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Atmospheric Environment 37 (2003) 5147–5156

ATMOSPHERIC ENVIRONMENT

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Simulations of atmospheric pollution in Greater Lyon an example of the use of nested models

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Received 11 November 2002; received in revised form 24 March 2003; accepted 31 March 2003

Abstract

Air quality in urban environments depends on numerous processes and phenomena, which cover a wide range of length scales, from the scale of the street to that of the region. In order to reproduce such a wide range of length scales, a modelling system based on nested models has been developed to compute atmospheric pollution in the Greater Lyon region. Regional scale calculations are performed using the models SAIMM for meteorological conditions, and UAM-V for pollutant transport; the calculations are performed for a domain measuring 208 km square, with a resolution of 4 km. Urban scale calculations are performed using the code MERCURE, on a domain measuring 32 km^2, with a resolution of 500 m. More detailed local scale calculations are performed using ADMS-3 and SIRANE. This system has been used to simulate NO_X concentrations for a 24 h period during the field measurement campaign ELO (June 1999) and the results are compared with measured data for that period. The comparison demonstrates the value of an approach based on nested models; in particular, the inclusion of a local scale simulation improves the accuracy of the calculations for near field locations. The local scale model needs to be chosen according to the source type and the characteristics of the domain.

Keywords: Urban air pollution; Scale nesting; 3D model; Plume model; Street network model

1. Introduction

Urban air quality depends on many different physical processes, over a wide range of length and time scales, from the scale of the street to that of the region. No single model is capable of reproducing such a wide range of length and time scales, and it is therefore necessary to construct a modelling system based on a set of nested models to represent different phenomena and different scales. There are two possible approaches for constructing such a modelling system. The first is based on the use of a single three-dimensional Eulerian model, nested at several different scales; this is the approach adopted in METPHOMOD (Perego, 1999) and RAMS (Pielke et al., 1992), for example. The main advantage of this type of model is that it uses the same methodology for all the different scales, and this facilitates the exchange of information between calculations at the different scales; the main disadvantage is that the models are computationally intensive, requiring considerable computing time and resources. This approach is therefore not usually practical for applications where it is necessary to carry out calculations rapidly, with rather limited resources. Also is it really feasible to use the same modelling assumptions at all scales? If the model uses wall functions, for example, are they going to be valid at all scales? The second approach is based on the use of different types of models for different scales, with each model chosen to represent the dominant physical

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doi:10.1016/j.atmosenv.2003.03.002

processes at that particular scale. Such a modelling system might therefore consist of different models for calculations at the scale of the region, the city, the district and the street. In some situations it might also be necessary to add a specific model for a complex industrial site. The principal advantage of this approach is that each model can be chosen to reproduce the dominant processes at the relevant scale, and this usually means that they are much more efficient than a general 3-D model. The major disadvantage is that the models often use very different approaches, so that, for example, a modelling system might consist of a combination of Eulerian, box, Gaussian plume and Lagrangian stochastic models. It is extremely difficult to couple such a disparate ensemble of models, particularly when the coupling needs to be both up-scale and down-scale. For this reason, most current modelling systems which use a variety of different models do not implement any strong coupling between the models. This simplification is acceptable when the phenomena of interest are only weakly dependent on processes at other scales, but in many cases it is necessary to model several different scales simultaneously, or quasi-simultaneously.

If it is necessary to carry out multi-scale calculations for an operational model, for which computing resources and time are both important considerations, it is currently impossible to envisage the use of a single 3-D model, nested at several different scales. It is therefore necessary to develop ways of nesting different types of models. This paper describes the development of such a modelling system, based on the coupling of a range of different models, and the use of this system to compute atmospheric pollution in the city of Lyon. The basic structure of the modelling system is shown in Fig. 1.

Initially, the different components of the modelling system were used to compute atmospheric pollution in Lyon, without any explicit coupling (Soulhac et al., 1998; Duclaux et al., 2002). The group from TotalFinaElf used the regional scale model to compute photochemical pollution in the Lyon area for a period of several days in June 1999; this period was chosen so that the results could be compared with the detailed data obtained during the ELO campaign. The calculations agreed reasonably well with the field data obtained at altitude (LIDAR measurements) and outside the agglomeration, but there were significant differences between observed and predicted ground level concentrations within the agglomeration. This was principally due to the rather low spatial resolution ($4\,km \times 4\,km$) used for the regional scale calculations, which made it impossible to reproduce significant small-scale variations within the urban environment. In order to improve the resolution of these small-scale local variations, and thus to improve the agreement between the data and the model, we have coupled the regional scale model with a series of small scale models. The regional model is summarised in Section 2, and then in Section 3 we present the urban scale model and describe how it has been coupled with the regional scale model. The results from the combined model are then compared with the field data. In Section 4, we suggest some possible approaches for further improving the agreement between the data and the calculations. In particular, we show that the model predictions can be improved by the use of a model such as ADMS-3 for the surroundings of large-scale industrial sites, and a street network model such as SIRANE to account for vehicle emissions in inner city areas.

