VALIDATION OF THE AEROPOL MODEL AGAINST THE KINCAID DATA SET

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INTRODUCTION

This validation study is the next step in validation of the AEROPOL model against the Model Validation Kit established at the Mol workshop, 1994 (Olesen, 1994). Earlier the AEROPOL model was validated against two minor data sets from the Kit: the Lillestrøm (Kaasik, 2000) and the Copenhagen (Kaasik and Kimmel, 2004) data set, both with relative success compared to the five models validated earlier (Olesen, 1995). In this paper the validation against the arc-wise maximal concentrations of "Quality 3" (most unambiguous) subset of Kincaid data is presented and discussed.

The AEROPOL model 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, developed at Tartu Observatory, Estonia (Kaasik and Kimmel, 2004). AEROPOL model has been initially developed for power plants, which have stack parameters in the same range with Kincaid one and applied in several case studies and environmental impact assessments targeted at such sources (e.g. Sofiev et al., 2003). There was found reasonable agreement with deposition measurements, but no direct validation against dispersion of a highly buoyant plume still occurred. Thus, it is justified to ask, what is the probable accuracy of these applications and under which conditions that model may go wrong?

BASIC CONCEPTS

Model

The AEROPOL model is a local dispersion model based on the stationary Gaussian plume with reflections from the underlying surface and capping inversion. Details are described by Kaasik and Kimmel (2004). The contemporary version has options to determine the plume dispersion parameters (in Briggs' formulation) either from routine meteorological observations (wind, solar elevation, cloud amount) or applying the sensible heat flux data and two-level wind speed. As sensible heat flux was measured in the Kincaid experiment, the later option (expected more accurate) is applied. Wind data at 10 m and 100 m levels were used.

The initial plume rise is calculated relying on the basic concepts of Briggs' empirical approach (Stern et al., 1984). The basic quantity for estimation is the buoyancy flux F, which is calculated as

$$F = \frac{g w_s D^2 (T_s - T)}{4T_s} \tag{1}$$

where D, w_s and T_s are respectively the stack diameter, gas velocity and temperature and T is the ambient air temperature. The plume is rising gradually with distance x (km) from the source by the "two-third law":

$$H(x) = H_0 + \frac{160 F^{1/3} x^{2/3}}{u} \tag{2}$$

where H_0 is the stack height and u is the wind velocity. The final plume rise $\Delta H = H - H_0$ (limit for Eq. (2), meters) was initially given by Briggs as

$$\Delta H = \frac{21.425 F^{3/4}}{u} \qquad \text{for } F<55 \text{ m}^4/\text{s}^3 \tag{3}$$

$$\Delta H = \frac{38.71 F^{3/5}}{u} \qquad \text{for F>55 m}^4\text{/s}^3 \qquad (4)$$

Eq. (3), (4) have been empirically derived from field data with buoyancy fluxes not exceeding 1000 m^4/s^3 (Pasquill & Smith, 1983). On the basis of field studies carried out near Narva power Plants, Estionia, it was suspected that Eq. (3), (4) result in too high plume rises for larger buoyancy fluxes. Thus, in the AEROPOL model those were replaced with a formula, matching both Eq. (3), (4) with 10% precision within their scope and giving remarkably lower values for F>1000 m^4/s^3 (Kaasik, 2000):

$$\Delta H = \frac{40[\ln(1+F)]^2}{(1+160/F)^{1/2} u} \qquad (5)$$

Data set

The Kincaid data set, including 1284 arc-hours is much more extensive than the Lillestrøm (22 arc-hours) and Copenhagen (23 arc-hours) ones. Even the "Quality 3" subset (only arc-hours with a single, clear and continuous maximum) includes 338 arc-hours that are about 15 times more than any of former ones. 315 arcs of them were applied for AEROPOL runs, as the rest 13 have gaps in initial meteorological data set that cannot be processed by AEROPOL without ambiguous extrapolation. Nevertheless, the results are compared below with validation results of five models reported by Olesen (1995) claimed to be based on the full "Quality 3" data set, as the missing about 4% of data cannot be fatal to the results.

