QUANTIFICATION OF UNCERTAINTIES ASSOCIATED WITH AN INTEGRATED GAUSSIAN LINE SOURCE MODEL USING ENSEMBLES

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INTRODUCTION

Atmospheric dispersion models will always be uncertain due to the inevitable uncertainties associated with input data and physical formulations. This paper deals with calculations of uncertainty in association with a newly developed dispersion model for open roads called WORM (Weak Wind Open Road Model).

THE WORM MODEL

The WORM model is an integrated Gaussian puff/plume model for calculation of hourly average concentrations from open roads and highways in a set of arbitrary receptor points.

The model consists of the following system components:

- An emission pre-processor
- A pre-processor for meteorological data
- A background concentration pre-processor
- An integrated Gaussian puff/plume dispersion model

The emission pre-processor generates hourly emission data (Q in g/ms) for each lane of the roadway based on traffic data (*AirQUIS*, 2005). The background concentration pre-processor generates hourly background concentrations for the road, based on using nearby (upwind) background stations, or urban/regional scale models (*AirQUIS*, 2005). Background concentrations are added to the WORM model concentrations to make them comparable with local (roadside) air quality observations.

A meteorological pre-processor calculates several meteorological parameters including:

- Friction velocity (u_*), temperature scale (θ_*) and Monin-Obukhov length scale (L)
- Horizontal and vertical diffusivities (σ_u, σ_v, σ_w)
- Mixing height (H_{mix})

based on Monin-Obukhov similarity theory, and hourly data for local wind speed and stability (vertical temperature gradient) (*AirQUIS*, 2005; *Walker, S.E. and J. Berger*, 2007). For the cuurent version of the WORM model, a minimum value of horizontal plume diffusivity (σ_u and σ_v) equal to 0.5 m/s is used.

The concentration in a receptor point r = (x_r, y_r, z_r) is calculated by:

$$C_r = \int_{s=0}^{S}\int_{t=0}^{T} \frac{Q}{(2\pi)^{3/2}\cdot\sigma_x(t)\cdot\sigma_y(t)\cdot\sigma_z(t)} \cdot \exp\left(-\frac{(x_r(s) - U_{eff}\cdot t)^2}{2\sigma_x^2(t)}\right)\cdot\exp\left(-\frac{y_r^2(s)}{2\sigma_y^2(t)}\right)\cdot \left\{\exp\left(-\frac{(z_r - H_{eff})^2}{2\sigma_z^2(t)}\right) + \exp\left(-\frac{(z_r + H_{eff})^2}{2\sigma_z^2(t)}\right)\right\} \mathrm{dsdt} \quad (1)$$

where Q is the emission intensity (g/ms), U_{eff} is the plume effective wind speed (m/s), H_{eff} is the plume effective height above ground (m), and where the coordinates of the receptor point and dispersion parameters in the integrand generally depends on the position s on the road, and time t since release. The integral is calculated numerically by using a highly accurate Gaussian quadrature routine.

Growth of dispersion parameters $\sigma_x = \sigma_y$ and σ_z are calculated based on atmospheric background turbulence (*AirQUIS*, 2005; *Walker, S.E. and J. Berger*, 2007), with initial sizes of puffs or plumes, $\sigma_{x0} = \sigma_{y0}$ and σ_{z0}, calculated by the same semi-empirical equation for traffic-originated turbulence as used in the CAR-FMI model (*Härkönen, J. et al.*, 1996). A comprehensive evaluation of the WORM model is given in *Berger, J. et al.* (2007).

QUANTIFICATION OF UNCERTAINTIES

The model value C_r is uncertain due to inevitable uncertainties associated with the model variables $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_n)$, and with the model formulation itself. These can generally be described using Bayesian statistics (*Box, G.E.P. and G.C. Tiao*, 1992). If $\boldsymbol{\theta}^t = (\theta_1, \theta_2, \ldots, \theta_n)$ denotes the correct (best input or true) values of the model variables for the current hour, and T_r denotes the correct or true concentration in receptor point r, we may write

$$T_r = C_r(\theta^t) + \varepsilon_r = C_r(\theta_1^t, \theta_2^t, ..., \theta_n^t) + \varepsilon_r \quad (2)$$

where ε_r denotes the model formulation error, i.e., the error induced by the model equations themselves, and not due to errors in the model data. If we are willing, and able, to put Bayesian subjective (prior) probabilities on all the model variables θ_i, for i = 1,…,n, and on model formulation errors ε_r, we obtain a Bayesian subjective (prior) probability distribution function (pdf) $\pi_r(T)$ associated with the true concentration T_r.

Generating $\pi_r(T)$ in the form of an explicit function, is a difficult task. Instead an approximation is sought based on using a discrete set of points, or ensemble, $\{T^{(1)}, T^{(2)}, \ldots, T^{(N)}\}$, produced by simulating from $\pi_r(T)$, i.e., to draw values from it, where N denotes the number of ensemble members (or ensemble size).

