Application of a methodology to validate atmospheric dispersion models

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keywords: validation tool, dispersion model, nuclear emergency, Kincaid

1 Introduction

A wide variety of atmospheric dispersion models is presently available and applied for regulatory purposes in various countries. The models are used for short and/or long range dispersion of chemicals, aerosols and/or radionuclides. Due to the high variability of relevant atmospheric conditions the real time calculations of spatial and temporal distributions of short-range and long-range dispersion are rather complicated. Real time prediction of ordinary emission and dispersion situation is distorted by for instance the inadequacy of applied dispersion algorithms and limitations in the available meteorological information.

In order to validate and intercompare these dispersion models it is necessary to have a model validation tool. A model validation tool can be used to assess the agreement between predicted and observed air concentrations (and/or the deposition), and to intercompare various models. Olesen[1, 2] developed his Model Validation Kit (MVK) which validates real time atmospheric models using frequency distributions and maximum arcwise concentrations. In the software package several statistical parameters are incorporated. An other approach is followed by Irwin[3] who introduced crosswind-integrated concentrations in his ASTM90 methodology.

At the 6th conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes several comments and suggestions were made by various researchers regarding the MVK of Olesen as well as the ASTM90 methodology of Irwin.
In an attempt to overcome several drawbacks a different methodology, which validates multiple aspects of the air dispersion modelling including an evaluation of the spatial distribution, has been developed[4]. Using this evaluation tool it is possible to rank models and to pinpoint some crucial flaws of the modelling results. Furthermore, using the methodology, it is possible to evaluate the consistency of an observed data set.

The validation methodology, which is based on ten statistical indices, is shortly described and is applied to the models TADMOD and TSTEP[4].

2 Methodology

By pairing observations and predictions per receptor point and time interval one creates often an apparent random scatter plot, due to the inherent problems of deterministic air dispersion modelling. Validation of air dispersion models with experimental data sets is therefore rather difficult. In a previous paper[4] an extended model validation method, which evaluates multiple aspects of air dispersion modelling, is described in detail. In addition to the statistical indices some non-statistical parameters such as the differences in the direction and distances of the centres of mass of the predicted and observed puffs are introduced in order to understand some basic dispersion modelling properties.
The ten statistical parameters of the validation method are in fact taken from ETEX[5] and the method is completed with non-statistical spatial information. The formulae of the statistical parameters are

given in Appendix 1. An overall ranking parameter is calculated using the ten statistical parameters each of which are scaled from 0 to 100 points (0 – high quality, 100 – poor quality).
The model validation tool is dedicated for use with daily-integrated concentrations, which are related to relevant quantities in the radiation protection community. It also smoothes the turbulent effects on shorter time scales. Nevertheless, the tool can also be applied to hourly values.
In order to assess the statistical and non-statistical data a) the Kincaid data are integrated per day per receptor point, b) the model output is integrated per day and interpolated to the Kincaid receptor points. The non-statistical parameters are the observed and predicted distance of the centre of mass and the angle between the two (error-angle).
By evaluating the modelled data with respect to an observed data set using the model validation tool, it is possible to characterise a) the prediction of maximum values, b) the spatial distribution of the concentration, c) sensitivity of a model with respect to its input, d) model performance with respect to other models.

3 Results and discussion

The air dispersion models TADMOD and TSTEP are evaluated using the model validation tool. These two models and the behaviour of several parameters are described in a previous paper[4]. In this paper the influence of the input variable, the wind direction at 100 m, on the ranking is shown; in this respect it is a quick sensitivity study.
The results of the ranking parameter for TADMOD and TSTEP are shown in Figure 1. From the figure it can be concluded that TADMOD is performing better with respect to the Kincaid data set (Appendix 2). Averaged over 19 days the ranking parameter for TADMOD is some 20 points lower (= better) than for TSTEP. An other point to be noted is the behaviour of the ranking parameter of TADMOD on day numbers 8, 11 and 15: high value, opposed to day numbers 3, 14 and 19: low value. In the previous paper it was concluded that the wind direction for day number 11 as delivered with the Kincaid data set within the MVK should be re-evaluated. One indication was given by the error-angle, giving the angle between the predicted and observed centre of mass, which could be underpinned by a Geographical Information System (GIS). Therefore, it was interesting to study the effects of varying the wind direction at 100 m on the resulting ranking parameter.
In order to establish an ‘ideal’ situation the wind direction at 100 m for each hour was corrected for the calculated error-angle. It must be mentioned that the error-angle is determined by the projection of the predicted and observed centres of mass on the Kincaid receptor points. It is possible that the predicted centre of mass as calculated on the model grid is not on the Kincaid grid. As a result, it is

