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APPLICATION OF SILAM MODEL ON AIRVIRO PLATFORM

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Abstract: *SILAM atmospheric chemistry-transport model was recently implemented in Estonian Environmental Research Centre for computations in a domain fitted to the area of Estonia. Database of pollution sources combined from CAMS and Estonian national inventory OSIS is used. This paper presents the results of first validation exercise based on yearly run (October 2022 – September of 2023). The results were compared with observations in nine monitoring stations (diversity of site types from rural background to street), applying a subset of statistical procedures recommended by HARMO initiative. The results include overestimation of NOx (possibly due to bias in database of sources), but adequate performance for ozone and carbon monoxide. Reasons for daily course of particulate matter $PM_{2.5}$ concentrations, sharply different from observations, has to be clarified.*

Key words: *SILAM model, model validation, nitrogen oxides, ozone, carbon monoxide, particulate matter.*

INTRODUCTION

Airviro, an integrated software platform of air quality monitoring and modelling, developed by Apertum AB, Sweden, is in use in institutions of several countries and municipalities (see e.g. Gidhagen, 2015). One of long-term Airviro users is Estonian Environmental Research Centre (EERC). In 2023, the SILAM atmospheric chemistry-transport model (Sofiev et al., 2008), version 5.8, developed in Finnish meteorological Institute (FMI), was installed to the Airviro platform in EERC. This application is considered a pilot project for wider use of SILAM joint with Airviro.
The dimensions of modelling domain fitted to the area of Estonia are 380 by 250 km with usual resolution 2 km in horizontal dimensions and 11 layers (layer thicknesses from bottom to top: 20, 50, 100, 200, 400, 500, 600, 800, 900, 1000, 2000 m) in vertical. With such resolution, the model time step is 2 minutes.
A variety of pollutant emission data, including NOx, SO_2, aerosol components and precursors and CO (among others) was used in the model runs. The data for NOx (point, area and road sources for GNFR sectors A-L) originates from the Estonian national inventory OSIS. All other emission data is gridded and originates from CAMS-REG-AP v5.1 emission inventory (Denier van der Gon, 2023). The inventory includes emissions from GNFR sectors A-L, including road transport (categories F1-F4) and residential heating based on heating degree days (Chdd). The SILAM boundary fields are provided by FMI and ECMWF meteorological fields by Estonian Environment Agency.

VALIDATION EXPERIMENT

Experimental setup

Using SILAM through the Airviro user interface, validation experiments were carried out in the Estonian modelling domain with "full chemistry" setup, which takes into account aerosol dynamics and both organic and inorganic chemical reactions in the atmosphere, including secondary organic aerosols and linear chemistry for SO_2 and SO_4. A full-year run, 01.10.2022 – 30.09.2023, was performed for NOx, SO_2, $PM_{2.5}$, O_3 and CO. A spin-up period of 4 days was used in the runs. The hourly concentrations for comparison with measurements were extracted from model output in locations of nine monitoring stations of different types described in Table 1. All modelled pollutants are measured in monitoring stations, except $PM_{2.5}$ in Tallinn-Rahu and CO in Saarejärve and Vilsandi.

Table 1. Monitoring stations used for validation of SILAM model

Station	Type	Latitude (deg.)	Longitude (deg.)
Tallinn-Liivalaia	Street	59.431003	24.760449
Tallinn-Rahu	Urban-industrial	59.447299	24.715117
Tallinn-Õismäe	Urban background	59.414043	24.649738
Tartu	Urban background	58.370604	26.734853
Kohtla-Järve	Urban-industrial	59.409649	27.278625
Narva	Urban-industrial	59.372207	28.200687
Lahemaa	Rural background	59.501934	25.936151
Saarejärve	Rural background	58.725292	26.507043
Vilsandi	Rural, maritime	58.376285	21.844561

Statistical procedure

For comparison of predicted concentrations C_p and observed concentrations C_o, three statistics of set recommended by HARMO initiative (Chang & Hanna, 2004) were used.

