft measurements Roach (1961) concluded that heating rates in excess of 10 K day\(^{-1}\) would occur in heavily polluted atmospheres.

The effect of radiative participation on the thermal structure of the PBL are illustrated in Fig. 5. It is seen that the reduction of solar flux at the surface gives rise to a decrease in the surface temperature during the simulation period. This temperature deficit reaches a maximum of about 1°C at 1800 hours. We also note that the aerosol absorption increases the mixed layer temperature. This is to be expected as the soil-mixed-layer system has a reduced albedo in the presence of aerosols and a reduction of surface temperature has to be accompanied by an increase in mixed layer temperature. It is easy to see that the warming of the soil-PBL system can result in three different
situations depending upon aerosol properties and characteristics of the air-soil interface. First, both the surface and mixed-layer temperature can increase. Secondly the surface temperature can increase with the PBL temperature decreasing. The third situation corresponds to the simulation described in this paper. The possibility of any one of the situations occurring can be best understood by examining the surface and PBL energy budgets.

Fig. 6 shows the turbulent (surface plus inversion) and radiative (solar heating—thermal cooling) heating rates for simulations P and NP. We note that the turbulent heating of the mixed layer varies from about 27 K day⁻¹ at 0600 hours to 0 K day⁻¹ at 1800 hours. Radiative participation by aerosols decreases the turbulent heating rate by about 5 K day⁻¹ on an average. On the other hand, aerosol absorption increases the radiative heating rate by about 7 K day⁻¹. It is clear from the net heating curves that the increase in solar heating exceeds the reduction in turbulent heating throughout the simulation period. It is quite conceivable that the reduction in turbulent heating is not compensated by the increase in solar heating in which case the mixed-layer temperature would decrease. Of course, the surface temperature would then increase.

The details of the surface energy budget are shown in Figs. 7 and 8. We note that aerosol participation decreases the sensible heat flux by as much as 80 W m⁻² around noon. This relatively large reduction of 25% is related to the aerosol-induced modification of the surface and mixed-layer temperatures. The decrease in surface temperature and the increase in mixed-layer temperature reinforce each other in reducing the temperature difference driving the sensible heat flux. Also, this relative stabilization of the surface layer leads to a decrease in the surface heat transfer coefficient (Cₕ) which in turn decreases the surface heat flux. Thus, the reduction in the sensible heat flux is associated with three synergistic effects induced by aerosols. It is interesting to note that aerosol participation causes transition (zero turbulent heating) to occur earlier by about 2 h. This reversal of sensible heat flux is also related to the plateau in the θₑ(φ) curve around 1630 to 1700 during which period θₑ is barely above θₑ. When θₑ drops below θₑ, the heat transfer coefficient Cₕ undergoes a rapid change to a much smaller value and θₑ drops sharply as the surface cools. The latent heat flux is also reduced by aerosol participation but to a smaller degree than the sensible heat flux. This decrease is related to the lower surface water vapor concentration (associated with the lower surface temperature) and the lower heat transfer coefficient.
From Fig. 8 we see that the heat flux into the soil is reduced in simulation P, but the decrease is smaller than we would expect it to be. Aerosol participation decreases the soil heat flux by less than 10% at 1200 hours, and the maximum reduction is about 15% around 1400 hours. Clearly, in this case the reduction in the absorbed solar flux is larger than the decrease of heat flux away from the air-soil interface. From the discussion we can see that the surface temperature can also increase. It might be useful to point out that previous investigators (Bergstrom and Viskanta, 1973; Zdunkowski et al., 1976) have primarily related aerosol extinction to a decrease in surface temperature. It is interesting to note from Fig. 7 that the latent heat flux reaches its maximum an hour after the sensible heat flux does so. For both numerical experiments (P and NP) the latent flux becomes larger than the sensible heat flux at some time during the simulation and stays larger during the rest of the simulation period. This suggests that a Bowen ratio approach to the parameterization of the latent heat flux would have produced considerably different results.

After the discussion of the previous paragraphs it is appropriate to ask the question: do aerosols cause warming or cooling? The answer cannot be a simple yes or no. In the presence of absorbing aerosols the soil-PBL system absorbs more energy than when aerosols are not present, and in this sense aerosols are warming. However, a reduction in surface temperature translates into cooling, an effect which seems to have been emphasized by previous studies (Bergstrom and Viskanta, 1973; Zdunkowski et al., 1976). On the other hand, the accepted semantics dictates that we associate the increase in mixed-layer temperature with warming. Thus it is clear that aerosol effects cannot be related to temperature changes without some difficulty. In our particular case, aerosols cause an increase in solar energy absorption by the soil-PBL system. The direction of the associated temperature changes of the surface and the PBL are functions of the soil-air interface properties. Probably, the aerosol effect could be best related to an average of the PBL and surface temperatures. A glance at Fig. 5 shows that this average temperature does show a slight decrease in simulation P.

