Developments in Short Range Atmospheric Dispersion Modelling

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This short review briefly describes some of the developments in the 1990s of practical and regulatory models for short range atmospheric dispersion. We cover the recent research results on the Atmospheric Boundary Layer and on the spatial and time dependence of atmospheric flows in complex terrain including the structure of turbulence. We consider the consequences of these developments and the better understanding of atmospheric chemistry processes for improved dispersion and transformation of pollutants. Finally some outstanding issues are mentioned about future application and methodologies.

1 INTRODUCTION

Several fast codes for small 'personal' computers were developed in the late 1980s and 1990s for 'regulatory' types of models of dispersion from localised sources in the atmospheric boundary layer (ABL). Some examples of these codes with references, are listed in Table 1. Essentially these are based on the implementation of international research conducted in the 1980s and 90s. This involved theory, computation (especially Large Eddy Simulation LES (eg, Mason [17])), field and laboratory experiments on all aspects of the meteorology and dispersion in the ABL. The key result was the description in non-dimensional form of the variation with height z and with stable/unstable stratification (as defined by the Monin-Obukhov length L_{MO}) of the turbulence and mean profiles (as a function of z/h and h/L_{MO}) in the boundary layer or 'mixed' layer with depth h. Modelling the depth h of the layer is particularly important as this defines the scale of the eddies in the convective layer and the behaviour of buoyant plumes (eg, from tall chimneys or accidental releases) near the top of the layer, which in turn has a sensitive influence on the ground level concentration.

Changes to the modelling of diffusion processes were also introduced with these changes in the meteorology, especially by allowing for non Gaussian vertical profiles of mean concentration in the convective boundary layer. This led to significantly higher (typically by a factor of 2) predicted concentrations in the maximum ground level concentration at a location significantly closer to the source. Another change was a reduction in stable conditions $(h/L_{MO} > 1)$ in the vertical rate of diffusion from elevated sources. In addition stochastic simulation and field experiment with new fast response instruments (Mylne [19]) showed that the statistics of concentration *fluctuation* have a sufficiently repeatable form that they could be parameterised and included in dispersion models. As it turned out, they have a close relation to the mean concentration statistics. (CERC [5])

Other key developments in regulatory dispersion modelling have been the inclusion of the effects of flows over buildings and complex terrain, using algorithms that are simple enough for PC level computations to be completed in a few minutes for each flow/source situation. This required considerable simplification. In the case of buildings the main objective was to provide useful approximate formulae for isolated or effective buildings of typical shape and in typical clusters (as in industrial plant buildings). (It took 10 years to transfer the basic concept presented in the UK by Hunt & Robins and in the USA by Huber & Snyder into reasonably well validated modules in the general dispersion codes ADMS and AERMOD (Robins et al [22]). Despite the general availability of CFD codes for flows as complex as these over arbitrarily shaped hills or buildings, and their greater accuracy (especially for groups of structures), these codes still require more computer time (by factors of 10 to 100 or more) and more capacity than are available for a typical air pollution dispersion calculation for one particular meteorological situation. Such calculations have to be repeated hundreds or thousands of times to derive long term averages needed to meet regulatory requirements. Another important development in regulatory models was the work of Berkowicz [2] and comparable studies which accounted for the effects of dispersion of vehicle exhausts in typical city streets between rows of multi-storey buildings (or 'street-canyons'). This enabled the dispersion models developed for industrial stacks to be used for urban air pollution situations to predict the location where concentrations are highest and as a corollary where they are significantly less only a small distance away from the busiest streets. (McHugh et al [18]). It is possible that these models could be applied to the dispersion of local releases of toxic contaminants in urban areas, a problem of urgency with the increased threat of bio-terrorism.

Studies of air quality in urban areas have also shown that people's health is affected by many types of gases and particles resulting from chemical reactions between exhaust gases and the atmosphere. This has led to new regulatory requirements and caused some urban communities and transportation agencies to base their future plans and daily decisions on computations combining dispersion and chemical reactions in urban areas (eg, Carruthers et al [3]). As with other regulatory calculations they also need to be fast enough to meet the timetable of decision makers, but detailed enough to guide practical decisions about emissions, traffic planning, etc (the models used for the decisions are often operated by planning specialists who have limited training in air pollution and meteorology).

