Science, Engineering & Education, 3, (1), 2018, 11-16

Evaluation of Delta Tool for comparison of different Air Quality Prediction models

Dejan Gradišar[1]*, Hua Shao[2], Boštjan Grašič[3]

[1]Department of Systems and Control, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana
[2]University of Wisconsin-Madison, 1415 Eng. Drive Madison, WI, USA, E-mail: hshao5@wisc.edu
[3]MEIS d.o.o., Mali vrh pri Šmarju 78, Šmarje-Sap, Slovenia, E-mail: bostjan.grasic@meis.si

Received 30 May 2018, Accepted 06 July 2018

ABSTRACT

This paper describes how to use Delta tool, a software for the assessment of air quality model applications to evaluate ozone prediction models. These models aim to improve the accuracy of forecasting ozone concentration in urban locations in Slovenia. As Delta tool was built in the frame of the EU Air Quality Directive, it is essential and conducive to evaluating the prediction models within regulation and policy. In this work, we demonstrate the procedure for implementing model data, developed previously, into the Delta tool and we show some examples of validation results.

Keywords: Delta tool, model validation, ozone prediction, air quality.

INTRODUCTION

Forecasts of various meteorological and air-quality parameters are produced based on previously developed prediction models. As these predictions are important for informing the population, the models have to be validated in order to comply with the standards defined by the public administration, e.g. the Environmental Model Guidance document of the US-EPA [1], the UK-DEFRA report [2], and the European Air Quality Directive 2008 [3].

Model evaluation involves various steps such as scientific evaluation, code verification, sensitivity analysis, model validation, etc. [4]. There are various methodologies and software packages of this complex procedure that have been developed in the past decades. For example, the BOOT software [4] was developed for assessing the dispersion model; however, it only supports statistic metrics without any graphic data results. The ENSEMBLE web-based platform [5], used for dispersion model and inter-comparison and evaluation of atmospheric chemistry transport, is widely used for research purposes or periodic model evaluation exercises. It has been used to support emergency response situations.

Delta tool, which is based on the IDL software environment, is developed as an easily handled

**Correspondence to: Dejan Gradišar, Department of Systems and Control, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, E-mail: dejan.gradisar@ijs.si*

and commonly used evaluation tool for air quality models. It is designed within the framework of FAIRMODE (Forum for Air quality Modeling, http://fairmode.jrc.ec.europa.eu/), which provides a procedure for benchmarking air quality models [6]. Tested on Linux and Windows systems, *Delta* tool applies a graphical user interface which helps users to understand and use all of the functions. Relying on the EU Air Quality Directive (AQD) [3], it supports pollutants and scales such as ozone, Particulate Matter, and Nitrogen, with data spanning an entire calendar year. For our research prediction models, we focus only on the prediction validation of ozone.

Delta tool works on pairs of modeled-observed data at surface level. Thus, the modeled data should be inserted at the surface level at each station location. The station should be carefully analyzed based on the grid resolution and data availability. The minimum available data over the selected time should be 75 percent, which is defined in [3]. *Delta* tool not only can compare the modeled and observed data within one model, it also supports the function of comparison with different models. The structure of *Delta* tool includes four modules: an input module, which contains both modeled and measured data; a configuration module, which connects the input files with statistical elaboration; the analysis module shows the benchmarking and exploration; and, an output module, which produces the diagrams and summary reports. Fig. 1 shows the sequences of the four main modules.

Because of EU directives, which define levels of air quality for the protection of human health, it is essential to generate a precise prediction model for assessment. At the same time, ozone pollution is one of the air pollutants that poses the greatest threat to human health in Slovenia. Thus, some models have been built to improve the accuracy of forecasting ozone concentration in urban locations in Slovenia, including Gaussian Process models with online updated data presented in [7], a hybrid Model discussed in [8], and an integrated model with empirical and deterministic models described in [9]. Because the *Delta* tool is built based on the EU AQD (2008), it can be a useful tool for comparing the prediction results. In this paper, we use the prediction results from the Gaussian Process in [7] as an example to show how the *Delta* tool works with our models.