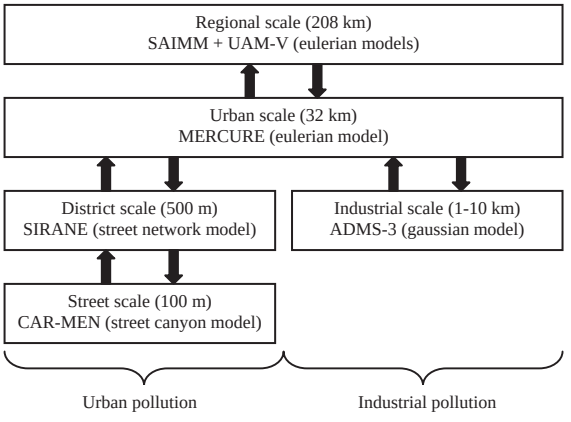

Fig. 1. The modelling system.

2. The regional scale model

The regional scale calculations were performed using the meteorological model SAI Mesoscale Model (SAIMM; ICF Kaiser, 1995) coupled with the Variable grid Urban Airshed Model (UAM-V; Morris and Myers, 1990). SAIMM is a hydrostatic model, based on a four-dimensional data analysis (FDDA) "nudging" scheme, in order to drive model predictions closer to observations. It uses a prognostic equation for the turbulent kinetic energy, from which vertical exchange coefficients are calculated. The results of these calculations provide the input data for the second model—UAM-V—which calculates the transport, dispersion and chemical transformation of atmospheric pollutants. The UAM-V Model is a three-dimensional, multi-scale photochemical grid model that calculates concentrations of pollutants by simulating the physical and chemical processes in the atmosphere. UAM-V uses an updated "Carbon-Bond IV" chemical mechanism to simulate the photochemical reactions between NO_X and ozone (Gery et al., 1989). Transport and turbulent diffusion are calculated using hourly values for the wind field and the vertical diffusivity, simulated with SAIMM. The UAM-V calculations also require temperature, pressure, water

vapour, cloud cover and precipitation for all grid points within the computational domain.

The computational domain measured 208 km × 208 km × 10 km, centred on Lyon, and extending to the Alps and to the Jura (see Fig. 2a). The resolution of the model was 4 km horizontally, with 22 grid points vertically; the first point was located 25 m above the ground, and the highest grid point was at a height of 10,000 m relative to the surface. The meteorological calculations were driven by the hourly data from 94 surface meteorological stations within the domain, the vertical profiles from two sodars (one providing hourly data up to an altitude of 400 m and the other providing half-hourly profiles up to an altitude of 1000 m), and a profile obtained from a radio sounding every 12 h. The boundary conditions for the calculations were derived from the results of the numerical model ARPEGE, run by Météo-France, which operates with a spatial resolution of 0.25°.

The time varying emissions were obtained from a detailed emissions inventory for the entire domain (Pajot, 2000). Vehicle emissions are represented as line sources, based on the results of a traffic model coupled with the COPERT II methodology for the emissions estimation (Ahlvik et al., 1997). Industrial emissions are modelled as point sources, whose characteristics are given by regulatory inventories. Biogenic and anthropic emissions (other than those due to industrial installations and vehicles) were evaluated as area sources, with emissions rates estimated for each soil class of the CORINE Land Cover database. All these emissions were aggregated on a grid mesh with a resolution of 4 km. The quantities of Ozone advected into the domain by wind transport were estimated from the results of the model CHIMERE (Vautard et al., 1999) which is a continental scale model.

The model was used to simulate atmospheric pollution over the period 22–25 June 1999, which corresponds to the period for which data are available from the ELO campaign. Preliminary comparisons between the simulations and data obtained from stations situated well outside the agglomeration and from LIDAR profiles showed that the model reproduced the variations in pollutant concentrations that were measured in these locations. In this article, therefore, we concentrate on the computation of ground level concentrations within the city, and in the neighbourhood of a large industrial site. The results of these calculations for NO_X concentrations are compared with data obtained from a variety of pollution monitors, for the 24th June 1999. In particular, three different measurement sites were selected, to characterise different types of environment. Fig. 3 shows the corresponding concentration measurements over the same 24 h period, for these different sites,