The effect of hills and mountains are increasingly factored into regulatory air pollution models; these are based on the flow patterns which are broadly characterised by the value of the non-dimensional Froude number $(F = U/(NH) \approx 100U/H$ for typical meteorological situations. When F > 1 (as is usual in most UK situations) the air flow passes over the hill and descends in a slow moving turbulent wake on the lee sides. The air flow also depends on how the surface roughness elements (eg, trees, rocky outcrops etc) are distributed over the hills. Typically the concentrations at the ground are changed by up to a factor of 2 or 3 in these flows compared to dispersion over level ground. For mountains, generally higher than about 300 m there are often much larger changes in the airflow and the dispersion especially in stable low wind conditions. The kinetic energy is not high enough for the wind to pass over the mountain and so plumes can impact directly onto its surface leading to large increases in maximum ground level concentration. The US EPA programme of research focused on the latter problem. The current 'advanced' UK and USA models (ADMS and AERMOD) include both neutral and stable types of complex flow, but only ADMS includes the wake down-wash effect.

As the number of different systems has increased, an increasing number of users including regulatory organisations, have called for systematic and open methods for comparing the codes and for testing them against experimental data, especially those obtained in field experiments. This has resulted in standard quality assured data sets that are widely available, and, equally as important methods for comparing the models against the data. (eg, Olsen [20] ASTM [1]] However there have also been less open studies by different organisations (eg, Environment Agency) comparing the different computational regulatory models. The results of these studies have sometimes been released publicly even though they were not open to general comments by all those involved in the code development or the experimentalists and thus contained inaccuracies. Perhaps this aspect of the governance of regulatory air pollution models will need to be examined in the future? Another qualitative development in regulatory air pollution modelling is that the application of models is being applied to forecasting air pollution in local areas using as input meteorological forecasts. This will become a growing trend and, as with weather forecasts, the regular comparison of such predictions with measurement will act as a rigorous test of the computational models particularly in special atmospheric conditions.

2 ATMOSPHERIC BOUNDARY LAYER RESEARCH

2.1 Over level surfaces

Recent research on the atmospheric boundary layer in the 1990s has provided further evidence to confirm the earlier conclusions about the variation of the structure of the layer in the different meteorological conditions. However there has been significant further understanding of the details of the structure and how it changes in varying or complex conditions, and how these changes affect turbulent diffusion.

In neutral conditions recent re-examination of field data, together with theoretical and numerical simulation has shown that over flat terrain in the lowest 50 m of the boundary layer the stream wise and transverse length scales of horizontal eddy motions are much larger than are currently assumed in models of spectra. These long scales are generated by downward impinging eddies scraping along the surface producing 'cats paws' and generating low wave number velocity spectra proportional to $u_*^2\kappa^{-1}$ (Hunt & Morrison [13]) - This may have implications for turbulent diffusion by explaining why the transverse plume width as increases linearly with distance x up to a distance of about 15 km from a source - as is assumed in current $\sigma_y(x)$ models but not hitherto explained. It is not clear whether these results can be applied to flow over very rough mountains or urban terrain because there are opposing influences that both increase and decrease length scales.

In stable conditions (when the Monin-Obukhov length L_{MO} is positive) the density gradient tends to suppress and transform atmospheric turbulence but this is a complex process and is more variable and intermittent than in neutral or convective conditions. It is also much more sensitive to terrain slope and to the time variation of the surface temperature. Field experiments, radar observation and local measurements have demonstrated the existence of various types of vertical mixing events, mostly confined to thin layers, including those very close to the ground. This leads to vertical diffusion being somewhat larger in the lower surface layer (on slopes in open terrains) than it is above about 30 m, at which level elevated plumes can travel for long distances with little vertical diffusion. These research results should improve the interpretation and application of dispersion models to these situations, which are important because they lead to large fluctuations in the concentration.

