BOUNDARY-LAYER DIFFUSION MODELLING: THE GAUSSIAN PLUME APPROACH VERSUS THE SPECTRAL SOLUTION

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Abstract. The equation of turbulent diffusion is solved for a vertical area source within the planetary boundary layer. The traditional Gaussian-plume approach is compared with the spectral solution of the diffusion equation used together with the barotropic boundary-layer model of Lettau and Dabberdt (1970). The results of the numerical computations are presented and the differences between the solutions are discussed.

List of Symbols

x, y, z	coordinates
u, v	wind components
I	concentration of contaminants
F	source area
L_y, L_z	lateral and vertical boundaries of the model
H	height of inversion layer
H_1	source height
Z	height of the boundary layer
σ_y, σ_z	deviations in the Gaussian profile
a, b, c, d	parameters for the σ_y, σ_z depending on stability
τ	travel time
Q	source strength
α	factor of proportionality between K_y, u
A, B, C	functions of x, y, z
l, λ, λ'	eigenvalues
β_0	angle between shearing stress and departure of the actual wind from the geostrophic value
$\mathbf{v}_g$	geostrophic wind
g	continuous function satisfying the boundary conditions
f_n	components of the linear combination for g
a_n	coefficients of f_n in the linear combination
m, n, p, r, s	natural numbers, indices

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1. Introduction

The equation of turbulent diffusion describes the space and time variations of the concentration of contaminants added to the atmosphere. In a Lagrangian coordinate system, a simple solution of this equation can be obtained assuming a Gaussian distribution of the concentration, the standard deviation of which depends on the prevailing meteorological conditions. However, concentration profiles deviating from the Gaussian plume cannot be handled as simply. The boundary conditions at the earth's surface or at an inversion layer have to be considered by adding mirror-image sources to the system, which leads to multiple reflection and thereby reduces the clarity of the statistical approach.

These disadvantages do not exist for analytical solutions of the diffusion equation in an Eulerian system. But, analytical solutions are known only for a few special cases. They crucially depend on the distribution of the turbulent diffusion coefficient and the wind field, which are related to the meteorological conditions governing the diffusion process. Additionally, the lateral decrease of the concentration at greater distances from the source has to be artificially prescribed.

A numerical solution of the diffusion equation in the Eulerian coordinate system has the same advantages as the analytical solution, but it is possible to account for the vertical structure of the atmosphere in more detail. Experimentally and theoretically derived configurations of the turbulent diffusion coefficient and wind components can be applied.

The following note shows the results of some calculations of atmospheric diffusion models. The discussion of these results concentrates on the Gaussian-plume approach and the spectral solutions of the diffusion equation for a barotropic boundary with varying angular wind spiral and for vertically-constant coefficients. These models have been designed for and applied to the diffusion process of water (liquid and vapor) and sensible heat as an interacting system which occurs subsequent to the convective phase of a cooling tower plume (Fraedrich *et al.*, 1977). A comparison of these methods is presented here under more general aspects.

2. Equation of Turbulent Diffusion

The turbulent transport of a concentration I within a planetary boundary layer can be described by

$$u\frac{\partial I}{\partial x}+v\frac{\partial I}{\partial y}=\frac{\partial}{\partial x}\left(K_x\frac{\partial I}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial I}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial I}{\partial z}\right) \tag{1}$$

assuming steady-state conditions, horizontal homogeneity of the wind field and negligible vertical motion and density variations. Two additional simplifications can be introduced: (a) in the forward (x) wind direction, the mean transport is significantly greater than the diffusion process (turbulent transport), which is valid for $u > 1\ \mathrm{m\,s^{-1}}$; (b) the contribution of the mean horizontal transport divergence along the main direction is larger than in the normal direction (McCormick and Gutsche, 1973). This can easily be verified if the wind at the top of the boundary layer is directed along the x-axis with a wind spiral underneath. Thus, a simplified equation of the turbulent diffusion process can be obtained

$$u\frac{\partial I}{\partial x}=\frac{\partial}{\partial y}\left(K_y\frac{\partial I}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial I}{\partial z}\right). \tag{2}$$

The lateral diffusion term is kept because a fully two-dimensional treatment appears to be too restrictive for our purposes. Different approaches to solve this equation will be discussed in later sections according to the following boundary conditions:

(i) At the surface ($z=0$), there is no absorption of the substance (reflectivity condition):

$$\left.\frac{\partial I}{\partial z}\right|_0=0; \tag{3}$$

(ii) At the top of the layer, two different conditions can be introduced depending on the meteorological situation which is related to the thermal stratification of the atmosphere influencing the turbulent fluctuations:

$$\begin{aligned} &z=L_z \quad \text{(without inversion):} \quad I=0\\ &z=H \quad \text{(with inversion):} \quad \partial I/\partial z=0; \end{aligned} \tag{4}$$

(iii) At the lateral boundaries ($y=\pm L_y$), the concentration is assumed to vanish:

$$I\,|_{L_y}=0; \tag{5}$$

(iv) At the upwind boundary ($x=x_0$), a puff of a given concentration $I(x_0, y, z)$ moves with wind speed u into the system so that the total area source at this boundary yields

$$Q=\int_0^{L_z}\int_{-L_y}^{+L_y} uI\,\mathrm{d}y\,\mathrm{d}z. \tag{6a}$$

This is a conservation condition which holds for all x. For the spectral approach, the area distribution of the source density rather than the total area source (6a) is to be prescribed:

$$uI\,|_{x=x_0}, \tag{6b}$$

where the concentration $I(x=x_0, y, z)$ within a cross-section of a Gaussian plume is spectrally approximated.

3. The Gaussian Plume

All particles originating from a distant point source contribute to the diffusion process by way of their random fluctuations (Sutton, 1953). They move along finite paths at the end of which they lose their identity. These mixing-length vectors of a large number of particles can be described by a Guassian distribution, whose standard deviations (σ_y and σ_z) are different for the y- and z-components normal to the mean wind and dependent on the downwind travel distance x according to the following power law (Singer and Smith, 1960):

$$\sigma_y = ax^b, \quad \sigma_z = cx^d. \tag{7}$$

The parameters a, b, c, d depend on the thermal stability of the atmosphere as specified in Section 5. Neglecting the fluctuation of the mean (vertically averaged) wind component

$$\bar{u} = \frac{1}{L_z} \int_0^{L_z} u \, dz, \tag{8}$$

all particles fluctuate in the y-z directions while drifting with the mean wind $\bar{u}$ for a representative travel time $\tau = x/\bar{u}$. The coefficient of turbulent diffusion (Equation (2)) can be directly derived (see e.g., McCormick and Gutsche, 1973):

$$K_{y,z} = \frac{1}{2} \frac{d}{d\tau} \sigma_{y,z} = \frac{1}{2} \bar{u} \frac{d}{dx} \sigma_{y,z}. \tag{9}$$

For a point source, the solutions of Equation (2) are now obtained in agreement with the boundary conditions (Section 2; with $L_y = \infty$).

Without inversion ($L_z = \infty$);

$$I = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left[-\frac{y^2}{2\sigma_y^2}\left\{\exp\frac{-(z-H_1)^2}{2\sigma_z^2} + \exp\frac{-(z+H_1)^2}{2\sigma_z^2}\right\}\right]. \tag{10a}$$

With inversion and multiple (n) reflexion ($L_z = H$);

$$I = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left[-\frac{y^2}{2\sigma_y^2} \sum_n \left\{\exp\frac{-(z-H_1+2nH)^2}{2\sigma_z^2} + \exp\frac{-(z+H_1+2nH)^2}{2\sigma_z^2}\right\}\right] \tag{10b}$$

where H_1 is the height of the point source.

For a vertical area source, similar solutions are applicable if a virtual point source of the same intensity Q can be introduced, the upwind distance being derived from the following condition. The elliptical area of the Gaussian plume within the closed boundary of the 10% concentration isoline

$$F = \pi \times 2 \times 15^2\, \sigma_y \sigma_z \tag{11}$$

should be as large as the area of the area source (Pasquill, 1961).

Given the area (or point) source, the thermal stability, and the mean wind, then the three-dimensional field of the concentration of air contamination can be calculated.