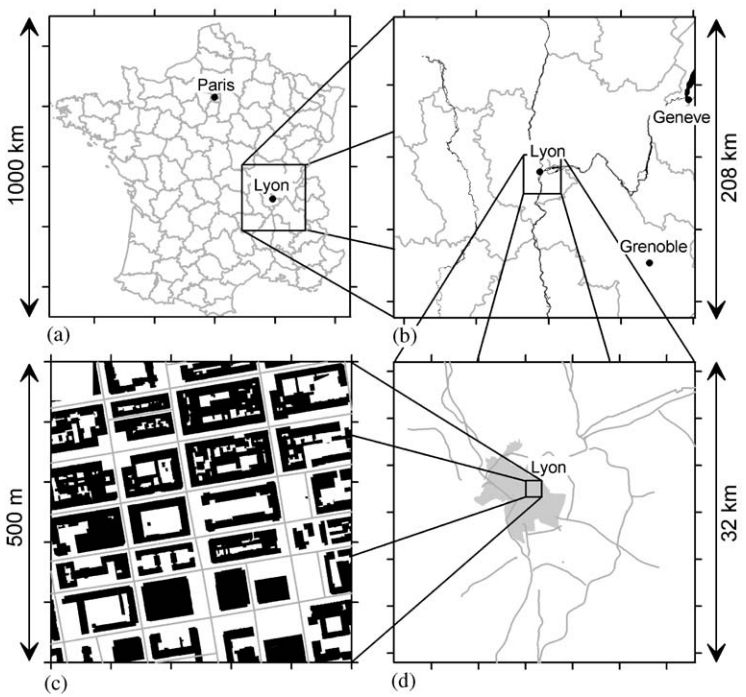

Fig. 2. The different computational domains used in this study. (a) Location of the regional domain within France. (b) Details of the regional scale domain and location of the urban scale model. (c) Details of the urban scale model and location of the city district model. (d) Details of the city district scale model.

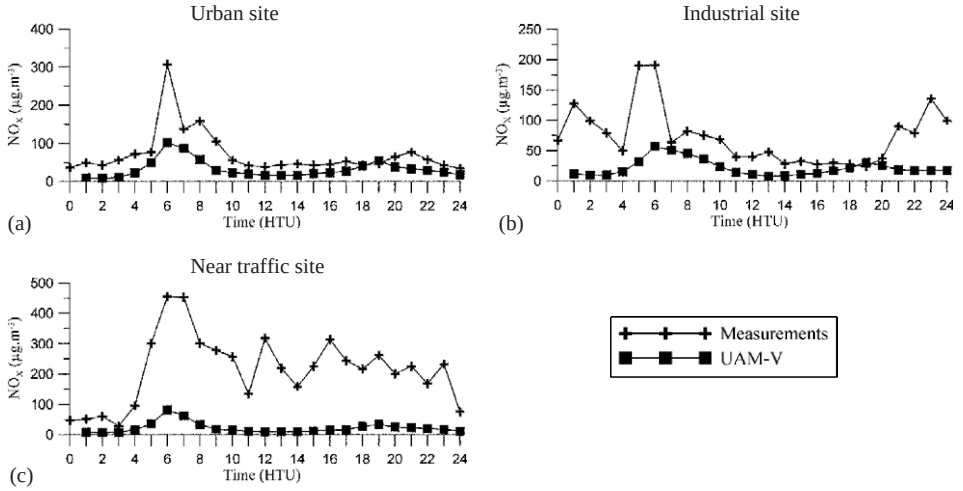

Fig. 3. Comparison between numerical simulations performed using UAM-V and field data (provided by the COPARLY) for three sites in Lyon. (a) Urban site, distant from main roads, (b) Urban site, downwind of a petrochemical plant, (c) Urban site, in a street canyon, with high traffic flows.

and it is clear that they exhibit significantly different behaviour. The first site (Fig. 3a) is located far from major industrial emitters and heavily trafficked roads, so that it is broadly representative of the background concentration in urban environment. The second site (Fig. 3b) is located close to a major petrochemical refinery, and the measured concentrations are heavily influenced by industrial emissions from a small number of highly localised sources. The third site (Fig. 3c) is situated beside a very busy city centre road, and the street geometry is similar to that for a classic "street canyon".

In all three cases, the model UAM-V significantly underestimates the measured concentrations. This is principally due to the size of the grid cells used in the calculation ($\Delta x = \Delta y = 4\,\mathrm{km}$): all emissions are unavoidably averaged over the grid cell in which they are located, leading to a rapid and fictitious initial dilution. This effect is particularly noticeable in Fig. 3b (the industrial site) and Fig. 3c (the city street), where the highly localised nature of the emissions is particularly adversely affected by this averaging. Another contributory factor is the impossibility of reproducing small-scale processes such as building effects or plume rise.

