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THE BASIS AND LIMITATIONS OF ESTIMATES OF POLLUTION FROM METEOROLOGICAL DATA*

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The purpose of this paper is to review briefly the position regarding the fundamental basis on which air pollution levels may be estimated from meteorological data, and also to bring out the uncertainties which appear to be unavoidable in practice.

1. The fundamental basis

The background of theoretical study in atmospheric dispersion of airborne material is now well-documented. Table 1 lists the main frameworks and certain of the relations involved. This is taken from a recent review[1] which gives further details and discussions of the conceptual problems. Features which have been more or less established and important questions which remain to be clarified are as follows (fuller discussions of many of these will also be found elsewhere[2].)

In circumstances of quasi-steady, quasi-homogeneous turbulence the turbulent spread of inert passive material has been found to be related to the observable intensity and scale of turbulence essentially in accordance with the statistical theory. The magnitude of the scale of turbulence is irrelevant close to a continuous point source but becomes increasingly important on the ratio of time of travel to Lagrangian time-scale increases. Allowance for this feature requires a working relation between Eulerian and Lagrangian features, and one such relation with some theoretical backing and a rough support from observations is now available.

(a) The dispersion relation which follows on these lines has been most clearly demonstrated in the lateral spread from a point source and the vertical spread from a source well away from the ground, over distances within about a kilometre downwind.

(b) The relation is questionable at longer distances, firstly in the respect that the observations have not included sufficient information on the crosswind scale of turbulence and secondly in the respect that further complication then arises from the systematic turning of the wind with height.

(c) The ultimate importance of the crosswind spread by the interaction of vertical mixing and turning of wind direction is strongly supported theoretically, but observational demonstration of this mechanism in the atmosphere is incomplete. On present evidence it appears unlikely to be of important consequence within a few kilometres of the source.

There are three major aspects of vertical diffusion to be noted.

(d) Regarding the use of the gradient-transfer hypothesis (for a source which is effectively at ground-level) an essential requirement is the explicit representation of the eddy diffusivity in terms of measureable properties of the flow. In the surface-stress layer the assumption of identity with the eddy viscosity expressed in terms of the wind profile has been given convincing support from diffusion observations in neutral conditions. Extension to a moderate degree of unstable and stable stratifications is still somewhat questionable but probably sufficiently realistic for many purposes. However in most respects the approach does not lead to any better representation of the effects of surface roughness and stratification than the simpler semi-empirical approach provided by similarity theory.

(e) For vertical diffusion extending above the surface-stress layer neither the momentum transfer analogy nor similarity theory at present offer a useful starting point. The most promising approach is now provided by the statistical theory arguments which, largely irrespective of stratification, prescribe an effective K profile in terms of the observable intensities and scales of turbulence. The greatest hindrance to progress on these lines is the need for turbulence measurements of a very sophisticated nature.

(f) For diffusion over appreciable depths of the atmosphere, apart from the indication that rapid vertical transport is usually effectively halted by an overhead stable layer, there is no well-developed theory or description of the detailed effect of the convective and large-scale vertical motions of the atmosphere.

For horizontal spread (and also vertical spread in regions clear of the ground or stable layers) the shape of the distribution of material from a maintained source is on average a close approximation to Gaussian form. However, individual cases display considerable irregularities and distortion from this simple form. There are indications that the vertical distribution from a ground-level source is systematically different from Gaussian. Furthermore, no useful details have yet been provided for the distribution developed within an expanding puff or plume.

The earlier treatment of the elevated source on the assumption of σ_y / σ_z constant with distance no longer appears to provide a satisfactory explanation of the results of surveys near power stations[1]. A useful fitting of such data has recently been offered by Moore[7] on the basis of σ_y and σ_z growths respectively proportional to x and $x^{\frac{1}{2}}$. There is some independent evidence for this sort of difference in the two components of spread by atmospheric turbulence but the fundamental position is not yet entirely clear, especially in regard to light wind convective conditions.

