3D adaptive unstructured meshes for air pollution modelling

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Abstract
High resolution models of air pollution transport and transformation are necessary in order to test possible abatement strategies based on pollution control and to forecast high pollution episodes. Models are especially relevant for secondary pollutants like ozone and nitrogen dioxide, which are formed in the atmosphere through nonlinear chemical reactions involving primary pollutant species, often far from their sources. Often we are trying to resolve the interactions between plumes from point sources such as power stations and regional pollution tides of ozone formed in other European countries. One method of tackling this problem of different scales is to use different grid sizes, using highly resolved grids in regions where the structure is very fine. Telescopic gridding is currently used in high emission areas or around sensitive receptor points. However, since meteorological conditions vary, this method cannot resolve a priori highly structured regions away from sources, e.g. along plumes. Such refinement can be achieved using adaptive methods which increase resolutions in regions of steep spatial gradients. This article describes the use of 3D adaptive gridding models for pollution transport and reactions using both a layered and a fully adaptive 3D tetrahedral approach and provides examples which show the effect of grid resolution on secondary pollutant formation.

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1. Introduction

One of the greatest numerical challenges in air pollution modelling is to achieve a high resolution solution without over-stretching current computational resources. This is a difficult task when often we are considering large numbers of species and many different scales of source types. An obvious way to tackle this problem is to concentrate the computational grid in regions where we gain accuracy from doing so and to use a coarse mesh elsewhere, thus reducing the total number of solution nodes. Adaptive gridding techniques have been developed as an attempt to automate the grid refinement process so that a priori decisions need not be made about where to place extra mesh elements. The effect of grid resolution on solution accuracy has been considered for advection schemes previously. In the context of air pollution modelling we are interested in two main areas – local concentrations and regional species budgets of reactive pollutants. This article aims to address a number of questions related to these two areas in the context of the effect of grid resolution in models describing the transport of chemically reacting species.

2. Model equations and solution strategy

The atmospheric diffusion equation in three space dimensions is given by:

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \frac{\partial}{\partial x}(K_x \frac{\partial c_s}{\partial x}) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right) + \frac{\partial}{\partial z}(K_z \frac{\partial c_s}{\partial z}) + R_s(c_1, c_2, ..., c_q) + E_s - (\kappa_{1s} + \kappa_{2s})c_s, \quad (1)$$

where c_s is the concentration of the s'th compound, u, v, w are wind velocities, K_x, K_y and K_z turbulent diffusivity coefficients and κ_{1s} and κ_{2s} dry and wet deposition velocities respectively. E_s describes the distribution of emission sources for the s'th compound and R_s is the chemical reaction term which may contain nonlinear terms in c_s. For n chemical species an n-dimensional set of partial differential equations (PDEs) is formed describing the rates of change of species concentration over time and space, where each is coupled through the nonlinear chemical reaction terms.

Two approaches have been adopted in the solution of the equation system. The first is to restrict the solution of equation (1) to two dimensions and describe the vertical transport using a parametrised approach similar to that used in the LOTOS model (van Loon, 1996). This is essentially a 2D approach using a triangular mesh but with four vertical layers describing the surface, mixing, reservoir and upper layers of the troposphere. The equations are discretised on a triangular unstructured mesh using the finite volume method of SPRINT-2D described in detail in Berzins and Ware (1996); Berzins *et al.* (1999); Tomlin *et al.* (1997) and Hart *et al.* (1998). Although the mixing layer height is diurnally varying the number of vertical layers remains at four and grid refinement is only possible in the horizontal direction. Operator splitting here is achieved at the level of the solution of the nonlinear equation system resulting from the method of lines, thus reducing splitting errors (Berzins and Ware, 1996; Tomlin *et al.*, 1997). The second approach uses a fully 3D unstructured mesh based on tetrahedral elements. A cell vertex finite volume scheme has been chosen so that the number of mesh elements and therefore flux calculations can be reduced when compared to a cell-centred scheme. The dual mesh is constructed by dividing each tetrahedron into four hexahedra of equal volumes, by connecting the mid-edge points, face centroids and the centroid of the tetrahedron. The flux evaluations are cast into an

edge-based operation. The advective flux is discretized using a second order upwind scheme with limiter (Barth and Jesperson, 1989). This scheme first performs a linear reconstruction to interpolate data to the control volume faces. Monotonicity principles are enforced to ensure that the reconstructed values are bounded by the values of a cell and its neighbours. To this end, multi-dimensional limiter functions are used. The diffusive term is discretized using a central differencing scheme. Operator splitting is here done using a standard approach, so that the chemistry and transport steps are treated separately.

