Sensitivity of DAUMOD (urban diffusion model) calculated air pollutant concentration to internal boundary layer parameterisation, surface roughness length and atmospheric stability

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1 Introduction

The urban diffusion model DAUMOD is a simple model that estimates surface background air pollution concentrations in urban areas. It has been developed and reported over last decade (Mazzeo and Venegas, 1991; Venegas and Mazzeo, 1998; Venegas and Mazzeo, 2000). The earliest version of this model estimates mean annual concentrations using climatological data as input and assuming neutral atmospheric conditions. The most recent version, referred to as DAUMOD, uses routine meteorological data and runs hourly. Evaluation of model performance has been reported in several studies (Venegas and Mazzeo, 1998; 2000; 2001). In this paper we study model results sensitivity to: roughness length, atmospheric stability and internal boundary layer height estimations.

2 Brief description of DAUMOD

In the air pollution model for an urban area that we have introduced in former papers (Mazzeo and Venegas, 1991; Venegas and Mazzeo, 1998) steady state conditions are assumed, the x - axis is in the wind direction and the air pollution concentration [C(x,z)] satisfies the bidimensional equation of diffusion:

$$u(z)\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left[K(z)\frac{\partial C}{\partial z}\right] \quad (1)$$

where u is the wind speed, K is the vertical eddy diffusivity for pollutants and z is the vertical axis. Considering a ground level source emitting continuously with strength (Q), the boundary condition at z=0 can be expressed by:

$$K(z)\frac{\partial C}{\partial z} = -Q \quad (2)$$

and assuming h as the top of the plume, the upper boundary condition (z=h) is given by:

$$K(z)\frac{\partial C}{\partial z} = 0 \quad (3)$$

The model uses the following wind and vertical eddy diffusivity profiles for surface layer (Arya, 1999):

$$u(z) = \frac{u^*}{k}\left[\ln\left(\frac{z}{z_0}\right) + \psi\left(\frac{z}{L}\right)\right] \qquad \text{and} \qquad K(z) = \frac{k\,u^*\,z}{\phi\left(\frac{z}{L}\right)} \quad (4)$$

where u* is the friction velocity, z_0 is the surface roughness length, k is the von Karman's constant (k=0.41), L is the Monin-Obukhov length and (see Wieringa, 1980):

$$\psi\left(\frac{z}{L}\right) = \begin{cases} 6.9\,\frac{z}{L} & \frac{z}{L} > 0 \\ 1 - \phi^{-1}\left(\frac{z}{L}\right) & \frac{z}{L} < 0 \end{cases} \tag{5}$$

and

$$\phi\left(\frac{z}{L}\right) = \begin{cases} 1 + 6.9\,\frac{z}{L} & \frac{z}{L} > 0 \\ \left(1 - 22\,\frac{z}{L}\right)^{-1/4} & \frac{z}{L} < 0 \end{cases} \tag{6}$$

$\Psi(0) = 0$ and $\phi(0) = 1$.

In the development of DAUMOD, the vertical distribution of pollutants is expressed by a polynomial form:

$$C(x,z) = C(x,0)\sum_{i=0}^{6} A_i\left(\frac{z}{h}\right)^i \tag{7}$$

where the coefficients (A_i) depend on atmospheric stability conditions (Mazzeo and Venegas, 1991). Substituting (4) and (7) into (2) and integrating we obtained the following equation:

$$C(x,0) = \frac{Q}{|A_1|\,k\,u{*}\,z_0}\,h\left(\frac{z}{L}\right) \tag{8}$$

The height (h) of the upper boundary of plume is obtained integrating the continuity equation:

$$\int_0^x Q\,dx = \int_0^h u(z)\;C(x,z)\,dz \tag{9}$$

with C(x,z) given by (7). The form of h(x) can be fitted with great accuracy to potential functions:

$$\frac{h}{z_0} = a\left(\frac{x}{z_0}\right)^b \tag{10}$$

where a and b are parameters that depend on atmospheric stability (Mazzeo and Venegas, 1991). Substituting (10) into (8),

$$C(x,0) = \frac{a\;\;Q}{|A_1|\;k\;u{*}\,z_0}\left(\frac{x}{z_0}\right)^b \tag{11}$$

Assuming an horizontal distribution of area sources, each square grid with an emission strength Q_i (i= 0, 1, 2,...N), the surface air pollution concentration is estimated by:

$$C(x,0) = \frac{a\left[Q_0\;x^b + \sum_{i=1}^{N}\left(Q_i - Q_{i-1}\right)\left(x - x_i\right)^b\right]}{|A_i|\;k\;z_0^{\,b}\;u{*}} \tag{12}$$

Present version of DAUMOD includes empirical expressions for $a(z_0/L)$, $b(z_0/L)$ and $A_1(z_0/L)$ and runs using hourly meteorological data as input.