In unstable conditions (when $L_{MO} < 0$) convective eddy motion occurs above the surface layer (where $z < |L_{MO}| \sim 50 - 100$ m). The statistical distribution of the vertical velocity in these convective eddy structures differs significantly from that in the neutral and stable boundary layer, and affects the profiles of mean concentration downwind of sources in the convective boundary layer or CBL. It is usually non-Gaussian with a negative value of the 'mode', ie, the most frequent values, which causes the maximum of the ground level concentration are nearer the source than with Gaussian profiles. This effect, which has been confirmed in field and laboratory experiments, has been incorporated in modern dispersion models. However recent research (suggested much earlier by Scorer [24]) has confirmed that in certain conditions (eg, cool air over warm ground with no solar radiation and over slopes) eddies in the CBL are more like puffs and the probabilities may be more Gaussian. These differences in eddy dynamics not only affect diffusion, but also affects the entrainment processes at the top of the mixed layer and thence momentum transport in the whole boundary layer (Hunt [10]).

2.2 Complex and mesoscale flows

Since most of the earth's surface is sloping and the surface roughness and temperature is varying, the idealisation of a steady ABL flow over a flat surface is not, in principle, widely applicable. Consequently research on the ABL has continued into questions concerning the validity of this idealisation and what kinds of correction might be introduced to account for complex flows both on the microscale (< 10 km) and mesoscale (up to 100 km). Small slopes (a) do not greatly affect the structure of convective turbulence (eg, Hunt *et al* [12]), but they do affect the mean wind speed *U* if the geostrophic wind is weak (< 3 ms^{-1}). Recent field and laboratory experiments in the USA have provided extensive data on flows over slopes that adjoin a flat plain. In daytime convective conditions the mean wind varies little with the magnitude of the slope ($U \sim 3w_*\alpha^{1/3} \sim 2$ ms^{-1} for $\alpha < 0.1$, where w_* is the convective velocity). In narrow 'Alpine' valleys pressure gradients lead to lower wind speeds (Hunt *et al* [14]). In the evening the timing of the cessation of the upslope wind varies; it is usually at sunset either if the valley is wide enough or in confined 'Alpine' valleys. But in some open valleys the wind direction does not change during the day *and* near the equator it continues for several hours after sunset; this seems to occur when the valley sides are steep enough to reduce Coriolis induced turning of the wind during the day.

Again, as Scorer observed in the UK with his experiments using rockets in the Welsh valleys, in stably stratified conditions, downslope flows driven by gravity currents, continue outwards onto the adjoining planes. The local structure of the stable turbulence here is similar to that on level surfaces so that dispersion models can be applied (eg, Hunt *et al* [12]; Hunt and Morrison [13]). However the combination of up and down slope winds greatly affects patterns of air pollution movement in urban areas on sloping terrains, especially in weak wind conditions so that it may not be appropriate to use models which ignore the variation of the wind direction. In one US city (Phoenix) this has caused the peak in concentration to occur after midnight when downslope winds return the pollution to the air that had been advected up slope in the early evening. But in other cities where the upslope winds cease at sunset, the maximum evening pollution occurs at that time.

Research on airflow and dispersion in urban areas has finally led to new measurements and to new concepts for developing models that are appropriate for regulatory purposes. In neutral conditions investigations conclude that a *displaced* logarithmic velocity profile $U = \frac{u_*}{L}\ln\left(z-d\right)/z_0$ is appropriate above the urban 'canopy', but there is still some uncertainty about how the value of the displacement height d and roughness length scale z_0 vary with the height H and spacing of the buildings, and the distance (x) into the urban area. The latter factor is found in field experiments to determine how the average wind speed U_c varies *below* the roof tops ($z < H$). Some models assume an equilibrium in which case U_c is determined by the wind above the canopy. A key development has been the introduction of the street canyon vortex, which determines the local patterns of pollution at street level (Berkowicz [2]).

In convective conditions recent research shows how the increased buoyancy forces, caused by the heat flux increases over urban areas, increase the velocity fluctuation in the centre of the CBL, but less so near the ground because of the large roughness length z_0 produced by buildings. Models for flat terrain can be applied to these situations taking suitably large values of w_* and z_0.