4. The Spectral Approach

Assuming that the horizontal turbulent diffusion coefficient is proportional to the main wind component

$$K_y = \alpha\, u, \tag{12}$$

and letting the following product represent the solution of Equation (2)

$$I(x, y, z) = A(x)B(y)C(z), \tag{13}$$

one obtains two eigenvalue problems

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(K_z \frac{\mathrm{d}C}{\mathrm{d}z}\right) + \lambda u C = 0 \tag{14}$$

$$\alpha \frac{\mathrm{d}^2 B}{\mathrm{d}y^2} + lB = 0 \tag{15}$$

and an ordinary first-order differential equation which depends on the eigenvalues l, λ:

$$\frac{\mathrm{d}A}{\mathrm{d}x} + (\lambda + l)A = 0. \tag{16}$$

The solution of Equation (2) with respect to the boundary conditions (Section 2) and the above assumptions yields

$$I = \sum_n \sum_m I_n^m \exp -(\lambda_m + l_n)x \cos \frac{(2n-1)\pi y}{2L_y}\, C_m(z), \tag{17}$$

where the eigenvalues

$$l_n = \left(\frac{(2n-1)\pi}{2L_y}\right)^2 \alpha \tag{18}$$

are given by Equation (15) with respect to the boundary conditions (Section 2). The coefficients I_n^m are chosen in order to fulfil the windward boundary condition

(6b) of the vertical area source, which was shown to be possible by Courant and Hilbert (1968):

$$I_n^m = \frac{\int_0^{L_z, H} \int_{-L_y}^{+L_y} I(0, y, z) B_n(y) u(z) C_m(z) \, dy \, dz}{\int_0^{L_z} \int_{-L_y}^{+L_y} B_n^2 C_m^2 u(z) \, dy \, dz} . \tag{19}$$

An average error of less than 2% allows the spectral series to be cut off after wave number 10 (which holds for both directions x, y). The vertical eigenfunctions C_m and the related eigenvalues λ_m (14) depend on the vertical profiles of u and K_z which are specified in the following.

4.1. u AND K_z VERTICALLY CONSTANT

The vertical eigenfunctions C_m can simply be derived.
With inversion $(z = H)$;

$$C_m(z) = \cos \frac{m\pi z}{H}, \quad m = 0, 1, 2, \ldots \tag{20a}$$

and the related eigenvalue

$$\lambda_m = \left(\frac{m\pi}{H}\right)^2 \frac{\bar{K}_z}{\bar{u}}. \tag{20b}$$

Without inversion $(z = L_z)$:

$$C_m(z) = \cos \frac{(2m-1)\pi z}{2L_z}, \tag{21a}$$

and the eigenvalue

$$\lambda_m = \left(\frac{(2m-1)\pi}{2L_z}\right)^2 \frac{\bar{K}_z}{\bar{u}}. \tag{21b}$$

4.2. A BAROTROPIC BOUNDARY LAYER WITH VERTICAL K_z AND u PROFILES

The wind field and the turbulence structure of this planetary boundary layer are given by a model of Lettau and Dabberdt (1970). They assume a linear height dependence of the angle β_0 between stress and departure from the geostrophic wind $\mathbf{v}_g$ so that analytical solutions are able to describe realistically the boundary-layer structure. The coefficient of turbulent diffusion is obtained from a fourth-order polynomial and the main wind component can also be represented by such a polynomial:

$$u(z) = \sum_{n=0}^{4} u_n z^n$$

$$K_z(z) = \sum_{n=0}^{4} K_n z^n.$$

TABLE I
Parameter values (see Section 5.1), metric units

	Gaussian plume				Barotropic boundary layer			Constant coefficients		Inversion height H
	a	b	c	d	β_0	v_g	L_z	$\bar{u}$	$\bar{k}_z$	
Stable	0.273	0.691	0.217	0.610	43°	5	300	4.2	0.41	210
Neutral	0.306	0.885	0.072	1.021	35°	10	1000	8.1	15.7	210

The dependence of the external parameters β_0, $\mathbf{v}_g$ and additional coefficients on the thermal stratification of the atmosphere is shown in Table I (Section 5). The related vertical profiles of the wind and the turbulent diffusion coefficient are shown in Figure 1.

The eigenvalue Equation (14) is self-adjoint and positive definite so that the Rayleigh and Ritz-method can be applied for its solution (Collatz, 1963). After Rayleigh, the first eigenvalue is given by the minimum of the following quotient:

$$R(g) = \frac{\int_0^{L_z,H} g \frac{\mathrm{d}}{\mathrm{d}z}\left(K_z \frac{\mathrm{d}g}{\mathrm{d}z}\right) \mathrm{d}z}{\int_0^{L_z} g^2 u \,\mathrm{d}z}, \tag{22}$$