Correlation *R*, the linear correlation coefficient of modelled and observed hourly values:

$$\boldsymbol{R} = \frac{\overline{(C_p - \overline{C_p})(C_o - \overline{C_o})}}{\sigma_o \sigma_{C_p}} \qquad (1)$$

Fractional bias *FB*, which gives a symmetrical measure of over- and underestimation:

$$\boldsymbol{FB} = \frac{(\overline{C_o} - \overline{C_p})}{0.5(\overline{C_o} + \overline{C_p})} \qquad (2)$$

Fraction in factor two *FA2*, which is defined as the factor of cases, when the modelled concentration is two times smaller to two times bigger than observed one.

In addition to the hourly average values, the same statistics were applied to daily minimum, maximum and average values, hourly values with daily course eliminated (subtracted) and for daily course only.

RESULTS

Nitrogen dioxide

Concentrations of NO_2 appear highly overestimated. FB based on hourly values is -0.77 to 1.25 (i.e. roughly overestimated by factor 2 – 4). Only case of moderate overestimation, by factor of 1.5 (FB=- 0.42) appears in Vilsandi, a remote small island in Baltic sea. On the other hand, the modelled and observed hourly concentrations appear rather well correlated, being highest (R=0.65) in Tallinn-Õismäe urban background site, nearly 0.5 – 0.6 in other urban sites and 0.4 – 0.5 in rural background sites. Only in Narva and Kohtla-Järve industrial sites the model results are almost uncorrelated with observed values, R=0.1. FA2 values 0.09 (Tallinn-Õismäe) to 0.41 (Lahemaa & Tartu) reflect the high overestimation. When daily course is removed, the statistics do not change remarkably and they remain rather similar even when analysing the daily course only. Thus, SILAM is capable to predict both quasi-periodical daily pattern and changes that occur mostly due to weather patterns in longer time scale. Statistics based on daily average concentrations show nearly same pattern of overestimation and correlations as the hourly one, but correlations are somewhat higher, up to 0.77 in Tallinn-Õismäe. Higher correlations related to longer averaging time may refer to short pollution events, which were represented by the model in principle, but shifted slightly forward or backward in time by the model. Daily minima are even more overestimated (by factor of 30 in extreme case of Tallinn-Õismäe). It is remarkable that validation for 2023 in European domain carried out by Finnish Meteorological Institute (FMI), operational run v58x, which is used in Estonian simulations as boundary conditions, gives moderate overestimation only in rural background of Estonia, not in urban areas.

Nitrogen monoxide

Both in modelled and observed values, NO constitutes a minor part of NOx (=NO+NO_2). However, as most of NOx is emitted in form of NO and gradually oxidized in the atmosphere, the fraction of NO is larger in urban centres and marginally low in most remote rural areas. For urban sites in Tallinn, SILAM suggests average fractions of NO and NO_2 in total NOx to be nearly half to half. In contrary, observation gives 76-83% of NO_2 in air of Tallinn. The modelled and observed fractions of NO_2 are quite similar, about 0.8, in Tartu, Narva and Kohtla-Järve. In agreement with its large fraction in NOx, the concentrations of NO in urban stations are even more overestimated than of NO_2. The correlations between modeled and observed hourly concentrations are rather low in general, reaching values close to 0.5 only in Tallinn. The lowest, nearly zero correlations are for industrial Narva and Kohtla-Järve. It is remarkable that SILAM reproduces the daily course very well for Vilsandi (R=0.96), Saarejärve (0.89) and Lahemaa (0.72) rural background stations, Tartu urban (0.87) and even for Narva (0.60) and Kohtla-Järve (0.71) urban-industrial stations. In stations of Tallinn, the daily course is predicted less accurately (correlations 0.38-0.56). In line with NO_2, the daily average concentrations are somewhat better correlated than hourly values, most remarkably in Tallinn. The daily minima are even more severely overestimated than hourly values. Both maxima and minima are less correlated with observations than the daily average. The European domain validation results by FMI show rather pronounced overestimation, suggesting that proportion of NO to NO_2 is larger in that simulation.

