

H14-116

COMPARISON AND EVALUATION OF THE 1KM AND 5KM RESOLUTION FRAME MODELLED ANNUAL CONCENTRATIONS OF NITROGEN OXIDES

Maciej Kryza¹, Anthony J. Dore², Małgorzata Werner¹, Marek Blas¹

¹Wrocław University, Department of Climatology and Atmosphere Protection, Wrocław, Poland

²Centre for Ecology and Hydrology, Edinburgh, UK

Abstract: The aim of this paper was to compare and evaluate the modelled annual NO_x air concentrations calculated for the same area at two different grid resolutions of 1km x 1km and 5km x 5km. The Fine Resolution Atmospheric Multi-pollutant Exchange model (FRAME) was used for this issue and the domains were defined to cover the entire area of Poland. Two simulations were performed for the year 2005 and 2008. The input files for the model were provided separately for both 1km and 5km grids, but it was assured that the emission, meteorological and boundary condition data were kept constant in terms of e.g. total mass. This was done by aggregation of 1km data into the 5km model grid.

The 1km and 5km model runs resulted in a similar spatial pattern and country average value of NO_x air concentrations. The maximum values were significantly higher for the 1km x 1km domain. For the high resolution domain the emission source areas were also distinctly separated from the background regions of low concentrations. For the 5km domain, 3rd quartile of gridded air concentrations was higher than for 1km x 1km run. The evaluation of the 1km and 5km results shows that the model – measurement agreement is improved for the high resolution simulations. The mean bias and average error statistics were decreased. The correlation coefficient was also higher for the 1km domain, with the exception of the urban stations in year 2008, which was attributed to the higher uncertainty of the emission inventory.

Key words: spatial resolution, air quality model, nitrogen oxides, FRAME

INTRODUCTION

Atmospheric transport models (ATM) are important tools supporting environmental management and provide spatially continuous information on current, past and future air quality. The ATM provided gridded information is used, among others, for the assessment of the critical levels and loads exceedances and population exposure to protect human health and ecosystems (IIASA, 2005; RoTAP, 2009). The large number of models and their various configuration often leads to different results of estimated spatial patterns of concentration and deposition of atmospheric pollutants. Hallsworth et al. (2010) show that the various resolutions used for calculation of ammonia air concentrations leads to significant differences in areas with critical level exceedances for ammonia and may further results in insufficient or unnecessary and costly protection of the ecosystems. The reason for this is the spatial averaging of the model input and output information with the increasing grid size. Denby et al. (2011) reported that insufficient spatial resolution of the air quality model results in significant underestimation of the urban background exposure for nitrogen dioxide. The spatial resolution of the model mesh is also important for deposition of nitrogen and sulphur compounds, especially in a complex terrain or in the vicinity of the emission sources (RoTAP, 2009).

The aim of this paper is to present and compare the results of NO_x air concentration modelling with the Fine Resolution Atmospheric Multi-pollutant Exchange (FRAME) model applied for Poland with the spatial resolutions of 1km x 1km and 5km x 5km. The simulations are run for the years 2005 and 2008. The results are compared both visually and statistically. The model estimates of annual average NO_x are compared with the air quality measurements gathered at background rural and urban stations.

DATA AND METHODS

Description of the FRAME model

FRAME is a Lagrangian statistical trajectory model that is used for the United Kingdom and Poland to support environmental management and protection. A detailed description of the model is provided by Singles et al. (1998), Fournier et al. (2005), and Dore et al. (2007). Details on the model configuration specific for Poland are provided by Kryza et al. (2010). The model provides information on annual air concentrations and deposition of nitrogen and sulphur compounds and primary particulate matter. Here the 8.3 version of the model is applied, and the simulations are run for the two domains covering the area of Poland with 1km x 1km (D1km) and 5km x 5km (D5km) spatial resolutions. The D1km mesh is composed of 800 x 800 grids, and D5km is of size 160 x 160 grids. The spatial extent of the D1km and D5km domains are the same. For each domain, separate input data on emission, precipitation and landuse were prepared. For the D5km, the emission, rainfall and landuse data were developed by aggregation of the D1km files, to assure spatial homogeneity e.g. in terms of mass of emitted pollutants or amount of annual precipitation. The boundary conditions were calculated with the FRAME-Europe model, and applied for D1km and D5km after re-gridding into 1km x 1km and 5km x 5km grid, respectively. The re-gridding process did not affect the total mass of the pollutants imported into the D1km and D5km domains.

