Validation of the improved AEROPOL model against the Copenhagen data set

Marko Kaasik
Researcher, Institute of Environmental Physics,
University of Tartu, 50090 Tartu, Estonia
E-mail: mkaasik@ut.ee

Veljo Kimmel
Researcher, Institute of Environmental Physics,
University of Tartu, 50090 Tartu, Estonia
E-mail: kimmel@ut.ee

Abstract: The improved Gaussian dispersion model AEROPOL (University of Tartu, Estonia) is validated against the Copenhagen air pollution dispersion dataset belonging to the Model Validation Kit of the Initiative on ‘Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes’. Model updates include the application of (1) surface heat flux instead of indirect indicators of surface layer stability and (2) two-level wind data instead of one (10 m) level. Validation results show a fair agreement of modelled and measured concentrations. In comparison with several models validated earlier, the scatter of modelled versus measured data is moderate, but a systematic deviation is small. Thus, the AEROPOL model is recommended for urban dispersion calculations in nearly neutral conditions. Best results are expected for long-term average pollution levels.

Keywords: atmospheric dispersion model; model validation; Copenhagen dispersion experiment; Model Validation Kit; AEROPOL; urban air quality.

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Biographical notes: Marko Kaasik graduated in basic courses (physics) in 1989, followed by an MSc in 1995 and PhD in 2000 in Environmental Physics at the University of Tartu, Estonia. Marko was a junior researcher at the University of Tartu (1986–1992), project researcher in Tartu Observatory, Estonia (1993–1997 and 1998–2001), and Head of the Environmental Service, Tartu City Government (1997–1998). From 2001, Marko is a researcher at the Institute of Environmental Physics, University of Tartu. Experience includes modelling of air pollution transport and atmospheric dynamics, model validation (including field experiments) and environmental impact assessment. Marko’s 36 publications include 7 in peer-reviewed international journals.

Veljo Kimmel graduated in basic courses (physics) in 1990, followed by an MSc in 1994 and a PhD in 2002 in Environmental Physics from the University of Tartu, Estonia. An M.Sc. was also obtained in Environmental Sciences and Policy from Manchester University in 2000. Veljo was Data Processing Manager at the University of Tartu (1987–1990), and Head of the Air Quality Department, South Estonian Environmental Protection Laboratory.

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1 Introduction

The international agreement represented by COM [1] sets certain criteria for the results of air pollution modelling. Usually there does not exist enough spatial information about pollution field – thus, validation of the model is complicated. International data sets for the validation of models are good alternatives – they represent pollution field in different meteorological conditions and pollution patterns.

The aim of the current study is to validate the Gaussian plume AEROPOL model against the Copenhagen data set and thus check its applicability in typical weather conditions in urban environment. The triggering reasons for this study were (1) improvement of the model and (2) extensive use of AEROPOL for urban planning applications in Estonia.

2 Model

The AEROPOL model (developed at Tartu Observatory, Estonia) is a Gaussian plume model, which includes the reflection and partial adsorption of the pollutant at the underlying surface, wet deposition, and the initial rise of buoyant plumes [1]. The model is applicable for gaseous pollutants and particles from stacks, transport and area sources like domestic heating [2,3].

The basic formula for concentration $C$ is:

$$C = \frac{Q}{2\pi \sigma_y \sigma_z u} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \sum_{n=-2}^{0} \left\{ a_n \exp\left[-\frac{(z-H+2nl)^2}{2\sigma_z^2}\right] + a_{-n} \exp\left[-\frac{(z+H+2nl)^2}{2\sigma_z^2}\right]\right\},$$

where $Q$ is the source strength, $y$ and $z$ are respectively, the lateral and vertical dimensions, $\sigma_y$ and $\sigma_z$ are the respective dispersion parameters, $u$ is the wind speed, $H$ is the source height and $l$ is the height of the capping inversion. Negative reflection indexes $n$ in equation (1) correspond to the plume first reflected from the capping inversion, $n = 0$ means that the plume is coming directly from the source (most intense component), and positive ones belong to the components first reflected from the underlying surface. The maximal reflection index $n = \pm 2$ is taken as a compromise between modelling precision and computing time.