A simple way to describe $\pi_r(T)$, and to make random draws from it, is to define $\pi_r(T)$ using a series of conditional pdfs associated with the model variables θ_i and formulation errors ε. This can be done recursively, viewing the model variables and calculations as a directed acyclic graph, as depicted in Fig. 1, showing a conceived fragment of the model, where a model variable θ_k is calculated based on other model variables θ_1, θ_2, …, θ_j, indexed here from 1 to j for simplicity of notation.

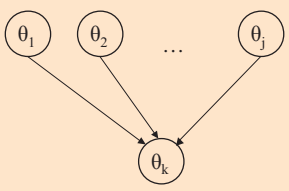

Fig. 1. Model calculation fragment (part of a directed acyclic graph).

The conditional pdf $\pi_k(\theta_k \mid \theta_1, \theta_2, \ldots, \theta_j)$ can then be defined recursively as follows. Assuming that the joint unconditional pdf $\pi_{1,j}(\theta_1, \theta_2, \ldots, \theta_j)$ is already defined in the acyclic directed graph for the variables $\theta_1, \theta_2, \ldots, \theta_j$, and that a pdf is locally defined for the local model formulation error ε_k, the conditional pdf for $\theta_k = \theta_k(\theta_1, \theta_2, \ldots, \theta_j) + \varepsilon_k$ is uniquely defined. The argument is repeated until a (conditional) pdf has been defined for all model variables in the graph, and subsequently for the last model variable calculated, the model output concentration.

The graph oriented recursive definition of the prior pdf $\pi_r(T)$ enables us also to easily draw samples from it. If we assume that we already have obtained a sample $(\theta_1, \theta_2, \ldots, \theta_j)$ from $\pi_{1,j}(\theta_1, \theta_2, \ldots, \theta_j)$, we may draw a sample of θ_k from $\pi_k(\theta_k \mid \theta_1, \theta_2, \ldots, \theta_j)$ by drawing a sample ε_k from the distribution of the local model formulation error, and adding this to the function value $\theta_k = \theta_k(\theta_1, \theta_2, \ldots, \theta_j)$. We then continue this process of calculating samples of model variables until we obtain a sample of the model output concentration $T^{(i)}$. By repeating the procedure N times we obtain our desired ensemble of N model concentrations, representing a set of N independent and identical (exact) samples from the prior pdf $\pi_r(T)$.

It is important to use available air quality observations to calibrate and adjust the prior pdf $\pi_r(T)$ to make sure that calculated p% confidence intervals contains observed concentrations about p% of the time.

RESULTS

Fig. 2 shows the result of running the WORM model for NO_x, using data from an 850 m long 4-lane roadway at Nordbysletta, close to Oslo, Norway (*Walker, S.E. and J. Berger*, 2007).

The graph contains hourly average observed concentrations (blue line), for a station situated 17 m from the roadway at a height of 3.5 m above the ground, together with model calculated concentrations for the same receptor point, in the form of an ensemble mean (red line), together with a 90% confidence interval (green lines). The period covered is 3 February – 10 February 2002, but only hours with wind direction towards the station are included. The number of ensemble members used is N = 1000.

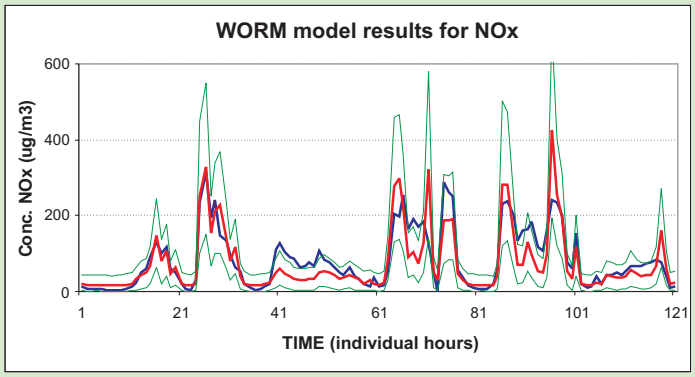

Fig. 2 WORM model results for NO_x

Individual ensemble members are created by drawing the following model variables: U_{10m} (wind speed at 10 m), u_*, θ_*, L, $\theta_v = \tan^{-1}(\sigma_v/u))$, $\theta_w = \tan^{-1}(\sigma_w/u))$, and initial size of plume σ_{y0} ($\sigma_{z0} = \sigma_{y0}/2$) using Gaussian pdfs around each nominal or model calculated (derived) value, with standard deviations set to 10% of respective mean values, except for U_{10m}, which is locally observed, and where the standard deviation has been set to 0.15 m/s. The standard deviation of model formulation error has been set to $\sqrt{20^2 + 0.3^2 \cdot C_r^2}$, where C_r is the corresponding model calculated concentration. Using this uncertainty model, 90% confidence intervals have been calculated using the ensembles (green lines in Fig. 2), and empirically here they contain the observed concentrations (blue line in Fig. 2) in about 85% of the hours.

SUMMARY AND CONCLUSION

A new integrated Gaussian line source model for open roads (WORM) is presented, which produces its output not as single concentration values, but rather as ensembles of values based on quantification of uncertainties associated with the model. Mean values and p% confidence intervals for the true concentrations can then be calculated based on the ensembles. Some preliminary, but encouraging, results using data from a 4-lane roadway at Nordbysletta, close to Oslo, Norway is presented.

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