Emission inventory for the year 2005 and 2008, available from Dębski et al. (2009) were used in this study. The emission data were provided at 1km x 1km grid resolution, and aggregated into 5km x 5km grid for the D5km model runs. For both years selected, the year specific wind and precipitation data were used. Similarly to the emission inventory, meteorological data for D5km were developed by aggregation of the D1km files. It should be noticed that for emission calculation from road traffic, detailed information on traffic intensity were available only for the year 2005. This information was also used to develop the emission map for the year 2008. Therefore the uncertainty related with emission inventory is higher for the year 2008, especially over the areas where road transport is the major source of nitrogen oxides for the atmosphere (e.g. large urban areas).

Evaluation of the model results

Annual average NO_x air concentrations calculated by the FRAME model were compared with the measurements performed on Polish air quality network and provided through the AriBase database. The completeness of the measurements used for calculation of annual average value was above 90% for all stations. For the model – measurement comparison, only background urban (BU) and background rural (BR) stations were used. For each year, configuration of the measuring network differ significantly, both in terms of total number of sites and fraction of urban and rural stations (Table 1). There was a significant increase in total number of measuring sites from year 2005 to 2008. However, the increase was mainly in the number of background urban sites, while the BR sites remained sparse. The new stations in year 2008 were located mainly in large cities (Fig. 1).

Table 1. Summary of the NO_x measuring sites for year 2005 and 2008 used for model evaluation

| Type of station | Year 2005 | Year 2008 |
|-----------------------|-----------|-----------|
| Background urban | 44 | 81 |
| Background rural | 14 | 21 |
| Total number of sites | 58 | 102 |

The model error was calculated for each site as a difference between model (M_i) calculated and observed (O_i) value. To summarize the model performance, the following error statistics were used (Yu et al. 2006):

$$\text{Mean Bias } MB = \frac{1}{N} \sum_i (M_i - O_i) \quad (1)$$

$$\text{Mean Absolute Gross Error } MAGE = \frac{1}{N} \sum_i |M_i - O_i| \quad (2)$$

$$\text{Root Mean Squared Error } RMSE = \sqrt{\frac{1}{N} \sum_i (M_i - O_i)^2} \quad (3)$$

The error statistics were calculated separately for BU and BR sites. The set of error metrics was complimented by the Pearson correlation coefficient (R). The modelled – measured values are also presented on the scatter plots. For each measuring site, relative error (RE) was calculated and marked on maps, according to the formula:

$$RE_i = \frac{|M_i - O_i|}{O_i} \quad (5)$$

RESULTS

In general, both D1km and D5km model runs give similar spatial pattern of NO_x annual average air concentrations. Main cities are the areas of the highest air concentrations (Fig. 1), and the main roads are recognizable on both D1km and D5km maps. For the D1km model setup, there is a strong separation of the emission source areas with high values of NO_x air concentrations from the background regions, especially along the main roads crossing the relatively clear areas. There is no tendency for clustering the stations with large or small relative errors, e.g. in the cities or over the background regions. The highest RE has been calculated for the same stations for D1km and D5km. In year 2005 the station with the highest RE is the urban station (Torun) for which the RE is 1.9 and 0.9 for D1km and D5km, respectively. For the year 2008, the maximum RE is for mountainous Sniezka station (SW Poland), with the RE equal to 3.2 and 3.5.

