Air quality modelling in Urban Regions using an Optimal Resolution Approach (AURORA)

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Keywords: urban air pollution, emission modelling, advection, diffusion, chemistry, street canyons

1 Introduction

Cities experience increasing signs of environmental stress, notably in the form of poor air quality. A vast majority of the urban and suburban population is exposed to conditions that exceed air quality guidelines established by the World Health Organisation (WHO, 1999). A thorough knowledge of the present and future air quality in cities and of the parameters that determine the air quality is considered to be the necessary base for the development of urban air quality management policies and programmes. This is also expressed by EU directive 96/62/EEC, in which air quality assessment in urban agglomerations is recommended. The directive recognises that air quality models are valuable tools for the assessment and forecast of air pollution.

For the assessment of air quality in cities, Vito introduced an *integrated model system*, known as AURORA (**A**ir quality modelling in **U**rban **R**egions using an **O**ptimal **R**esolution **A**pproach). This urban air quality management system has been designed for urban and regional policy support and reflects the state-of-the-art in air quality modelling, using fast and advanced numerical techniques. The model input consists of terrain data (digital elevation model, land use, road networks) that are integrated in a GIS system. Meteorological input data are provided, with a resolution up to a few hundred meters, by a separate meteorological model (ARPS). The emission input data are resulting from a detailed inventory and acquisition of existing emission data in combination with emission modelling (Mensink *et al.*, 2000). In this way the emissions are described as a function of space, time and temperature.

The physical and chemical processes are modelled in a modular way (see Figure 1) following the state-of-the-art in urban air quality modelling and involving large-scale computations. Every module was tested and validated individually before integration in AURORA. The most important parts of the model system are the modules for physical transport phenomena (advection, diffusion, deposition, etc.) and the modelling of photochemical processes and chemical reactions. These modules include some advanced and improved numerical solvers. Concentrations at the street level are estimated by means of the Street module (Mensink and Lewyckyj, 2001), using the 3D spatial configuration of the considered street and the related traffic information.

Calculated pollutant concentrations are coupled to specific dose-response functions in order to assess both health effects and ecosystem (or material) degradations. Using the ExternE methodology (1995), estimations of the related costs can be provided. A scenario module allows the decision-maker to evaluate possible future remedial actions in both qualitative and quantitative ways. Finally, a comparison of the model results with both the European and national regulations is also included.

The model system is implemented in the cities Antwerp and Hasselt (B) and is being applied in various EU 5th framework projects (BUGS, DECADE,…). In this article the general concept of model system is presented and some of the validated modular units are briefly described. In particular this concerns some characteristics of the urban transport emission model (section 2), some computational aspects of the newly implemented advection-diffusion scheme (section 3), the development of compact chemistry mechanisms to reduce computational time (section 4) and the "street box" module, allowing a fast evaluation of concentrations in street canyons (section 5).