This preliminary comparison leads to two important conclusions:

- The comparison with rural and elevated measurements shows that coupled transport-transformation models such as SAIMM/UAM-V are reasonably well adapted to modelling the temporal evolution of photochemical pollutants (particularly Ozone) on a regional scale, over periods of several days.
- The comparisons with data from different types of urban site show that these same models are not at all suitable for studying small-scale phenomena that determine concentrations at a local scale, for which much finer scale models are necessary.

We have therefore investigated ways of coupling the SAIMM/UAM-V model with different small-scale models, so as to take account of local phenomena. The results of these studies are presented in Sections 3 and 4.

3. Urban scale modelling

3.1. The simulations

The transport and dispersion of pollutants within the Lyon agglomeration was simulated in more detail using the atmospheric boundary layer code MERCURE (Carissimo et al., 1995). MERCURE is a three-dimensional non-hydrostatic model, solving the Reynolds-Averaged Navier Stokes equations, with a $k-\varepsilon$ type turbulence closure model. It includes specific model for heat, mass and momentum transfer at the ground. The transport and dispersion of pollutants is computed by solving the advection-diffusion equation for non-reacting species; at the moment it does not include any models for atmospheric chemistry.

The domain measured $32\,\mathrm{km} \times 32\,\mathrm{km} \times 2.5\,\mathrm{km}$, and was centred on Lyon. The horizontal resolution was 500 m, and the vertical resolution varied between 20 m at the ground, and 400 m at the top of the computational domain. Within the domain, the ground elevation varied between 150 and 600 m above datum. The surface boundary conditions (roughness, radiation, heat and moisture fluxes) were estimated from a preliminary

classification of the surface into 7 different categories. The meteorological conditions in the model were imposed through boundary conditions imposed on the sides of the domain, and derived from the regional scale calculations described in Section 2. This provided a time-evolving forcing of the system, with a time step of 1 h. (No forcing term was included in the model equations, so the flow within the domain adapted to the temporal variation in the forcing on the domain boundaries.) The emissions data were taken from the inventory used for the regional scale model, but discretised at the resolution of the urban model (500 m × 500 m); the emissions also varied in time, with a temporal resolution of 1 h.

This model was used to simulate 24 h during the period of the ELO campaign—the 24th June 1999. Meteorological conditions were anti-cyclonic, with little or no cloud cover over the entire domain, and temperatures that reached 26°C in Lyon. The wind was from the North-West in the morning, and from the North-East in the afternoon. Measurements for the period show high concentrations of primary pollutants, which resulted in high levels of Ozone, because of the strong sunshine and the high temperatures. In order to test the coupling between the two models we have examined the transport and dispersion of the primary pollutants, particularly NO_X. Fig. 4 shows the ground level concentrations of NO_X computed for four instants during the day. Simple visual inspection of these figures shows that, at least in the centre of the city, the ground level concentrations are principally associated with vehicle emissions; this observation has been confirmed quantitatively by simulating concentrations due to vehicle emissions and other sources separately. Since these emissions are highly localised, it is likely that local refinement of the spatial resolution of the model would improve the quality of the predictions significantly, at least in those regions where the road network is relatively dense, since the process of averaging the emissions over large grid squares tends to smooth out these local variations.

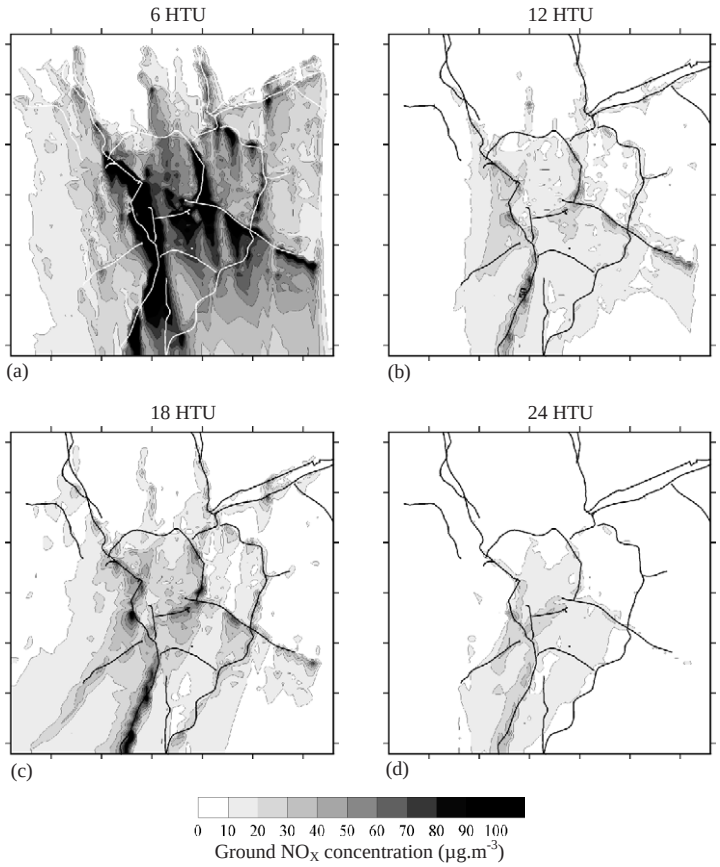

Fig. 4. Ground level concentrations of NO_X at urban scale (32 km × 32 km), computed using MERCURE at four instants during the 24th June 1999. The main roads are shown in white (a) or black (b, c and d).