Ozone

Despite well-pronounced overestimation of NO and NO_2, the secondary pollutant O_3 is predicted rather well. Slight overestimation by 20-30% (FB=0.19 to 0.27) occurs in three stations of Tallinn, whereas even slighter overestimation occurs at rural background. Even industrial sites do not show big discrepancies. FA2 based on hourly values is bigger than 0.5, except in three urban stations in Tallinn. Correlations of modelled and observed hourly values are highest in Vilsandi (R=0.68), Saarejärve (0.61) and Lahemaa (0.57) background stations and in the range of 0.43-0.54 in other sites. In most of sites, the modelled average daily course of O_3 is perfectly correlated (R=0.93 to 0.99) with observations and FA=1.00, i.e. all modelled values differ less than two times from observed ones.

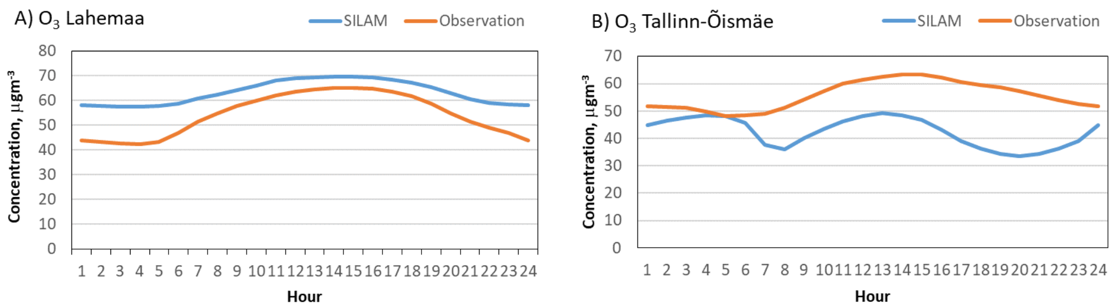

Figure 1. Yearly average daily course of ozone in Lahemaa rural background station (A) and two-maxima model prediction in Tallinn-Õismäe urban background station (B) that does not agree with measurements.

Unexpectedly, city stations in Tallinn show nearly-zero correlation in daily course, although still FA2=1.00. The reason found is the unconventional shape of average daily course predicted by SILAM for these sites: besides usual after-midday maximum there is another maximum in early morning, also the main maximum lasts shorter (Figure 1). In line with regulatory requirements, SILAM model results agree well with the average value of measured daily maxima of O_3. In all the stations, absolute value of FB is not bigger than 0.12 (i.e. difference no more than 13%), whereas FA2 ranging from 0.91 to 1.00. Daily-based correlations are bigger (0.74-0.82) in rural sites and small cities (Tartu and industrialized Narva) and lower in Tallinn and in another industrial town Kohtla-Järve (0.65-0.66).

The European simulation shows similarly highly accurate concentrations of ozone, compared to monitoring sites in Estonia.

Carbon monoxide

On average, CO is station-wise underestimated by factor 1.5 or less. Another indicator of rather good model performance is FA2, which ranges from 0.94 (Narva) to 0.99 (Kohtla-Järve), with an outlier Tartu (0.76). CO is not measured in Saarejärve and Vilsandi rural background monitoring stations. The correlation coefficients of hourly values range from 0.48 to 0.70, without any clear indication of less or more polluted areas. Daily course of CO is well predicted by SILAM: all hourly values are in range of two (FA2=1.00) and correlation ranges between 0.44 and 0.75, except high value 0.9 in Narva. With daily course removed, the results do not substantially differ from initial hourly values, thus the model performs rather well for weather patterns beyond the daily cycle. Daily minimal and average modelled concentrations of CO agree considerably better with observations than the hourly values, possibly indicating the pattern of peaks and lows modelled in sub-daily scale, although not with perfect timing. The statistics of daily maxima do not differ substantially from the initial statistics, based on hourly values. The simulation in European domain, in contrary, shows moderate overestimation of CO concentrations in Estonia.