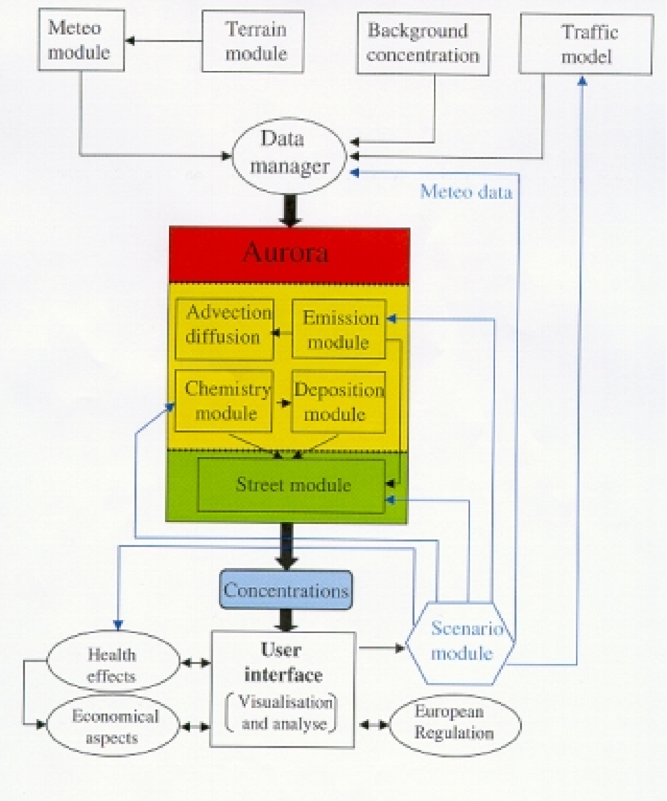

Figure 1 Flowchart of the modular designed AURORA model.

2 Emission modelling

Urban emission inventories describe in a very detailed way the stationary and mobile emission sources that can contribute to any form of air pollution within the urban canopy. For urban air quality modelling an emission inventory should provide the input data with a sufficient time resolution and an adequate spatial resolution. For the urban situation this means that at least hourly variations in emissions can be described within a small grid domain (max. 1 x 1 km^2) or even at street level. Also the sensitivity of emissions with regard to temperature variations is important, not only for emissions stemming from spatial heating, but for traffic emissions as well. The required dynamic character and spatial accuracy with which emission variations have to be described resulted in the development of an urban transport emission model (Mensink et al., 2000). Its design is based on the results of an urban traffic flow model (Nys, 1995), which is actually used by the Antwerp City authorities. The urban traffic flow model provides hourly traffic volumes for each element in a network of 1963 streets and road segments in Antwerp. It was implemented in a GIS environment. By combining the hourly traffic volumes computed per road segment with fleet statistics and the corresponding emission factor, the hourly urban transport emissions can be obtained. The emission E(t) ($g \cdot h^{-1}$) calculated for pollutant i, vehicle class j, road type k and road segment n, can be expressed by:

$$E_{i,j,k,n}(t) = EF_{i,j,k} \cdot F_{m,d,h}(n, t) \cdot L(n) \tag{1}$$

where EF is the emission factor ($g \cdot km^{-1}$) for pollutant i, vehicle class j and road type k. F is the time dependent traffic flow rate (h^{-1}) and L the road length (km) per road segment. The model substances are CO, NO_x, NMVOC (42 components), PM, SO_2 and Pb.

The emission factors for hot running vehicles as defined in the COPERT II methodology (Ahlvik, 1997) are a function of vehicle speed, vehicle class, fuel type and cylinder capacity. For the specification of vehicle classes, the UN-ECE classification was followed, restricted to the vehicle types Passenger Cars (PC), Light Duty Vehicles (LDV) and Heavy Duty Vehicles (HDV). The last category includes urban busses and coaches. An assessment of the uncertainty in the model was carried out partially by comparing the computed hot and cold start emission factors for CO, NO_x and VOC with measured values for urban driving conditions during an on-the-road measurement campaign (De Vlieger, 1997). In addition modelled and observed traffic flows were compared for in several streets in and around the city of Antwerp (Mensink, 2000).

3 Advection-diffusion

Modules for advection and vertical diffusion in AURORA were completely re-designed, leading to a more accurate and much faster (factor 25 speed-up) version of AURORA's Eulerian Dispersion Module (EDM). In the new version, advection is treated with a recently developed algorithm by Walcek (2000). While being positive definite, mass conserving, and highly accurate, the algorithm is very fast. The superior capability of this scheme to preserve sharp concentration gradients is demonstrated in Figure 2. Both panels show advection of the initial concentration profile (dashed line at the left) over approximately a hundred grid cells towards the right. The dots are corresponding to the algorithm's solution and the solid line to the analytical solution: the upper panel corresponds to Walcek's scheme, and the lower panel to Zalesak's scheme (1979), used in the old version of EDM.