The grid average NO_x concentrations are at similar levels for both domains (Fig. 2), reaching 6.9 and 7.0 μg m⁻³ in year 2005 for D1km and D5km, and 7.7 and 7.8 μg m⁻³ in year 2008. For both years, the D1km simulations results in significantly higher maximum and lower minimum values of NO_x (68.1 for D1km and 52.6 μg m⁻³ for D5km in 2005, for year 2008 the respective values are 83.3 and 63.8 μg m⁻³). This is related to the mentioned above strong separation of the source and background areas. For the D5km model domain, the concentrations are averaged over the larger grids, and this is the reason for decreased maximum values if compared to D1km. For the same reason, the 3rd quartile is shifted towards the high values for D5km runs.

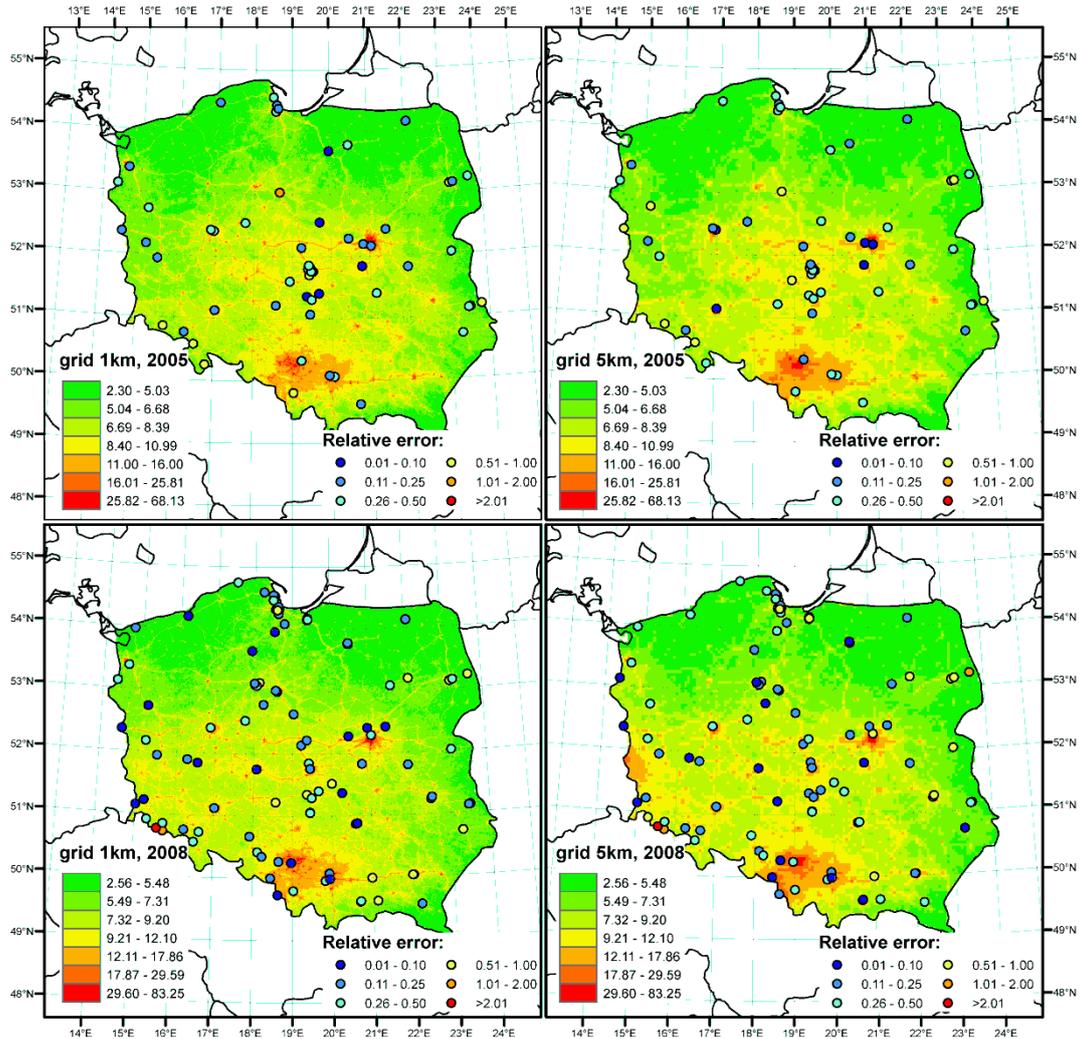


Figure 1. Modelled 1km and 5km NO_x concentrations for years 2005 and 2008 and RE for each of the NO_x measuring sites

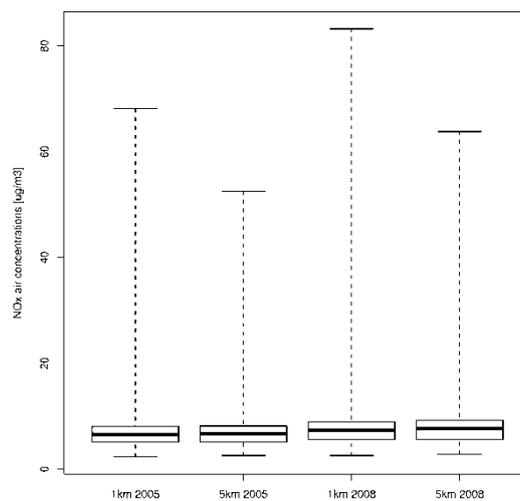


Figure 2. Statistical summary of the modelled 1km and 5km NO_x air concentrations for years 2005 and 2008

The model – measurements comparison is presented in Fig. 3. For the D1km, the number of sites that fall below or above 1:2 and 2:1 lines is lower than for D5km for both years. The D1km model run gives overall higher NO_x air concentrations for urban stations, which results in decreased MB (Table 2), especially for the year 2008, and for some sites this is the reason for

the overestimation of the observed values. However, the D1km model still have a general tendency for underestimation of the annual NO_x air concentrations for both urban and rural stations, reflected in the negative mean bias for both years 2005 and 2008, with the exception of the rural sites for the year 2008.

Both statistics of the average error, MAGE and RMSE, suggest the improved performance of the D1km over the D5km. The average errors are lower for both urban and rural stations. For the rural stations, the correlation coefficient is also higher for the D1km model run than for 5km grid. However, there is relatively poor correlation for the urban sites in year 2008, and the R value is smaller for the D1km. The smaller R for the year 2008 can be explained by the uncertainty in the traffic emission inventory, which brings the majority of emitted nitrogen oxides, and is based on traffic flow measurements performed in year 2005 and rescaled to the year 2008. The greater uncertainty in mapping high resolution emissions data can be also the reason for smaller R for the year 2008 D1km simulation, if compared with D5km, for which the errors may be averaged out resulting in an improved R value