Intensive research is now re-evaluating the earlier estimates (eg, Oke [20]) on how the heat flux and the urban heat island depend on radiation balance and heat transfer to and from buildings, roads etc. . When the ABL outside urban areas is stably stratified, (eg, at night), because of the heating in urban areas, there is usually a transition to convective condition analogous to movement of stable marine air onto warm land in a sea breeze, so that regulatory-type coastal models could be applied to this situation.

Research on the ABL near coasts in wide valleys and roughness changes has shown that some of the significant changes on scales of order 10 km or less, are determined by mesoscale dynamics, although these also affect the flow over much longer length scales, of the order 100 km or more (on the Rossby deformation scale (the distance for an internal wave to travel in a rotational period) $L_R = hN/f$). These sharp changes occur in and above the ABL to the height at which the atmosphere is stably stratified (even quite weakly). The most significant effects for dispersion modelling are the sharp variations *parallel* to roughness changes of mean wind speeds and turbulence intensities and in the vertical variation of isopycnals which causes systematic local variation of cloudiness and surface solar radiation [Hunt, Olafsson & Bougeault [14]].

3 DEVELOPMENTS ON MODELLING OF DISPERSION AND TRANSFORMATION OF POLLUTANTS

3.1 Extensions of existing methods

The essential basis of most current regulatory models is the calculation of the mean concentration produced by a steady source with strength Q (say over 1 hour) along the mean streamline(s) from the source(s) (determined by the distribution of the mean wind field U) using information about the turbulence to derive the plume dimension Anal, so that $C \sim Q/(U\sigma_z\sigma_y)$). This elemental formula has been extended to be applied in quite complex flows, such as plumes impinging onto mountains or around buildings (when the effect of dispersion in the wake is estimated either by moving the source upwind or in the more recent models by introducing a new source in the wake and depleting the strength of the plume coming from the original source, eg, Robins, Carruthers & McHugh [28]). This approach of defining effective values of U, σ_z, σ_y is now being applied to even more complex flows such as those in urban areas. [Hanna & Britter [9]].

For dispersion from steady local sources over level terrain, the statistics of fluctuating concentrations can be related to those of the mean concentration in field, [Thomson [26]]. There has only been limited research into these relations in non-neutral and complex flows (eg, Mylne [19]). But these have yet to be incorporated into regulatory models.

When sources are unsteady the dispersion is also now computed using analytical algorithms and these situations are included in regulatory models. However when the meteorological conditions are changing and when dispersion from plume sources is to be computed over several hours, the present quasi-steady plume/puff methods are not applicable. Either they need to be adapted or entirely different methods are necessary. One possible form of adaptation is the puff-model (such as RIMPUFF from Risø) in which matter from a continuous source is divided into finite volume elements and these are tracked over several hours, as they are advected by the mean velocity and dispersed by the turbulence as the meteorology evolves. To adapt current quasi-steady models to this approach would require substantial reprogramming and recalibration of the existing quasi-steady systems. However there are more straightforward and computationally faster methods to adapt these systems reasonably economically to account for changing meteorological conditions, Fig 1. One way being developed at present at CERC is a mixed Eulerian-Lagrangian scheme (similar to the semi-Lagrangian method used for numerical integration in some numerical weather prediction (NWP) schemes.

This first requires defining a grid within the computational domain of the flow with sides $\Delta x, \Delta y, \Delta z$ (eg, 00 m). At the end of each time interval (eg, 1 hour) the concentration field $C(x, y, z, \Delta t)$ in each grid box is averaged over the box, so that in the next time interval the pollutants in the flow consist of the new pollutants being emitted from actual sources plus the pollutants left over from the previous hour. These are now considered as sources distributed over the grid boxes using the standard dispersion formulae for the quasi-steady method (which is already applied to modelling dispersion in urban areas to account for multiple sources which cannot be individually treated). Then in the example of the urban area with upslope and downslope winds the pollutants being carried out the urban area are distributed over grid boxes at the end of each hour and then, when the wind reverses, this material is advected back towards the area. This regridding method is also necessary to account for chemical reactions of pollutants that take place over several hours even when meteorological conditions do not change. Where the flows are also highly inhomogeneous, eg, in coastal/mountainous urban areas it is practical also to use the Lagrangian-Eulerian method with the updated fields computed over a larger grid scale ΔX ΔY (eg, 3 km) (using fast approximate methods or mesoscale models).