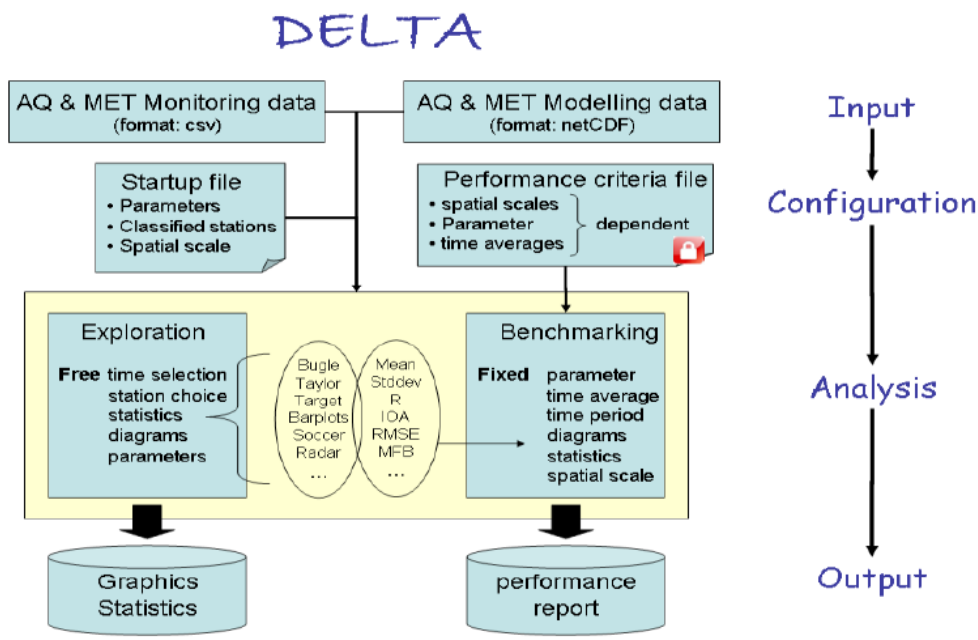

Fig. 1. *Delta* tool structure.

STEPS TO RUN *Delta* TOOL

To test our prediction model by using the benchmarking *Delta* tool, it is necessary to create several input files in the Delta tool folder. These input files are (i) *INI* file, (ii) monitoring data files, and (iii) modeling data files. Additionally, it is also essential to make some modifications in the *MyDeltaInput.dat* file to point to the correct directory. After preparation of all files, we can open the *Delta* tool and check their integrity.

A. Preparation of input files

1) INI file: The *startup.ini* file is usually located in the source folder. It is used to give general information about the spatial scale, the parameters and the characteristics of the monitoring stations. For our model validation, we only need to show a maximum of five stations, which are Koper, Ljubljana, Nova Gorica, Celje, and Zagorje. The information about these stations can be found in our research article ”Improving of local ozone forecasting by integrated models” [9].

2) Observation data files: Every station should have its own *CSV* format file containing measured data for one entire year. Because the measured data provided to us are stored in Matlab *mat* files, it is necessary to rewrite them into *CSV* format files with columns: year, month, hour, and the observed parameters. It should be noted that all missing data must be set to -999. Since daily values with all hours from 0 to 23 must be included, the daily data we have has been repeated 24 times for each day. Finally, it is important to make sure that the file name for each station should be the same as the name in the *startup.ini* file.

3) Model data file: *Delta* tool requires the model output data to be given in *netcdf* format. To help with that, *Delta* tool provides the conversion tool to change *CSV* format files to *netcdf*. First we have to convert the Matlab data to a *CSV* format file, similarly, as with the observation data. Then we can use the conversion tool to get the *CDF* file. We can combine all the stations into one *CDF* file. Here, we should first change the directory definition in the *InfoMODcsv2cdf.txt* file, which is located in the ”conversion” folder. Then, open the conversion tool widget available under the help menu and click ”ReadInfo” to import the new *InfoMODcsv2cdf.txt* file.

4) MyDeltaInput.dat: The *MyDeltaInput.dat* file, located in the *./resource* directory, aims to show the locations of the three inputs, which are *startup.ini*, prediction data *CDF* files, and observation data *CSV* files. This file should be modified according to the following instructions [10]:

- first line: put the name of the *startup.ini-/* file in the *./resource* directory,
- second line: put the location of the model data in the *./data* directory,
- third line: put the location of the monitoring data in the *./data* directory.

B. Data Integrity Check

Delta tool can help us to check the consistency and integrity of all the input files. Select the item ”Help”>”Data check integrity tool” from the *Delta* tool top menu and the data check integrity process will run automatically. If there are any problems, it stops immediately and shows where and what the problems are.

C. Data Selection and Analysis Window

The users should make selections in the ”Data selection” and ”Analysis” window interfaces in order to get the final reports. The data selection interface contains model selection, parameter selection, and station selection. We will use the prediction model of 8-h average ozone concentration as an example to demonstrate the results in the next section.

