Diagnostic evaluation of two atmospheric dispersion models against a roadside dataset

A contribution to subproject SATURN

Jaakko Kukkonen[1], Dietmar Öttl[2], Raimund Alfons Almbauer[2], Peter Johann Sturm[2],
Mia Pohjola[1] and Jari Härkönen[1]

[1]Finnish Meteorological Institute, Air Quality Research, Helsinki, Finland, Jaakko.Kukkonen@fmi.fi
[2]Institute for Internal Combustion Engines and Thermodynamics, Graz University of Technology, Graz, Austria

Summary

This study utilizes the results of a previous measurement campaign near a major road at Elimäki in southern Finland in 1995 that was specifically designed for model evaluation purposes. Numerical simulations were performed with a Gaussian finite line source dispersion model CAR-FMI and a Lagrangian dispersion model GRAL, and model predictions were compared with the field measurements. We analyzed especially the difference between the model predictions and measured data in terms of the wind speed and direction. The performance of the CAR-FMI model deteriorated as the wind direction approached a direction parallel to the road, and for the lowest wind speeds. However, the performance of the GRAL model varied less with wind speed and direction; the model simulated better the cases of low wind speed and those with the wind nearly parallel to the road.

Introduction

In some European countries, national air quality guidelines give recommendations on specific dispersion models, or types of dispersion models, which should be used in environmental impact assessments. It is therefore useful to compare the performance of various categories of dispersion models against field data.

For a more detailed description of this study, the reader is referred to Öttl et al. (2001) and Kukkonen et al. (2001).

Objectives

The objective of this study is to compare the predictions of two dispersion models with an experimental dataset. Such a comparison yields information on the reliability and the limits of validity of these models. Simulations were performed with a Gaussian finite line source model (CAR-FMI, Contaminants in the Air from a Road - Finnish Meteorological Institute) and a Lagrangian dispersion model (GRAL, Graz Lagrange Model).

Activities

A description of the roadside data set utilised in this study has been published by Kukkonen et al. (2001). The road itself is a straight line for a distance of more than a kilometre in both directions from the measurement site and its orientation is 30° east of north. The surroundings are characterized by flat terrain; the roughness length was estimated to be about $z_0 = 0.20\,\mathrm{m}$.

The data set comprises electronically-performed traffic counts, measured and pre-processed meteorological data and the concentrations for NO_x, NO_2 and O_3 at three locations and at various heights. As the monitoring stations were located on both sides of the road, background concentrations could be determined for all wind directions. Traffic volumes were automatically classified as heavy-duty and light-duty traffic, for both driving directions.

We have utilized the on-site measurements of wind speed and direction, temperature and solar radiation. However, the atmospheric stability parameters and mixing height were evaluated using a meteorological pre-processing model MPP-FMI (Karppinen et al., 1997). We applied emission factors of NO_x that are functions of the vehicle driving speed, and correspond to a vehicle speed of 100 km/h.

The CAR-FMI model includes an emission model, a dispersion model and statistical analysis of the computed time series of concentrations (Härkönen et al., 1995 and 1996; Karppinen et al., 2000a and 2000b). The dispersion equation is based on an analytic solution of the Gaussian diffusion equation for a finite line source.

For a detailed description of the Lagrangian dispersion model GRAL, the reader is referred to Oettl et al. (2000). The vertical dispersion was treated according to Franzese et al. (1999). The algorithm is based on the following equations, which satisfy the well-mixed criterion (Thomson, 1987) in stationary and horizontally homogeneous turbulence:

$$w'(t+\Delta t_v) = w'(t) + a(w',z)\cdot\Delta t_v + [C_0\cdot\boldsymbol{e}(z)]^{1/2}\cdot\Delta W, \qquad (1)$$

$$z(t+\Delta t_v) = z(t) + w'(t+\Delta t_v)\cdot\Delta t_v, \qquad (2)$$

where w' is the vertical velocity of a particle, C_0 is a universal constant set at a value of 2.1, $\boldsymbol{e}(z)$ is the ensemble-average rate of dissipation of turbulent kinetic energy, ΔW are the increments of a Wiener process with zero mean and variance Δt_v, and Δt_v is the time-step. The deterministic acceleration term $a(w',z)$ is assumed to be a quadratic function of the vertical velocity.

Results

We utilised the original models (CAR-FMI and GRAL) without any modifications. For comparison purposes, a number of statistical measures were computed, including fractional bias (*FB)*, normalized mean-square error (*NMSE*), correlation coefficient (*COR*), index of agreement (*IA*) and the factor of two (*F2*). These have been defined in, e.g., Willmott (1981) or Kukkonen et al. (2001).