3.2 Real time forecasting and long range methods

In order to calculate the dispersion of pollutants that travel from a source for more than a few hours firstly requires information about the overall wind fields derived from NWP. Whereas in the past this information was restricted to those working in National Meteorological Services (NMSs) it is now widely available from US and European distributions for both archived data or even real-time. The NERC Atmospheric Data Centre provides a convenient service however as is common with many data sources there are restrictions for non academic users which inhibits widespread use of these data. Nonetheless this type of data is now used for air quality forecasts in urban areas using short range quasi-steady dispersion models. For longer range dispersion these data have been applied by NMS to dispersion over thousands of kilometres from actual or simulated nuclear reactions and to debris from volcanic eruptions. Maryon & Buckland [16] applied this technique in a basic study to determine the different patterns of long range dispersion in a range of meteorological conditions varying on synoptic space and time scales. This study provides a useful guide as to what to expect when short range dispersion models are applied outside their range of validity over much longer distances and times.

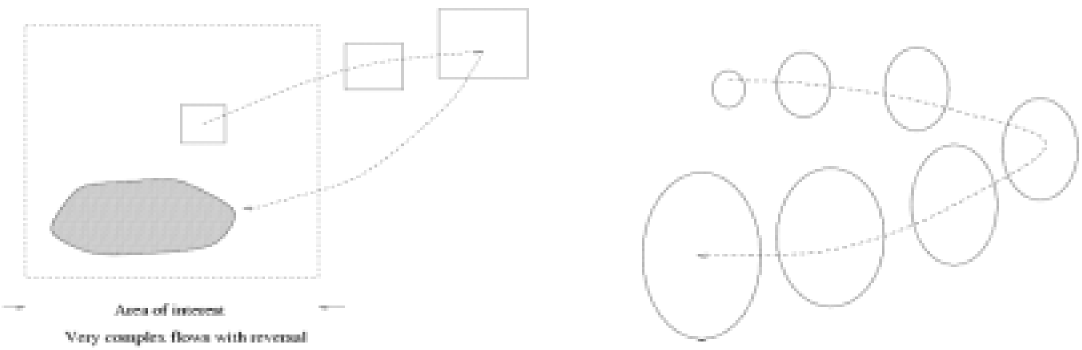
The method used for these dispersion calculations is based on combining the results of NWP models and the random walk method used for research into short range dispersion. Particles move with the average wind at that point (as averaged over a typical grid box and time interval from NWP) and with a short range random element determined by the velocity scale of the turbulence. Since there is a continuous spectrum between the 'resolved scale' motion of the NWP and sub-grid scale velocity fields there is some uncertainty about how best to derive the random displacements from the observed spectra (see Sakai et al [23]; Maryon & Buckland [16]). But the verification and intercomparison of these and large scale 'dispersion' simulations (eg, as organised through the World Meteorological Organisation) has given confidence about these methods.

3.3 Dispersion combined with other processes

One of the early applications of regulatory dispersion models was the prediction of the concentration of elements and their decay along the path of a plume. Since then there have been other applications involving the combined modelling of dispersion and other processes. Many of these models may need to be reconsidered in the light of recent research. For example the mean velocity of settling of small particles in the atmosphere, which hitherto has been assured to be independent of turbulent velocity fluctuations (with rms value u_0), has in fact been found to be amplified by up to about 80% for particles of the order of 20 μm (for which V_T is of the order of u_0). For slightly larger particles V_T is reduced by turbulence (Davila & Hunt [6]). For regulatory calculations an increase in V_T is likely to produce an increase in the rate of deposition of certain small particles at the ground. These calculations are significant for many environmental processes including agricultural assessments of the chances that pollen from transgenic plants grown in one field can be deposited at significant rates on plants in adjoining fields (Hunt *et al* [11]).