3.2. Comparison with field data

We have compared the results from MERCURE with meteorological data and with pollution measurements made at ground level within the agglomeration for the corresponding period. Fig. 5 shows a comparison of model results with meteorological data obtained from a measurement station outside the city. The model reproduces the variations in wind speed and direction reasonably well, but slightly underestimates the temperature during the afternoon. We have also compared the height of the mixed layer with that predicted by the regional scale model and with the measured value obtained from a radio-sounding taken at 12 h UCT. The two models and the data agree reasonably well at midday, but in the afternoon the layer thickness computed by MERCURE is rather greater than that computed by the regional scale model. This is almost certainly due to the finer resolution of the forcing term at the urban scale, compared with the regional scale.

The computed pollutant concentrations have been compared with those measured at ground level by pollution samplers located in three different areas of the city. Each of these points was chosen to be characteristic of a particular type of situation that is often encountered in urban areas. The first sampler (Fig. 6a) is located within the city, sufficiently far from the main roads that its measurements are not directly influenced by any particular source of emissions. The graph shows that the model calculations agree rather well with the data, and that, in particular, the model reproduces the peak in concentrations produced by the morning rush hour traffic. So the scales of atmospheric movement which principally determine what is measured by this type of sampler are reasonably well resolved by a calculation with a spatial resolution of 500 m.

The second sampler (Fig. 6b) is located downwind of a petrochemical plant which emits significant quantities of NO_X. The principal source of these emissions is a chimney with a height of 90 m. The figure shows that the model overestimates the ground level concentrations; this is almost certain, because the rather coarse resolution of the model leads to an overestimate of the initial dispersion of the pollutant (the pollutant fills the whole grid square) and prevents any explicit modelling of plume rise. Consequently, in the region immediately downwind of the chimney, the pollutant is diffused down to the ground much too rapidly (compared with the reality) and ground level concentrations are overestimated. The only way of correcting this is to use an explicit model for the chimney plume in the near source region; this approach is discussed in Section 4.1.

The third sampler (Fig. 6c) is located in the centre of the city, in a street with high traffic flows (which can exceed 20,000 vehicles/day) and a geometry which is typical of a "street-canyon". It can be expected that the concentrations measured by this sampler will be heavily influenced by the local traffic. The figure shows that MERCURE alone severely underestimates the concentrations, compared with the observed values. This is caused primarily by the local small-scale structure of the flow within a street canyon, which cannot be reproduced by a calculation with MERCURE at the scale of the city. In reality, the rather high concentrations within a street are caused by the fact that the pollutants are emitted in a highly confined, badly ventilated space and this severely limits their lateral dispersion. In order to maintain a sufficient pollutant flux from the street into

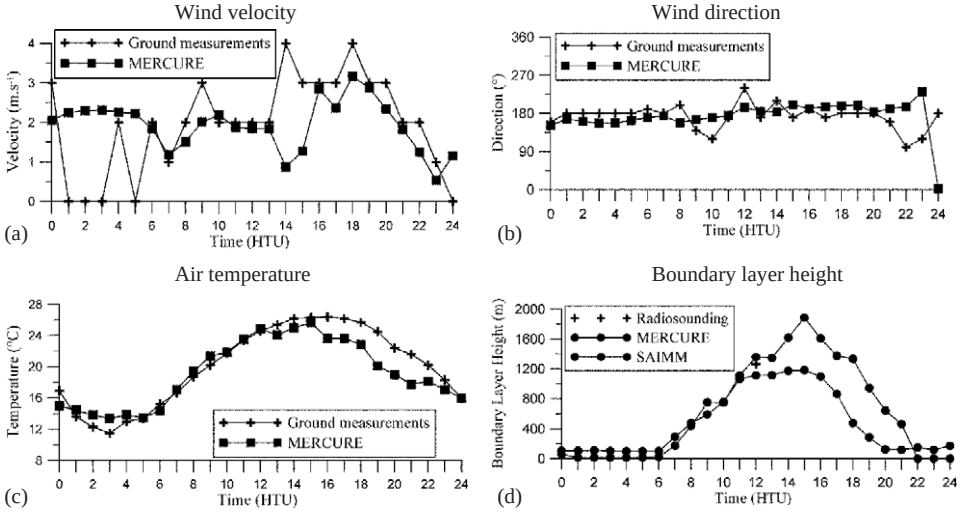

Fig. 5. Comparison of the results of the calculations performed using MERCURE with data obtained from the meteorological station at Bron. (a) Wind speed, (b) wind direction, (c) air temperature at ground level and (d) boundary layer height computed by MERCURE and SAIMM, and the value measured by radio sounding at Lyon Saint-Exupéry.