Despite the large number of arc-hours the applied data set did not cover the full range of dispersion conditions, but only neutral-to-unstable part with some shift towards unstable stratification: 107 arc-hours belong to the Turner class 4 (nearly-neutral), 128 to class 3 (slightly unstable), 68 to class 2 (moderately unstable) and 12 to class 1 (strongly unstable). Class 1 never occurs and class 2 is seldom at high latitudes, where AEROPOL model was used for practical purposes. Stable classes 5 and 6 do not occur in the subset, but they were rather frequent in past applications of AEROPOL. Thus, that validation does not result in a comprehensive valuation of model's applicability. The compendium of validation exercises against the Kincaid, the Copenhagen (neutral) and the Lillestrøm (stable) data sets looks more like that, although there are no buoyant plumes in later two of them.

RESULTS

Standard validation

There were established some standard validation procedures and quantities for validation against the Model Validation Kit (Hanna et al., 1991). The results of validation in comparison with five models validated earlier (Olesen, 1995) are presented in Table 1.

In the comparison of all statistics, the AEROPOL model performs fairly at level. Despite rather poor correlation (but not the worst; all models except HPDM had severe problems with that) the mean value is only slightly biased and fraction in factor 2 is not far from the best (IFDM).

The scatter plot of normalised concentration does not differ substantially from those models listed by Olesen (1995). The quantile-quantile plot indicates that model tends to "nullify" some concentrations (these are near the stack) and does not produce as high concentrations as measured, disagreement appears at concentrations more than $100 \cdot 10^{-9}$ s/m^3 (Figure 1).

Performance relevant to dispersion conditions

The "Quality 3" data set of arc-hours was divided into sub-samples representing maximums at each downwind distance separately. Thus, each sub-sample includes 20 – 51 arc-hours except for 1 km distance, which consist only of 7 arc-hours. 40 km sub-sample consisting of only one arc-hour was neglected. Dimensionless statistics NMSE, COR, FA2 and FB (see Table 1) for these sub-samples are presented in Figure 2. Fractional bias is high and normalised mean square error exceptionally high at low distances, indicating that in model calculation the plume usually did not reach the ground at distances less than 3 km. Both of these statistics and also fraction in factor 2 suggest best fit at 2 – 20 km from the source. At 30 – 50 km the overestimation appears, possibly due to too poor modelled dispersion. The complicated behaviour of correlation coefficient is a matter of further investigations, but rather small sub-samples and narrow range of concentrations in each of them may play a certain role.

Table 1. Statistics for maximum arc-wise concentrations (normalised with emission, unit 10^{-9} s/m^3). Sigma – *standard error,* NMSE – *normalised mean square error,* COR – *linear (Pearson) correlation coefficient,* FA2 – *fraction in factor 2,* FB – *fractional bias,* FS – *fractional standard deviation.*

Model (country, comparison year)	Mean	Sigma	Bias	NMSE	COR	FA2	FB	FS
Observations (315 arc-hours)*	53.69	40.78	0.0	0.00	1.000	1.000	0.000	0.000
AEROPOL (Estonia, 2005)	42.05	31.90	11.64	1.09	0.126	0.572	0.243	0.244
Observations (338 arc-hours) **	54.34	40.25	0.0	0.00	1.000	1.000	0.000	0.000
HPDM (USA, 1994)	44.84	38.55	9.50	0.75	0.441	0.565	0.192	0.043
IFDM (Belgium, 1994)	29.42	26.03	24.92	2.00	-0.132	0.423	0.595	0.429
INPUFF (Romania, 1994)	34.61	26.76	19.72	1.29	0.140	0.497	0.443	0.403
OML (Denmark, 1994)	47.45	45.48	6.89	1.24	0.146	0.547	0.135	-0.122
UK-ADMS (UK, 1994)	86.32	103.78	-31.99	2.45	0.228	0.518	-0.455	-0.882