It is worthwhile to examine the effect of aerosol participation on the growth of the mixed layer which is one of the more important variables in air pollution meteorology. In Fig. 9 we illustrate the variation of the mixed-layer height in the numerical experiments. We notice that aerosols do not affect mixed-layer growth to the extent we would expect it to be in light of the substantial reduction in the surface heat flux. This insensitivity of the mixed layer to aerosol participation can be understood by examining (8a). We see that the rate of mixed layer growth is roughly proportional to the surface heat flux \( H \) (varies very slightly after 2 h of simulation) and inversely proportional to the temperature jump \( \Delta \theta \) (sometimes referred to as the intensity) across the inversion. We have noted previously that the presence of aerosols decreases the surface heat flux; thus for \( \partial h/\partial t \) to remain unaffected \( \Delta \theta \) has to become smaller. We note from Fig. 10 that this is indeed the case. The inversion intensity in simulation P is smaller than in simulation NP throughout the period under consideration. For NP, \( \Delta \theta \) increases monotonically reaching a maximum of about 2.8°C at 1800 hours. This indicates that \( \gamma \partial h/\partial t \) is always greater than \( \partial \theta_m/\partial t \) during the 12 h of simulation. This is not the case for the numerical experiment with aerosol participation. We see that \( \Delta \theta \) reaches a maximum of about 1.5°C and then decreases. What is important to notice is that aerosol participation decreases \( \Delta \theta \), and in the case considered this reduction amounts to 2°C at a maximum. Clearly, the decrease in \( \Delta \theta \) is related to the increase in the mixed layer temperature \( \theta_m \) caused by aerosol absorption of solar energy.

To put the argument in more physical terms, in the presence of aerosols buoyant elements reaching the top of the mixed layer have less kinetic energy but have a smaller potential energy barrier to overcome in order to entrain the stable layer above the PBL. Thus,
Fig. 7. Effect of aerosol participation on sensible and latent heat fluxes for Case I. The curves corresponding to the initial adjustment period during which the fluxes vary haphazardly are not shown in the figure.

Fig. 8. Variation of soil fluxes (into the soil) for Case I in simulations P and NP for Case I.
aerosol participation induces two principal effects which tend to offset each other.

As expected, the very small modification of mixed-layer height by aerosols is accompanied by small changes in aerosol concentration and wind as can be seen from an examination of Table 3. The aerosol concentration is increased by a maximum of 7% (7 μg m⁻³) in simulation P while the velocity field is hardly affected. It is suspected that the insensitivity of these variables to radiative participation by aerosols is a consequence of the built-in inertia of the mixed-layer model.

8. Effect of surface properties

This part of the study was motivated by a paper by Mitchell (1971) which suggested that aerosol effects are very closely tied to air-soil interface properties such as albedo and wetness. In this section we present the results of a limited number of simulations conducted to study the effect of surface properties on surface and mixed-layer temperatures. The roles played by surface wetness (M) and albedo ($r_s$) in increasing or decreasing aerosol-induced effects can be explained as follows. When $r_s$ is increased a greater fraction of the solar flux incident at the surface is reflected into the polluted mixed layer. Thus, a larger
amount of energy is absorbed by the mixed layer and consequently $\theta_m$ is increased to a greater extent when $r_s$ is large. A larger $r_s$ also means that less solar energy is absorbed by the surface. Thus surface temperature becomes relatively insensitive to changes in incident solar flux when $r_s$ is large. The effects of surface wetness are similar. When $M$ is large, a large fraction of solar energy incident on the earth's surface contributes toward evaporation and a relatively small fraction goes into sensible heating. Thus, surface temperature is not sensitive to changes in surface solar flux caused by aerosol absorption in the mixed layer. Therefore, direct solar heating in the mixed layer is not counteracted by a reduction in sensible heating to the same extent as when $M$ is relatively small; the aerosol induced effect on $\theta_m$ is increased when the surface wetness is increased.