where g is obtained from a set of continuous functions satisfying the boundary

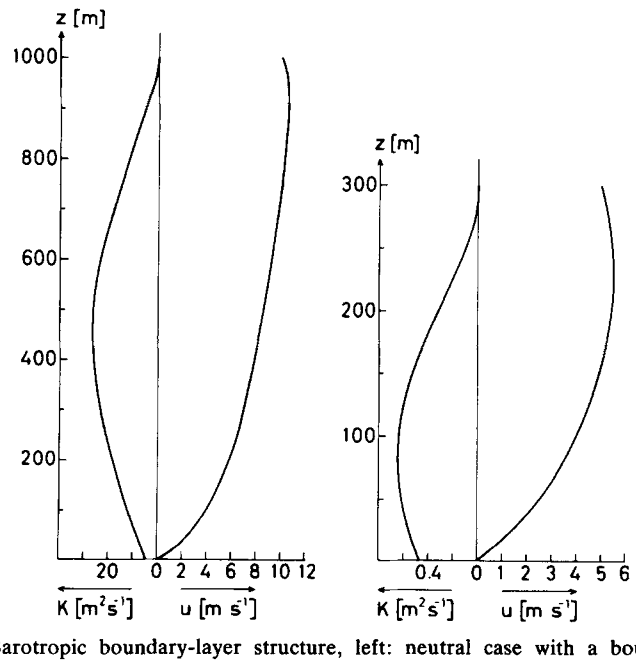

Fig. 1. Barotropic boundary-layer structure, left: neutral case with a boundary-layer height of 1000 m. right: stable case with a boundary-layer height of 300 m.

conditions. They are represented by a linear combination of p linearly-independent functions

$$g(z) = \sum_{n=1}^{p} a_n f_n(z), \tag{23}$$

the coefficients a_n of which are defined for R_g being a minimum. This variational problem leads to the Galerkin-equations (Collatz, 1963):

$$\sum_{s=1}^{p} a_s \left[\int_0^{L_z} f_r \frac{\mathrm{d}}{\mathrm{d}z}\left(K_z \frac{\mathrm{d}f_s}{\mathrm{d}z}\right) \mathrm{d}z - \lambda' \int_0^{L_z} f_r u f_s \, \mathrm{d}z \right] = 0, \tag{24}$$

$r = 1, \dots p$

$s = 1, \dots p$

which is a linear and homogeneous system for the p unknowns a_s. A non-trivial solution exists for a vanishing determinant of the coefficients.

Thus, the problem of solving the differential equations has been reduced to a matrix problem:

$$\int_0^{L_z} f_r \frac{\mathrm{d}}{\mathrm{d}z}\left(K_z \frac{\mathrm{d}fs}{\mathrm{d}z}\right) \mathrm{d}z = \lambda' \int_0^{L_z} f_r u f_s \, \mathrm{d}z, \quad r = 1, \dots, p; \quad s = 1, \dots, p. \tag{25}$$

As the matrices are symmetric and positive definite, all eigenvalues λ' are real and positive.

The functions f_n are prescribed by the eigenfunctions of Equation (14) with vertically constant u and K_z, as solved via Equations (20) and (21) with respect to the boundary conditions (Section 2). The eigenfunctions for vertical profiles in u and k_z (i.e., for the barotropic boundary layer described above) are obtained if the eigenvectors g_s of the system (24) are substituted into Equation (23). The following relation holds for the eigenvalues of the matrix approximation λ' and of the differential equation λ:

$$\lambda'_m \geq \lambda_m. \tag{26}$$

In our numerical calculations, the value of p was continuously increased until the first ten eigenvalues (needed for the spectral representation of the solution by ten wave numbers) no longer diminished. These eigenvalues are thereby exact, which was the case for $p \geqslant 30$.

5. A Comparison

5.1. The Input Parameters

Some specifications have to be introduced to make the different solutions of the diffusion Equation (2) compatible.

(a) The vertically-averaged u-component of the barotropic boundary-layer model is used for the Gaussian-plume approach and one of the spectral solutions (Section 4.1) which also incorporates the vertically-averaged diffusion coefficient.

(b) The maximum strength of the source is situated at 150 m above the surface; its shape is described by the profile of a Gaussian-plume which, for the spectral approach, is represented by the eigenfunctions of Equation (13).

