MULTI-SCALE ATMOSPHERIC DISPERSION MODELLING BY USE OF ADAPTIVE GRIDDING TECHNIQUES

G. HART[*], A. TOMLIN[*], J. SMITH[☆], M. BERZINS[♦]
Department of Fuel and Energy[*], School of Computer Studies[♦] and School of Chemistry[☆]
University of Leeds, Leeds LS2 9JT, UK

Abstract

An accurate prediction of the transport-reaction behaviour of atmospheric chemical species is required to fully understand the impact on the environment of pollution emissions. Elevated levels of secondary pollutants such as ozone in the lower atmosphere can be harmful to the health of both plants and animals, and can cause damage to property present in the urban environment. Detailed models of pollution mechanisms must therefore be developed through comparisons with field measurements to aid the selection of effective abatement policies. Such models must satisfy accuracy requirements both in terms of the number of species represented, and the spatial resolution of species profiles. Computational expense often compels current models to sacrifice detail in one of these areas. This paper attempts to address the latter point by presenting an atmospheric transport-reaction modelling strategy based upon a finite volume discretisation of the atmospheric dispersion equation. The source terms within this equation are provided by an appropriate reduced chemical scheme modelling the major species in the boundary layer. Reaction and transport discretisations are solved efficiently via a splitting technique applied at the level of the non-linear equations. The solution grid is generated using time dependant adaptive techniques, which provide a finer grid around regions of high spatial error in order to adequately resolve species concentration profiles. The techniques discussed are applied in two dimensions employing emissions from both point and area sources. Preliminary results show that the application of adaptive gridding techniques to atmospheric dynamics modelling can provide more accurately resolved species concentration profiles, accompanied by a reduced CPU time invested in solution. Such a model will provide the basis for high resolution studies of the multiple scale interactions between spatially inhomogeneous source patterns in urban and regional environments.

1 Introduction

The prediction of primary and secondary pollution generation and transport is required in order to fully understand the impact upon the environment of a range of source types. Elevated levels of ozone in the lower atmosphere can be harmful to animal and plant life and can cause extensive damage to property. Detailed models of pollution mechanisms must therefore be developed to aid effective abatement policies thus ensuring compliance with national and international environmental legislation. The complex interaction of pollutants with atmospheric species, together with the additional effects of meteorological phenomena can cause species production, destruction and dispersion to take place at a long range from the pollutant source. On the other hand the pollution source itself may be of a very small scale, such as a power station plume. This presence of multi-scale behaviour in the atmosphere requires detailed computational grids, in order to resolve concentration profiles over the whole range of dispersion. Comparisons can then be made with field measurements and used in model validation. Such comparisons are useful as they inevitably promote a better understanding of the behaviour of pollutants when released into the atmosphere.

Early Eulerian models of the 1970's only utilised sparse uniform grids over which to solve the atmospheric diffusion equations. Resolution has been improved in second generation (Peters 1995) models due to increases in computer power and memory, and

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the application of selectively refined regions of grid points. Regions of high concentration gradient are predicted a-priori and grid points concentrated accordingly, nesting regions of high density grid within the overall domain. These have generally been concentrated in regions of high emissions. However, the complex nature of pollutant species interaction with prevailing meteorological conditions can cause high concentration gradients at a long range from the pollutant source. This makes the use of nested gridding methods more difficult and less effective. There is therefore a need for the application of methods which can refine the grid according to where the solution requires it i.e. time dependent grid adaptive algorithms. There have recently been some applications of adaptive grids for environmental modelling, e.g. Skamarock *et al.* (1989), although as yet these methods have not been implemented in standard air quality models. The present work describes how adaptive gridding techniques, which automatically refine the mesh in regions of potentially high spatial error, can improve on the telescopic or nested approach. The aim of this work is to show that the use of such techniques will lead to a better understanding of the complex multi-scale phenomena that arise from regional scale models.

We have not attempted to develop a comprehensive regional model, but rather to apply a set of numerical modelling tools to a particular test case in order to demonstrate their advantage over traditional techniques. We therefore investigate the solution of the atmospheric transport-reaction problem described by an Eulerian formulation of the atmospheric dispersion equation and a reduced chemical reaction scheme. This problem is solved using a finite volume method over an unstructured grid generated using adaptive techniques. Solution methods presented specifically concentrate upon the release of NO and NO_2 and the subsequent reaction of this effluent with existing atmospheric species to generate secondary pollutants such as ozone.

