ADMS Urban
- an integrated air quality modelling system for local government

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Abstract
Under the (UK) Environment Act 1995, each local authority in the UK has a duty to review and assess air quality. Modelling is one of the tools available to Environmental Health Officers to assist in this process. Many of the models available are, however, difficult to use and often do not reflect the current understanding of dispersion within the atmospheric boundary layer. ADMS Urban is an example of a new generation of Windows based systems which aims to bring the latest modelling techniques to the non-specialist user. At the heart of the system is an extensively validated, receptor specific model (ADMS) for calculating concentration from point, line, area and volume sources. This is enhanced by an integrated street canyon model derived from the Danish model OSPM and a simplified model of atmospheric chemistry. ADMS is characterised by the use of boundary layer similarity profiles to parameterise the variation of turbulence with height within the boundary layer and the use of a skewed-Gaussian concentration profile, which can bring material from elevated sources rapidly down to the surface, as observed in the field. The model is integrated with an emissions inventory relational database framework within a GIS system, in this case ESRI's ArcView. The use of a commercially available GIS system significantly enhances the possibilities for display and analysis of model predictions and, if part of a networked system enables air quality data to be shared between different departments within the local authority.

ADMS Urban is now being used in cities throughout the UK, including Oxford, Cambridge, Bristol, Birmingham, Cardiff and Newcastle.

1. Introduction
ADMS-Urban is a development of the UK Atmospheric Dispersion Modelling System (ADMS) which now has more than eighty users worldwide. The original industrial source version of ADMS has already been well described elsewhere [1 & 2] and an outline of ADMS-Urban was presented along with the current generation of industrial model (ADMS-2) at the Fourth Workshop on Dispersion Model harmonisation in Ostende in 1996 [3]. The aim of this
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paper is to summarise the main characteristics of the ADMS family and to look at the new features of the Urban model in more detail.

In common with other members of the ADMS family of dispersion models, ADMS-Urban applies up-to-date physics, using parameterisations of the boundary layer based on the Monin-Obukhov length and the boundary layer height. The Monin Obukhov length is defined as

\[ L_{MO} = \frac{-u^2}{\kappa g F_{\theta_o} / (\rho c_p T_o)} \]

where \( u \) is friction velocity at the earth's surface, \( \kappa \) (=0.4) is the von Karman constant, \( g \) is the acceleration due to gravity, \( F_{\theta_o} \) surface heat flux, \( \rho \) and \( c_p \) are respectively the density and specific heat capacity of air and \( T_o \) the surface temperature.

This method allows for a realistic representation of the changing characteristics of dispersion with height within the boundary layer. Defining the boundary layer structure in terms of these measurable physical parameters generally results in a more accurate and soundly based prediction of the concentrations of pollutants than for other models which characterise the boundary layer imprecisely in terms of the Pasquill-Gifford stability category or equivalent.

2. Model Features

ADMS-Urban has been designed as a practical modelling tool to assist local authority environmental health officers to fulfil their duty to review and assess air quality under the (UK) Environment Act 1995. It requires a high specification Pentium PC running Windows 95 or Windows NT. The model features an intuitive graphical interface which is integrated with ESRI's ArcView Geographical Information System (GIS). Microsoft Access is used for an emissions inventory database and output from the model is easily imported into other standard applications such as Microsoft Excel for post-processing of results.

The main features of ADMS-Urban are summarised below:

- an advanced dispersion model in which the boundary layer structure is characterised by the height of the boundary layer and the Monin-Obukhov length, a length scale dependent on the friction velocity and the heat flux at the surface
- a non-Gaussian vertical profile of concentration in convective conditions which allows for the skewed nature of turbulence within the atmospheric boundary layer that can lead to high concentrations near the source
- a meteorological pre-processor which calculates boundary layer parameters from a variety of input data: e.g. wind speed, date, time, cloud
cover or, wind speed, surface heat flux and boundary layer height. Meteorological data may be statistically analysed or raw hourly averaged data:

- **point, line, area and volume** sources.
- an integrated **street canyon model**
- realistic calculation of flow and dispersion over **complex terrain**
- modelling of **chemical reactions** involving NO, NO₂ and O₃
- a unique ability to model **odours** using **short-term concentration fluctuations**
- **easy to use** graphical user-interface
- integration with **Geographical Information Systems (GIS)** and an **Emissions Inventory Database**

## 3. Dispersion

In ADMS the concentration profile from a point source is a Gaussian plume with reflections at the ground and the inversion layer, i.e.