The statistical measures indicate the good overall performance of both models. This is also an indication of the good quality of the observed data. A perfect agreement between measured and predicted values would result in an IA value of 1.0. In all data, the IA values range from 0.76 to 0.87 and from 0.81 to 1.00 for the CAR-FMI and GRAL models, respectively. All of these values correspond to fairly good or good agreement between predicted and measured values. The CAR-FMI model tends to slightly overestimate the NO_x concentrations, averaged over all data, FB = + 14 %, while the GRAL model has a tendency to underestimate, averaged over all data, FB = - 16 %.

A diagnostic evaluation of the measured and predicted concentrations in terms of meteorological parameters was also performed, focusing on the influence of wind speed and direction. The analysis was carried out for the measurements at a distance of 34 m from the road, as this station included the most comprehensive dataset.

Figure 1 shows the dependency of the ratio of predicted and observed concentrations on wind speed and direction for the CAR-FMI (top) and GRAL (bottom) models. The figure shows data gathered in one specific wind direction quadrant, extending from a wind direction perpendicular to the road (air flow from a direction of 120°) to a wind direction parallel with the road (air flow from a direction of 210°). For simplicity, wind direction has been normalised, with a direction of 0° corresponding to the direction parallel to the road and 90° to that perpendicular to the road.

Both models underestimate concentrations in the regime of higher wind speeds and non-parallel wind directions; this underprediction is more pronounced for the GRAL model. The CAR-FMI model overestimates concentrations in low wind speed conditions, regardless of the wind direction, and in near-to-parallel wind conditions. This overprediction cannot therefore be entirely caused by the assumption of steady-state, homogeneous wind flow (for a perpendicular-to-road wind, this has only a minor influence). Both of these trends accumulate to produce relatively high inaccuracies in a regime with a lower wind speed and a nearly parallel wind direction. The performance of the GRAL model varies less in terms of the wind speed and direction; the model better simulates cases with low wind speed and wind direction the nearly parallel to the road, as compared with the CAR-FMI model.

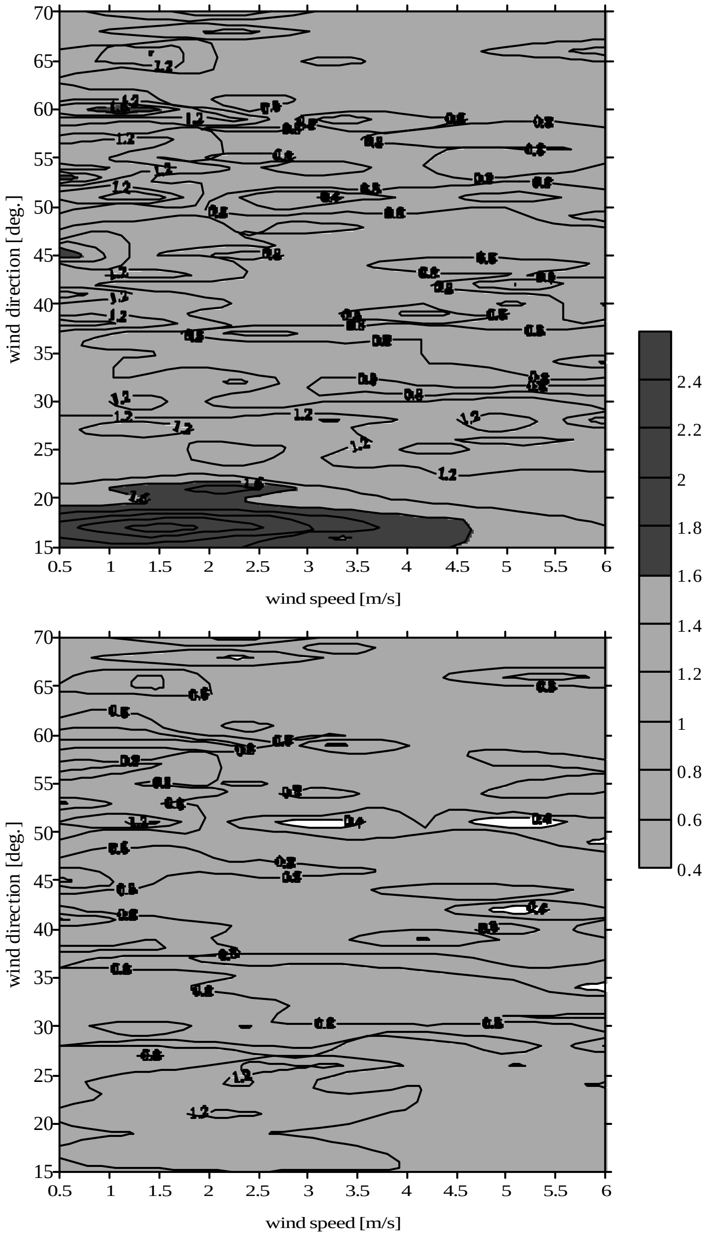

Figure 1. The dependency of the ratio of predicted and observed concentrations on wind speed and direction for the CAR-FMI (top) and GRAL (bottom) models for the measurement site at Elimäki, at a distance of 34 m from the road. Data from all measurement heights were used.