The paper is structured as follows. In sections 2.1 - 2.3 we briefly introduce the equations which describe the atmospheric transport and reaction problem and the test case over which these equations are solved. Section 2.4 introduces the numerical scheme used to solve these equations. Section 2.5 provides details of the adaptive gridding technique and the criteria for mesh refinement is briefly described. Section 3 presents a comparison of results of the test case using both constant density and adaptive gridding techniques. Finally in sections 4 and 5 we present a discussion and conclusions about the use of adaptive methods in air pollution models.

2 Code Structure

2.1 TRANSPORT-REACTION EQUATION

The 2D transport-reaction behaviour of atmospheric species is modelled by solving the atmospheric diffusion equation for each species ,

$$\frac{\partial c_s}{\partial t} = -\frac{\partial uc_s}{\partial x} - \frac{\partial wc_s}{\partial y} + \frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right) + R_s(c_1, c_2, \ldots, c_n) + E_s - (k_{1s} + k_{2s})c_s \qquad 2.1$$

where:
- c_s = the concentration of the s'th compound.
- u,w = wind velocities.
- K_x, K_y = diffusivity coefficients.
- k_{1s}, k_{2s} = dry and wet deposition velocities.
- E_s = distribution of emission sources for s'th compound
- R_s = source due to chemical reaction .

The above transport-reaction model is solved for n chemical species. This generates an n dimensional set of partial differential equations, each coupled through the non-linear chemical reaction terms.

2.2 CHEMICAL SCHEME

The initial chemical reaction scheme used for code development was introduced by Azzi *et al* (1992). The mechanism, shown in equation 2.2, contains only 7 species and therefore enables fast turn around time in terms of developing the numerical code. Despite its simplicity it represents the main features of a tropospheric mechanism, namely the competition of the fast equilibrating inorganic reactions 3) and 4) with the chemistry of volatile organic compounds, which occur on a much slower time-scale. This separation in time scales generates stiffness in the resulting equations so that sophisticated ordinary differential equation (ode) solvers must be used to solve such schemes. The voc reactions are represented by reactions of a single lumped species, ROC. This is unrealistic in terms of the actual emissions generated in the environment, but the investigation of fully speciated vocs is not the purpose of the present study.

							Reaction rates	
ROC	+	hv	$\xrightarrow{O_3}$	RP	+	ROC	$jp[1] = 1000\exp(-4710 / T) jp[3]$	(1)
RP	+	NO	→	NO_2			$kr[2] = 3.7098\times10^{-12} \exp(242 / T)$	(2)
NO_2	+	hv	→	NO	+	O_3	$jp[3] = 1.45\times10^{-2} \exp(-0.4 \sec\theta)$	(3)
NO	+	O_3	→	NO_2			$kr[4] = 1.7886\times10^{-12} \exp(-1370 / T)$	(4)
RP	+	RP	→	RP			$kr[5] = 6.7673\times10^{-12}$	(5)
RP	+	NO_2	→	SGN			$kr[6] = 1.00\times10^{-13}$	(6)
RP	+	NO_2	→	SNGN			$kr[7] = 1.00\times10^{-13}$	(7)

2.2

where:
- ROC = Reactive Organic Compounds.
- RP = Radical Pool.
- SGN = Stable Gaseous Nitrogen Products.
- SNGN = Stable Non-gaseous Nitrogen Products.
- jp[n] = Photolosis rates parameterised as a function of solar zenith angle, θ.
- kr[n] = Reaction rate.
- T = Temperature.

The rate constants have been chosen to be in agreement with those used by Derwent *et al.* (1990). The solar zenith angle θ is calculated as a function of the time of day, the time of year and the latitude. Temperature dependant rate constants are represented by a

standard Arrhenius expression, the temperature calculated as a parameterised function of time of day.