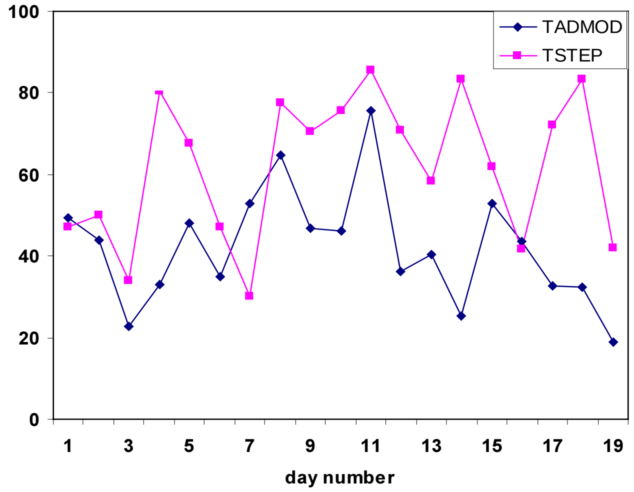

Fig. 1 Ranking for day sums for TADMOD and TSTEP

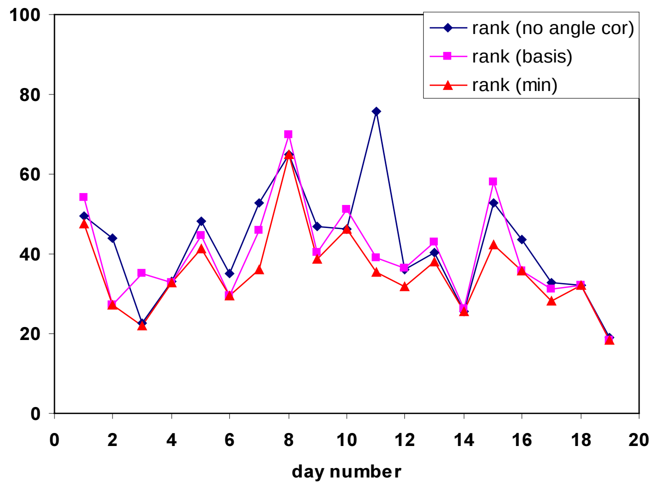

Fig. 2 Ranking for day sums for TADMOD, using no angle corrections, ‘ideal’= basis situation, minimum ranking (all angles).

possible that the calculated error-angle is smaller than the ‘real angle’. The ‘ideal’ situation is evaluated with the model validation tool, as well as situations where the input wind direction is altered from -20^o to +20^o (step 10^o) with respect to the ‘ideal’ situation. In Figure 2 the ranking values are shown for the original wind directions, the ‘ideal’ situation and the minimum ranking values of all six situations. From this figure it is clear that the ranking parameter for day number 11 can considerably be improved (40 points) by changing the wind direction. For day numbers 2, 7 and 15 this was also the case, although less pronounced. On the other hand, the ranking parameter for day number 8 can not be improved and remains at a high value (65 points). Projecting the observed concentrations with GIS it turned out that high concentrations are found at many isolated receptor points, which probably can not be simulated by any model.

4 Conclusions

Air dispersion models can be ranked using the extended validation methodology. The validation tool is primarily based on the statistical parameters, which evaluate the spatial distribution of the predicted concentrations. Maximum predicted values can also be evaluated using specific cut off values for some of the parameters. The non-statistical parameters, such as the differences in direction and distances of the predicted and observed centres of mass, can be used as to explain the (mis)performance of a model.

In a quick sensitivity study employing only one variable, it turned out that the wind direction has a significant influence on the ranking parameter. It seems possible that the original wind direction for 25 July 1980 in the Kincaid data set can be estimated. Consequently, it is possible to examine the consistency of the observed data set as well by using the tool.