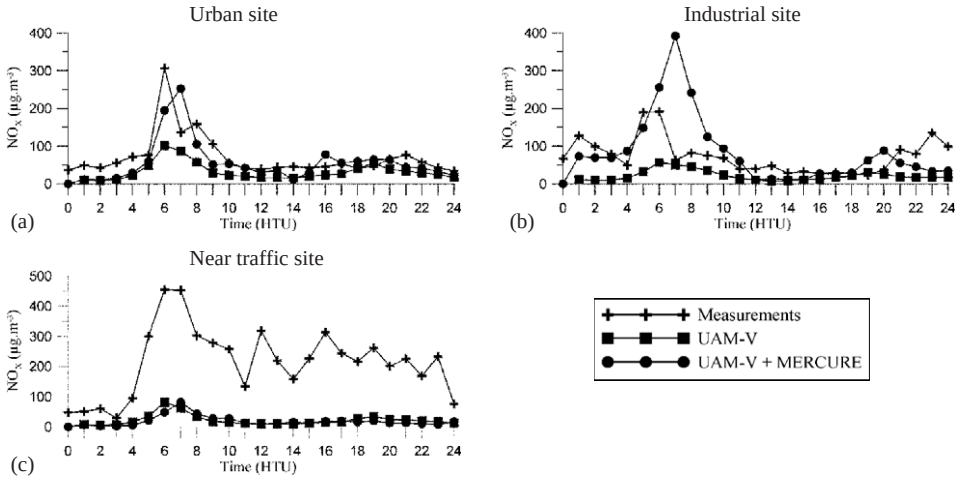

Fig. 6. Comparison between numerical simulations and field data (provided by the COPARLY) for three sites in Lyon. (a) Urban site, distant from main roads, (b) urban site, downwind of a petrochemical plant, and (c) urban site, in a street canyon, with high traffic flows. The numerical simulations were performed using UAM-V alone, UAM-V coupled with MERCURE.

the overlying atmosphere it is necessary to create a rather strong concentration gradient, and this therefore leads to relatively high concentration within the street. Since the horizontal grid size in the calculations is 500 m, these local effects cannot be modelled explicitly (the presence of buildings is modelled through an increase in roughness length) and so the initial dispersion is overestimated. In order to model the local effects correctly, it will be necessary to couple the model with a small-scale model adapted to the local geometry; this coupling is discussed in Section 4.2.

4. Local scale modelling

4.1. Coupling with a Gaussian plume model ADMS-3

In order to improve the modelling of major point sources, we have coupled MERCURE with the model ADMS-3 (CERC, 2000). This code, developed to simulate dispersion from point sources, uses a model for the wind field based on a Fourier transform solution of the linearised equation of motion (FLOWSTAR; Hunt et al., 1988). It assumes that the terrain is relatively flat, and it includes atmospheric stability effects. Dispersion is modelled using a modified Gaussian plume model, and it includes plume rise effects due to buoyancy or momentum.

The models are based on very different assumptions, and use very different approaches, so we have to develop some consistent basis for their coupling. The flow field model in ADMS-3 was applied to the same domain as that for MERCURE, with the same boundary conditions. We assume that the pollutant (NO_X) can be treated as a passive scalar (there are obviously reactions between NO and NO_2, but the total concentration of NO_X varies very little) so that we can treat the pollutant emitted by major point sources separately from that emitted by other, more diffuse sources. Then MERCURE is used to compute the transport and dispersion of pollutants emitted by the diffuse sources, and ADMS-3 is used to model the transport and dispersion of pollutant emitted by the major point sources. The total concentration is then obtained from the sum of the two contributions:

$$C_{\mathrm{Total}} = \underbrace{C_{\mathrm{Indust.}}}_{\text{ADMS-3}} + \underbrace{C_{\mathrm{Traffic}} + C_{\mathrm{Biogen.}} + C_{\mathrm{Anthrop.}}}_{\text{MERCURE}}$$

This method improves the model significantly, compared with the results obtained from a calculation with MERCURE alone (cf. Fig. 7). In particular, the prediction of the peak concentration around the time of the morning rush hour is much closer to the measured value, because the emissions from the chimney are not artificially diffused over the grid cell in which the chimney is located.