3 Results

One objective of a sensitivity study is to obtain a measure of the error in the predicted pollutant concentrations as a function test is measure the error in the estimated pollutant concentrations, as a function of the error in input variables. Furthermore, the analysis of model results sensitivity to different model assumptions or parameterisations is also of interest.

We evaluated the performance of the model using a Copenhagen (Denmark) two years data set kindly made available to us by Berkowicz. We used a typical diurnal variation of NOx emission data subdivided into a grid net with a resolution of 2km x 2km. Hourly meteorological data and measured concentrations were taken at an urban background station located on the roof of a building at the centre of the grid. In addition, regional background concentrations obtained at a rural site were also available.

3.1 DAUMOD calculated concentration sensitivity to z_0

We studied the sensitivity of model predictions to surface roughness length, estimating hourly NOx background concentration in Copenhagen for 1994-1995, assuming z_0 = 1m, 2m, 3m. Mean hourly values, mean daily values and mean monthly values obtained from DAUMOD estimations were compared with observations. Table 1 shows the output from the BOOT statistical analysis (Hanna et. al, 1991; Olesen, 1995) for all DAUMOD data, for the three averaged time values.

The results show that z_0= 3m gives the best agreement. It is not easy to parameterise urban terrain by one characteristic roughness length. The value of z_0= 3m may be at least twice larger than other found literature values but it is similar to the roughness length applied by the urban airshed model (UAM-IV) (Morris and Myers, 1990).

Table 1 Statistics for concentrations estimated assuming different roughness length: mean, standard deviation (sigma), bias, normalised mean square error (nmse), correlation coefficient (cor), fraction within a factor two (fa2), fractional bias (fb), fractional variance (fs).

a) Mean hourly values N= 48

	Mean	sigma	bias	nmse	cor	fa2	fb	fs
Obs.	16.70	4.62	---	---	---	---	---	---
Z_0=1 m	63.10	30.05	-46.41	2.70	0.837	0.188	-1.163	-1.467
Z_0=2 m	30.70	14.54	-14.00	0.63	0.787	0.542	-0.591	-1.036
Z_0=3 m	17.53	8.45	-0.84	0.13	0.691	0.958	-0.049	-0.587

b) Mean daily values N= 680

	Mean	sigma	bias	nmse	cor	fa2	fb	fs
Obs.	16.63	9.20	---	---	---	---	---	---
Z_0=1 m	62.70	30.52	-46.07	2.67	0.627	0.035	-1.162	-1.073
Z_0=2 m	30.50	14.48	-13.87	0.63	0.621	0.547	-0.589	-0.446
Z_0=3 m	17.42	8.19	-0.79	0.22	0.589	0.868	-0.047	0.116

c) Mean monthly values N= 24

	Mean	sigma	bias	nmse	cor	fa2	fb	fs
Obs.	16.49	3.55	---	---	---	---	---	---
Z_0=1 m	62.51	12.70	-46.02	2.14	0.916	0.000	-1.165	-1.127
Z_0=2 m	30.42	6.71	-13.93	0.41	0.917	0.750	-0.594	-0.616
Z_0=3 m	17.38	4.44	-0.89	0.02	0.885	1.000	-0.053	-0.223

3.2 DAUMOD calculated concentration sensitivity to atmospheric stability

Last version of DAUMOD takes into account the hourly atmospheric stability condition in the estimation of u* from wind profile and also includes algorithms to estimate coefficients a, b and A_1 in function of the Monin-Obukhov length. We estimated the NOx background concentrations applying the actual DAUMOD version and also considering neutral conditions at every hour, assuming z_0 = 3m. Statistical parameters of the evaluation of model performances are included in Table 2.

These results indicate that the inclusion of atmospheric stability condition improves model predictions even for large averaged time concentrations.