The sum at the right in equation (1) represents the effect of multiple reflections from the surface and the capping inversion. For gases, the reflection coefficients $a_n$ are calculated multiplying all the fractions remaining after the previous reflections of current component:
\[ a_n = \prod_{j=0}^{n} \max\left(0, \frac{u \tan \alpha_{j-1} - v_j}{u \tan \alpha_j}\right) \quad \text{if} \quad n \geq 0 \]
\[ \prod_{j=1}^{n} \max\left(0, \frac{u \tan \alpha_j - v_j}{u \tan \alpha_j}\right) \quad \text{if} \quad n < 0 \]

where

\[ \tan \alpha_j = \frac{f}{|\gamma|} \frac{H + z + 2jl}{\sigma_z} \frac{\partial \sigma_x}{\partial x} \quad (3) \]

Thus, each \( a_n \) is a function of the deposition velocity \( v_j \) and the number of reflections from the ground. A perfect reflection is assumed at the capping inversion. In the case of stable stratification (Pasquill classes E, F) there is no upper boundary, all \( a_n \) except \( a_1 \) are zeros and, therefore, only two members remain in the formula (1). Empirical values of the mixing height are applied for unstable and neutral stratification: \( l = 1500 \text{ m} \) for Pasquill A, B, C and \( l = 900 \text{ m} \) for Pasquill D.

The described approach is asymptotically equivalent to the Overcamp’s formulation [4] for small deposition velocities, but avoids too low concentrations in the case of large ones. The \( x \)-dimension (towards the plume centreline) is included into the Biggs’ formulae [5] (urban ones in this case) for the dispersion parameters. The initial plume rise, depending on buoyancy flux and momentum, is included, and Biggs’ approach [5] is applied.

The AEROPOL model was earlier validated against the Lillestrøm data set (expressing predominantly very stable stratification) with a relative success [6]. In recent years the AEROPOL model has intensely been applied for urban planning purposes in Estonia.

The recent updates of the AEROPOL model include two-level wind data (instead of the earlier 10 m wind only) and the heat-flux-based method to determine the atmospheric stability conditions (instead of the earlier determination by the cloud amount and solar elevation).

In the new model version the wind speed for the plume is interpolated (extrapolated) logarithmically and the wind direction linearly between two levels, approximating the Ekman law by simple measures. It is recommended to have the plume centreline between these two heights or close to one of them to avoid large distortions.

Both the initial and recently updated model versions apply the Pasquill stability classes [7, Table 6.V] to calculate the dispersion parameters. Earlier, the estimation of stability was based only on the data routinely collected at meteorological stations: wind speed and cloud amount (and solar elevation). In the updated model version the stability classes are derived from their relation with the 10 m wind speed and the surface heat flux [7, Figure 6.1]. The Copenhagen experimental data set (see next section) includes the surface heat flux. Thus, application of the updated model version is appropriate.
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The AEROPOL model requires the following data for each run:

- source data – position (Cartesian coordinates), height, stack opening diameter, gas velocity and temperature (for the buoyant and upward momentum plumes), source strength (g/s) and the dimensions of buildings or other obstacles near the source (if any);
- admixture data – deposition velocity and the coefficients for washout calculations (for gases), particle density and diameter (for particles);
- meteorological data – wind speed and direction, temperature, cloud amount (or the surface heat flux for updated version), date and time.

The model output constitutes a ground-level concentration field in a user-defined rectangular grid. The deposition fluxes at each grid point are available as well.

3 Experiment and validation procedure

The conditions of the dispersion experiment in Copenhagen (1978–1979, [8]) correspond well to a typical situation, in which the AEROPOL model is applied: urban elevated (115 m) release, mid-latitude maritime climate with quite strong winds and neutral or slightly unstable stratification.

The improved AEROPOL model was validated against the Copenhagen data set (observed data [9]). Wind speeds at 10 and 115 m height were applied for model runs. As the plume was non-buoyant and the upper wind measurement height matched with the plume centreline height, actually no interpolation was needed. 10 m wind was used to determine the Pasquill stability class (see previous section). The measurement arcs were always oriented downwind and no wind direction was reported in the data set. Following the site description, no significant obstacles near the emission source were assumed.

The deposition velocity for an inert tracer (sulphur hexafluoride, SF₆) was assumed zero, thus applying a perfect reflection of the plume from the ground. As no data on rainfalls were reported in the Copenhagen data set, no wet deposition was assumed in model runs.