In Figs. 11 and 12 we have illustrated the effects of changing surface wetness and albedo on the surface and mixed layer temperatures. We should note that aerosol optical thicknesses for all the three simulations are identical at any given time as we have used a constant pollutant source strength. Thus, the albedo ($R$) variation of the soil-PBL system for Case II is identical to that of Case I. In other words the warming influence of aerosols from the point of view of excess solar energy absorption does not differ in Cases I and II. However, the change in surface wetness does make a substantial difference to energy transfer to the soil and PBL. We note that for Case II the surface temperature difference between simulations P and NP ($\Delta\theta_{NP-P}$) is less than that of Case I; the maximum value is about 0.8°C while that of Case I is 1.5°C. We also note from Fig. 12 that the maximum temperature excess of the mixed layer is 1.5°C for Case II while it is 1°C for Case I. In terms of the average temperature $[\theta_a = (\theta_m + \theta_s)/2]$ change Case I shows a cooling of 0.25°C while Case II shows a warming of 0.35°C. We could go a step further and relate $\theta_a$ to the screen level temperature. Then, the aerosol effect in Case I would be cooling and that in Case II would be warming. This discussion points out the necessity of defining what we mean by cooling or warming. The definition used in climatic studies is not readily applicable to the smaller scales of the urban area. We feel that an appropriate temperature such as $\theta_a$ should be an indication of the aerosol effect. It should be clear that conclusions about aerosol effects on the urban scale should be qualified by statements about soil-interface properties. This aspect of the aerosol problem has been discussed by other investigators (Mitchell 1971; Russell and Grams, 1975) in reference to simple climate models but the literature on small-scale studies (Bergstrom and Viskanta, 1973; Zdunkowski et al., 1976) does not seem to have emphasized it.

We have also investigated the effect of changing the surface albedo on aerosol-induced modifications of the surface and mixed layer temperatures. We see from Figs. 11 and 12 that a doubling of $r_s$ from 0.2 to 0.4 in Case III decreases the sensitivity of the surface temperature to solar flux changes considerably over that of...
Case I; the maximum $\Delta \theta_{\text{PPLP}}$ is less than 0.4°C. On the other hand, the maximum mixed layer temperature increase is almost 2°C indicating a $\theta_a$ increase of about 0.8°C. We recall that $\theta_a$ decreases by 0.25°C when $r_s=0.2$. The greater sensitivity of the soil-PBL system to aerosol participation when the surface albedo is increased is a well known result (Mitchell, 1971; Russell and Grams, 1975) which our study confirms in the context of temperature changes.

9. Summary and conclusions

The model presented in this paper does not pretend to be as detailed as those formulated by previous investigators (Bergstrom and Viskanta, 1973; Zdunkowski et al., 1976). However, we believe that it retains the principal physics of the modeled situation and can be gainfully utilized to study the radiative effects of pollutants. The simplicity of the model allows us to gain the type of insight into the problem which is not readily forthcoming from more detailed models.

The aerosols modeled in this study reduce the effective albedo of the soil-PBL system and are thus warming from the point of view used in climatic studies (Russell and Grams, 1975). However, we have seen that the albedo-based criterion is not readily applicable to the smaller scales of this investigation. In our case aerosol effects have to be related to changes in surface and mixed layer temperatures. The results show that these temperature changes are at least as closely tied to soil-air interface properties as they are to aerosol properties. Generalizations such as “aerosols increase daytime temperatures” or “they decrease surface temperatures” might be misleading. Conclusions about aerosol effects have to be very carefully tempered by statements about soil-interface properties.

In the limited number of situations modeled in this paper, aerosols decrease the surface temperature and increase the mixed-layer temperature. The magnitude of these temperature changes are greatly dependent on surface properties. In this connection we have attempted to introduce a convenient indicator of aerosol effects in defining $\theta_a$. We realize that this definition is tailored to the outputs of our particular model. However, we believe that similar temperature indicators can be derived from the variables of multi-layer models. We note that $\theta_a$ is a function of the sensitivity of the soil-air interface to solar flux changes. Surfaces which are relatively wet or have high albedos are associated with increases in $\theta_a$ in the presence of aerosols which decrease the effective albedo of the soil-PBL system. On the other hand, dry surfaces with relatively low albedos tend to react to aerosol-induced reductions of surface solar fluxes by decreases in surface temperatures which are large enough to decrease $\theta_a$. As mentioned before this important aspect of aerosol induced modification of the PBL microclimate has been discussed before by Mitchell (1971) in connection with the climate of the troposphere. We have to point out that Mitchell’s approach which emphasized energy relationships was considerably different from ours. We have modeled the dynamics of the PBL and in doing so we have focused attention on the role of surface parameters which does not seem to have been given the attention it deserves in other similar investigations (Zdunkowski et al., 1976; Bergstrom and Viskanta, 1973).

