LINKING URBAN (STREET CANYON) MODELS WITH REGIONAL AIR QUALITY MODELS THROUGH URBAN BOUNDARY CONDITIONS

Clemens Mensink, Karen Van de Vel, Koen De Ridder, Peter Viaene and Stijn Janssen

Flemish Institute for Technological Research (VITO), Boeretang 200, B-2400 Mol, Belgium

Abstract: This contribution addresses the question of how detailed information from the urban canopy can be assimilated into regional models. This detailed information concerns, among others, road transport emissions, specific exchange and turbulence patterns in the built up canopy, and effects of roads and roughness elements on wind direction and wind speed. This information is typically obtained from detailed street canyon models in combination with traffic emission models. In order to integrate the dynamics of the urban canopy into regional air quality models, we propose the formulation of urban boundary conditions. The formulation has been tested and compared with measurements for benzene and NO_x in the city of Antwerp, Belgium.

Key words: Urban air quality, street canyons, NO_x , benzene, boundary conditions, emission and deposition fluxes

1. INTRODUCTION

In regional air quality models the exchange of pollutants between the surface and the atmosphere is generally represented by an emission source term and/or a deposition term. These terms are included in the governing equations. As a consequence, the emissions generated at the surface are instantaneously diffused into the grid cells. In this way the diffusion and many of the dynamics of the urban canopy are not represented in regional models, despite the fact that we nowadays have quite a lot of detailed information about these dynamics, e.g. on the canopy structure and roughness elements, on traffic emissions and on the street canyon dynamics (for an overview see e.g. Vardoulakis et al., 2003). In particular the emissions and concentrations due to road transport can be modelled hourly as a function of road type, vehicle type, fuel type, traffic volume, vehicle age, trip length distribution and actual ambient temperature. Furthermore it is becoming state of the art to obtain or verify this actual information by means of remote sending techniques.

We present a new approach in which we propose to replace the static emission (sources) and deposition (sinks) terms by a dynamic turbulent diffusive boundary flux describing the interactions between the urban canopy and the regional domain. The flux takes into account the streetwise road transport emissions, the road dimensions, the urban meteorology and atmospheric stability conditions as well as the turbulent intermittency in the urban canopy sub-layer. The turbulent diffusive flux is derived from the Prandtl-Taylor hypothesis and describes the vertical exchange of the pollutant over a characteristic length which can be associated with a typical mixing length, e.g. created by turbulent eddies shedding of at roof level. It can be implemented in the code by means of a Neumann type boundary condition.

The theoretical formulation of the methodology will be presented (section 2) and the methodology will be illustrated by model applications for benzene and NO_X in the city of Antwerp (section 3). Results are validated by means of measurements from an urban monitoring station in Borgerhout.

2. METHODOLOGY

The basic assumption in the concept to obtain a formulation for urban boundary conditions is a turbulent diffusive flux describing the interactions between the urban canopy and the regional model domain. This turbulent diffusive flux is derived from the Prandtl-Taylor hypothesis. The vertical exchange of mass and momentum takes place over a characteristic length which is associated with a typical mixing length, e.g. created by turbulent eddies shedding off at roof level. The street canyon(s) at which this exchange takes place is represented by a box or a number of boxes, dimensioned by the length and width of the street(s) and the height(s) of the built up area. Inside the box(es), only horizontal advection along the street(s) (x-direction) and vertical diffusion processes (z-direction) are considered, together with a continuous source term S. Net contributions of *horizontal* turbulent fluxes are neglected as well as diffusion in horizontal directions:

$$\frac{\partial \overline{c}}{\partial t} = -\frac{\partial}{\partial x} \left(\overline{v_x} \ \overline{c} \right) - \frac{\partial}{\partial z} \left(\overline{v_z} \ \overline{c'} \right) + D \frac{\partial^2 \overline{c}}{\partial z^2} + S$$
(1)

where the concentration c (µg m⁻³) has been replaced by a time-smoothed value c and a turbulent concentration fluctuation c', following the Reynolds decomposition concept. The same is applied to the velocity vector **v**. The first term on the right hand side in equation (1) represents the advective mass transport, the second term the mass transport due to turbulent fluctuations, and the third term the contribution due to diffusion at low wind speeds with coefficient D (m²s⁻¹). The vertical turbulent mass flux term in (1) is approximated by applying the eddy diffusivity concept in analogy to Fick's law (Bird et al., 1960):

$$\overline{v_z'c'} = -K\frac{\partial c}{\partial z} \tag{2}$$

For a turbulent free stream flow the eddy diffusivity $K (m^2 s^{-1})$ can be related to a characteristic length scale ℓ (m) and the free stream velocity gradient by applying the Prandtl-Taylor hypothesis (Hinze, 1987):

$$\overline{\mathbf{v}_{z}^{\prime} \mathbf{c}^{\prime}} = -\ell^{2} \left| \frac{\mathrm{d} \mathbf{U}}{\mathrm{d} z} \right| \frac{\partial \mathbf{c}}{\partial z}$$
(3)