2. The airflow parameters utilised in dispersion calculations

Table 2 lists the special properties of the airflow additional to the obviously relevant wind speed and direction, which are required in applying the theories of dispersion. These are all familiar in the subject of boundary layer meteorology. Certain of them deserve further comment here because of their over-riding importance in the estimation of vertical spread, which in turn is specially significant in considerations of area sources of pollution.

(i) The intensity and scale of the vertical component of turbulence

Prominent features, some of which are discussed in more detail elsewhere[3], are as follows. On the basis of the observational data available it seems that at present only the broadest generalisations about λ_m and l_E would be justified. Probably the most that can safely be stated is :

(a) in neutral flow λ_m / z is between 2 and 4 and effectively constant with height in the first 20m or so,

(b) in neutral flow l_E / z is uncertain in the range $\frac{1}{2}$ to 2 over this height range,

(c) the effect of thermal stratification is to increase or decrease the scales in unstable or stable conditions, and in effect to increase or decrease the height range with effectively linear increase. However, the precise magnitudes of the effects on scale, and the heights of occurrence of maxima in the scales, are still quite uncertain.

For the magnitude of the vertical component a large number of independent observations give values of σ_w / u_* in neutral conditions in the range 1.2 to 1.4 and suggest an overall mean value of 1.3 , in or near the surface-stress layer.

In thermally stratified conditions σ_w / u_* increases or decreases from the neutral value respectively according as the stratification is unstable or stable. The variation is most logically expressed in terms of z/L and for large -z/L i.e. in markedly convective conditions recent work[4] has demonstrated the approach to the relation

$$\sigma_w = A^1 \left(\frac{g}{\rho c_p T} \right)^{\frac{1}{3}} \left(zH(z) \right)^{\frac{1}{3}}$$

for heights up to 1km, with A^1 approximately unity, and H(z) being the local value.

(ii) The vertical eddy diffusivity

The form listed at (b) in Table 1 has been used to evaluate profiles of K throughout the depth of the boundary layer and these have been used in numerical solutions of the two-dimensional equation of diffusion to give σ_z as a function of distance up to 100km for a ground-level source. Full details of this work, by F.B.Smith and S.A.Matthews, are as yet unpublished but a preview of some of the final results has been given elsewhere[1]. These results for σ_z are being incorporated by F.B.Smith in a revised form of the Meteorological Office system,[5] originally formulated in 1961, for estimating diffusion.

(iii) Mixing depth

The concept of the 'mixing depth' has long been familiar in the context of air pollution meteorology. The essential feature is the severe reduction or complete suppression of vertical mixing by overhead layers of the atmosphere in which very stable stratification has been produced, usually either by large-scale subsidence or the gradual over-riding of relative warm air. Such stable layers have bases which may be as much as two or three kilometres in height but occasionally much lower. It becomes obvious, on considering the typical sequence of diurnal cooling and heating, that stable layers with a high base are likely to be effective only over limited periods of the day, according to the vigour of the convective mixing generated during the heating period. Thus, in general the height of a well-marked overhead inversion may be regarded as defining a potential mixing depth, but the mixing depth actually prevailing will typically start from the very small magnitude established during the night and build-up toward the potential value more or less rapidly during the morning and early afternoon. Simple models of this development are now available[6], and the idea of the developing mixing layer is being incorporated in the revised system referred to in the preceding paragraph.

3. Accuracy and limitations.

The accuracy achievable in calculating air pollution levels from meteorological data depends partly on the extent to which the properties of the airflow conform to the idealised form assumed in the theoretical treatments, and partly on the type of meteorological data available. An indication of the range of accuracies is provided in Table 3, which is accompanied by explanatory notes. In some of these examples the assessment is indirect, being based on the accuracy of estimating the lateral and vertical spreads and effective height of source, whereas in others the assessment is based on the concentration itself. The estimates are not claimed to be exact limits - they are partly speculative and subjective and are to be regarded only as a general guide. They should however be adequate to eliminate or prevent any gross misconceptions on the part of users of dispersion formulae.