3 Mesh generation and adaptation

3.1 The meshes

The choice of an unstructured mesh over a regular Cartesian mesh has been made so that resolution of small-scale structures such as those due to a point source can be achieved even in a large domain. There is, however, an overhead resulting from the more complex data structures required for an unstructured mesh, and from the complexity of the description of the numerical scheme.

The initial unstructured triangular meshes used in SPRINT-2D are created from a geometry description using the Geompack (Joe and Simpson, 1991) mesh generator. The initial tetrahedral meshes are generated by dividing the whole region into cuboids and then subdividing a cuboid into six tetrahedral elements. Extra mesh levels are placed in the lower regions of the boundary layer.

Local refinement of the mesh is then achieved by subdividing the triangles or tetrahedra using data structures to enable efficient mesh adaptation. For triangles, regular subdivision results in four sub-triangles, but this may leave some nodes which are unconnected on the edges of the refinement region. These nodes are removed by "Green" refinement which divides triangles into two. Figure 1 demonstrates regular and "Green" refinement for the tetrahedral mesh. Green refinement is used on the edges of the adapted region so that hanging nodes are removed and each node is connected in the mesh (Spears and Berzins, 1997).

3.2 Adaptation criteria

Two methods of adaptation criteria have been implemented. The first calculates a first and second order solution and bases the current spatial error on the difference between the two. The spatial error for the next time-step is then predicted using interpolation and compared to a user defined tolerance level. In regions where the spatial error is predicted to exceed the tolerance level, the mesh element is flagged for refinement. The details of this procedure are outlined in Tomlin *et al.* (1997). The second is somewhat simpler and is based on the calculation of the solution gradient between neighbouring nodes. Both techniques show similar refinement behaviour and adapt in regions of steep spatial gradients. For reactive problems we are interested in a number of species and a user decision has to be made about which species or group of species to refine around. Tolerance values are then set by the user for a single species or a group of species. The results shown here use gradients in total NOx (i.e. NO + NO_2) as the criteria and this seems to give good resolution of structures such as plume characteristics.

4. Test cases

The following test cases have been designed to investigate the effects of mesh resolution on the solution for situations representative of those found in regional scale air pollution models.

4.1 The effects of horizontal refinement for the layered mesh

As emissions inventories improve, it will become common to represent data as point, line and area sources on a regional basis. It is therefore important to investigate the effects of mesh resolution on the representation of transport and reaction from various source types. The following results show the effect of resolution for the transport and reaction from a single NOx source through a background of VOCs and ozone.

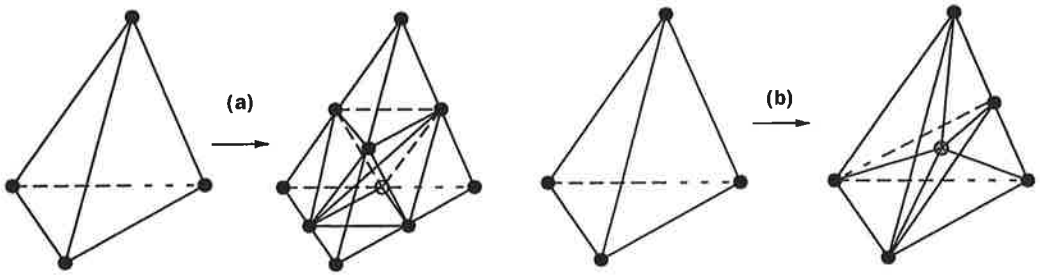
4.1.1 Passive dispersion

If we neglect chemical reaction terms we first see the effect of the mesh on turbulent transport. Figure 2 shows the dual mesh for the refined simulation.