Particulate matter PM2.5

$PM_{2.5}$ was chosen as the indicator of particulate matter, because it is measured in all stations except Tallinn-Rahu. Measurements of PM_{10} are rather scarce in Estonia. Hourly values of $PM_{2.5}$ in different stations are overestimated by 15-80% (FB=-0.16 to -0.57). Overestimation is biggest in Tallinn-Liivalaia and Tallinn-Õismäe urban stations. In all stations, except Narva, slightly more than a half of model results are found within the range of 2 with measured hourly values. Correlation based on hourly values is highest in Lahemaa and Tallinn-Liivalaia (0.62) and lowest in Vilsandi (0.38). The modelling system has obviously a problem with daily course of $PM_{2.5}$, as all the modelled-to-observed daily course correlations (except Vilsandi, R=0.41) were found low and some of them even strongly negative: -0.91 for Lahemaa, -0.50 for Kohtla-Järve and -0.45 for Saarejärve station. Measured and modelled daily minima and averages were found better correlated with observed values (R=0.59 to 0.73) than hourly values, but overestimated by nearly same range. Indeed, looking at average daily course in Lahemaa rural background station (Figure 2), a daytime maximum in observations is evident, whereas in model output a minimum appears at the same time. On the contrary, modelled daily course in Tallinn-Liivalaia street station has two distinct maxima, obviously related to rush hours of city traffic, but observations do not confirm such a course. The European domain validation gives nearly similar overestimation at Estonian monitoring sites.

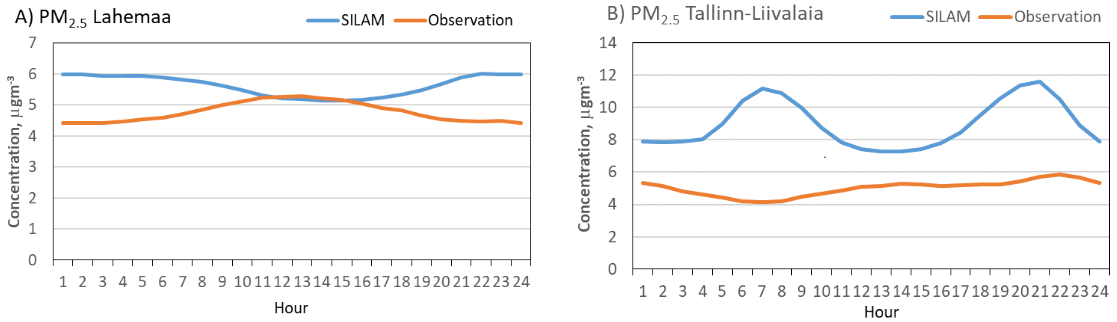

Figure 2. Modelled and observed yearly average daily course of $PM_{2.5}$ in Lahemaa rural background station (A) and Tallinn-Liivalaia street station (B).

Table 2. Linear correlation coefficients based on monthly averages

	Kohtla-Järve	Lahemaa	Narva	Saarejärve	Tallinn-Liivalaia	Tallinn-Õismäe	Tallinn-Rahu	Tartu	Vilsandi
NO_2	0.70	0.74	0.07	0.24	0.81	0.63	0.88	0.55	0.33
NO	0.39	-0.08	0.80	0.84	0.78	-0.05	0.81	0.57	0.87
O_3	0.45	0.57	0.57	0.72	0.43	0.36	0.49	0.43	0.82
CO	0.90	0.88	0.82		0.96	0.87	0.97	0.92	
$PM_{2.5}$	0.74	0.58	0.71	0.65	0.78	0.84	-0.05	0.88	0.43

Yearly performance through monthly averages

To represent, how well the yearly course of pollutants is estimated, the linear correlations of modelled and observed monthly average concentrations in all measurement stations were calculated (Table 2). It is remarkable that in this setting, carbon monoxide is predicted best. NO_2 is highly overestimated by the model, but usually well correlated with monitoring data, also as monthly means. SILAM predicts more or less pronounced minimum of NO_2 in July to September, whereas maximum ozone levels are predicted for the same season (Figure 3). In reality, the measured seasonal changes of NO_2 and O_3 are smoother than SILAM expects, while the maximum of ozone was found in early summer.