Background atmospheric sources are obtained from the Department of the Environment national atmospheric emissions inventory (Goodwin 1993). This provides NOx and ROC emissions inventories, measured over a 10km x 10km grid, across the UK. These emissions are included as source terms at each computational grid position by interpolating from the 10km x 10km mesh onto the current solution grid. Point sources are represented separately and are averaged over the grid cell in which they are contained. We assume a constant emission ratio of 90% NO and 10% NO_2 for all NOx sources.

An additional sink is included in the form of species dry deposition. Deposition sinks are included at present as a simple parameterised function derived from deposition velocities and the changing height of the boundary layer. Deposition velocities are assumed to be constant across the whole domain.

2.3 DOMAIN AND TEST CASE CONFIGURATION.

A power plant plume or urban plume is a highly concentrated source of NOx emissions which can be carried through the atmosphere for hundreds of kilometres, and so provides a stringent test of whether adaptive gridding methods can lead to more reliable results for complex multi scale models. Since power stations and urban transport provide some of the highest emission sources for NOx it is important to be able to generate an accurate understanding of their impact on not only the total NOx budget, but on the generation of secondary pollutants such as ozone. To achieve this we must consider the interaction of plumes with their surroundings

The model is currently applied over a 2-dimensional domain. This is a necessary simplification while the technique is developed and validated, allowing many of the numerical issues to be resolved before expansion to a more complex, but realistic, 3D case. The domain covers a 500km x 500km region stretching from the English midlands up to the Scottish highlands.

Meteorological data has been kept simple and constant in order to easily identify plumes and to optimise refinement procedures. At present the wind is considered to blow directly from the South at a constant speed of 5m/s. Diffusion only takes place perpendicular to this, the diffusion parameter being set to $50m^2s^{-1}$. Consequently no flow is permitted across the East and West boundaries, Neumann boundary conditions are applied to the North edge of the domain and Dirichlet along the South. At present the concentration at the Southern edge is assumed to be a constant background value, again for simplicity although somewhat unrealistic. In this test case we wish to demonstrate the differences between constant density, telescopic and fully adaptive meshes. We have therefore chosen to refine the initial base mesh around 3 power stations in Northern England to demonstrate the telescopic approach of refining around high emission areas. This can be

seen in Figure 2a. The other point sources are interpolated onto the standard background mesh i.e. constant density for two simple cases and a refined mesh for the adaptive case. For this test case the model is run over a two day period to identify diurnal variations in species concentration and is primarily used to develop an understanding of how NOx and ROC react within the atmosphere to form secondary pollutants such as ozone.

2.4 NUMERICAL DISCRETISATION

The atmospheric diffusion equation described by 2.1 is solved using the flux limited, cell centred finite volume discretisation scheme of Berzins and Ware (1996, 1995). The basis of this finite volume scheme is the space discretisation of the partial differential equation (pde) 2.1 which is reduced from a pde in three independent variables into a system of odes in the single independent variable of time. This is achieved by the integration of 2.1 over each finite volume, use of the divergence theorem and the evaluation of the line integral along the boundary of each volume using the midpoint quadrature rule.

This 'method of lines' approach with the above spatial discretisation scheme results in a system of odes in time which are integrated using the SPRINT2D software tool developed by Berzins and Ware (1996). The SPRINT2D software tool contains a number of solution techniques available for use. For much of the present study the Theta solution method has been utilised, with functional iteration used to solve the resulting system of equations. The Theta option is specifically designed for the moderate accuracy solution of stiff systems with automatic control of the local error in time. The large ode systems which result from the discretisation of flow problems with complex chemistry can result in excessive c.p.u processing times. An approach used here which overcomes this is to use a form of operator splitting based on a decomposition of the pdes into a set of flow terms and a source reactive term (Berzins and Ware, 1996).

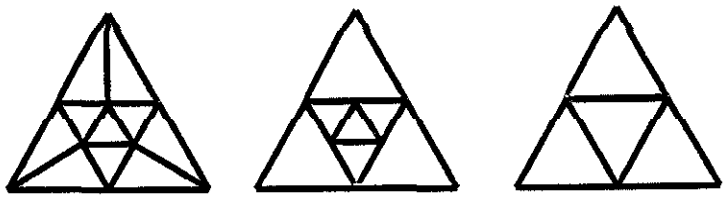
2.5 ADAPTIVE GRIDDING

The domain is represented by an unstructured mesh of triangular elements surrounding each grid point, thus forming a small volume over which the solution is averaged. The use of an unstructured triangular mesh more easily enables adequate resolution of the complex solution structures found within multi-scale dispersion modelling. This is especially relevant for cases where we wish to represent point source and urban plumes within a large scale background. The term unstructured represents the fact that each node in the mesh may be surrounded by any number of triangles, whereas in a structured mesh this number would be fixed. The initial unstructured meshes used in SPRINT2D are created from a geometry description using the Geompack (Joe 1991) mesh generator.