The characteristic length ℓ is associated with a typical mixing length, e.g. created by turbulent eddies shedding off at roof level. The velocity gradient over this mixing length is assumed to be constant and equal to the free stream velocity U_{\perp} (ms⁻¹) above the roof tops in the direction of the eddy shedding, i.e. perpendicular to the street direction, divided by the mixing length ℓ . Thus, conform Prandtl's mixing length theory, the eddy diffusion becomes equal to the product of a mixing length ℓ and some suitable velocity, expressed here by U_{\perp} :

$$\mathsf{K} = \ell \; \boldsymbol{U} \tag{4}$$

Substitution of (2) and (4) in Equation 1 and reformulation of (1) in terms of a flux balance assuming steady state conditions, i.e. no change in meteorological input, emissions and concentrations during a model time step, leads to:

$$C - C_{b} = \frac{Q}{U_{\pm} \cdot \left(\frac{H}{L}\right) \cdot W + (D + \ell U_{\perp}) \cdot \left(\frac{W}{H}\right)}$$
(5)

Where Q is the emission source strength per unit length (μ gm⁻¹s⁻¹), C_b is the background concentration (μ g m⁻³), H is the height (m), W the width (m) and L the length (m) of the street(s). In Equation 5 the wind speed parallel to the street U_z is responsible for the ventilation of the street box, whereas the wind speed perpendicular to the street U_⊥ is responsible for the vertical exchange of the pollutant over a characteristic length ℓ . As mentioned this length scale can be associated with a typical mixing length caused by turbulent eddies shedding off at roof level. It can also be expressed in function of atmospheric stability, e.g. by means of the Monin Obhukov length. This is a topic for further investigation. For the moment the value has been tuned and set to $\ell = 1$ m. Model results are not very sensitive with respect to this parameter, as has been shown by Mensink and Lewyckyj (2001). D is the diffusion coefficient at low wind speeds. Copalle (2001) has shown that at low wind speeds there still is a certain amount of diffusion. He suggests a value of D = 1.5 m² s⁻¹.

The associated vertical turbulent diffusive flux describing the interactions between the urban canopy and the regional model domain can be expressed as:

$$G = -L \cdot W \cdot \left(D + \ell U_{\perp}\right) \frac{C_{\rm b} - C}{H} \tag{6}$$

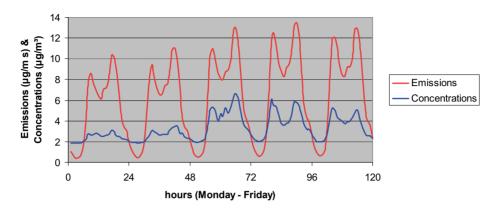
Note that this flux G can be implemented as a Neumann type boundary condition. Note also that the flux expressed by Equation 6 is bi-directional depending on the difference between the concentration C inside the canyon and the concentration C_b above the canyon, e.g. obtained from the associated grid cell in the regional model. It thus acts as an emission flux during daytime and possibly as a deposition flux during night time when traffic emission are low. Since in an urban context is difficult to describe a deposition flux in terms of the commonly used resistance analogy, expression (6) could be an alternative for defining a dry deposition flux in urban situations. Further details of the model formulation are given in a paper by Mensink et al. (2002).

3. RESULTS

Benzene and NO_X concentrations and fluxes have been calculated for the city of Antwerp for 4 periods of 5 days in 1998. For these periods diffusive sampler measurements were available from the MACBETH measurement campaign as carried out in 101 streets in Antwerp and at 4 regional background locations. The benzene measurement were used for an assessment of the whole urban canopy, whereas the NO_x concentrations and fluxes were calculated and measured for a single street canyon in Antwerp, i.e. the "Plantin en Moretuslei", where a regulatory monitoring station is located. Both benzene and NO_X concentrations were calculated on an hourly basis, from Monday to Friday for the following periods: 19–23 January 1998, 23–27 March 1998; 25–29 May 1998 and 28 September–2 October 1998. For 1963 road segments in Antwerp, benzene and NO_X emissions were calculated by a road transport emission model (Mensink et al., 2000). The concentrations and flux contributions were calculated using Equations 5 and 6 using the measured background concentrations obtained from the four background monitoring locations for benzene and from a background location outside Antwerp for NO_X . The hourly values for wind speed and wind direction were obtained from two meteorological towers located in the city. Wind speed at roof level was calculated from a wind profile described by a power law, with the exponent derived from the wind speeds measured at heights of 30 m and 153 m respectively.