The treatment of vertical turbulent diffusion equally underwent considerable changes. A semi-implicit diffusion scheme was implemented, yielding good performance at low computer cost. Comparisons with analytical solutions indicated a high level of accuracy. Particular care has been devoted to a transparent coding of the transport algorithms, in such a way as to allow straightforward coupling of advection and diffusion to other modules such as chemistry.

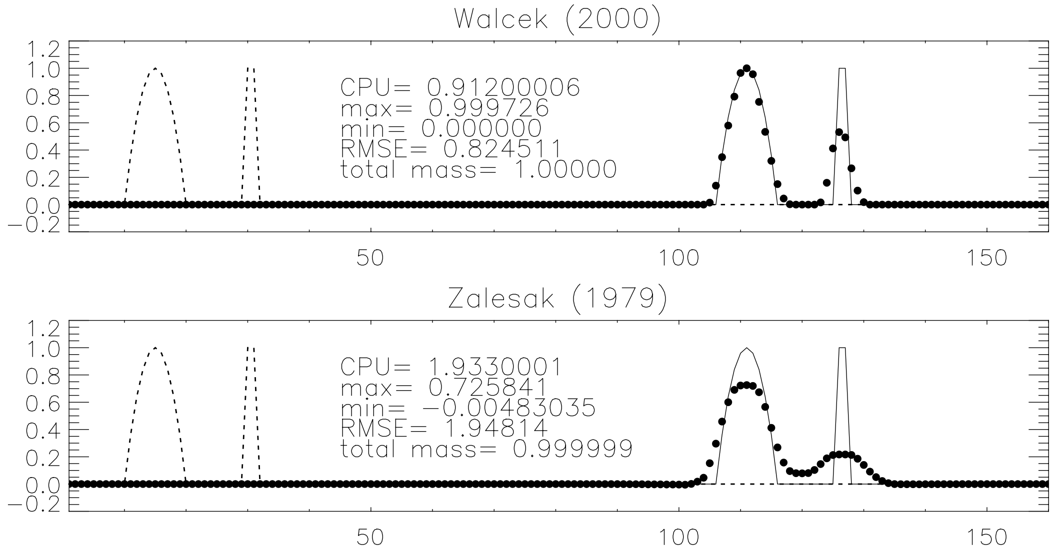

Figure 2 Comparison of the Walcek (upper) and Zalesak (lower) schemes with an analytical solution for advective transport.

4 Chemistry module

The chemical composition of the atmosphere is the result of the complex interaction of thousands of reactive (and less reactive) organic and inorganic species. In order to reduce the computing time for solving numerically the set of ordinary differential equations describing these interactions, the used chemical mechanisms are highly condensed, consisting of 100-200 reactions, and make use of molecular and/or structural lumping. Such a condensed chemical mechanism has been implemented in AURORA in order to simulate the chemical changes that occur over time within the urban atmospheric environment. The chemical module makes use of emissions and background concentrations of various atmospheric pollutants (NOx, VOC's, CO, …) and simulates the concentration of secondary pollutants such as ozone and PAN over time periods varying from a few minutes to several days.

The mechanism was implemented by means of CHEMC, a CHEMical Compiler. CHEMC has been tested and validated by means of a set of internationally accepted chemical reaction mechanisms such as RACM (Regional Atmospheric Chemistry Mechanism), EMEP (Co-operative programme for monitoring and evaluation of the long range transmission of air pollutants in Europe) and CB-IV (Carbon Bond IV). Several box tests were carried out (Derwent *et al.*, 1998). Figure 3 shows the results for the three mechanisms with respect to ozone. As the processing time is still substantial, attempts are made to develop a more compact chemical mechanism.