* for AEROPOL only
** for other models

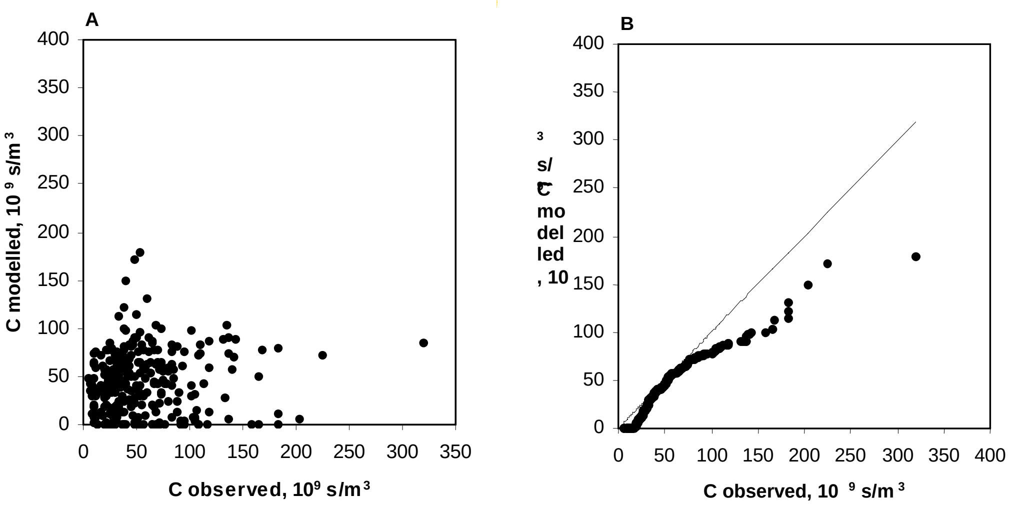

Fig. 1. Comparison of observed and modelled (AEROPOL) arc-wise maximum concentrations normalised with emissions, Kincaid "Quality 3" data set: A – scatter plot; B – quantile-quantile plot (solid line marks the one-to-one ratio).

To clarify the reasons of plume-height-dependent disagreement, the final plume rise by Briggs (Eq. (3), (4)) and Briggs & Kaasik (Eq. (5)) were examined (Figure 3). It appears that plume rise is highly variable, in the range of 100 – 2000 m in Briggs' original and 100 – 1200 m in updated formulation. It is known from Briggs' formulation that plume rise depends highly on thermal stability. Classifying these data by Taylor classes 1, 2, 3 and 4 (respectively 3, 25, 61 and 61 hours of experimental run), we see that average plume rise varies greatly: 635, 732, 415 and 235 m respectively.

To understand, how much the initial plume rise affects the accuracy of model results, the "Quality 3" data set was divided first into two nearly equal parts, with ΔH<300 m (average ΔH=198 m) and ΔH<300 m (average ΔH=643 m), and then into sub-sets by downwind distance. Results are presented in Figure 4.

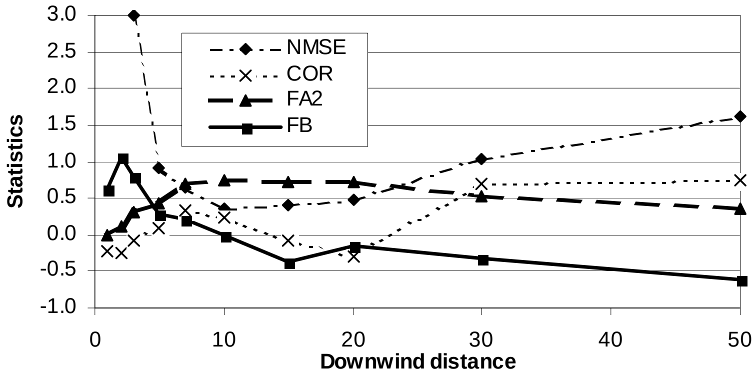

Fig. 2. Dimensionless statistics depending on downwind distance, "Quality 3" data set.