Analysis selection contains choices of all the graphs and plots from *Delta* tool, such as the standardized mean-squared error (SMSE), time series plots, and so on. It should be noted that some of the plots have specific requirements such as threshold numbers or limits of stations.

RESULTS

This section provides the validation of an ozone prediction model, described in [7]. The prediction model is developed with an evolving Gaussian Process model. These kinds of models

update online with new incoming measurements. The model is aimed at making predictions of the daily maximum ozone concentrations one-day ahead and predictions of the maximum 8-h-averaged ozone concentrations one-day ahead. The daily maximum value is defined as the maximum value of the hourly average ozone concentrations obtained between 1 and 24 h on a particular day. An 8-h-averaged value at the moment of consideration is the moving average of eight consecutive, hourly, average ozone concentrations, including the most recent one. The 8-h-averaged values from which the maximum for a particular day is determined are presented as moving averages, calculated between 1 and 24 h on the particular day.

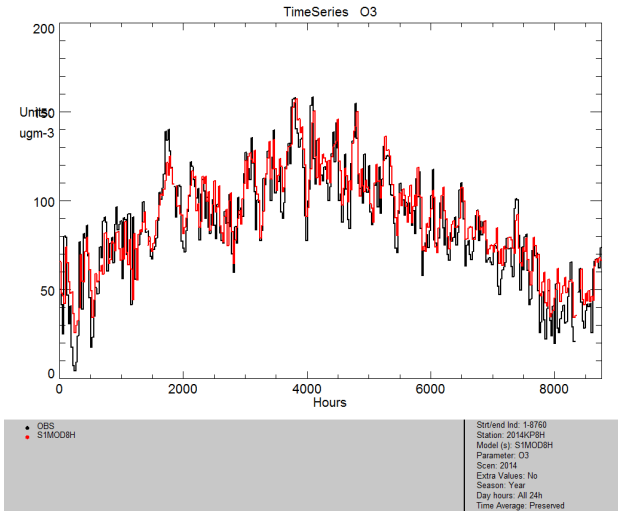

Fig. 2. Time series - Koper.

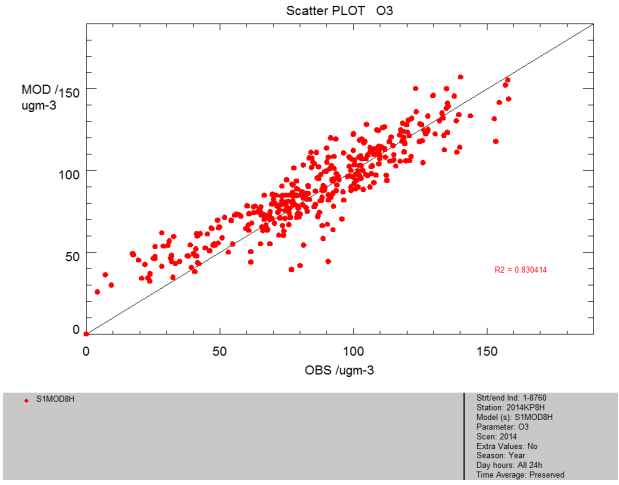

Fig. 3. Daily Model vs Observation values - Koper.

The benchmarking of air quality models is discussed within the framework of FAIRMODE. It is essential to design a method of model validation for policy requirement, as was previously discussed. The model performance report generated by *Delta* tool describes the strengths and weaknesses of a specific model. This report uses RMSE, R, NMB, NMSD and CRMSE, which are five core statistical indicators [11].

A. General reports

The time series in Fig. 2 shows observation (OBS) and prediction values for 8-h average daily ozone concentrations (S1MOD8H) over one year (2014) for the city of Koper. The prediction results can also be performed by scatter plots. The scatter plot indicates the predicted values versus the observation values for 8-h-average daily ozone concentrations (see Fig. 3). The scatter plot of mean values (Mean of Models Vs Mean of Observations) for four stations is showed in Fig. 4. Each single point represents average statistics for a given station.

There are several essential barplots we can get from the *Delta* tool. For example, a barplot of RMSE is showed in Fig. 5. Similarly, other measures can be represented such as Correlation coefficients (R), a Factor of two of the observations (FAC2), Normalised bias, and Standard deviation.