Figure 3 shows the down-wind concentrations of NO for different levels of mesh refinement ranging from 300m up to 10km in edge length. The difference in NO concentrations between the high and low resolution simulations is around a factor of four at a distance of 30km from the source.

The reason for this high level of error can be attributed to high levels of numerical diffusion from the coarse mesh. A simple calculation based on the determination of plume width for different meshes and a Gaussian approach demonstrates that the numerical diffusion for the coarsest mesh is

Figure 1
(a) Regular refinement based on the subdivision of tetrahedra by dissection of interior diagonal (1:8) and (b) "Green" refinement by addition of an interior node (1:6)



in fact eight times that represented by K_x and K_y. The conclusion from this simple test case must be that the types of meshes commonly used in regional and larger scale dispersion models seriously overestimate the levels of mixing from concentrated sources, and therefore underestimate down-wind concentrations. In fact, in most cases, the amount of numerical diffusion is probably greater than K_x and K_y.

4.1.2 Reactive plume

This smearing of the concentration profile will have an obvious effect on the chemical reaction rates and this can be demonstrated by studying profiles of secondary species such as NO_2 and O_3. Chemical reaction terms in the model are represented by both the GRS (Venkatram *et al.*, 1994) and a carbon bond type scheme (Heard *et al.*, 1998), showing similar local concentrations for O_3. The local concentrations of ozone are clearly affected by grid resolution, as shown in Figure 4 and the total species budgets for ozone across the domain as shown in Figure 5.

4.1.3 Regional scale model

The results from the layered model clearly demonstrate the effects of mesh resolution on

Figure 2
Dual mesh for passive dispersion from a single NO_x source showing refinement along plume centre

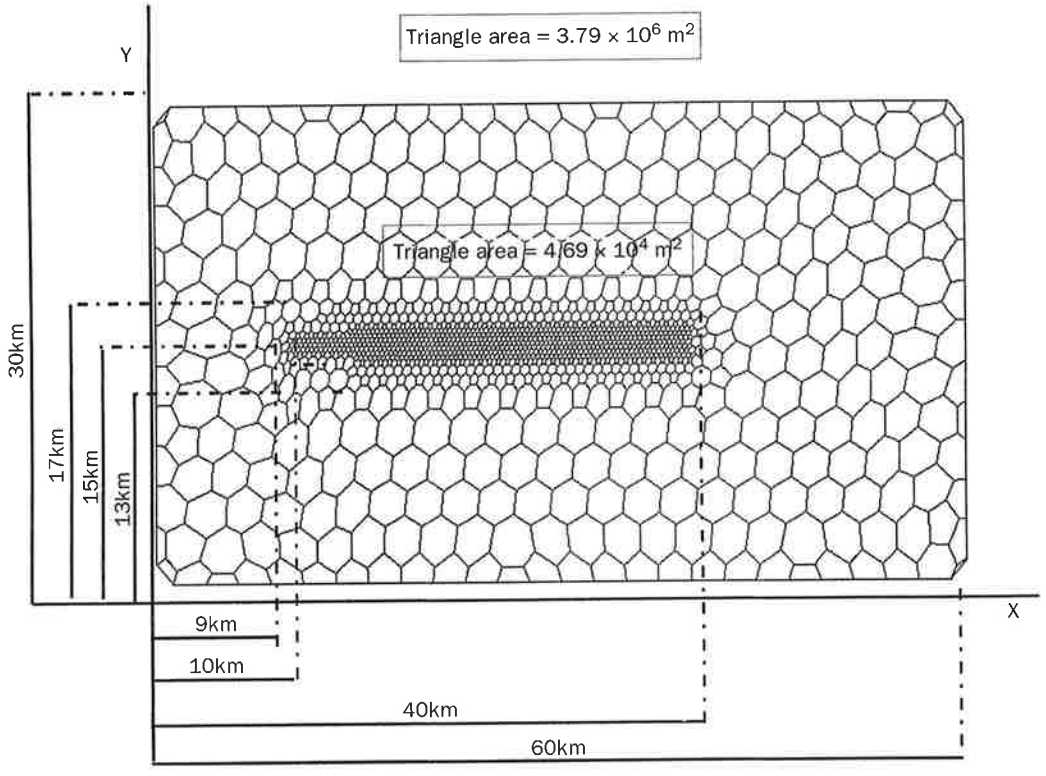
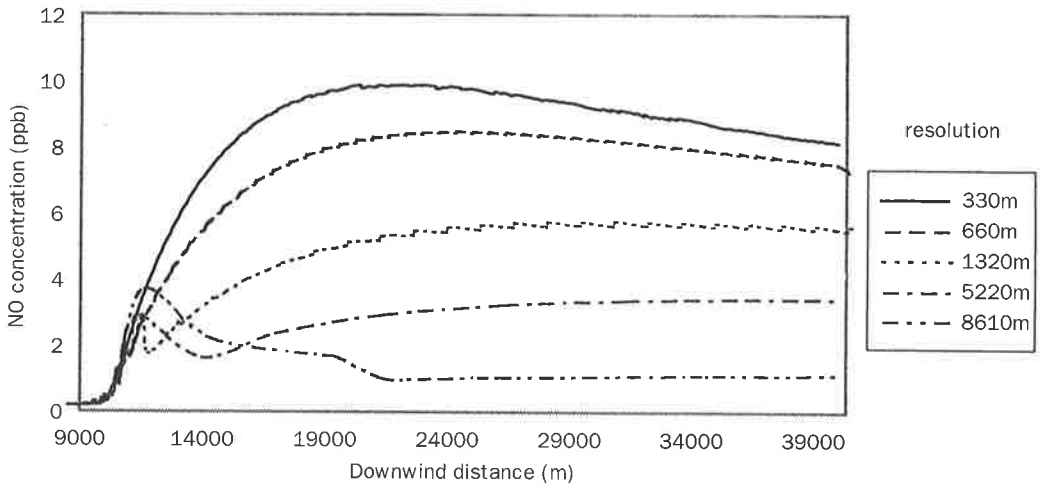