The complex nature of the atmospheric dispersion problem makes prespecification of grid density a problem as many complex reactions can take pace at some distance from the pollution source. To this end the dispersion code presented here utilises adaptive gridding techniques to quantitatively evaluate the accuracy of the solution and then automatically refine or derefine the mesh where necessary. This is achieved using a tree-like data structure with a method of refinement based on the regular subdivision of

triangles. Here an original triangle is split into four similar triangles (Figure 1) by connecting the midpoints of the edges. Hanging nodes are removed by joining with nearby vertices to produce the completed refinement. This finer grid may later be coalesced into the parent triangle to coarsen the mesh. This process is called local h-refinement, since the nodes of the original mesh do not move and we are simply subdividing the original elements.

Figure 1: Triangle refinement procedure



Once a method of refinement and derefinement has been implemented it remains to decide on a suitable criterion for the application of the adaptivity. The ideal solution would be that the decision to refine or derefine would be made on a fully automatic basis. In practice a combination of an automatic technique and some knowledge of the physical properties of the system is used. The technique used in this work is based on the calculation of spatial error estimates. This is achieved by first calculating some measure of error in each species concentration over each triangle. A reliable method for achieving this is to examine the difference between the solution gained using a high accuracy method and that gained using a method of lower accuracy. Clearly over regions of high spatial gradient the difference between high and low order solutions will be greater than over regions of relatively smooth solution and therefore refinement generally occurs in these regions. A refinement indicator for the jth triangle is defined by an average scaled error measured over all *npde* pdes using supplied absolute and relative tolerance:

$$serr_j = \sum_{i=1}^{npde} \frac{e_{i,j}(t)}{\frac{atol_i}{A_j} + rtol_i \times c_{i,j}} \qquad 2.3$$

where:
- $serr_i$ = average scaled error.
- npde = number of pdes.
- $e_{i,j}(t)$ = local error estimate of species i over element j.
- $atol_i$ = absolute tolerance applied to species i.
- $rtol_i$ = relative tolerance applied to species i.
- $c_{i,j}$ = concentration of species i over triangle j.
- A_j = area of jth triangle.

This formulation for the scaled error provides a flexible way to weight the refinement towards any species error, and for the user to control the extent of refinement by providing tighter or looser tolerances. An integer refinement level indicator is calculated from this scaled error to give the number of times the triangle should be refined or derefined. Since the error estimate is applied at the end of a time step it is too late to

make refinement decisions. Methods are therefore used for the prediction of the growth of the spatial error using linear quadratic interpolants. The spatial error estimate can also be used to indicate when the solution is being solved too accurately and can indicate which regions can be coarsened.

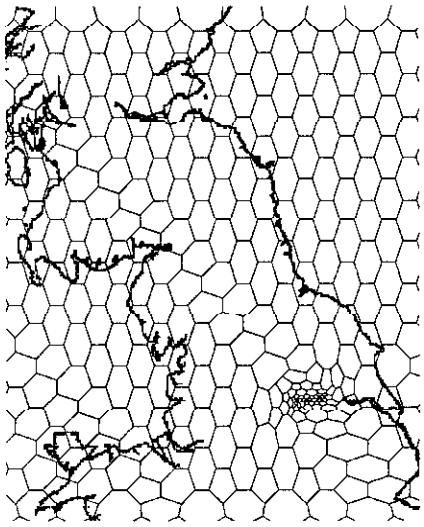


Figure 2a: Level 0 constant density dual mesh.