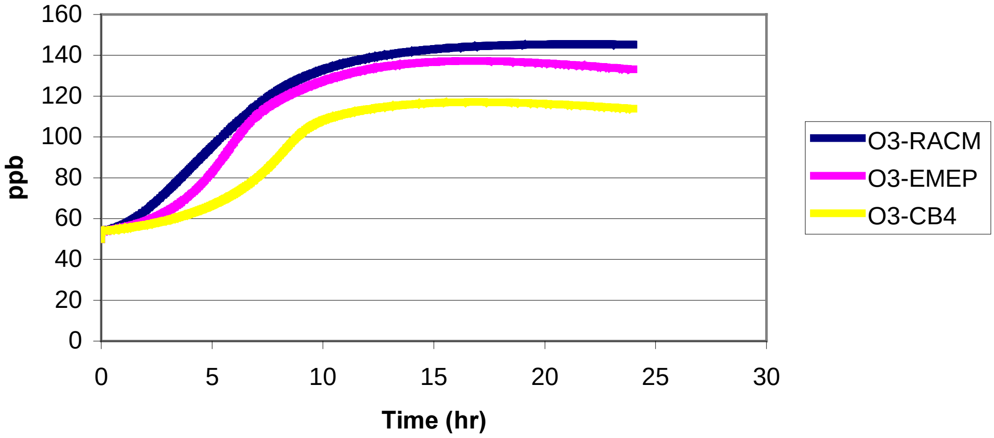

Figure 3 Comparison of ozone concentrations for three chemical reaction mechanisms RACM (upper), EMEP (middle) and CB-IV (lower) as implemented in CHEMC, using the same input data.

5 The street box model (street module)

The concentrations in the street are evaluated by a newly developed analytical model (Mensink and Lewyckyj, 2001). It assumes a uniform concentration distribution over the street and is therefore called « Street box » model, with the box dimensioned by the length and width of the street and the height of the surrounding built-up area. The concentration in the street is determined from a mass flux balance between a horizontal convective flux, a turbulent diffusive vertical flux and a continuous road transport emission source. In contrast with other models, like the Canyon Plume-Box Model (CPBM) developed by Yamartino and Wiegand (1986) and the Operational Street Pollution Model or OSPM model (Berkowicz, 1998), the "Street box" model does not necessarily assume re-circulation of the flow in the street canyon. It rather considers the turbulent intermittence in the shear flow shed from the upwind roof as the driving force. This concept is supported by measurements and observations made by Louka et al. (2000). The turbulent diffusive flux is described using the Prandtl-Taylor hypothesis. The result is a vertical exchange of the pollutant over a characteristic length, associated with a typical mixing length created by turbulent eddies shedding off at roof level, enhancing the exchange of mass and momentum:

$$C - C_b = \frac{Q}{U_{\equiv} \cdot \left(\frac{H}{L}\right) \cdot W + (D + \ell U_{\perp}) \cdot \left(\frac{W}{H}\right)} \qquad (2)$$

with C the calculated concentration in the street (µg m^{-3}), C_b the background concentration (µg m^{-3}). Q is the emission source strength per unit length (µg m^{-1} s^{-1}), H is the height (m), W the width (m) and L the length (m) of the street. In equation (2) the wind speed parallel to the street $U_{\equiv}$ (m s^{-2}) is responsible for the "ventilation" of the street box, whereas wind speed perpendicular to the street

$U_\perp$ (m s^{-2}) is responsible for the vertical exchange of the pollutant over a characteristic length ℓ. This characteristic length ℓ can be associated with a typical mixing length caused by turbulent eddies shedding off at roof level and is set to $\ell = 1$ m. D is the diffusion coefficient *at low wind speeds* (m^2 s^{-1}). Copalle (1999) showed that at low wind speeds this diffusion can play a role. He suggests a value of $D = 1.5$ m^2 s^{-1}.

6 Conclusions

For the assessment of air quality in cities, a modular integrated modelling system has been developed, known as AURORA (**A**ir quality modelling in **U**rban **R**egions using an **O**ptimal **R**esolution **A**pproach). This urban air quality management system has been designed for urban and regional policy support, using fast and advanced numerical techniques. Various modules in the system have been designed and refined, resulting in an air quality management tool that can provide reliable answers to policy makers and traffic planners. In order to minimise the computational burden, careful attention has been paid to the computational aspects of the AURORA model, in particular with respect to the advection-diffusion scheme and the chemistry module.

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