\[
C = \frac{Q_S}{2\pi \sigma_z U} e^{-\frac{y^2}{2\sigma_z^2}} \left\{ e^{-\frac{(z-z_i)^2}{2\sigma_z^2}} + e^{-\frac{(z+z_i)^2}{2\sigma_z^2}} + e^{-\frac{(z+2h-z_i)^2}{2\sigma_z^2}} + e^{-\frac{(z-2h+z_i)^2}{2\sigma_z^2}} + e^{-\frac{(z-2h-z_i)^2}{2\sigma_z^2}} \right\}
\]

Sufficiently far from the source, the vertical variation in concentration of the pollutant is so small as to be negligible, approximately where \( \sigma_z \approx h \) (in fact, where \( \sigma_z = 1.5h \)). Then the plume is considered to grow horizontally as a vertical wedge as if from a uniform line source of height \( h \), rather than as a cone. Upwind and downwind of this point different models are used which are referred to as the near-field and far-field models.

### 3.1. Stable and Neutral Boundary Layers

All the turbulence in the stable boundary layer is mechanically generated i.e. there is no generation of turbulence due to convective motions. Usually the level of turbulence decreases with height, as the relative effects of stratification increase, although it can be enhanced by wave motions at the top of the boundary layer. However, the effect of wave motions is not considered by ADMS Urban.

\( \sigma_z \), the vertical dispersion parameter at the mean height of the plume, \( z_m \), is linked directly to the vertical component of turbulence, \( \sigma_v \), and the travel time from the source, \( t \), by the relationship (Weil 1985; Hunt 1985)

\[
\sigma_z = \sigma_v t \left\{ \frac{1}{b^2} + \frac{N^2 t^2}{1 + 2\gamma^2 Nt} \right\}^{-\gamma/2}
\]
where $N$, $\sigma_\infty$ and $U(z)$ are the buoyancy frequency, r.m.s. vertical velocity and mean wind speed at height $z$. Thus parameter $\gamma$ represents the rate of mixing of the plume with the environment and the factor $b$ ensures a smooth transition between the solution for surface releases and elevated releases.

The transverse dispersion parameter, $\sigma_y$, is given by

$$\sigma_y^2 = \sigma_{y_s}^2 + \sigma_{y_v}^2.$$ 

in stable flows, $h/L_{mo} > 1$,

$$\sigma_y = \sigma_v t \left( 1 + (15.6)^{1/3} u_s t L_{MO} / h^2 \right)^{1/2}$$

and

$$\sigma_y = \sigma_v t \left( 1 + (15.6)^{1/3} u_s t / h \right)^{1/2}$$

in neutral flows, $-0.3 \leq h/L_{mo} \leq 1.0$. The spread due to variations in wind direction, $\sigma_{\theta}$, is equal to $\sigma_{\theta_x}$. $\sigma_{\theta}$, the standard deviation of the wind direction, is either specified as a met input parameter, or calculated using

$$\sigma_\theta = 0.65 \sqrt{T / U_{10}}$$

where $T$ is the averaging time in hours. The spreading due to turbulence $\sigma_s$ is assumed to become linear with respect to time in stable flows when $h/L_{mo}$ is large, as increasingly large scales diffuse the plume as it travels downwind.

3.2. Convective Boundary Layers

Field experiments of diffusion from elevated sources in the convective boundary layer (Briggs 1985) have confirmed earlier laboratory and computational studies (e.g. Lamb 1982) that the form of the vertical profiles of concentration are skewed and significantly non-Gaussian. This changes the distribution of concentration along the ground and is important for modelling processes such as wet or dry deposition. To allow for this effect ‘practical’ models have recently been adopted, by incorporating non-Gaussian profiles into the calculation of diffusions, as in the High Plume Diffusion Model (HPDM) of Hanna & Paine (1989), the Almanac code of National Power (Moore & Lee 1982) and the recent CTDM code of the USA EPA (Perry 1991). These models use non-Gaussian profiles to simulate ground-level concentrations, and that method is also used here.
In the convective boundary layer (CBL) the probability distribution of the vertical velocity and, hence, the concentration distribution is non-Gaussian, or skewed. The non-Gaussian distribution ensures that, for elevated sources, the height at which the concentration is maximum descends as the plume moves downwind while the mean plume height ascends. After the height of the maximum reaches the ground it can rise again.