4.2. Coupling with the street network model SIRANE

Many pollution monitors in urban areas are located in streets that behave as street canyons, and for which the measured concentrations are heavily influenced by the traffic in the street. To include this effect in the calculations, we have coupled MERCURE with the street network model SIRANE (Soulhac et al., 1998; Soulhac, 2000). In this model, the streets in a city district are modelled as a network of connected street segments (see Fig. 8a). The flow within each street is driven by the

component of the external wind parallel to the street, and the pollutant is assumed to be uniformly mixed within the street. The model contains two main mechanisms for transport in and out of a street segment (see Fig. 8b).

Diffusion across the interface between the air in the street and the overlying air. This is modelled by a standard concentration gradient diffusion approach, with a diffusion coefficient calculated from the external boundary layer properties (friction velocity and Monin-Obukhov length).

Exchanges with other streets, at street intersections, due to the advection along the street. Several detailed wind tunnel experiments and numerical simulations were performed to parameterise these exchanges. The model assumes the conservation of mass in each intersection, generating a vertical flux when horizontal advection fluxes into and out of the intersection are not equal (see Fig. 8c). The mixing rate of pollutants advected from the different upwind streets is related to the fluctuation of the external wind direction.

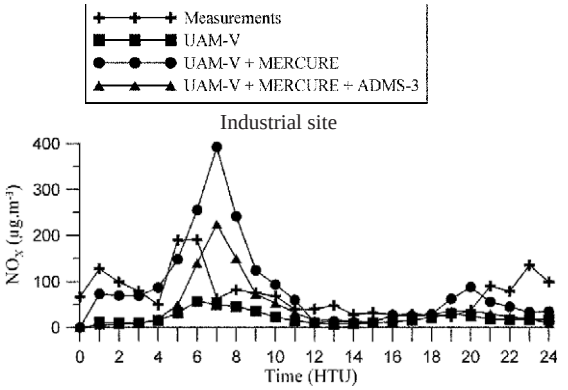

Fig. 7. Comparison between numerical simulations and field data for the industrial site. The numerical simulations were performed using UAM-V alone, UAM-V coupled with MERCURE and UAM-V coupled with MERCURE and ADMS-3.

The dispersion of pollutants advected or diffused into the overlying air is taken into account using a Gaussian plume model (see Fig. 8d), with the standard deviations σ_y and σ_z parameterised by similarity theory. The input data for the final model are the external wind (velocity and direction), the atmospheric stability, the concentration of pollutants advected into the model domain by the wind and the emissions within each street in the network. The model was tested against detailed wind tunnel measurements and numerical simulations of flow in a grid of streets, subject to an external wind of varying direction. The results confirmed that, although relatively simple, the model nevertheless predicted concentrations that agreed well with those obtained in the experiments and the simulations. The SIRANE model has also been validated by comparisons with field measurements (Soulhac et al., 2001).

SIRANE has been coupled with MERCURE, to improve the modelling of local effects in the city centre. The model domain was taken as the complete grid square in MERCURE (500 m × 500 m) in which the pollution monitor is located. MERCURE then provides the external wind field and the background concentrations for a more detailed calculation with SIRANE. Traffic emissions taken into account in the SIRANE domain were represented as line sources, provided by the traffic and the emission models (see Section 2). The total

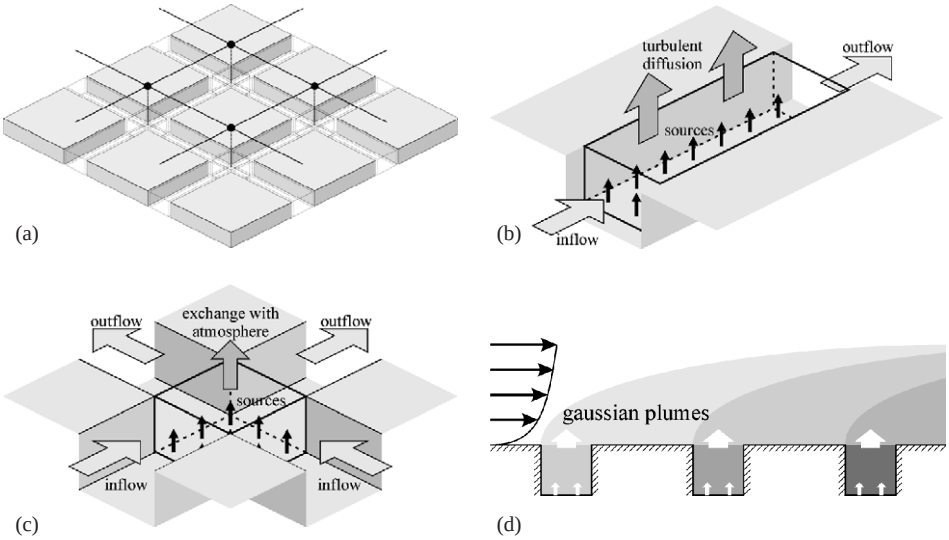

Fig. 8. The different components of SIRANE. (a) Modelling a district by a network of streets. (b) Box model for each street, with corresponding flux balance. (c) Fluxes at a street intersection. (d) Modified Gaussian plume for roof-level transport.