(c) The empirical constants incorporated into the Gaussian and spectral solutions as well as into the boundary-layer model are shown in Table I. The stability parameters a, b, c, d (Section 3) are classified according to Klug (1969). The free parameter $\alpha = 6$ of the spectral solution (Equation (12)) is chosen such as to fit optimally the diffusion of the Gaussian plume, because there is no direct transformation between the horizontally varying standard deviations and the diffusion coefficient. The parameters defining the internal structure of the boundary layer are the geostrophic wind v_g in the x-direction, its height Z, the angle between the surface stress and the geostrophic wind, which depends on the atmospheric stability, and the Coriolis parameter (50° N).

The vertically averaged wind and diffusion coefficient are also given. It should be noted that not the magnitudes but the vertical profiles are of major interest; the latter are hardly influenced by slightly varying parameter values.

(d) Two classes of thermal stability (neutral, stable) are discussed in the following, which are studied with and without an inversion. Without inversion, the top of the barotropic boundary-layer model is at 1000 m (300 m) for the neutral (stable) case. For both stability classes, the height of the boundary layer has been reduced to the height of the inversion, i.e. $H = 210$ m.

As the three methods of solution are hardly to be distinguished in the y-direction, only the vertical profiles are presented, depending on the downwind distances 0.5, 1.0, and 2.0 km from the area source. The concentrations are normalized by the area average.

5.2. The Results (Figures 2a–d)

(a) *Stable Stratification*

The diffusive process modelled by the Gaussian plume shows slightly stronger concentrations than the spectral solutions which certainly depend on the external parameters chosen. However, it is important to note that there is hardly any difference of the vertical profiles in the spectral solutions. Only at larger distances from the source the spectral solution of the vertically structured boundary layer produces higher concentrations near the ground compared with the other approaches.

(b) *Stable Stratification with an Inversion*

Also in this case the Gaussian plume shows higher concentrations, especially below the inversion. This is due to the effect that the inversion is (implicitly)