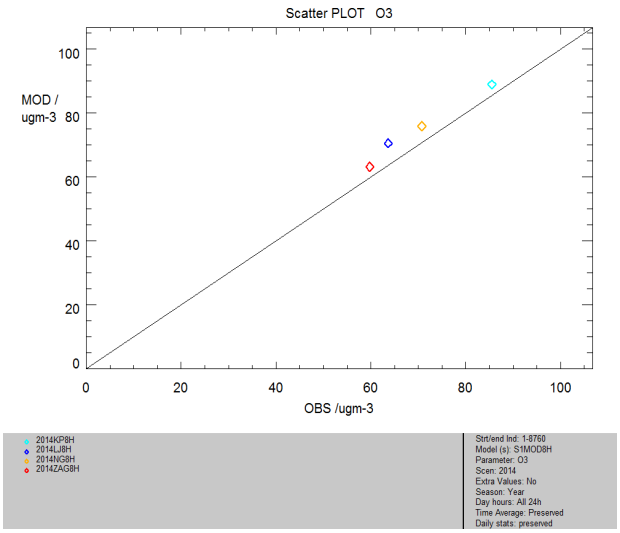

Fig. 4. Scatter plot of mean values (Mean Mods vs Mean Obs).

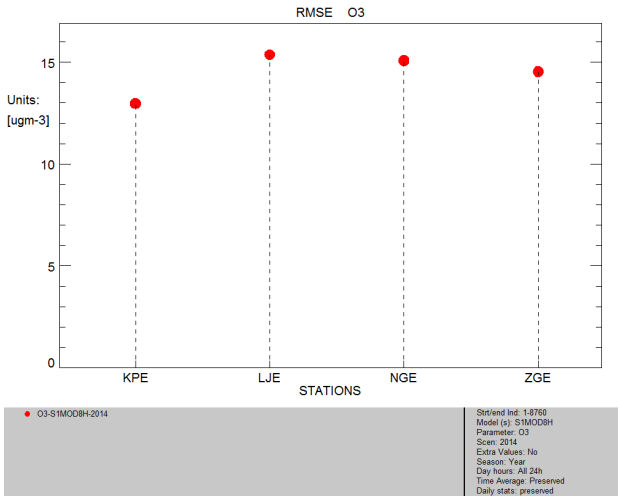

Fig. 5. The root mean square error (RMSE) of

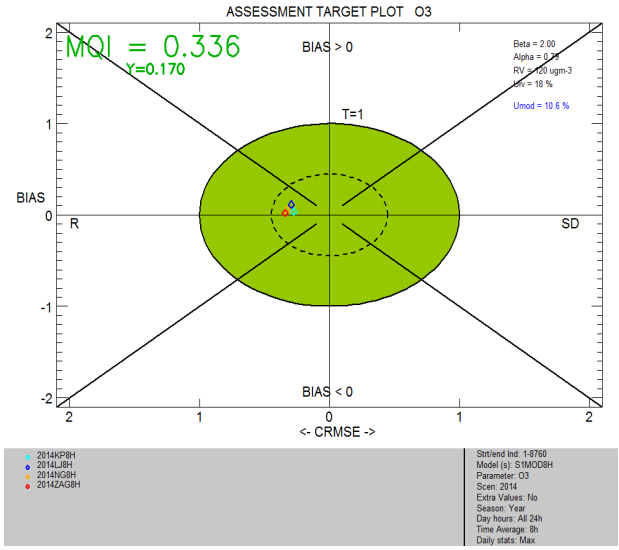

Fig. 6. Target diagram for O3 8h max values.

B. Target MQI diagram and summary report

The target diagram (Fig. 6) allows for the representation of different statistical indicators in a single plot - SD, BIAS, CRMSE, and R. These divide the screen into four areas. The CRMSE related error aims to express if it is dominated by SD or by R [10]. The target diagram gives the overview of model performance at every station. MQI (Model Quality Indicator) represents the distance between the origin and a given station point, shown in the upper left corner of Figure 6. The model is good if the MQI is less or equal to one, i.e. the green circled area. The dashed circle

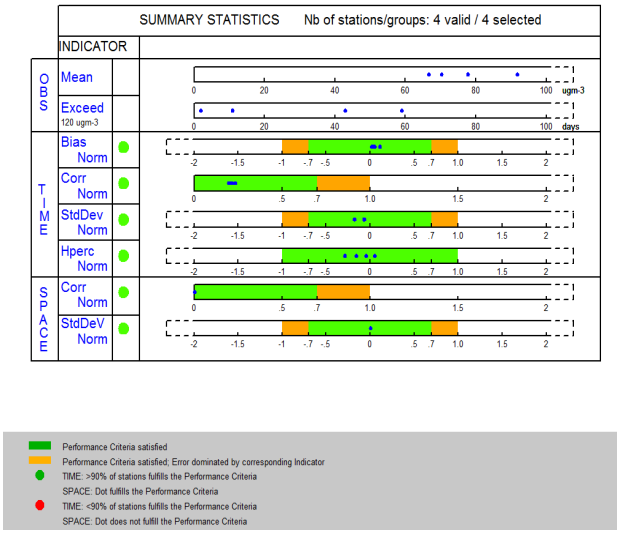

Fig. 7. Summary Report.

on Fig. 6 indicates an assessment of the general observational uncertainty [12].