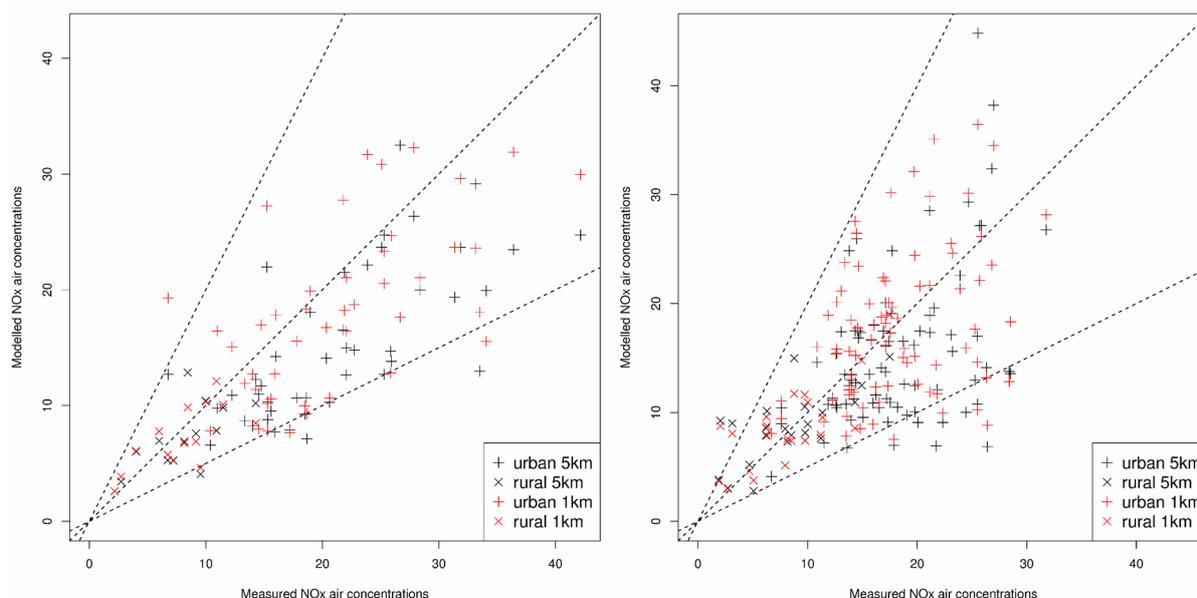


Figure 3. Modelled vs. measured NO_x air concentrations for urban and rural stations in year 2005 (left) and 2008 (right)

Table 2. Error statistics for urban and rural stations for 1km and 5km model runs

| Year | Model grid | Urban stations | | | | Rural stations | | | |
|------|------------|----------------|------|------|------|----------------|------|------|------|
| | | MB | MAGE | RMSE | R | MB | MAGE | RMSE | R |
| 2005 | 1km | -3.17 | 5.98 | 7.31 | 0.61 | -0.74 | 1.93 | 2.45 | 0.71 |
| | 5km | -6.05 | 6.89 | 8.27 | 0.69 | -0.83 | 2.10 | 2.59 | 0.69 |
| 2008 | 1km | -0.46 | 5.50 | 6.95 | 0.38 | 0.43 | 2.28 | 2.86 | 0.75 |
| | 5km | -2.76 | 5.58 | 7.27 | 0.44 | 0.54 | 2.42 | 3.09 | 0.69 |

SUMMARY AND CONCLUSIONS

The main aim of this paper was to compare the FRAME modelled annual air concentrations of NO_x for two domain of different spatial resolutions for the area of Poland. The model was run for two years: 2005 and 2008. Apart from the visual and statistical comparison of the estimated NO_x concentrations, the model results were evaluated by comparison with background rural and urban air quality measurements.

Both 1km and 5km simulations estimated similar country average values of annual NO_x concentrations. This is in accordance with the findings reported by Stroud et al. (2011) for organic aerosols with the AURAMS model running with three different spatial resolutions (42, 15 and 2.5 km). The 1km FRAME model gives locally significantly higher maximum values, but the 5km model estimate higher concentrations for larger areas of the country, what is described by the higher values of the 3rd quartile. This is important in terms of critical levels exceedances and may be the reason for insufficient or unnecessary protection of the area. This issue should be also examined for other atmospheric pollutants, especially for particulate matter, because of its strong adverse impact on human health and large spatial variation of emission of primary particles and gaseous precursors for the secondary aerosols (e.g. ammonia and sulphur dioxide).

There FRAME model runs for a high resolution mesh of 1km x 1km are in overall better agreement with the NO_x air concentrations measurements. The MB and average errors, MAE and RMSE, are decreased when higher spatial resolution is applied for both urban and rural sites. The only exception is the correlation coefficient calculated for the urban sites in year 2008, which can be attributed to the higher uncertainty related with the emission inventory used.