Conclusions

In comparison with corresponding results presented previously in the literature, the agreement between measured and predicted datasets, as indicated by various statistical parameters, was good for both models considered. For instance, considering all data, the IA values varied from 0.76 to 0.87 and from 0.81 to 1.00 for the CAR-FMI and GRAL models, respectively (N = 587).

The difference between model predictions and measured data were also analyzed in terms of the wind speed and direction. In cases of low wind speeds and for wind directions nearly parallel to the road, the Gaussian line source model overestimates concentrations, while for the Lagrangian dispersion model considered, there is almost no systematic bias. In parallel wind conditions, Gaussian line source models are much more sensitive to the assumption of steady-state, homogeneous wind flow (e.g., Benson, 1992). These differences are largest at low wind speeds or in calm situations, as then wind meandering is most pronounced and also most difficult to measure reliably (e.g., Kukkonen et al., 2001).

In parallel-to-the-road wind conditions, the background concentration measurements could also be influenced by traffic-originated pollution from the road. The modelling of Gaussian line source models could be improved in the case of low wind speed and parallel wind conditions, by utilizing meteorological results concerning the variation of wind direction in terms of wind speed and other relevant meteorological parameters.

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References

Benson P. (1992): A review of the development and application of the CALINE3 and 4 models. *Atmos. Environ.*, **26B:3**, 379-390.

Franzese P., A. K. Luhar, and M. S. Borgas (1999): An efficient Lagrangian stochastic model of vertical dispersion in the convective boundary layer. *Atmos. Environ.*, **33**, 2337-2345.

Härkönen J., E. Valkonen, J. Kukkonen, E. Rantakrans, L. Jalkanen, and K. Lahtinen (1995): An operational dispersion model for predicting pollution from a road. *Int. J. Env. Poll.*, **5**, Nos. 4-6, 602 - 610.

Härkönen J., E. Valkonen, J. Kukkonen, E. Rantakrans, K. Lahtinen, A. Karppinen, and L. Jalkanen (1996): A model for the dispersion of pollution from a road network. *Finnish Meteorological Institute, Publications on Air Quality* **23**, Helsinki.

Karppinen A, J. Kukkonen, T. Elolähde, M. Konttinen, T. Koskentalo and E. Rantakrans (2000a): A modelling system for predicting urban air pollution, Model description and applications in the Helsinki metropolitan area. *Atmos. Environ.* **34**, pp 3723-3733.

Karppinen A, J. Kukkonen, T. Elolähde, M. Konttinen and T. Koskentalo (2000b): A modelling system for predicting urban air pollution, Comparison of model predictions with the data of an urban measurement network. *Atmos. Environ.* **34**, pp 3735-3743.

Karppinen A., S. Joffre, and P. Vaajama (1997): Boundary layer parameterization for Finnish regulatory dispersion models. *Int. J. of Env. Poll.* Vol. 8, **3-6**, 557-564.

Kukkonen, Jaakko, Jari Härkönen, Jari Walden, Ari Karppinen and Kaisa Lusa, 2001. Evaluation of the dispersion model CAR-FMI against data from a measurement campaign near a major road. *Atmos. Environ.* **35-5**, pp. 949-960.

Thomson, D. J., 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech.*, **180**, 529-556.

Willmott C., Ackleson S., Davis R., Feddema J., Klink K., Legates D., O’Donnell J. and Rowe C., 1985. Statistics for the evaluation and comparison of models. *Journal of Geophysical Research*, **90**, C5, 8995-9005.

Öttl D., R. A. Almbauer, and P. J. Sturm, 2000. A new method to estimate diffusion in low wind, stable conditions. *J. Appl. Met.* (in print).

Öttl, D., J. Kukkonen, R.A. Almbauer, P.J. Sturm, M. Pohjola and J. Härkönen, 2001. Evaluation of a Gaussian and a Lagrangian model against a roadside dataset, with focus on low wind speed conditions. *Atmos. Environ.* **35**, pp. 2123-2132.