The model-measurement comparison statistics follow the formulae given by Hanna et al. [10]: normalised mean square error

\[
\text{NMSE} = \frac{(C_o - C_P)^2}{C_o C_P} \tag{4}
\]

fractional bias

\[
\text{FB} = \frac{C_o - C_P}{0.5(C_o + C_P)} \tag{5}
\]

fractional standard deviation

\[
\text{FS} = \frac{\sigma_{o} - \sigma_{p}}{0.5(\sigma_{o} + \sigma_{p})} \tag{6}
\]
In formulae (4–6) $C_0$ is the observed concentration, $C_P$ is the modelled concentration, the overbar means averaging over the ensemble, and $\sigma$ with its corresponding indexes is the standard deviation. Other applied statistics are the linear correlation coefficient (COR) and the factor of $C_P/C_0$ in the diapason 0.5–2 (or fraction in factor 2, FA2). The arc-wise maximal and cross-wind integrated concentrations from the Copenhagen data set were compared with their modelled counterparts.

4 Validation results

The summary statistics for the arc-wise maximal concentrations are given in Table 1 and for the crosswind integrated concentrations in Table 2. Both concentrations are normalised with the source emission (mass emitted in unit time).

<table>
<thead>
<tr>
<th>Model (country, comparison year)</th>
<th>Mean</th>
<th>Sigma</th>
<th>Bias</th>
<th>NMSE</th>
<th>COR</th>
<th>FA2</th>
<th>FB</th>
<th>FS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observations</td>
<td>632.7</td>
<td>450.3</td>
<td>0.0</td>
<td>0.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>AEROPOL (Estonia, 2002)</td>
<td>573.0</td>
<td>448.7</td>
<td>59.6</td>
<td>0.30</td>
<td>0.642</td>
<td>0.826</td>
<td>0.099</td>
<td>0.004</td>
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<td>HPDM (USA, 1994)</td>
<td>358.2</td>
<td>268.1</td>
<td>274.4</td>
<td>0.61</td>
<td>0.847</td>
<td>0.658</td>
<td>0.554</td>
<td>0.507</td>
</tr>
<tr>
<td>IFDM (Belgium, 1994)</td>
<td>551.9</td>
<td>345.3</td>
<td>80.8</td>
<td>0.19</td>
<td>0.843</td>
<td>0.870</td>
<td>0.136</td>
<td>0.264</td>
</tr>
<tr>
<td>INPUFF (Romania, 1994)</td>
<td>560.6</td>
<td>352.7</td>
<td>72.1</td>
<td>0.50</td>
<td>0.490</td>
<td>0.739</td>
<td>0.121</td>
<td>0.243</td>
</tr>
<tr>
<td>OML (Denmark, 1994)</td>
<td>283.6</td>
<td>251.1</td>
<td>349.1</td>
<td>1.12</td>
<td>0.823</td>
<td>0.217</td>
<td>0.762</td>
<td>0.568</td>
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<tr>
<td>UK-ADMS (UK, 1994)</td>
<td>177.1</td>
<td>138.5</td>
<td>455.5</td>
<td>2.84</td>
<td>0.891</td>
<td>0.043</td>
<td>0.125</td>
<td>1.059</td>
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<td>UK-ADMS extra (UK, 1994)</td>
<td>261.8</td>
<td>176.9</td>
<td>370.8</td>
<td>1.37</td>
<td>0.913</td>
<td>0.348</td>
<td>0.829</td>
<td>0.872</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Model (country, comparison year)</th>
<th>Mean</th>
<th>Sigma</th>
<th>Bias</th>
<th>NMSE</th>
<th>COR</th>
<th>FA2</th>
<th>FB</th>
<th>FS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observations</td>
<td>448.7</td>
<td>239.3</td>
<td>0.0</td>
<td>0.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>AEROPOL (Estonia, 2002)</td>
<td>386.5</td>
<td>183.6</td>
<td>62.2</td>
<td>0.19</td>
<td>0.624</td>
<td>0.913</td>
<td>0.149</td>
<td>0.263</td>
</tr>
<tr>
<td>HPDM (USA, 1994)</td>
<td>382.3</td>
<td>161.6</td>
<td>66.4</td>
<td>0.16</td>
<td>0.778</td>
<td>1.000</td>
<td>0.160</td>
<td>0.387</td>
</tr>
<tr>
<td>IFDM (Belgium, 1994)</td>
<td>443.3</td>
<td>193.4</td>
<td>5.43</td>
<td>0.16</td>
<td>0.681</td>
<td>0.957</td>
<td>0.012</td>
<td>0.212</td>
</tr>
<tr>
<td>INPUFF (Romania, 1994)</td>
<td>339.6</td>
<td>180.4</td>
<td>109.1</td>
<td>0.46</td>
<td>0.361</td>
<td>0.696</td>
<td>0.277</td>
<td>0.280</td>
</tr>
<tr>
<td>OML (Denmark, 1994)</td>
<td>249.2</td>
<td>131.7</td>
<td>199.5</td>
<td>0.52</td>
<td>0.893</td>
<td>0.565</td>
<td>0.572</td>
<td>0.580</td>
</tr>
<tr>
<td>UK-ADMS (UK, 1994)</td>
<td>207.1</td>
<td>110.7</td>
<td>241.6</td>
<td>0.86</td>
<td>0.912</td>
<td>0.348</td>
<td>0.737</td>
<td>0.735</td>
</tr>
<tr>
<td>UK-ADMS extra (UK, 1994)</td>
<td>297.0</td>
<td>122.5</td>
<td>151.6</td>
<td>0.34</td>
<td>0.856</td>
<td>0.783</td>
<td>0.407</td>
<td>0.646</td>
</tr>
</tbody>
</table>
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Like the models validated earlier [11], the AEROPOL model tends to underestimate slightly both concentrations (bias). The scatter of data is relatively large (moderate correlation coefficient COR), but large deviations from observed values are seldom (high FA2 and low NMSE). The overall scatter (Sigma) for the cross-wind integrated concentrations is somewhat underestimated, and for the maximum arc-wise concentrations it is almost perfect.