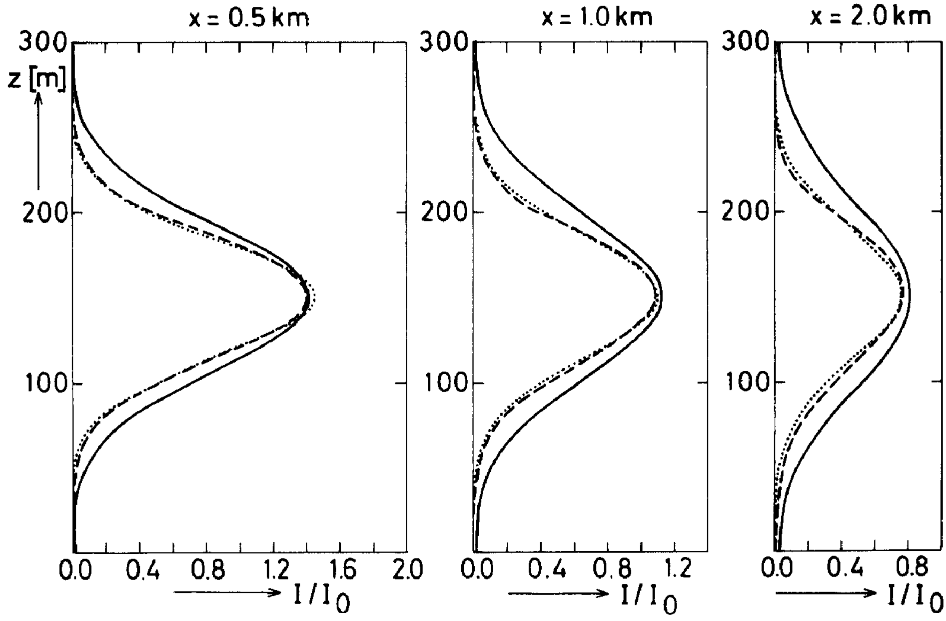

Fig. 2a

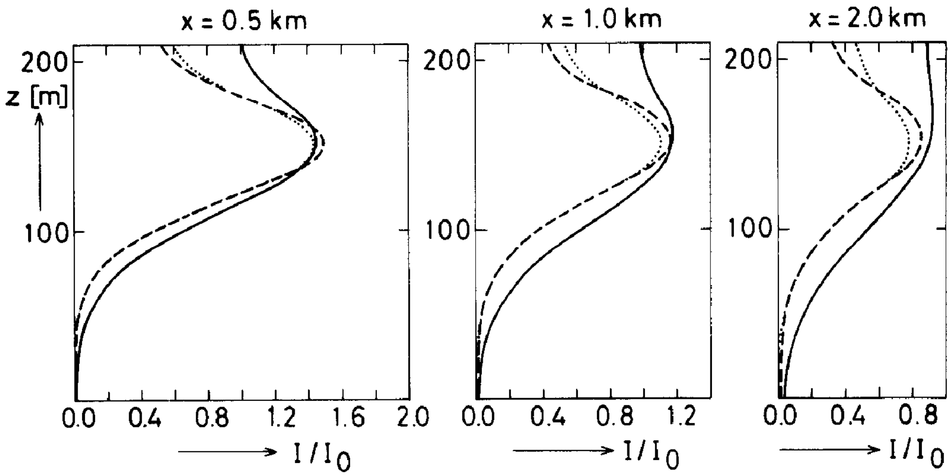

Fig. 2b.

Fig. 2a–d. Comparison of the vertical profiles of the normalized concentration at a distance of 0.5, 1.0, and 2 km from the vertical area source: Gaussian plume (full); spectral solution with constant coefficients (dotted), with vertically varying wind spiral (dashed). (a) stable, (b) stable with inversion (c) neutral, (d) neutral with inversion.

incorporated as a rigid lid in order to fulfill the boundary condition (4). Comparing the two spectral models, the case of variable coefficients shows a more pronounced vertical structure, as expected. At ≈210 m, the wind has its maximum whereas the diffusion coefficient is decreasing so that advective transport predominates over the vertically decreasing diffusive flux; thus, a maximum appears

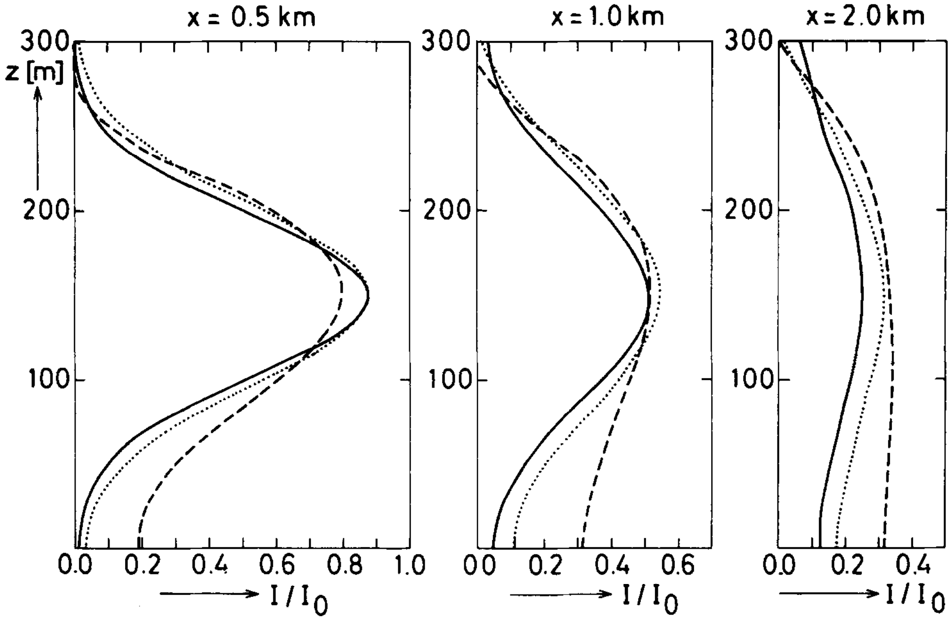

Fig. 2c.

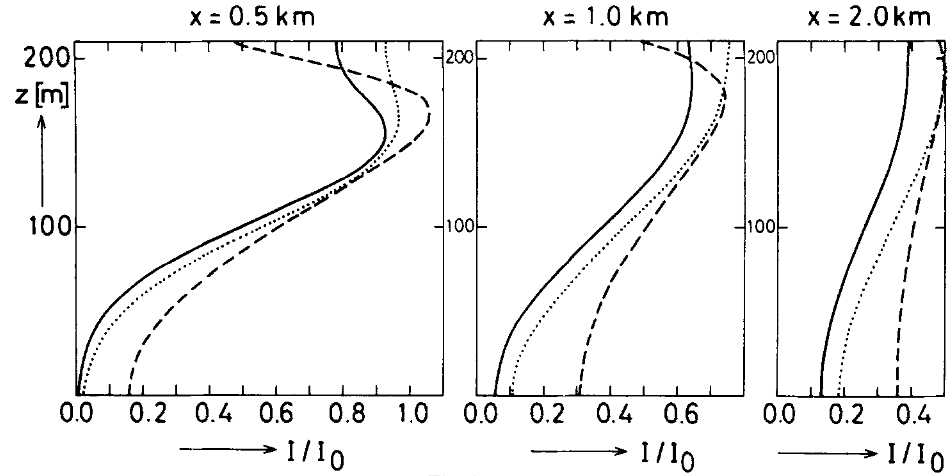

Fig. 2d.