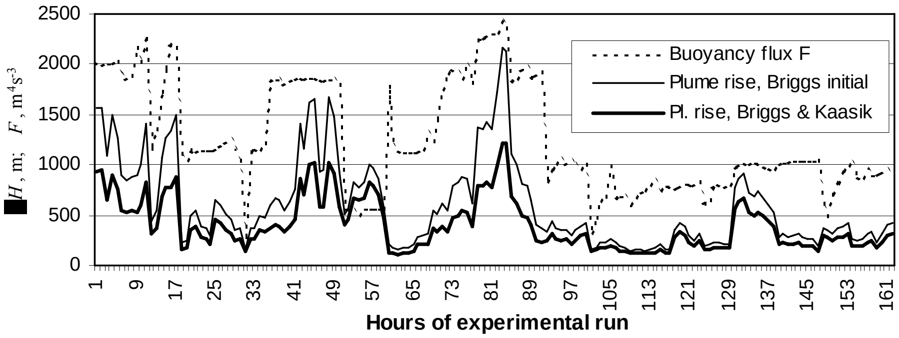

Fig. 3. Buoyancy flux and plume rise by Briggs initial formulae (3), (4) and Briggs and Kaasik (5) during the Kincaid experiment in time sequence, "Quality 3" runs only.

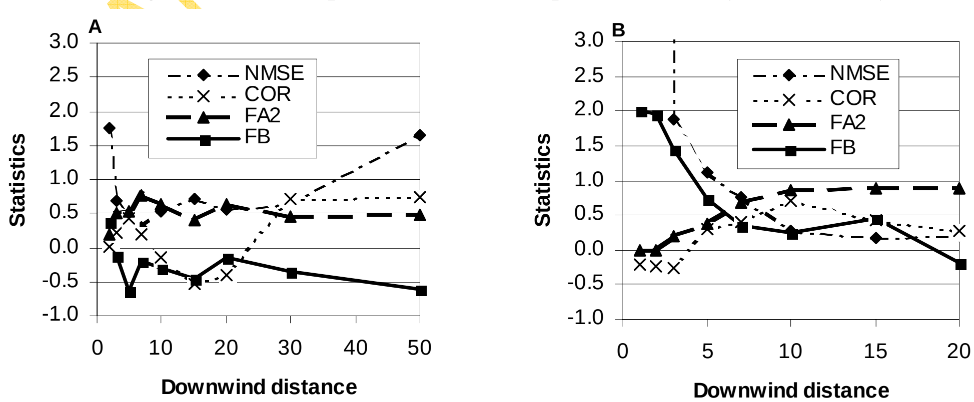

Figure 4. Dimensionless statistics depending on downwind distance, "Quality 3" data set: A –cases with ΔH<300 m only (153 arc-hours); B –cases with ΔH>300 m only (161 arc-hours).

It appears that at "low plumes" the concentrations are moderately overestimated everywhere except very close to the source. Thus, we have an impression that modelled dispersion (at least vertical) is slightly too poor in nearly-neutral conditions. The strongly negative correlation at mid-distances is a feature to be clarified further. It may be due to systematic wrong position of modelled down-wind maximum in respect to the measured one. The "high plume" graph repeats all main features of full data set (Figure 2), but coincidence is better at distances 10 – 20 km.
In order to introduce more variability in the plume height, there was made an AEROPOL run with zero plume rise, but this exercise resulted in severe overestimation of surface concentrations (in factor of 5 – 20 close to the sources and about twice at 10 km and further), indicating that true plume rises probably lie closer to those determined by Eq. (5) than to the zero-line.

CONCLUSIONS

The Briggs formulae overestimate severely the initial rise of a highly buoyant plume in the convective boundary layer. This conclusion concerns even the formulation with reduced dependence on the buoyancy flux, Eq. (5).
Regarding the Gaussian plume formula, it was not a surprise that hardly avoidable uncertainties in calculated plume rise may destroy the model accuracy despite of other well-tuned parameters, when plume rise is in the same order with stack height or larger. Nevertheless, that effect is proven with a common plume rise formulation and extensive high-quality data set now.
As the former applications of AEROPOL concern mainly stable and nearly-neutral stratification, the results above are not a reason for alarm. Nevertheless, these results must be considered in further development and applications of that model.

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