The transverse dispersion parameter is calculated as two parts, the first for dispersion due to convection $\sigma_{y_c}$, the second due to mechanically driven turbulence $\sigma_{y_m}$

\[
\sigma_{y_c} = \sigma_{v_c} t \left( 1 + \frac{t}{h} \frac{0.75^{1/3} w_*}{u_*} \right)^{-1/2}
\]

\[
\sigma_{y_m} = \sigma_{v_m} t \left( 1 + \frac{t}{h} (15.6)^{1/3} u_* \right)^{-1/2}
\]

$\sigma_{v_c}$ and $\sigma_{v_m}$ are the r.m.s. horizontal velocities due to convection and mechanically driven turbulence respectively. An additional term $\sigma_{ym}$ may be included to allow for the variation in the wind direction.

The total spread is given by

\[
\sigma_y^2 = \sigma_{y_c}^2 + \sigma_{y_m}^2 + \sigma_{ym}^2.
\]

The formulae given above reduce to forms suitable for neutral conditions, but the actual forms are not the same as the Gaussian plume formula for the neutral or stable boundary layer. Therefore a smooth transition from the convective boundary layer solution to the neutral and stable solution, is used.

4. Street Canyon

The street canyon model which is incorporated into ADMS Urban is based on the Danish model OSPM. OSPM (Operational Street Pollution Model) was developed at the Danish National Environmental Research Institute (NERI) and is described in a series of papers [10-13] and has been validated against Danish and Norwegian data. It uses a simplified flow and dispersion model, with a Gaussian plume model.

The canyon model is automatically used for points which lie in roads lined with buildings with heights greater than 2m. Concentrations inside the road tend to the non-canyon results in the limits as the canyon height is reduced to zero or the road width increased to over twice the canyon height. Concentrations at points
outside the canyon are identical with those which would be obtained if the road was not a canyon. The model ignores end effects such as junctions. It assumes a straight length of road which has a width $L$, and is lined on both sides by flat-roofed buildings of height $H_g$.

4.1. Recirculation Region

Figure 1 shows how, when the wind is not parallel to the axis of the street, a vortex is generated in the street canyon. The region occupied by the vortex is called the recirculation region and the velocity at street level in the recirculation region, $u_b$, is opposite in direction to the velocity at roof level $u_r$. The width of the recirculation region, $L_r$, is calculated as in the OSPM model. $L_r$ is a function of roof level wind speed and canyon height.

\[ L_r = \text{function of roof level wind speed and canyon height} \]

![Figure 1](image)

4.2. Concentrations

The concentration in the recirculation region, $C_r$, is determined from a balance of inflow and outflow of material.

\[ C_r = \frac{(Q / L)d_1 \sin \phi}{v_d d_2 + \sigma_w d_3} \]

where $d_1$ is the base length of the recirculating region, $d_2$ is the length across the top of the recirculating region, $d_3$ is the side length of the recirculating region, $v_d$ is the removal velocity at roof level given by
\[ v_d = \left(0.01 u_t^2 + 0.4 \sigma_w^2\right)^{1/2} \]

and \( \sigma_w \) is the street level turbulence given by

\[ \sigma_w = \left(u_b^2 + \sigma_w^2\right)^{1/2} \]

\( \sigma_w \) is the traffic induced turbulence described later.

The concentration at a point on the lee side of the canyon is given by the sum of \( C_k \) and a contribution, \( C_{\text{d,lee}} \), obtained by integrating across the recirculation region.

\[ C_{D_{\text{d,lee}}} = \sqrt{\frac{2}{\pi}} \frac{Q}{L \sigma_w} \left\{ \ln \left[ \frac{h_0 + \sigma_w d_\delta / u_b}{h_0} \right] + \frac{\sigma_w}{v_d} \left[ 1 - \exp \left[ -\frac{v_d d_7}{u_b H_B} \right] \right] \right\} \]

where

\[ d_\delta = \min(\max(L_{\text{Max}}, L_r), x_I) \]

\[ d_7 = \max(L_{\text{Max}}, x_I) - x_I \]

\[ x_I = u_b(H - h_0) / \sigma_w \]

\( x_I \) is the downstream distance from a source element at which \( \sigma_z = H_B \), when the plume escapes from the canyon.

At points on the wind side of the canyon the concentration is given by the sum of \( C_k \) and a direction contribution, \( C_{D_{\text{wind}}} \), from vehicles outside the recirculation region. This is given by

\[ C_{D_{\text{wind}}} = \sqrt{\frac{2}{\pi}} \frac{Q}{L \sigma_w} \left\{ \frac{h_0 + \sigma_w d_\delta / u_b}{h_0} + \frac{\sigma_w}{v_d} \left( 1 - \exp \left[ -\frac{v_d d_5}{u_b H_B} \right] \right) \right\} \]

where
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\[ d_4 = \text{Min}(L_{\text{Max}} - L_R, x_i) \]

\[ d_5 = \text{Max}(L_{\text{Max}} - L_R, x_i) - x_i \]

and \( h_i \) is the initial vertical spread due to the vehicles, assumed = 2m.