Another area of active research for models with regulatory applications is chemical transportation. Over the last decade substantial advances were made in the understanding of many VOC degradation pathways. Reaction rates are under constant review through authoritative panels drawn together by IUPAC and NASA. However substantial uncertainties remain in aerosol processes, in particular in the area of nucleation rates, and accurate mechanistic modelling of aerosols in 'regulatory' applications remains some time away.

Detailed measurements of biogenic and anthropogenic volatile organic compounds (VOCs) and their reactive by-products are increasingly common, whether in routine measurements such as those at Marylebone, London or in field campaigns such as in Houston, Texas in September 2000. Such measurements have enabled the use of increasingly complex models of atmospheric chemistry. These measurements are complemented by emissions inventories of increasing complexity, detailing the diurnal and seasonal variability of VOCs of varying reactivity. Such inventories are often formulated by cross correlating known biogenic emission profiles with land-use data derived from satellites or local knowledge. In urban environments detailed emissions inventories can be obtained by cross-referencing urban traffic volumes and velocities with laboratory measured vehicle emissions. Such methods have been much simplified by the increasing popularity of geographical information systems.



or

Figure 1: Exploring use of mixed point – Eulerian (grid) models (ie, receptor box becomes emitter for new conditions – eg, wind changes) – same method as for chemistry – efficient

These data have enabled the verification of many chemical mechanisms of varying complexity (Carter [4], Gery et al [8], Jenkin et al [15], Stockwell et al [25]), considering the reactions of anywhere from 30-2000 species. The most complex mechanisms are primarily research tools, though they can also be used in instances where the atmospheric activity of a novel compound needs to be estimated [Derwent et al [7]]. The computational expense of very complex mechanisms is prohibitive for 'regulatory' applications, but compact mechanisms involving 30-40 inorganic and organic species can be used. An advantage of these over earlier, simpler chemical mechanisms is that they allow for the varying reactivity of different VOCs, thus providing much more accurate estimates of changes in ozone and nitrogen oxides arising from to the diurnal and seasonal variability of VOC emissions. In addition these mechanisms improve the accuracy of aerosol models by supplying them with detailed air composition estimates.

	Country of origin	Reference
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HPDM	USA	Hanna SR and Paine RJ (1989) 'Hybrid Plume Dispersion Model development and evaluation', J *Appl.Meteor.,* Vol. 28, pp 206-224
ADMS	UK	DJ Carruthers, RJ Holroyd, JCR. Hunt, WS Weng, AG Robins, DD Apsley, DJ Thomson and FB Smith (1994) UK-ADMS: A New Approach to Modelling Dispersion in the Earth's Atmospheric Boundary Layer. J *Wind Engineering and Industrial Aerodynamics,* Vol. 52, pp 139-153. DJ Carruthers, RJ Holroyd, JCR Hunt, WS Weng, AG Robins, DD Apsley, DJ Thomson and FB Smith (1991) The United Kingdom Atmospheric Dispersion Modelling System - a new approach to modelling dispersion in the Earth's atmospheric boundary layer. In *Proc. CEC Workshop on Objectives for Next Generation of Practical Short-range Atmospheric Dispersion Models,* Ris0National Laboratory, Denmark, pp 143-146
AERMOD	USA	RF Lee, RJ Paine, SG Perry, AJ Cimorelli, JC Weil, A Venkatram, RB Wilson (1996) Development Evaluation of the AERMOD Dispersion Model. Proceedings of the 21st NATO/CCMS Conference 'Air Pollution Modeling and its Application', Baltimore, Maryland 6-10 November pp623-660. Also in Proceedings of American Meteorological Society/Air and Waste Management Association Joint Conference *(AMS 10th Conference on Air Pollution Meteorology 11-16 January, Phoenix, USA, pp ~25)* AMA Paper No. 1.5

Table 1: Examples of PC based models developed for regulatory purposes

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