at the height of the area source (150 m) and a minimum at the inversion; these are smoothed by the solution with vertically-constant wind and diffusive coefficients.

(c) *Neutral Stratification*

In comparison to the stable stratification, the following two examples of neutral stability (i.e., thermally well-mixed!) are calculated using a stronger wind (by a factor 2) and a larger diffusion coefficient (an order of magnitude). The Gaussian plume and the spectral solution with constant coefficients give essentially the same profiles. But the important result is the relatively high surface concentration determined by the vertically-structured spectral solution; in the lower layers, the wind is more rapidly decreasing than the diffusion coefficient, which leads to an increasing downward diffusive transport to be balanced by horizontal advection. Thus, the relatively weak surface wind has to be correlated with relatively large horizontal gradients (of the concentration) compared to the Gaussian plume or the spectral solution with constant coefficients, respectively. This result is in good agreement with tracer experiments (Vogt and Geiss, 1974), which yield higher surface concentrations than predicted by a Gaussian-plume model.

(d) *Neutral Stratification with an Inversion*

The Gaussian plume predicts generally smaller concentrations. Besides the effect of higher surface values, the vertically-structured model shows lower concentrations under the inversion (see Figure 2b).

(e) *The Unstable Stratification*

The unstable stratification is of no practical importance. After a short travel distance downwind, the calculations show a nearly uniform distribution of the concentration with, again, slightly higher values at the surface for the vertically-structured case.

6. Conclusions

In comparison with the Gaussian-plume approximation of the diffusive boundary-layer processes, the incorporation of a realistic vertical structure of the atmosphere leads to higher concentrations at the surface and lower values beneath the inversion. The effects appear weakest for stable conditions because it takes a greater distance for the stable plume to interact with the ground. Thus, under these circumstances the Gaussian plume is still quite a realistic approximation. For the other cases, however, if diffusive transports (e.g., of cooling-tower plumes) have to be realistically modelled, it appears reasonable to include explicitly the vertical structure of the planetary boundary layer.

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References

Collatz, L.: 1963, *Eigenwertaufgaben mit technischen Anwendungen*, Akademische Verlagsgesellschaft, Leipzig, 500 pp.

Courant, R. and Hilbert, D.: 1968, *Mathematische Methoden der Physik*, Band I, Springer Verlag, Berlin, 469 pp.

Fraedrich, K., Nitsche, H., Rudolf, B., Thommes, W., Wergen, W.: 1977, *Konvektion und Diffusion über einem Kühlturm-Entwurf eines Modells*, Bonner Meteorologische Abhandlungen, to be published.

Klug, W.: 1969, 'Ein Verfahren zur Bestimmung der Ausbreitungsbedingungen aus synoptischen Beobachtungen', *Staub-Reinhaltung der Luft*, **29**, 143–147.

Lettau, H. H. and Dabberdt, W. F.: 1970, 'Variangular Wind Spirals', *Boundary-Layer Meteorol.* **1**, 64–79.

McCormick, R. A. and Gutsche, B.: 1973, *Meteorologie der Luftbeimengungen*, Institut für Theoretische Meteorologie, FU Berlin, 126 pp.

Pasquill, F.: 1961, 'The Estimation of the Dispersion of Windborne Material', *Meteorol. Mag.* **90**, 33–49.

Singer, I. A. and Smith, M. E.: 1960, 'An Improved Method of Estimating Concentrations and Related Phenomena from a Point Source Emission', *J. Appl. Meteorol.* **5**, 631–639.

Sutton, O. G.: 1953, *Micrometeorology*, McGraw-Hill, New York, 333 pp.

Vogt, K. J. and Geiss, H.: 1974, 'Tracer Experiments on the Dispersion of Plumes over Terrain of Major Surface Roughness', Bericht der KFA Jülich, Nr. 1131.