Figure 1 shows the hourly benzene emissions and concentrations as averaged over the whole city domain (1963 road segments) for the first period. Due to relatively high average wind speeds on Monday (8.1 ms⁻¹) and Tuesday (6.2 ms⁻¹), the concentrations are somewhat lower (more ventilation in the streets) than on the other week days, i.e. Wednesday (2.5 ms⁻¹), Thursday (3.1 ms⁻¹) and Friday (3.6 ms⁻¹). Figure 2 shows a comparison of ensemble averages of measured benzene concentrations (101 locations in Antwerp) with ensemble averages of calculated concentrations in the streets of Antwerp (1963 road segments). The error bar shows the standard deviation for the 101 measurements. Figure 2 shows that for the ensemble average the benzene concentrations are well predicted. The

benzene background contributions for the city as a whole varies between 50% and 58% depending on the period considered.



Benzene emissions & concentrations in Antwerp (19-23 January 1998)

Figure 1. Calculated hourly benzene emissions and concentrations as averaged over the Antwerp domain for 19-23 January 1998.

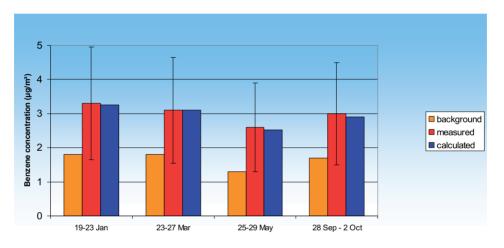
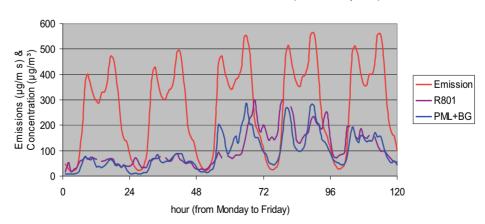


Figure 2. Comparison of ensemble averages of measured benzene concentrations (101 locations) and background concentrations (4 locations) with ensemble averages of calculated concentrations in the 1963 streets of Antwerp for the four measurement periods.



NOx emissions & concentrations in the PM-lei (19-23 January 1998)

Figure 3. Calculated hourly NO_x emissions and calculated and measured NO_x concentrations for a street canyon in the "Plantin en Moretuslei" (R801) in Antwerp for the period of 19–23 January 1998.

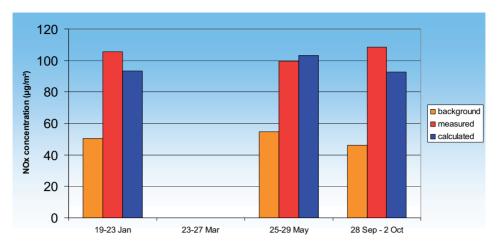


Figure 4. Comparison of the measured NO_X concentrations, measured background concentrations and calculated NO_X concentrations inside a street canyon in the "Plantin en Moretuslei" in Antwerp for three of the four measurement periods.

Figure 3 shows NO_x emissions and NO_x concentrations in the "Plantin en Moretuslei" as calculated and measured for the period in January. Calculated NO_x emissions and concentrations show the same pattern as for the benzene emissions and concentrations, presented in Figure 1. The computed concentration pattern with lower concentrations on Monday and Tuesday is in very good agreement with hourly observed values. Figure 4 shows the average NO_x concentrations as calculated and measured over the four periods (no measurements available for 23–27 March). The NO_x background contribution to the street canyon was found to be 48% for the period in January, 55% for the period in May and 48% for the autumn period.

4. CONCLUSIONS

We showed a formulation of a Neumann type boundary condition that can be used to calculate a turbulent diffusive boundary flux. It can replace the static source (emissions) & sink terms in the governing equations. This bidirectional flux can take into account some of the dynamics in the urban canopy (traffic, roughness elements, vertical exchange, wind, temperature). It allows a two way interaction between the urban canopy and the regional model domain.

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