In the presented study the dispersion characteristics of models using high stacks are evaluated. In the near future other experimental data sets (low stacks, and low heat content) must be included in the validation tool to complement it.

References

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Appendix 1. Formulae of the used statistical parameters

The formulae are constructed using the following variables:
N=number of receptor points,
P_i=predicted value at receptor point i,
M_i=observed value at receptor point i,
$\overline{P}$ =grid-averaged predicted value,
$\overline{M}$ =grid-averaged observed value,
$N_{(P_i > M_i)}$ = number of receptor points at which $P_i > M_i$,
$N_{\left(\frac{M_i}{\alpha} < P_i < \alpha \cdot M_i\right)}$ =number of receptor points at which $P_i > M_i / \alpha$ and also $P_i < \alpha M_i$,
N_{params}=number of used statistical parameters,
A_i=area of predicted (i=1) or observed (i=2) values in which the value of the concentration is above some specified threshold (10% of the maximum value on grid),
$prob(P(x_b))$, $prob(M(x_b))$ =probability of occurence of predicted or observed values not higher than x_b.

$$bias = \frac{1}{N}\sum_i (P_i - M_i)$$

$$NMSE' = \sum_i \frac{(P_i - M_i)^2}{(P_i + M_i)^2}$$

$$VG\ (geometric\ mean\ variance) = \exp\left[\frac{1}{N}\sum_i \left(\ln\left(\frac{M_i}{P_i}\right)\right)^2\right]$$

$$MG\ (geometric\ mean\ bias) = \exp\left[\frac{1}{N}\sum_i \ln\left(\frac{M_i}{P_i}\right)\right]$$

$$FOEX = \left[\frac{N_{(P_i > M_i)}}{N} - 0.5\right] \cdot 100$$

$$FMS = \frac{A_1 \cap A_2}{A_1 \cup A_2}$$

$$KS\ (Kolomogorov\ Smirnov\ parameter) = N \cdot MAX\ |\ prob(P(x_b)) - prob(M(x_b))\ |$$

$$P_{corr} = \frac{\sum_i \left(M_i - \overline{M}\right)\cdot\left(P_i - \overline{P}\right)}{\sqrt{\sum_i \left(M_i - \overline{M}\right)^2}\sqrt{\sum_i \left(P_i - \overline{P}\right)^2}}$$

$$FA\alpha = \frac{N_{\left(\frac{M_i}{\alpha} < P_i < \alpha \cdot M_i\right)}}{N}$$

$$ranking = \frac{1}{N_{params}} \cdot \left(\frac{|bias|}{\overline{P} + \overline{M}} \cdot 100 + NMSE' \cdot 100 + \frac{\ln(MG)}{\left| \ln\left(\frac{\overline{M}}{\overline{P}}\right) \right|} \cdot 100 + \frac{\ln(VG)}{\left| \ln\left(\frac{\overline{M}}{\overline{P}}\right)^2 \right|} \cdot 100 + 2 \cdot |FOEX| + \right.$$

$$\left. (1 - FMS) \cdot 100 + (1 - FA2) \cdot 100 + (1 - FA5) \cdot 100 + \frac{KS}{N} \cdot 100 + (1 - Pcor) \cdot 100 \right)$$

Note that *NMSE'* is used in stead of the standard $NMSE = \frac{1}{N} \sum_i \frac{(P_i - M_i)^2}{\overline{P} \cdot \overline{M}}$, because of the possibility of scaling *NMSE'* from 0 to 100.

<u>Treatment of zero's or very low values</u>

In a previous paper[4] details about the treatment are given.

Appendix 2. Day numbering for this validation tool and actual days in Kincaid data set

day number	date
1	1980-04-20
2	1980-04-25
3	1980-05-01
4	1980-05-04
5	1980-05-05
6	1980-05-07
7	1980-05-09
8	1980-07-11
9	1980-07-13
10	1980-07-24
11	1980-07-25
12	1981-05-16
13	1981-05-22
14	1981-05-23
15	1981-05-24
16	1981-05-25
17	1981-05-28
18	1981-05-29
19	1981-05-31