In cases 1-4 of Table 3 uncertainties in the source strengths have been assumed negligible compared with those arising in the estimation of dispersion and of effective height of source. However, the assessment in case 5 does include the uncertainties which must arise in practice in specifying a multi-source inventory of emissions. Case 6 is an example of the approach in which for practical reasons estimates of the emission inventory and direct application of the detailed dispersion formulae are not attempted. Instead, the past history of the levels of pollution as actually observed is used in deriving more-or-less detailed regressions between current levels of pollution and meteorological factors. In effect the history of the air pollution levels is being used to represent the emission inventory.

The broad implication of the examples considered in Table 3 is that an accuracy as good as $\pm$ 10 per cent in the estimate of pollution concentration may be envisaged only for certain special ensemble averages in the most ideal combination of circumstances, with complete information on source strength and air flow properties. An accuracy of 10-20 per cent may be achievable for certain long-term averages in practical circumstances, though still excluding cases of stagnant or confined airflow. For short term estimates at individual sites however, the uncertainties may at best be several tens of per cent (root mean square), and factors of two or more on particular occasions.

4. References

(1) Pasquill, F., 1971 Atmospheric dispersion of pollution, Quart. J. R. Met. Soc., 97, 369-395.

(2) Pasquill, F., 1962 Atmospheric Diffusion, D. van Nostrand.

(3) Pasquill, F., 1972 Some aspects of boundary layer description, Quart. J. R. Met. Soc., 98, 469-494.

(4) Caughey, S.J. and Readings, C.J., 1973 The vertical component of turbulence in convective conditions, 2nd IUTAM-IUGG Symposium on Turbulent Diffusion in Environmental Pollution, Charlottesville, U.S.A.

(5) Pasquill, F., 1961 The estimation of the dispersion of windborne material, Met. Mag., 90, 33.

(6) Carson, D.J., 1973 The development of a dry inversion-capped convectively unstable boundary layer, Quart. J. R. Met. Soc., 99, 450-467.

(7) Moore, D.J., 1973 Observed and calculated magnitudes and distances of maximum ground-level concentration of gaseous effluent material downwind of a tall stack, 2nd IUTAM-IUGG Symposium on Turbulent Diffusion in Environmental Pollution, Charlottesville, U.S.A.

(8) Islitzer, N.F. and Dumbauld, R.K., 1963 Atmospheric diffusion-deposition studies over flat terrain, Int. J. Air Water Poll., 7, 999.

(9) Pasquill, F., 1966 Lagrangian similarity and vertical diffusion from a source at ground level, Quart. J. R. Met. Soc., 92, 185.

(10) Briggs, G.A., 1969 Plume Rise, US Atomic Energy Commission Div. Tech. Inf.

(11) Pasquill, F., 1970 Prediction of diffusion over an urban area - current practice and future prospects, Proceedings of Symposium on Multiple Source Urban Diffusion Models, US Environmental Protection Agency.

(12) Smith, F.B. and Jeffrey, G.H., 1971 The prediction of high concentrations of sulphur dioxide in London air, Meteorological Office Boundary Layer Research Branch Turbulence and Diffusion Note No. 19.

TABLE I: BASIC THEORETICAL FRAMEWORKS

Type of theory	Gradient - transfer	Statistical	Similarity
Basic quantities	Eddy diffusivity K	R.m.s., eddy velocity and Lagrangian auto-correlation $R(\xi)$	Friction velocity u_* Vertical heat flux H
Limitations	Small-scale action implied. K-field to be specified	Homogeneity. Specification of $R(\xi)$ or equivalent spectral properties	Surface stress layer
Suitable aspects	σ_z (ground source)	σ_y, σ_z (elevated source) σ_y (ground source)	σ_z (ground source at short range)
Measurements and relations	(a) wind and temperature profiles - providing for $K = ku_* z/\phi(\frac{Z}{L})$ (b) intensity and scale of turbulence - providing for $K \simeq \frac{\beta i}{4.4}\sigma_w \lambda_m$ $\simeq \frac{\beta i}{6.6}\varepsilon^{\frac{1}{3}}\lambda_m^{4/3}$	Spectrum of Turbulence $\sigma_y = \sigma_v T f_1(\frac{T}{t_L})$ $\sigma_z = \sigma_w T f_2(\frac{T}{t_L})$ $t_L = \beta t_E$	Wind and temperature profiles $\frac{d\bar{Z}}{dt} = bu_*\psi(\frac{\bar{Z}}{L})$ $\frac{d\bar{X}}{dt} = \bar{u}(c\bar{Z})$