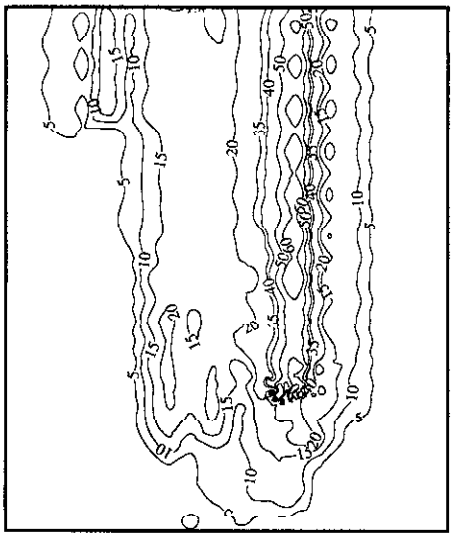


Figure 2b: Level 0 const. density solution.

3.0 Results

To demonstrate the application of adaptive gridding techniques to the reaction-dispersion problem, three different scenarios are presented, and the subsequent effects upon solution accuracy, run time and storage requirements discussed.

The first two solutions presented demonstrate the performance of constant density gridding techniques at low and high grid resolution. The first solution is solved over a coarse constant density grid without refinement, i.e. level 0 except for the telescopically refined area which is refined to level 4 (Figure 2a). The second solution presented is solved over a more refined grid with a density of level 2 over the whole domain (Figure 3a). The third solution presented used adaptive gridding techniques to refined from a constant density level 0 grid, adapting where necessary up to level 2 (Figure 4a). The adaptive gridding technique is configured to adapt around steep spatial NO gradients and thus track and envelop the NOx plumes as they advect Northwards. In Figures 2a, 3a and 4a the vertices of each polygon represent the centre of a triangle on the computational mesh.

3.1 SPATIAL SPECIES DISTRIBUTION

Figure 2b presents the NO solution generated over the level 0, constant density grid. This snapshot of the spatial NO distribution is taken at 12:00 noon on day 2 of the simulation. Contour levels display NO concentrations in parts per billion (ppb). Several plumes can

Figure 3a: Level 2 constant density dual mesh.

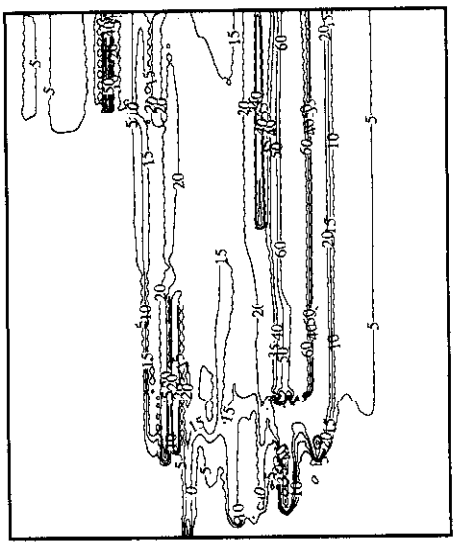


Figure 3b: Level 2 constant density solution.

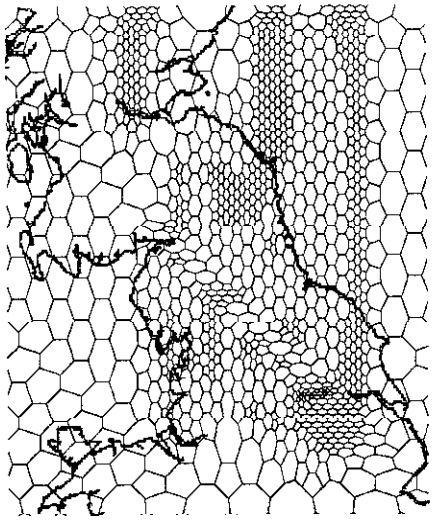


Figure 4a: Adaptive dual mesh.