Figure 3
Downwind concentration of NO for passive plume for varying mesh resolutions



secondary species predictions. Regional scale comparisons have also been made using the same approach and multi-scale emissions data – EMEP emissions data on a European scale and point and area emissions data (10km × 10km) from NETCEN for the UK region. Dry deposition and vertical dispersion are included following the approach of van Loon (1996). The meshing approach here has been to use a large scale grid over Europe, in order to provide boundary conditions for the regional scale model. A nested region with some refinement has been defined over the UK and transient refinement to finer meshes is allowed in this region according to the spatial error of the solution. A maximum refinement level has to be provided by the user since point sources will otherwise reach high gradients leading to further refinement requirements. Usually there are about five to six levels of refinement from the European to the local scale, with mesh elements ranging from 150km to 2km in terms of edge length. Space does not permit a detailed discussion of the effects of mesh on the regional scale model. In essence, the results are similar to the simple test case. Refinement generally takes place in regions with high spatial gradients, such as along the edges of power station and urban plumes. Figure 6 shows a typical mesh for a regional scale calculation.

Local concentrations are significantly affected by the mesh resolution as demonstrated by the NO_2 profile across the UK region shown in Figure 7. Any

Figure 4
Cross-plume ozone profile

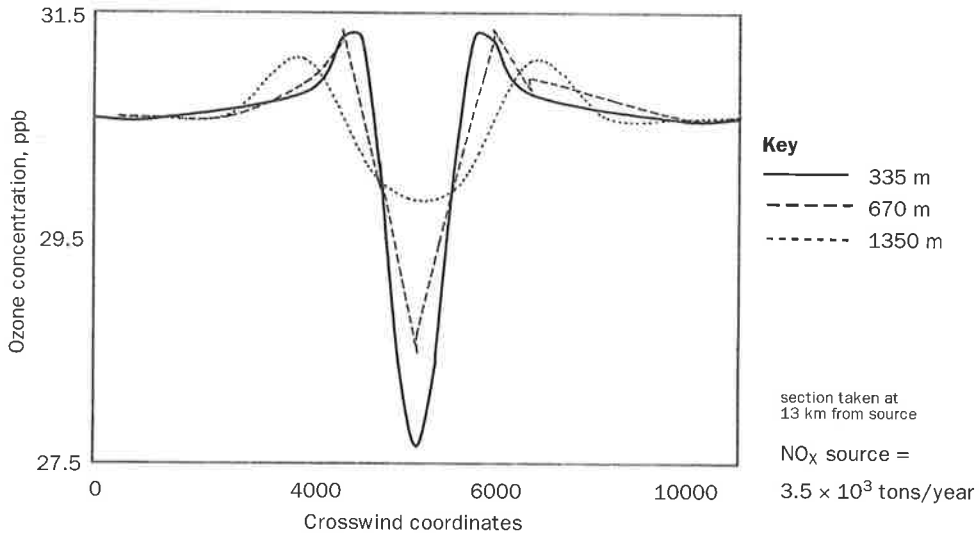
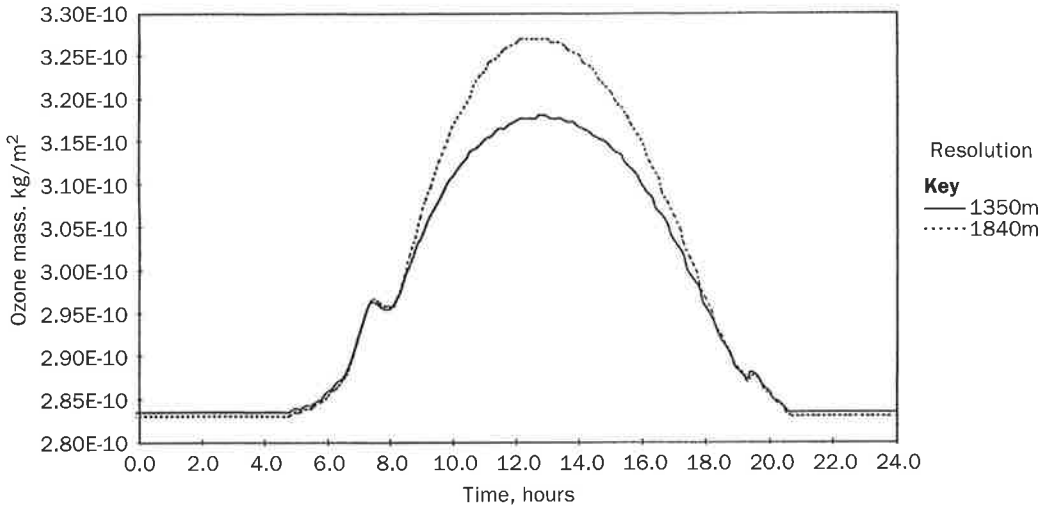
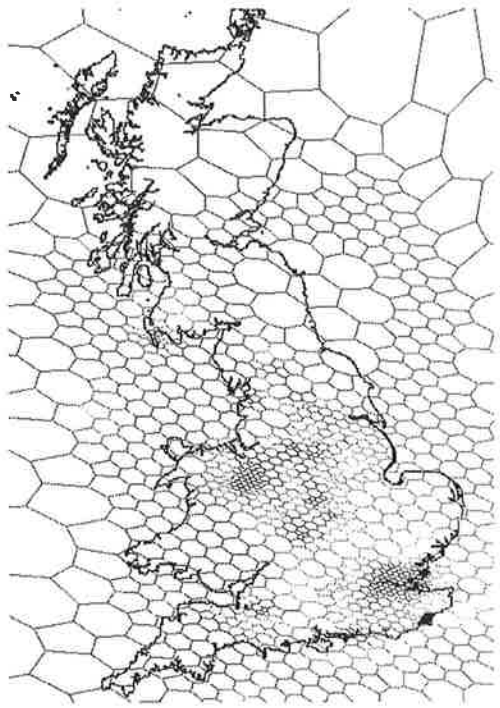


Figure 5
Total ozone concentration in the surface layer for the whole domain showing the effects of mesh resolution on total species budgets using the carbon bond scheme



comparison with measured data will be better achieved using better resolved meshes. As in the simple test example, there is some effect on the total ozone concentration integrated over the entire refinement region, especially when extremely coarse meshes are used. The effect is not as significant, however, as for local concentrations, suggesting that coarse resolution models are a reasonable way to estimate general ozone trends over large time-periods but will not be suitable for local ozone forecasts and for comparison with monitored data, particularly in areas where many sources of different scales are present.