Nomenclature:

- b, c — numerical constants
- k — von Kàrmàn's constant
- L — Monin-Obukhov length
- R_ξ — autocorrelation of eddy velocity in Lagrangian sense
- t_L, t_E — Lagrangian and 'fixed-point' integral time-scales of turbulence
- $\bar{Z}$, $\bar{X}$ — mean vertical and alongwind displacements of particles after a given time of travel T
- σ_y, σ_z — crosswind and vertical root-mean-square displacements of particles
- σ_v, σ_w — root-mean-square eddy fluctuations of the crosswind and vertical components of velocity
- λ_m — equivalent wavelength for peak in product of spectral density S(n) and frequency n
- ε — rate of dissipation of turbulent kinetic energy
- ϕ — Monin-Obukhov function
- ψ, f_1, f_2 — other functions to be specified

Table 2 The special meteorological factors

Property and significance	Parameter	Definition / Further details
Aerodynamic roughness. Determines vertical profile of wind and mechanical maintenance of turbulence in boundary layer	Roughness parameter z_o	$\overline{u}(z) = \frac{u_*}{k} \ln \frac{z}{z_o}$ in neutral conditions
	Friction velocity	$u_* = (\tau_o/\rho)^{\frac{1}{2}}$
Thermal stratification. Represents magnitude of buoyancy forces which enhance or diminish turbulence and mixing	Richardson No.	$Ri = \frac{g}{T} \frac{\partial\overline{\theta}/\partial z}{(\partial\overline{u}/\partial z)^2}$
	Vertical flux of sensible heat, H	$H = \rho c_p \overline{w'\theta'} = - \rho c_p K_H \frac{\partial\overline{\theta}}{\partial z}$
	Monin-Obukhov length scale	$L = - \frac{\rho c_p T}{k g} \frac{u_*^3}{H}$
	Height of elevated inversion	determining potential mixing depth
Turbulence. Directly represents mixing quality of the air. May be used more or less directly to prescribe rate of diffusion of windborne material	R.m.s. fluctuation of eddy velocity	$\sigma_w = (\overline{w'^2})^{\frac{1}{2}}$ etc
	Intensity of turbulence	$i = \sigma/\overline{u}$
	Rate of dissipation of turbulent kinetic energy ε	related to shearing stress and heat flux.
	Integral scales of turbulence	$t_s = \int_0^\infty R(t)dt$, $\ell_s = \int_0^\infty R(x)dx$ etc
	Equivalent wavelength for peak nS(n)	$\lambda_m = \overline{u}/n_m = a\overline{u}t_s$, a depending on spectrum shape
	Lagrangian/Eulerian scale ratio	$\beta = t_L/t_E = \overline{u}t_L/\ell_E$
Diffusivity. Represents ratio of diffusion relative to gradient	Eddy diffusivity	K = Flux/Gradient. Representable in terms of σ_w, λ_m, ε.

TABLE 3 Uncertainties in pollution estimates based on meteorological data. The figures are fractional deviations, from the mean or actual values, of (a) ensemble average estimates in particular conditions (e.g. of wind speed or stability), (b) individual values (r.m.s.) of cases forming the ensemble averages, (c) long-term average estimates. Figures labelled (d) are extreme ratios 'estimate/actual' or its reciprocal.