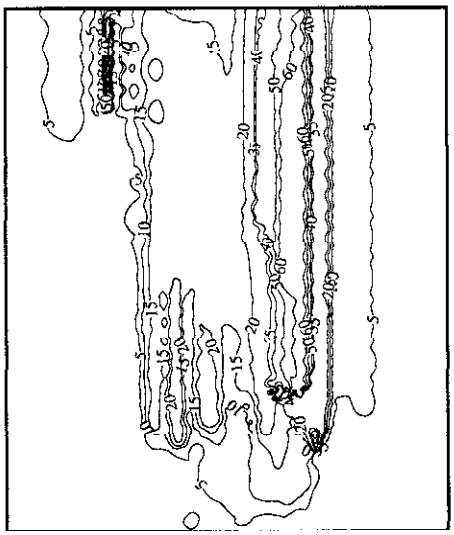


Figure 4b: Adaptive solution.

clearly be identified advecting northwards from high emission sources in urban areas. The most prominent plumes originate from the region around the Yorkshire power stations which was telescopically refined. Figure 3b presents the NO solution at the same instant in time but solved over the much finer level 2 constant density grid. This solution is clearly much less dispersive than the level 0 solution, the plume widths are smaller and much higher NO concentrations are found in the plume cores. The finer grid reduces the artificial spreading of the plumes. This effect is especially marked for plumes originating from sources which were not telescopically refined on the base mesh. The level 2 output is therefore considered to represent a more accurate solution to the scenario described due to the use of a higher resolution grid. However, as the level 2 solution has sixteen times as many more grid points demanding solution, this configuration takes considerably longer to solve. In addition, if the time dependant solution at every grid point is to be saved, much more storage space is required. So, improved performance in terms of solution resolution and accuracy clearly results in greatly increased computational expense.

Figure 4b represents the case where the grid is generated using adaptive techniques. At the start of the simulation the initial mesh is constant density level 0. The code then refines the grid around regions of high spatial error in NO concentration up to a level 2 density. Again, the gross features of the plumes are represented. The effect of using adaptive methods on solution accuracy is perhaps most prominent around the main plume where refinement has occurred around the plume edge (Figure 4a). This has the effect of reducing the artificial dispersion of species via the solution averaging process. The solution achieved using the adaptive gridding process therefore more closely follows that generated by the level 2 constant density grid. If the smaller plumes are examined we see that the level of definition obtained is higher than that achieved by the level 0 grid. The loss of definition obscuring these smaller plumes found in the coarse grid does not arise to such an extent in the adaptive case. Examination of 2D solution profiles alone suggests that a level of accuracy near that of the high resolution constant density grid can be obtained by an adaptive grid using far fewer grid cells. This results in reduced run time and storage requirements.

3.2 CROSS PLUME PROFILES

If a slice is taken through the 2D domain a 1D profile of the solution can be extracted. This profile is useful because it provides a more clear representation of local concentrations. Figures 5 a and b present the cross plume profiles for the three solution strategies obtained by taking a slice across the domain in a West to East direction, 230 km downwind of the 3 main pollution sources. Profiles generated are viewed from a Northerly direction, effectively reversing East and West on the x-axes.

In Figure 5a the level 2 constant density solution is represented by the dashed line and is compared to the level 0 constant density solution. The high resolution solution resolves the high, narrow NO peaks, the main plume represented by the highest peak just East of centre. The level 0 solution can clearly be seen attempting to follow the high resolution

profile but falls short of the main plume peak concentration. In addition the more dispersive level 0 solution smears out the solution profile to the extent that the smaller scale peaks are not represented at all. Figure 5b again presents the solution achieved using level 2 constant density grid but here it is compared to the solution produced using adaptive gridding techniques. The adaptive solution seems to more adequately attain the peak concentration of the high resolution solution. Furthermore the adaptive solution also resolves many of the smaller peaks accompanying the main plume. However, it should be noted that the very small scale plume peaks, such as the peak situated 300km from the Eastern edge, are still not adequately represented. These areas could be resolved using tighter tolerances.

3.3 TOTAL INTEGRATED CONCENTRATION.

As grid density affects the degree of species dispersion the amount of species mixing will be grid dependant which will ultimately alter the total rate of species reaction. The mesh dependency of total species budgets is therefore assessed by examining the total integrated quantity of species over the course of the simulation.