4.3. Vehicle Induced Turbulence

The vehicle induced turbulence, \( \sigma_{w_0} \), has been determined experimentally. It is given by

\[ \sigma_{w_0} = b \left( \frac{N N_H V_H S_H^2}{L} + \frac{N N_C V_C S_C^2}{L} \right)^{1/2} \]

where \( NN \) is the number of vehicles passing a point in the street each second, \( V \) is the vehicles’ average speed, and \( S \) is the horizontal area occupied by each vehicle. The subscripts \( H \) and \( L \) refer to heavy and light vehicles respectively. \( b = 0.3 \).

5. Chemistry

Vehicles and industrial sources emit a complicated mixture of chemicals including many organic compounds e.g. VOCs (Volatile Organic Compounds) and oxides of Nitrogen which are involved in reactions with Ozone.

It is beyond the scope of a practical model to model all the chemical reactions, therefore a scheme is used which models the important reactions involving Nitrogen, VOC’s and Ozone. The Generic Reaction Set of equations (GRS) [14] is a semi-empirical photochemical model which reduces the complicated series of chemical reactions involving NO, NO\(_2\), Ozone and many hydrocarbons to just seven:

1. ROC + h\( \nu \) \( \rightarrow \) RP + ROC
2. RP + NO \( \rightarrow \) NO\(_2\)
3. NO\(_2\) + h\( \nu \) \( \rightarrow \) NO + O\(_3\)
4. NO + O\(_3\) \( \rightarrow \) NO\(_2\)
5. RP + RP \( \rightarrow \) RP
6. RP + NO\(_2\) \( \rightarrow \) SGN
7. RP + NO\(_2\) \( \rightarrow \) SNGN

where:
ROC = Reactive Organic Compounds
RP = Radical Pool
Equations (3) and (4) represent exact chemical reactions, which happen very quickly. The other equations are approximations.

The chemistry scheme in ADMS-Urban consists of two modules. The first models chemical reactions that occur only in the main model domain. The main model domain contains all individually defined sources, receptor points and output grids. For each set of input meteorological data, the time taken (Δt) for background pollutants to travel from the most upwind point of the main model domain to the first (most upwind) source is calculated. The chemistry scheme is then applied to the background pollutants over the period Δt to calculate background concentrations at the first source. All background concentrations downwind of the first source are assigned the values that occur at the first source, so that chemical reactions are not applied twice to these pollutants.

A weighted mean age of pollutant is calculated for each point in the plume(s) downwind of each source in the main model domain. The minimum (non-zero) value is used to determine the time period over which the GRS scheme of chemical reactions is applied. The scheme is only applied to points that are affected by source emissions within the main model domain to provide a receptor specific value of pollutant concentration.

The second module consists of a simple lagrangian box model which is used to calculate background concentrations for the air approaching the main model domain. This allows the main ADMS model to be nested within a larger domain such as a large urban conurbation, where the effects of NOx and VOC emissions over the whole area need to be considered - Figure 2.

Computational time is a major restriction on the complexity of the box model, as it is used for a large number of sequential meteorological datasets. For this reason a single layer ‘Box’ model with a regular grid is used. Meteorological parameters and emissions are assumed to be constant over the grid square. Removal of pollutants from the atmosphere is by way of dry deposition at the surface.

The governing equation for the box model is

\[
\frac{dC(t)}{dt} = \frac{F_e}{H_{mix}} - \frac{V_d C(t)}{H_{mix}}
\]
where \( C(t) \) is the concentration of the chemical species at time \( t \), \( H_{mix} \) is the depth of the atmospheric boundary layer, \( V_d \) is the applied deposition velocity and \( F_e \) is the emission flux of the species. The solution of this equation for a time period \( \Delta t \) (assuming steady state conditions) is given by

\[
C(t_0 + \Delta t) = C(t_0) \exp\left\{-\frac{\Delta t \cdot V_d}{H_{mix}} \right\} + \frac{F_e}{V_d} \cdot \left[1 - \exp\left\{-\frac{\Delta t \cdot V_d}{H_{mix}} \right\}\right]
\]