Nature of source and terrain †	Conditions	Meteorological data available	Distance of travel km	Property estimated	Uncertainty	Notes
1. Passive ground level source on flat unobstructed ground.	Overcast steady wind	u z_o σ_θ	0.1 - 1	Peak of time-mean (few minutes) crosswind distribution	a < 0.1 b 0.1	(i)
	generally unstable	u z_o σ_θ Ri	< 3		b 0.2	(ii)
2. As 1 but source moderately elevated (50-100 m).	generally unstable	u z_o σ_θ σ_ϕ	1	Distance of maximum Magnitude of maximum	b 0.3 b 0.35	(iii)
3. Power station on terrain without marked irregularities. Heat emission known.	unstable or windy	u, Temp gradient		Distance of maximum hourly average	a 0.3 b 0.45	(iv)
			10	Maximum hourly average	a 0.35 b 0.5	(iv)
	any*	u, Temp gradient and wind direction statistics		Long-term average maximum	c 0.1	(v)

TABLE 3 (cont.)

4. Plume in mixing layer.	unstable with stable cap, definite wind field.	u,	Turning of wind direction with height, depth of mixing layer	100	Peak of time-mean (∽1 hr) crosswind distribution.	d	2	(vi)
5. Multiple sources in urban industrial complex.	any*	u,	z_o σ_θ σ_ϕ	10	Long-term spatial mean.	c	0.2	(vii)
					Individual site, value averaged over few hours.	b	1.0	(vii)
					Extreme (on say 1 percent of occasions) of few-hour average at individual site.	d	2	(vii)
					<u>Daily mean</u>			
6. As 5, but source inventory not specified.	any*		Duration of light wind, minimum temperature, mixing depth; (also long-term mean concentration).	10	Averaged over 100 sites.	b	0.25	(viii)
					At 1 site.	b	0.35	(viii)

See following page for notes (i) - (viii).

Notes on Table 3

† Marked topographical effects excluded.

* Except stagnant conditions of airflow.

(i) Based on comparison between early Porton data and recently recommended formulae.[1]

(ii) Based largely on comparison between crosswind spread measurements and estimates from wind direction fluctuation[8] and of limited experience on vertical spread[9]. An ensemble-average uncertainty is not attempted here because of certain unresolved anomalies in the data on concentration distribution at the longer ranges[1]. The formulae referred to in (i) tend to give concentrations progressively too high with increasing distance. The r.m.s. uncertainty quoted here represents only the scatter which would exist in estimates even if these were correct in ensemble average.

(iii) From treatment of elevated source, χ_m is determined essentially by $1/H\sigma_y(x_m)$. The figures given for x_m are based on Bowne and Islitzer's sample of observations of x_m.[5] and those for χ_m on the σ_y figures used in (ii), H being assumed accurately known.

(iv) As in (iii) but now assuming, on the basis of the practical experience with plume-rise formulae[10] that H is specifiable as an ensemble average at best within 10 percent, but that individually short-term means may have r.m.s. deviations from the ensemble average of 20 percent. Also assuming that x_m is given by taking $\sqrt{2} \leqslant H/\sigma_z(x_m) \leqslant \sqrt{3}$ and that $\sigma_z \propto x^{\frac{1}{2}}$. It then appears that the uncertainty is essentially in respect of x_m, being increased only marginally from this in respect of χ_m. Moore's[7] recent 'optimised' fitting of the observational data collected for the Tilbury and Northfleet power stations gives uncertainties broadly consistent with the present estimates for x_m , but considerably less for ensemble average values of χ_m and somewhat greater for r.m.s. deviations of individual values of χ_m .

(v) The long-term maximum effect from a power station will be determined by the crosswind integral of the distribution of concentration (hence by 1/H) and by the frequency of occurrence of wind direction from the stack. Assuming the latter is well-known the uncertainty is simply that in H ;

(vi) If the mixing layer 'h' is well-mixed vertically, as assumed, the peak time-mean concentration at sufficiently long distance will be determined by $1/h'\sigma_y$. If the magnitude of 'h' is known only within say $\pm$ 50 % , the likely uncertainty of a factor of 2 in σ_y at say 100km (based on limited experience of relating σ_y to wind direction turning with height) will be the dominant contribution.

(vii) Based on the experience of the Reading, England study by British Petroleum[11].

(viii) From preliminary evaluations of the model proposed for forecasting daily levels of SO_2 in a city.[12]