Figure 6 a-d presents the species budgets for all three gridding schemes showing , NO2, NO, O3 and RP. These plots present total integrated species quantities in molecules, within a 1cm layer of the mixing height, against simulation time. Comparison shows that for diurnal variations in NOx-Ozone exchange differences between the gridding regimes are small. Total area under the adaptive and high density NO solutions show only a 0.09% difference. Similar comparison of the adaptive and low density NO solution shows a larger 3% difference, demonstrating that average centreline concentration is a mesh dependant property adequately resolved by the adaptive technique. The most significant differences in total species budget lie in the reactive pool. Large differences in RP quantity exist between solutions gained using the high and low resolution constant density grids. The solution gained using the adaptive gridding regime more closely follows those generated by the low resolution constant density grid. This is because we have chosen to refine around NO concentrations in order to simplify the demonstration of the technique and have consequently not resolved RP structures adequately. This problem is easily solved by applying appropriate tolerance values to RP.

4.0 Discussion

Comparison of the solutions for the two constant gridding scenarios provides a clear demonstration of the effect of grid density on solution. Results demonstrate that as resolution improves clearer identification of small scale structures is possible. In addition, refinement of the grid reduces artificial dispersion of species and therefore the smearing out of detail. Furthermore, examination of cross plume profiles shows that fine