It is instructive to point out the role of aerosols in affecting energy distribution in the soil-PBL system. We note that aerosols increase solar energy absorption in the PBL and decrease it at the surface. The surface reacts to this loss of energy by allowing less sensible heat to flow away from it. At the same time the increase in energy of the PBL is offset to an extent by the decrease in sensible heat flowing into the PBL from the surface. In a sense the surface acts like a relief valve in counteracting the tendency of the PBL temperature to increase and the surface temperature to decrease.

The compensating mechanism associated with the soil-PBL system is also evident in the behavior of mixed-layer growth. Radiative participation by aerosols leads to a decrease in the surface turbulent heat flux, an effect which would tend to reduce the rate of mixed-layer growth. However, the inversion intensity is decreased by the absorption of solar energy in the PBL, an effect which tends to increase mixed layer growth. Thus, in a sense the soil-PBL system acts to regulate the stresses induced by the extra solar energy absorbed by aerosols. In reference to the modification of mixed-layer growth it is important to note that aerosol participation advances the transition to stable conditions (see Fig. 7) when the mixed layer collapses to small heights. This implies that aerosols increase the pollution potential in an indirect way by decreasing the period during which the “flushing factor” (mixed layer height $\times$ PBL velocity) is relatively high.

At this point, we will discuss some of the shortcomings of the model used in this study. Although the slab model of the PBL bypasses the use of eddy diffusivities it cannot handle the effects of local radiative heating or cooling which might be important from the point of studying elevated layers of pollutants.

It is clear that the assumption of uniform distribution of pollutants inside the mixed layer is not entirely satisfactory. We know (Deardorf and Willis, 1975) that dispersion in the daytime PBL is controlled by $h$ as well as the velocity scale $w_0$. In this study we have not been able to take the effect of changing $w_0$ into account in predicting aerosol-induced modification of pollutant distributions. As the surface heat flux is reduced considerably by aerosol absorption of solar energy, we would suspect that surface pollutant concentrations would be more sensitive to aerosol participation than this study would indicate. However, any attempt at
more satisfactory modeling of aerosol distribution would necessitate a detailed model of turbulence. We feel that the presently available simpler models of turbulent transport (eddy diffusivity models) are based on arbitrary assumptions much more objectionable than those of the mixed-layer model. It is necessary to utilize numerically cumbersome second-order models in order to make a satisfactory resolution of the problems associated with studying radiative effects in a turbulent boundary layer.

Although we have used a "realistic" aerosol model in this study, the considerable uncertainty in determining aerosol properties would require an exhaustive study of the effect of aerosol properties on the magnitude of radiative effects. The results of such a study will be discussed in a forthcoming paper.

Acknowledgments. Part of this research was supported by the Meteorology and Assessment Division of the U. S. Environmental Protection Agency under Grants R801102 and R803514 to Purdue University.

APPENDIX

Numerical Method

The numerical solution of the momentum equations (1) and (2) is greatly facilitated by defining the complex variable \( \tilde{a} \)

\[
\tilde{a} = (u + iv - G) \exp(i\beta)
\]

(A1)

Then using \( \tilde{a} \), Eqs. (1) and (2) can be combined to yield

\[
\frac{d\tilde{a}}{dt} = u^2 \exp[i(\beta + \alpha)].
\]

(A2)

Thus, the coupled momentum equations are reduced to a single, complex, first-order differential equation which can readily be solved on the computer using complex arithmetic.

The governing equations were solved numerically using a predictor-corrector scheme which can be illustrated by considering the equation

\[
\frac{dx}{dt} = F(x),
\]

(A3)

where \( x \) is a vector.

Then, the procedure to advance \( x \) in time \( t \) is given by

\[
x^{n+1}(t+\Delta t) = x(t) + \left\{ F[x(t)] + F[x^n(t+\Delta t)] \right\} \Delta t/2
\]

where \( x^n(t+\Delta t) \) is the value of the vector at the \( (n+1) \)th iteration. The iterative cycle is terminated using the criterion

\[
\left| \left[ x^n_{j+1}(t+\Delta t) - x^n_{j}(t+\Delta t) \right]/x^n_j(t+\Delta t) \right| < \epsilon
\]

(A5)

where \( x_j \) is a component of \( x \), and \( \epsilon \) is a convenient error limit. In our computations we took \( x_j \equiv h \) and \( \epsilon = 1.0 \times 10^{-3} \). In most of the cases considered in the paper, it was not necessary to continue the iteration beyond three cycles.

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