**Figure 2** Schematic showing the main model nested within a larger area-wide box model.

The Box model is employed in the following way. For each prevailing weather condition the most upwind point of the main model domain is calculated and this point is designated as the receptor point for the Box Model. A back trajectory is calculated from the receptor point to the edge of the Box Model domain. The box model is initialised using concentrations from automatic monitoring sites or values specified by the user. Different sites may be used for different prevailing wind directions. The Box Model is then run along the trajectory from the edge of the domain to the receptor point, grid square by grid square. The time period required to cross the grid square is estimated, and by assuming steady state conditions in each grid square, the change in concentration due to emission and dry deposition is computed easily using the above formulation. The algorithms used to determine values in the current grid square are the same used by the FRAME atmospheric transport model[15].
Once the new concentrations have been calculated for the current grid square, the GRS chemistry scheme is applied to calculate the change in concentrations due to chemical processes. Because the transport and chemistry are uncoupled, the scheme estimates the age of the pollutant which increases with advection and decreases with new emissions. The chemistry scheme uses an adaptive time stepping scheme which determines the timestep dependent on the maximum rate of change of concentration occurring amongst all the pollutants. This allows the chemistry module to proceed quickly when concentration changes due to chemical reactions are low, and more slowly when detailed and rapid chemistry is occurring.

For a time period $\Delta t$, the age of a pollutant in the air column is calculated by

$$\text{Age} = \frac{1}{C(t_0 + \Delta t)} \left( \frac{\Delta t}{V_d} F_c * \left[ 1 - \exp\left( -\frac{\Delta t V_d}{H_{mix}} \right) \right] \right) + \frac{C(t_0)}{V_d} H_{mix} * \left[ 1 - \exp\left( -\frac{\Delta t V_d}{H_{mix}} \right) \right]$$

where the first part of the equation in parenthesis refers to material emitted from the current grid square (which is relatively new material), and the second term refers to material advected in from the previous grid square (which is relatively older material).

This scheme is used for each grid square on the trajectory. For the final grid square, which contains the receptor point, a smaller time step is estimated to be the time of travel from the edge of the grid square to the receptor point. Pollutant concentrations at the receptor point are then used as background values in the main ADMS model domain.

### 6. Model Output

Model output can be given as a time series of pollutant concentrations at specified locations or as contour plots. Tables of numerical values are also available. Concentrations may be calculated based on a range of averaging times, including rolling averages, corresponding to existing EU, WHO and EPAQS(UK) limits and guidelines. Annual average, 24 hour, 8 hour, hourly and 15 minute averages are all available. Different averaging periods may be specified for each pollutant. The model also has a statistical facility for generating percentiles of concentration over a large number of sequential meteorological datasets.
7. GIS

During the development of ADMS-Urban, it was felt that the integration of emissions and air pollution data with other geographical information was of great importance to the usability and application of the system. Rather than repeat the development of many functions already available elsewhere, it was decided to design ADMS-Urban to work with an existing, widely used Geographical Information System. ArcView was chosen as it offers powerful standard tools for thematic mapping, querying and analysis of data together with database connectivity and extensible software architecture in a relatively low-cost package. Different types of data can be used in the system, including vector map data in ARC/INFO libraries and various CAD formats, and combined with images such as aerial photographs.

ArcView’s built in development environment, Avenue, was used along with Visual Basic to customise ArcView’s standard interface. ArcView’s basic functionality was extended to allow the user to create a geographically referenced emissions inventory database. Model output can also be represented within ArcView as pollution contour maps overlaid with base mapping data - Figure 3 - or as time series graphs at specific locations. All data displayed within ArcView can be made available to other ArcView and ARC/INFO users across a network. ArcView’s built in publishing facilities provide an easy
means to create impressive hard-copy maps which can also be made available over the internet with ESRI’s ArcView Internet Map Server Extension.

8. Emissions Inventory Database

The emissions inventory is a relational database developed using Microsoft Access for the storage of source and pollutant information. This database has been seamlessly integrated with ArcView for entry and geographical representation of source information. The use of standard Windows applications has allowed data gathered for other purposes to be readily made available for use by ADMS-Urban. The database structure is flexible enough to allow emissions inventories such as those produced by the London Research Centre for Birmingham and London to be accessed and used by the system.

9. Conclusions

ADMS-Urban is a practical modelling tool which applies the current understanding of dispersion to the problem of assessing air quality in urban areas. It has now been installed in a number of towns and cities in the UK. Comparisons with other models and measured pollutant concentrations is underway in these areas as part of a trial scheme testing the available methods for reviewing air quality. The final results of this work should be available towards the end of 1997.

References

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