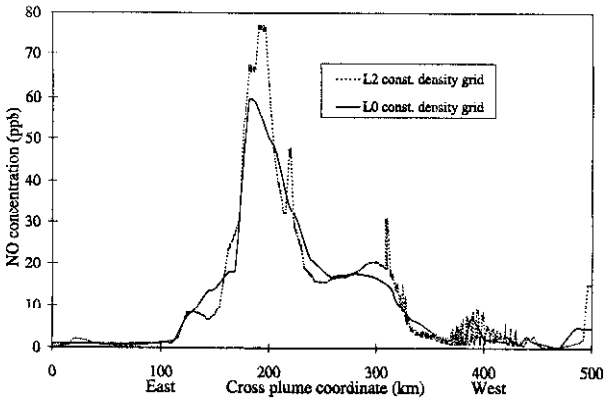


Figure 5a: Level 2/Level 0 cross plume profiles

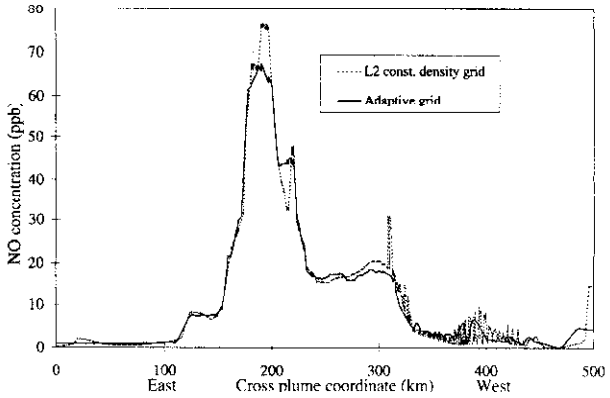


Figure 5b: Level 2/Adaptive cross plume profiles

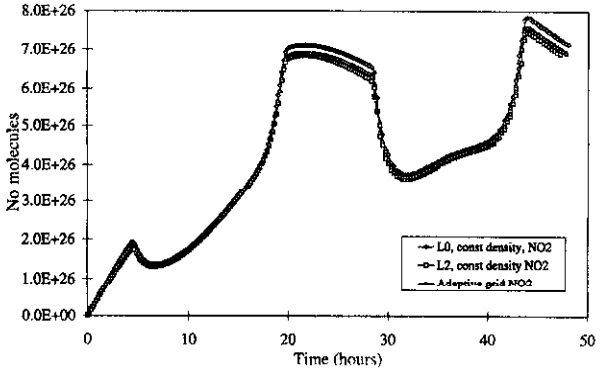


Figure 6a: NO_2 total species budget

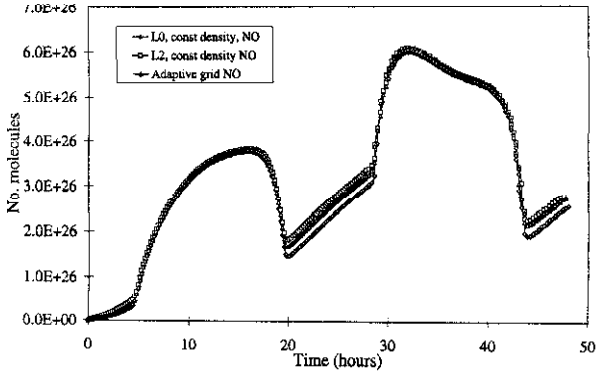


Figure 6b: NO total species budget

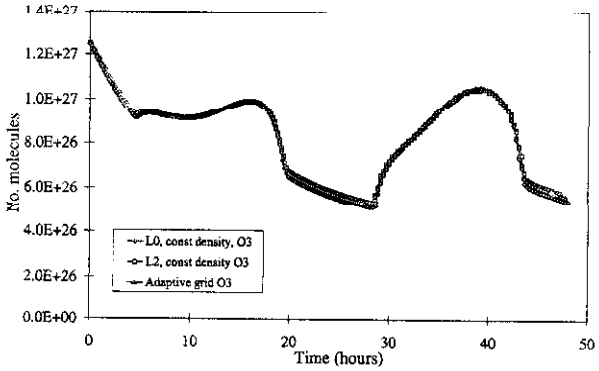


Figure 6c: O_3 total species budget

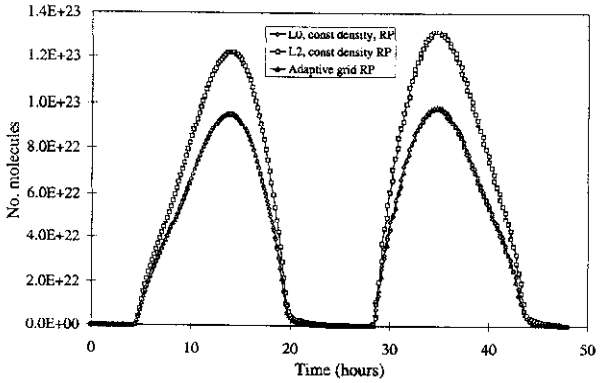


Figure 6d: RP total species budget

structures within the solution can lead to localised regions of very high species concentration. The resolution of these small scale structures may become very important when comparing numerical results to sparse monitoring data. The large differences between total reactive pool budgets yielded by the different grids are explained in Tomlin (1995) as the result of averaging the non-linear reaction rate over a single finite volume for the coarse grid. The reaction rate averaged over a single volume will only yield an accurate result if the concentration over the surrounding region is smooth, so in regions of steep spatial gradients there are likely to be large errors induced by the non-linear terms. Equation 2.2 shows that RP undergoes several non-linear reactions, accounting for the large discrepancy between high and low resolution results.

Despite improved solution accuracy, code performance is degraded in terms of processing time and storage requirements when using high density grids. This problem has been addressed using time adaptive gridding algorithms. The grid generated using adaptive techniques clearly clusters grid points in regions of potentially high spatial error such as plume edges. Such a grid configuration resolves rapidly changing solution profiles,

identifying structures only represented on a small spatial scale. This degree of accuracy is achieved using far fewer grid points than a constant density grid of similar resolution. In addition, more complex meteorology would make the prespecification of such a grid virtually impossible. The use of adaptive gridding therefore results in a higher accuracy solution solved in less time and requiring much reduced storage. The telescopic approach has shown to be useful in resolving structures close to the high emission areas selected. It is, however, incapable of resolving plume structures as they develop downwind of these sources.

5.0 Conclusion

In this paper we have presented a methodology based upon adaptive gridding techniques which could potentially reduce the computing cost of solving the dispersion problem while maintaining solution accuracy. The code presented successfully detects regions of potentially high spatial error and clusters grid points in these regions. The solutions yielded using such techniques were compared to those achieved using constant density gridding. They were found to be comparable to those gained using higher density grids, and successful in resolving gridding problems which telescopic models only partially address.

Lower resolution grids fail to resolve the small scale structures which may become important when comparing numerical results to monitoring data and in addition disperse species to such an extent that detail is smeared and indistinct. Grid dependency of non-linear reactions has been discussed and the errors possible demonstrated. Total species budgets for NOx and O_3 were not sensitive to grid structure but are highly sensitive for non-linear species such as the radical pool. For our simple scheme these errors did not feed back into major species but this may not be true for other chemical schemes. Local concentrations are far more sensitive to the grid and may require high levels of adaptivity in certain areas in order to be resolved. To achieve adequate solution accuracy using constant grids a high density must clearly be used. However, there is a price to pay in terms of run time and storage requirements when using such grids.

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