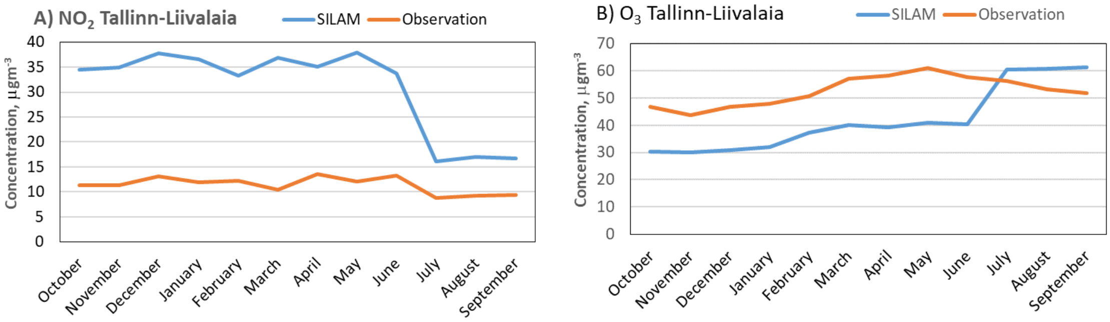

Figure 3. Monthly average modelled and observed concentrations (October 2022 – September 2023) of nitrogen dioxide (A) and ozone (B) in Tallinn-Liivalaia street monitoring station.

CONCLUSIONS

The Estonian application of SILAM highly overestimates the concentrations of NOx, although the yearly and daily courses and weather-related patterns of intermediate range are represented reasonably well. Assuming that SILAM as an atmospheric chemistry-transport model has been extensively validated against numerous data before, including very recent validation in European domain for 2023, which did not show that big deviations from observations, we can expect a bias in input source data. Database should be critically checked. Despite obvious bias in NO and NO_2 emission data, the related secondary pollutant ozone is predicted rather accurately, with slight overestimation in rural and slight underestimation in urban areas. Carbon monoxide (CO), emitted mostly from heating sources, is best reproduced by SILAM among considered primary pollutants. The concentrations are slightly underestimated, correlations show rather adequate performance both for daily course and longer-term weather patterns. SILAM tends to moderately overestimate the concentrations of $PM_{2.5}$ particles. Reasons of inadequate, often opposite daily course in respect to observations have to be clarified.

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REFERENCES

Chang, J.C. and Hanna, S.R., 2004: Air quality model performance evaluation. *Meteorol. and Atmos. Phys*., **87**, Nos. 1–3, pp.167–196.

Denier van der Gon, H., Gauss, M., Granier, C., 2023: CAMS2_61 – Global and European emission inventories. Documentation of CAMS emission inventory products. 109 p. [DOI: 10.24380/q2si-ti6i](https://doi.org/10.24380/q2si-ti6i).

Gidhagen, L., Bennet, C., Segersson, D., Omstedt, G., 2015: Exposure Modeling of Traffic and Wood Combustion Emissions in Northern Sweden. In: Denzer, R., Argent, R.M., Schimak, G., Hřebíček, J. (eds) Environmental Software Systems. Infrastructures, Services and Applications. ISESS 2015. IFIP Advances in Information and Communication Technology, vol **448**, 242-252. Springer, Cham. https://doi.org/10.1007/978-3-319-15994-2_24.

Sofiev, M., Galperin, M., Genikhovich, E., 2008: A Construction and Evaluation of Eulerian Dynamic Core for the Air Quality and Emergency Modelling System SILAM. In: Borrego, C., Miranda, A.I. (eds) Air Pollution Modeling and Its Application XIX. NATO Science for Peace and Security Series Series C: Environmental Security. Springer, Dordrecht. https://doi.org/10.1007/978-1-4020-8453-9_94.