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SOME VIEWS ON MODELLING DISPERSION AND VERTICAL FLUX

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In conventional dispersion modelling we are concerned with semi-empirical predictions of the vertical (σ_z) and lateral (σ_y) spread of a point source plume, and of the effective height of the source in the case of hot chimney effluent. The resultant errors in concentration which arise in practice from the combination of the separate errors in estimating these three parameters have been discussed previously (Pasquill 1973).

For surface releases and short range (ca 1 km) over uniform terrain experience suggests that each of the spreads might be estimated (semi-empirically) with a r.m.s error of 10-15% for individual occasions with sampling over some minutes at least. For elevated sources of given height the most important error is in estimating the distance (x_m) of maximum concentration, (implying an error in estimating σ_z), and may be $\pm$ 35% (r.m.s) in unstable conditions. This error largely determines the final error in the magnitude (C_m) of the ground-level maximum concentration. These r.m.s errors are increased still further when the effective height of the source has to be calculated semi-empirically and then are estimated to reach around 50% for the hourly average ground-level maximum concentration. An even more dramatic increase in error (to near 100%) appears when the interest is in the concentration at a <u>fixed receptor</u> within a multiplicity of sources, presumably a consequence mainly of the combination of all the foregoing errors with errors in the assumed wind direction.

In considering these errors it is worth remembering that the conventional approach, with plume geometry specified in terms of σ_y and σ_z , implicitly contains the basic physical principle represented in the conservation expression, e.g. for the two-dimensional (line source) case

$$\bar{u}\frac{\partial C}{\partial x} = \frac{\partial F}{\partial z}$$

where F is the vertical turbulent flux. $C(x,0)$ therefore has to be evaluated through $\partial F/\partial z$ at $z = 0$. In certain simple situations when it is valid to assume that u is constant with height and that vertical profiles are similar irrespective of distance (i.e. a universal function of z/σ_z) it follows that $C(x,0) \propto (\bar{u}\,\sigma_z)^{-1}$.

The value of σ_z may be obtained by any one of several methods, one of which may in fact be solving directly a simplified integrated form of the conservation equation itself. The alternative methods also imply, albeit implicitly, a conservation of material C and it is worth re-emphasising that essentially the so-called plume-model approach simply represents a convenient simplification of the problem of finding a general solution which, although it may introduce an error (which is often only marginal), is fundamentally equivalent to solving the full basic diffusion (i.e. conservation) equation.

However in a more complex situation such as over a heterogeneous city-complex this simple approach may be acceptable no longer and we are forced back to a direct solution of the fundamental equation :

$$u \frac{\partial C(x,0)}{\partial x} = \left(\frac{\partial F}{\partial z}\right)_{z=0}$$

Much interest is now being developed in modelling of the flow field itself, and in the avoidance of the suspect gradient-transfer theory, the implication being that it should be possible thereby to reduce the errors in conventional dispersion modelling. But even for a prime flow property such as wind direction it has not yet been established how far flow-modelling may be expected to succeed in important practical circumstances, such as those mentioned above of a large urban-industrial area with variations in topography, aerodynamic roughness and buoyancy effects. For the more complex effects which determine the <u>dispersion</u> of injected material it seems even more a matter of wishful thinking.

The formulation of higher-order equations for turbulent transport in the hope of avoiding the gradient transfer approach is no doubt an important step, but closure approximations and assumptions are still required. We consider it important to keep these in mind stage by stage, and to design observational tests of the most searching nature, rather than to construct a whole closed hierarchy of equations and test the net effect against a whole practical survey in a multi-source situation.

As an example of what we have in mind we offer the following preliminary considerations of the vertical flux in the one-dimensional time-dependent case. Physically, for example, this corresponds to the non-steady evaporation from a uniform effectively infinite area of evaporating surface, and is also the time-analogue of the advective build-up of pollutant concentration over an area source with non-uniform emission.