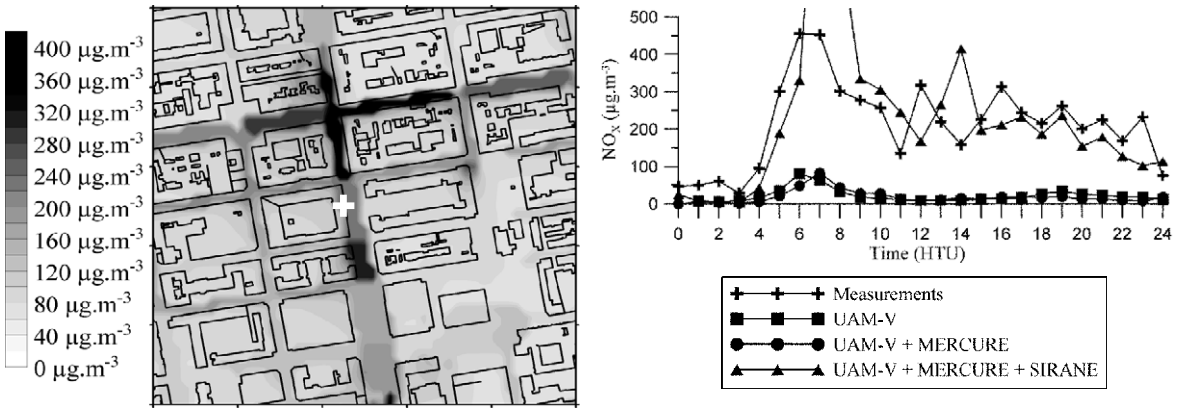

Fig. 9. Comparison between numerical simulations and field data in the near traffic site. The numerical simulations were performed using UAM-V alone, UAM-V coupled with MERCURE and UAM-V coupled with MERCURE and SIRANE.

concentration is the sum of the contribution from MERCURE and from SIRANE:

$$C_{\text{Total}} = \underbrace{C_{\text{District}}}_{\text{SIRANE}} + \underbrace{C_{\text{Background}}}_{\text{MERCURE}}.$$

The results presented in Fig. 9b show that this approach leads to a significant improvement in the model predictions; the predicted values are close to those measured by the sampler, except during the morning rush hour, when the combined model overestimates the concentration, by a factor of about 2. A comparison of the results obtained with and without SIRANE shows that the background concentration contributes very little to the overall value for this site in the city centre (this is not necessarily true for all the streets in the network). As the results presented in Fig. 9a show, the concentration in the street depends principally on emissions within the street and emissions within some heavily polluted neighbouring streets. This underlines the importance of considering a network of streets rather than simply an isolated street canyon, which could not include the influence of neighbouring streets.

5. Conclusions

We have developed a modelling system composed of different, coupled models, to enable us to compute atmospheric pollution in the urban canopy. This system consists essentially of a regional scale model (SAIMM/UAM-V), an agglomeration scale model (MERCURE) and two local scale models (ADMS-3 and SIRANE). The modelling system has been applied to the city of Lyon, and used to compute the temporal variation in NO_X for a 24 h period in June 1999, for which extensive measurements are also available. The comparison between the model calculations and the data confirm the importance of intermediate and small scale effects in many typical situations; the predictions from the combined model are significantly better than those from the agglomeration scale model on its own.

In these calculations, we have only used one-way (downscale) coupling—the larger scale models have been used to define boundary conditions for the smaller scale models. The next step of this project is the development of a full two-way coupling to allow the transfer of information from the small scales to the large scales. An important aspect of the work currently in progress concerns the modelling of buildings and other obstacles in the urban scale calculations. The results presented here show that a simple modification of roughness length is not sufficient to reproduce local effects, but it is not currently feasible to model an entire city such as Lyon using a street network model like SIRANE. We are therefore investigating an intermediate approach, in which the buildings are represented as source terms (for momentum and turbulence) distributed over the lowest grid cells. The fundamental difficulty with this approach lies in the correct parameterisation of the source terms, as a function of the building geometry and spacing, and the imposed external wind field. We are currently studying these problems using wind tunnel experiments and numerical simulations. The results from this work should provide an improvement in the urban scale simulations.

Acknowledgements

We gratefully acknowledge the financial support provided by TotalFinaElf (J.-P. Boch).

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