Figure 6
Typical mesh used in the refinement region for the UK



5. Vertical refinement using tetrahedral meshes

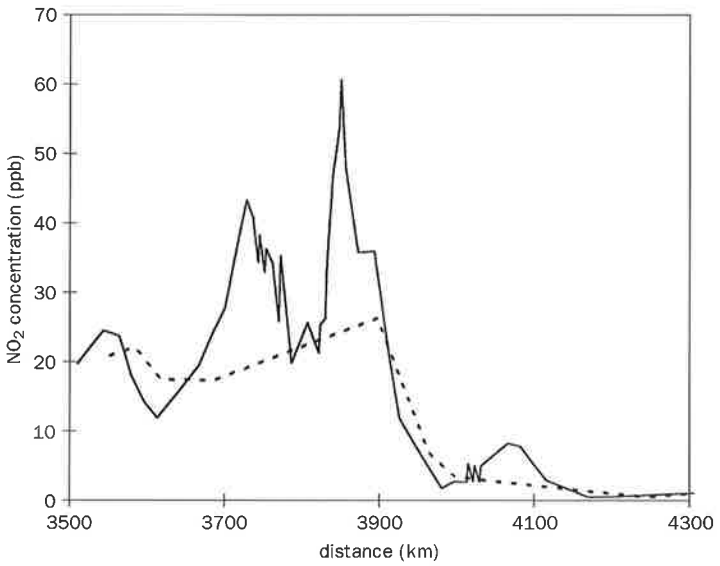
The layered model uses highly parametrised description of mixing in the vertical direction. This will have a large effect on near source concentrations as enhanced mixing caused by coarse layering will change the vertical profile of concentrations. A tetrahedral model has therefore been developed which can adapt in the vertical plane. The advection and chemical schemes have first been tested using a standard rotation problem.

5.1 Test examples

For test purposes, we have kept the chemical mechanism simple but it produces the same numerical difficulties which might be often encountered in other photochemical models. One such simple description (Hov *et al.*, 1989) of the atmosphere is given in Table I. The solution to the advection part is known: the concentration c_1 of a certain species located at some point X_1 is moved to another point X_2 after a certain time. Conversely, if no advection is taking place, but the chemistry is activated, the concentration at X_1 will be changed to c_2 during the same period of time. Therefore, if both advection and chemistry are applied, then the concentration at X_2 should be c_2.

The dimensions of the base grid in the horizontal, lateral and vertical directions are

Figure 7
Cross mesh profile for NO_2 for a sample regional-scale UK calculation. The bold line represents three levels of refinement over the base mesh, represented by the dashed line



200km, 120km and 3km respectively. The initial grid consisted of 4,576 nodes and the grid is refined by four levels if the concentration gradient and concentration value of HCHO exceed some tolerance parameters. The number of nodes after refinement is 15,460 which varies little as the peaks are rotated around a circle although the position of the refinement region moves with the peak. The vertical levels are refined near the ground. The solar zenith angle, θ is kept constant at 71.5° throughout. Four species, HC, HCHO, NO and NO_2 have peaks located at 80km, 60km, 0.15km and their background concentrations are set equal to 2.5 per cent of the peak values. Here HC is a lumped hydrocarbon molecule. For computational efficiencies, an operator splitting technique is used to decouple the chemistry from the transport as follows:

Transport

$$\frac{\partial c_i}{\partial t} + (y - y_1)\omega\frac{\partial c_i}{\partial x} + (x_1 - x)\omega\frac{\partial c_i}{\partial y} = 0,$$

where (x_1, y_1) = 100km, 60km and ω is chosen so that the period of the rotation is 24 hours.