As we have noted, the interest is especially in $\left(\frac{dF}{dz}\right)_{z=0}$. Consider this quantity F ($= \overline{w'C'}$) for passive material (concentration $C = \overline{C}+C'$) in terms of the 2nd order equation (e.g. see Donaldson 1973). The full equation in the one-dimensional context is

$$\overline{w}\,\frac{\partial \overline{w'C'}}{\partial z}^{(1)} + \frac{\partial \overline{w'C'}}{\partial t}^{(2)}$$

$$= -\overline{w'^2}\,\frac{\partial \overline{C}}{\partial z}^{(3)} - \overline{w'C'}\,\frac{\partial \overline{w}}{\partial z}^{(4)} - \frac{\partial \overline{w'^2C'}}{\partial z}^{(5)}$$

$$-\frac{1}{\rho}\,\frac{\partial (\overline{p'C'})}{\partial z}^{(6)} + \overline{\frac{p'}{\rho_0}\,\frac{\partial C'}{\partial z}}^{(7)}$$

$$+ g\,\frac{\overline{C'T'}}{T_0}^{(8)} + \nu\,\frac{\partial^2 \overline{w'C'}}{\partial z^2}^{(9)} - 2\nu\,\overline{\frac{\partial w'\,\partial C'}{\partial x_i\,\partial x_i}}^{(10)}$$

Simplifying to zero-divergence of the flow terms (1) and (4) are eliminated. The pressure fluctuation terms (6) and (7) are of unknown magnitude but for a passive property it is difficult to see any reason for important magnitudes. The 'molecular' terms (9) and (10) are also of unknown significance - presumably (10) is a 'decorrelation' term analogous to the dissipation of turbulent fluctuations of velocity, but estimation thereof is at present problematical.

We see therefore that even with a simplified situation the position as regards solving the equation for $\overline{w'c'}\,(z)$ as a function of time is not straightforward and the best we can now do, hopefully, is to consider the equation as essentially reduced to

$$\underset{(2)}{\frac{\partial \overline{w'c'}}{\partial t}} = -\underset{(3)}{\overline{w'^2}\frac{\partial \overline{C}}{\partial z}} - \underset{(5)}{\frac{\partial \overline{w'^2c'}}{\partial z}} - \underset{(8)}{\frac{g}{T}\overline{c'T'}} + \underset{(10)}{\text{'decorrelation'}}$$

A useful next step would be to examine the magnitudes of the terms (2), (3), (5), and (8) observationally, and to consider further and theoretically term (10). For the observational study we could use humidity mean profile and humidity/vertical component fluctuations at two or more low heights above a near-ideal large area of grassland, in the morning regime of build-up of evaporation.

Some estimates may be made without further ado for the terms (2) and (3), for despite the suspicions about the gradient-transfer approach we know that realistic estimates of $\overline{w'C'}$ are thereby provided for water vapour at low heights and we can also make quite good estimates of $\overline{w'^2}$ at low height, e.g. from a specification of z_o and u_*. Following this line in terms of humidity profile data and evaporation estimates published by one of us (Pasquill 1949) we find that typically in the forenoon rise of rate of evaporation term (3) is 10^4 times term (2) at a height of roughly 0.5 metres.

It is of course evident from the typical diurnal trend in evaporation that shortly after noon the rate of evaporation is a maximum, while $\frac{\partial \overline{C}}{\partial z}$ is large, and it is then obvious that term (2) is a negligible term in the balance. However, what was not immediately obvious is the typically low relative order of this term in the important morning phase of the diurnal cycle.

In our present context this has an immediately disconcerting implication if we are set on the course of estimating $F(z,t)$ without using the gradient-transfer assumption in a 1st-order closure. From the results above it would appear that assumptions made about the component terms in the 2nd-order equation (e.g. the 3rd-moment term at (5)) must be correct to the order of 0.01 per cent !! We do not have immediately any numerical data for the analogous case of $\frac{dF}{dx}$ over a large area source with source strength q building-up to a maximum at some position. However, at first sight there seems no reason to expect radically different relative magnitudes of the terms which determine $\frac{dF}{dx}$.

To summarise, the purpose of our discussion is to bring out three main points :

1. Conventional dispersion modelling has fairly clearly defined limitations and inaccuracies.
2. In its most practical form (plume modelling) the basic 1st-order conservation equation is fully implied.
3. Use of 2nd-order conservation equations, to circumvent the objections to closure at the 1st-order, may require closure assumptions which would have to be valid to an accuracy which we cannot visualise ever being attained.

References

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