Looking at the plots of modelled Vs. observed concentrations (Figure 1) we see, that both the cross-wind integrated and the arc-wise maximal concentrations are randomly scattered. The deviations from the one-to-one line are bilateral and balanced (which is consistent with the small bias) and increase nearly in proportion with the concentration, i.e. the relative error is nearly constant. The maximal arc-wise concentrations are slightly more scattered than the cross-wind integrated ones.

Figure 1  Plots of modelled and observed cross-wind integrated concentration (a) and maximal arc-wise concentration (b). Concentrations are normalised with the source emission rate, one-to-one line is added to the graphs

5 Discussion and conclusions

As there are no systematic differences between modelled and measured data, the scatter of data points (Figure 1) is nearly proportional to the absolute value of concentrations and thermal stratification did not change dramatically (not far from neutral), we assume that the discrepancies between modelled and measured values are not of deterministic nature. As most of compared models performed quite similarly, we assume that the simplicity of field data for the model input (single-point time-averaged meteorological data only, no detailed data on the underlying surface etc.) is limiting the model performance. An inhomogeneous urban landscape can cause spatial and temporal variations, which are not controlled by these parameters. More complex models would probably not perform significantly better with the same initial data set.

As 91% of the cross-wind integrated and 82% of the arc-wise maximum concentrations are fitting in the fraction of factor 2 and the bias is respectively 16% and 10% only, we can conclude that AEROPOL performs satisfactorily for practical use in nearly-neutral stratification.
We have to conclude that the AEROPOL model performs fairly for elevated releases in urban area during neutral or slightly unstable stratification. The systematic error of results is relatively small – a significant advantage from the operational point of view. Therefore, the best performance is expected for the long-term average concentrations.

Most of the models give higher correlations with observation than the AEROPOL model, but tend systematically to underestimate the concentrations (especially UK-ADMS). These models, however, were validated eight years earlier and therefore this comparison does not reflect the present state of their development. Nevertheless, as these models were in operational use already in the middle of the 1990s during the validation at the Mol workshop, we have to conclude, that AEROPOL performs well at level with the models applied in Europe and USA during the last decade.

The assessment of air pollution levels by measurements is well determined through standard methods and procedures set by COM [1] and later directives. Although we cannot expect that the assessment of air pollution by modelling is standardised, we can expect that the validation of models is somehow standardised. Intensified practice of validating models against available international data sets, and creating newer and better data sets can accelerate the ongoing process of standardisation and improve the comparability and quality of air pollution modelling.

References