Chemistry

$$\frac{\partial c_i}{\partial t} = a_i - b_i c_i,$$

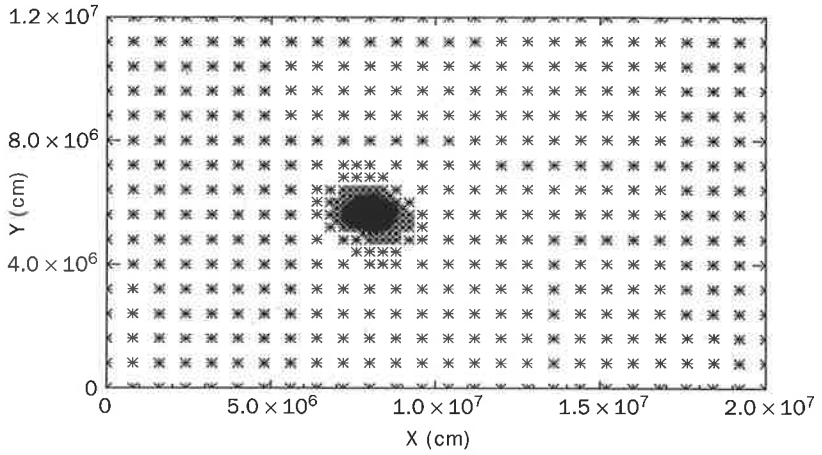
where a_i is the production and $b_i c_i$ is the loss rate for species i. These two operators are applied in sequence in order to step the solution in time. The advection part calculates a time step according to the CFL condition, whereas the chemistry routine chooses its time step automatically (Berzins *et al.*, 1999).

Figure 8 shows the grid points at the $z = 0.15$km plane after one rotation with advection only. The grid points are clustered

Table I
Simplified chemical mechanism used in the model

Reaction			Rate
HC + OH	→	4 RO_2 + 2 HCHO	$k_1 = 6 \times 10^{-12}$
HCHO + hν	→	2 HO_2 + CO	$k_2 = 7.8 \times 10^{-5}e^{-0.87/\cos\theta}$
RO_2 + NO	→	NO_2 + HCHO + HO_2	$k_3 = 8 \times 10^{-12}$
NO + HO_2	→	NO_2 + OH	$k_4 = 8.3 \times 10^{-12}$
NO_2 + hν	→	NO + O_3	$k_5 = 1.0 \times 10^{-2}e^{-0.39/\cos\theta}$
NO + O_3	→	NO_2 + O_2	$k_6 = 1.6 \times 10^{-14}$
O_3 + hν	→	O_2 + O(1D)	$k_7 = 1.9 \times 10^{-4}e^{-1.9/\cos\theta}$
O(1D) + H_2O	→	2 OH	$k_8 = 2.3 \times 10^{-10}$
NO_2 + OH	→	HNO_3	$k_9 = 1.0 \times 10^{-11}$
CO + OH	→	CO_2 + HO_2	$k_{10} = 2.9 \times 10^{-13}$