Table 2 Statistics for concentration estimations considering neutral conditions (NEUTRAL), actual DAUMOD version and the modified version (Garratt): mean, standard deviation (sigma), bias, normalised mean square error (nmse), correlation coefficient (cor), fraction within a factor two (fa2), fractional bias (fb), fractional variance (fs).

a) Mean hourly values	N= 48							
	Mean	sigma	bias	nmse	cor	fa2	fb	fs
Obs.	16.70	4.62	---	---	---	---	---	---
NEUTRAL	31.30	17.50	-14.60	0.75	0.919	0.542	-0.609	-1.165
DAUMOD	17.53	8.45	-0.84	0.13	0.691	0.958	-0.049	-0.587
Garratt	54.39	41.64	-37.69	3.46	0.084	0.333	-1.060	-1.601
b) Mean daily values	N= 680							
	Mean	sigma	bias	nmse	cor	fa2	Fb	fs
Obs.	16.63	9.20	---	---	---	---	---	---
NEUTRAL	31.11	15.27	-14.49	0.69	0.599	0.540	-0.607	-0.496
DAUMOD	17.42	8.19	-0.79	0.22	0.589	0.868	-0.047	0.116
Garratt	54.01	41.02	-37.38	3.04	0.571	0.226	-1.058	-1.267
c) Mean monthly values	N= 24							
	Mean	sigma	bias	nmse	cor	fa2	fb	fs
Obs.	16.49	3.55	---	---	---	---	---	---
NEUTRAL	31.01	5.01	-14.52	0.44	0.702	0.583	-0.611	-0.341
DAUMOD	17.38	4.44	-0.89	0.02	0.885	1.000	-0.053	-0.223
Garratt	53.69	25.53	-37.20	2.14	0.862	0.083	-1.060	-1.512

3.3 DAUMOD calculated concentration sensitivity to internal boundary layer parameterisation

The DAUMOD parameterisation of internal boundary layer is given by eq.(10). However, according to Garratt (1992) for practical application it can be assumed that $h \propto x^{1/2}$ under thermal stratification effects and $(h/z_0) = 0.38\ (x/z_0)^{0.80}$ in neutral condition. Assuming z_0 = 3m, we estimated NOx background concentrations for Copenhagen using last version of DAUMOD and a modified version which includes the potential forms of h suggested by Garratt (1992). Table 2 also includes the statistical parameters concerning the modified version (Garratt). Model estimations do not improve by including the alternative parameterisations of h considered in this analysis. At present, model performance is better considering the fitted forms of h given by eq.(10).

4 Conclusions

DAUMOD results are sensitive to the roughness length input value. The best agreement with Copenhagen data set is obtained for z_0 = 3 m. The model estimations of mean concentration values improve if hourly atmospheric stability conditions are taken into account. DAUMOD estimations including the potential variation of the internal boundary layer height with distance derived from the equation of mass continuity show better agreement than when considering other well known potential forms of h(x).

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References

Arya, S.P. ,(1999), '*Air Pollution Meteorology and Dispersion'*, Oxford University Press, pp.310.

Garratt, J.R., (1992), '*The Atmospheric Boundary Layer'*, Cambridge University Press, pp.316.

Hanna, S., Strimaitis, D., Chang, J.,(1991),'*Hazard Response Modelling Uncertainty (A Quantitative Method)*, Vol. I: User's Guide for Software for Evaluating Hazardous Gas Dispersion Models', Sigma Research Corp., pp. 71.

Mazzeo, N.A., Venegas, L.E., (1991), 'Air Pollution model for an Urban Area', *Atmos. Research*, Vol.26, 165-179.

Morris, R.E., Myers, T.C., (1990), *User's Guide to the Urban Airshed Model*, Vol.I-V, Environmental Protection Agency.

Olesen, H.R., (1995), 'The Model Validation Exercise at Mol: overview of results', *Int. J. Environment and Pollution*, Vol.5, 4-6, 761-784.

Venegas, L.E, Mazzeo, N.A. (1998) 'Urban Diffusion-Deposition Air Pollution Model', *Proc. 11th World Clean Congress*, Vol.2, 6E-4.

Venegas, L.E, Mazzeo, N.A., (2000), 'Estimación de la concentración de fondo y del depósito de contaminantes en áreas urbanas', *XI Congresso Brasileiro de Meteorologia*, CDROM, QA00006. (in Spanish)

Venegas, L.E, Mazzeo, N.A., (2001), 'An Evaluation of DAUMOD Model in Estimating Urban Background Concentration', *Third Int. Conference on Urban Air Quality*, Loutraki, Greece.

Wieringa, J.,(1980), 'A revaluation of the Kansas mast influence on measurements of stress and cup anemometer overspeeding', *Boundary-Layer Meteorol.*, Vol. 18, 411-430.