All the findings summarized above indicate the importance of the spatial resolution of the domain setup for the final results that the model can provide. The better model – measurement agreement calculated for the 1km domain suggest that the increase of resolution may result in improved estimates of chemical composition of the air. However, the increase in resolution must go together with the quality of the input data, as the errors resulting e.g. from the wrong spatial allocation of emission are not averaged out at high resolutions.

ACKNOWLEDGEMENTS

The work was funded by the Polish Ministry of Science and Higher Education grant nr N N306 140738.

REFERENCES

- Denby, B., M. Cassiani, P. De Smet, F. De Leeuw, J. Horalek, 2011: Sub-grid variability and its impact on European wide air quality exposure assessment. *Atmos. Environ.*, **45**, 4420-4229.
- Dębski, B., K. Olendrzyński, J. Cieślińska, I. Kargulewicz, J. Skośkiewicz, A. Olecka, K. Kania, 2009: Inwentaryzacja emisji do powietrza SO₂, NO₂, CO, NH₃, pyłów, metali ciężkich NMLZO i TZO w Polsce za rok 2005. IOŚ, KCIE.
- Dore, A.J., M. Vieno, Y.S. Tang, U. Dragosits, A. Dosio, K.J. Weston, M.A. Sutton, 2007: Modelling the Atmospheric Transport and Deposition of Sulphur and Nitrogen over the United Kingdom and Assessment of the Influence of SO₂ Emissions from International Shipping. *Atmos. Environ.*, **11**, 2355-2367.
- Fournier, N., Y.S. Tang, U. Dragosits, Y. De Kluizenaar, M.A. Sutton, 2005: Regional Atmospheric Budgets of Reduced Nitrogen over the British Isles Assessed Using a Multi-Layer Atmospheric Transport Model. *Water Air Soil Pollut.*, **162**, 331-351.
- Hallsworth, S., A.J. Dore, W.I. Bealey, U. Dragosits, M. Vieno, S. Hellsten, Y.S. Tang, M.A. Sutton, 2010: The role of indicator choice in quantifying the threat of atmospheric ammonia to the 'Natura 2000' network. *Env. Sci. Policy*, **13**, 671-687.
- IIASA, 2005: CAFE Scenario Analysis Report Nr. 6, "A Final Set of Scenarios for the Clean Air For Europe (CAFE) Programme". URL (2011) http://ec.europa.eu/environment/archives/cape/activities/pdf/cape_scenario_report_6.pdf.
- Kryza, M., M. Werner, M. Błaś, A.J. Dore, M. Sobik, 2010: The Effect of Emission from Coal Combustion in Nonindustrial Sources on Deposition of Sulfur and Oxidized Nitrogen in Poland. *J. Air & Waste Manage. Assoc.*, **60**, 856-866.
- RoTAP, 2009: Review of transboundary air pollution. Acidification, Eutrophication, Ground Level Ozone and Heavy Metals in the UK. URL (2001) <http://www.rotap.ceh.ac.uk>
- Singles, R., M.A. Sutton, K.J. Weston, 1998: A Multi-Layer Model to Describe the Atmospheric Transport and Deposition of Ammonia in Great Britain. *Atmos. Environ.*, **32**, 393-399.
- Stroud, C.A., P.A. Makar, M.D. Moran, W. Gong, S. Gong, J. Zhang, K. Hayden, C. Mihele, J.R. Brook, J.P.D. Abbatt, J.G. Slowik, 2011: Impact of model grid spacing on regional- and urban- scale air quality predictions of organic aerosol. *Atmos. Chem. Phys.*, **11**, 3107-3118.
- Yu., S., B. Eder, R. Dennis, S. Chu, S. Schwartz, 2006: New unbiased metrics for the evaluation of air quality models. *Atmos. Sci. Lett.*, **7**, 26-34.