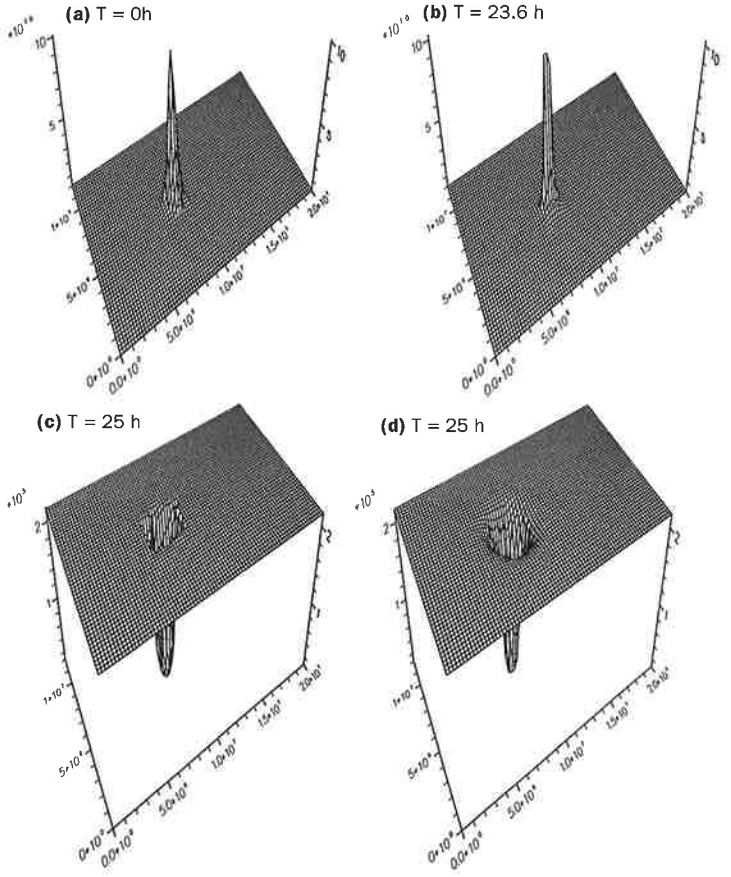
Figure 8
The grid nodes in the z = 0.15km plane after one rotation with advection only



together around the peak of the solution due to the adaptation of the mesh in the high gradient region.

Figure 9(a) shows the NO concentrations at t = 0 and figure 9(b) approximately after one rotation with advection only at the $z = 0.15$km plane. The final peak is almost the same as that of the original, showing that little numerical diffusion is taking place. The concentration after 25 hours with chemistry alone is shown in Figure 9(c) and with chemistry + advection in Figure 9(d). The

Figure 9
(a) Initial NO concentration. (b) NO concentration with advection only, (c) with chemistry only and (d) with advection + chemistry after one rotation. The x-y axes are in cm and the z-axis in molecules/cm^3



peak concentrations are within 2 per cent of each other, showing the high accuracy in predicting the peaks. The mesh is refined or derefined after every 24 minutes and uses a safety layer around the high resolution region. This means that as well as adapting mesh elements of high spatial error, their neighbours are also refined. The advantage of this is that as the region of steep gradients advances due to advection, the cells ahead of the front are already of high resolution and the plume front is not diluted into large cells. Without the safety layer, the mesh remains coarse since as the steep gradient is advected into a large grid cell, the solution is smeared and the gradients become low. Further refinement will then be prevented. This might imply that the best strategy to start a model with multiple source points and a complex initial concentration field would be to use a refined mesh and then coarsen the mesh as the solution proceeds where the gradients are low. This way it will be certain that initial steep gradients are maintained throughout the simulation.

A small amount of vertical numerical diffusion resulting from a horizontal advection scheme is a side-effect of using fully unstructured meshes. As Cartesian meshes are usually aligned to the surface, we would not expect them to demonstrate this problem for modelling dispersion over flat terrain. However, the results show that the total overall diffusion can be kept small if sensible mesh refinement is used.

6. Discussion and conclusions

The test cases studied clearly demonstrate the need for finer meshes when predicting local concentrations. For ozone, total species budgets are not as mesh sensitive but highly coarse meshes will show some inaccuracies. Preliminary studies have shown that adaptive methods can be successfully applied in regional and larger scale models. Standard test problems show solutions to be far less diffusive than using coarse meshes. There are a number of issues which still need to be resolved regarding the use of unstructured meshes. Errors due to the interpolation of wind field data onto the unstructured mesh need to be quantified, although methods are available for mass conserving interpolation (Mathur and Peters, 1989). The resolution of initial data seems to be a crucial factor here. Using standard advection schemes, the time-step is chosen according to a CFL condition and for small meshes the time-step necessarily becomes smaller in order to preserve stability. There are limits to the amount of refinement possible therefore if long-time runs are to be carried out. The need for sophisticated refinement and derefinement criteria to resolve species of interest accurately for different problem types should be investigated. Initial results demonstrated here, however, indicate that further research is warranted in these areas and that adaptive methods would seem to be well-suited for air pollution problems.

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