The summary report (see Fig. 7) provides a complementary source of information to the target diagram to identify the model strengths and weaknesses. From Fig. 7, the first two rows show the mean value of measurement and the number of exceedances with threshold value 200 $ug = m^3$ for the 8 h daily ozone maximum. Rows 3 to 6 show the statistics of bias, correlation, and standard deviation. The green area indicates criteria fulfillment. The orange area shows the criteria fulfillment with some error related to the particular indicator. The last two rows show the overview of correlation and standard deviation, which are calculated with the average values of a particular time period. The single point on every bar shows the spatial correlation of the selected stations [10].

CONCLUSIONS

Delta tool, as an IDL based model validation software, compares modeled and observed data with pairs. Thus, there are two data files in the *Delta* tool folder that are monitoring and modeling the data folder. These data files are prepared in *CSV* format. Because *Delta* tool is generated based on the EU AQD [3], it evaluates all the data based on the annual ozone concentration measurement. The modeling

data files are converted to *netcdf* format by the conversion tool that has been installed in *Delta*.

The data from the prediction model, discussed in [7], is prepared for the evaluation. Depending on different statistical indicators, *Delta* tool can generate various graphical diagrams such as bar plots showing RMSE, R, NMB, NMSD, and CRMSE; scatter plots and time series with entire calendar year data; Taylor diagrams; target MQI diagrams; summary reports and so on. The target MQI diagram is one of the most important visual graphs to express the model validation results. This diagram can indicate almost all previously mentioned statistical results and shows the analysis of the model performance in one place. Moreover, the summary report is a supplement of the target diagram, so that it gives more detailed and numerical results of assessment.

Delta tool provides relevant comparison results of every model. It also can be used to compare several different model results at the same time. In addition, *Delta* tool is not difficult to use even by a semiskilled researcher. Because this tool is newly released, there are still some inapplicable functions such as the planning tab. Moreover, this application can only compare the results of prediction data, the other elements of model evaluation, such as sensitivity analysis, are still lacking.

Acknowledgments

This work was supported by the Slovenian Research Agency with Grant Method for the forecasting of local radiological pollution of atmosphere using Gaussian process models, ID L2-8174 and Grant Systems and Control, P2-0001.

REFERENCES

1. EPA, Guidance Document on the Development, Evaluation, and Application of Regulatory Environmental Models. No. EPA/100/K-09/003. U.S. Environmental Protection Agency, 2009.
2. D. Derwent, A. Fraser, J. Abbott, P. Willis, T. Murrells, Evaluating the performance of air quality models, Department for Environment and Rural Affairs, UK, 2010.
3. EU-Commission, Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe, Official Journal of the European Communities, v. L 152, 2008, 1-44.
4. C.J. Chang, R.S. Hanna, Air quality model performance evaluation, Meteorology and Atmospheric Physics, 87, 2004, 167-196.
5. S. Galmarini, R. Bianconi, G. de Vries, R. Bellasio, Real-time monitoring data for real-time multi-model validation: coupling ENSEMBLE and EURDEP, Journal of Environmental Radioactivity, 99, 2008, 1233-1241.
6. S. Janssen, C. Guerreiro, P. Viaene, E. Georgieva, P. Thunis, Guidance Document on Modelling Quality Objectives and Benchmarking, FAIRMODE, 2017.
7. J. Kocijan, D. Gradišar, M.Z. Božnar, B. Grašič, P. Mlakar, Online algorithm for ground-level ozone prediction with a mobile station, Atmospheric Environment, 131, 2016, 326-333.
8. D. Gradišar, B. Grašič, M.Z. Božnar, P. Mlakar, J. Kocijan, Improving of local ozone forecasting by integrated models, Environmental Science and Pollution Research, 2016, 1-12.
9. D. Gradišar, B. Grašič, M.Z. Božnar, P. Mlakar, J. Kocijan, Local ozone prediction with hybrid model, in Simultech 16, July 2016.
10. P. Thunis, C. Cuvelier, DELTA Version 5.4, Concepts / Users Guide / Diagrams. Brussels: Joint Research Centre, Ispra, 2016.
11. P. Thunis, A. Pederzoli, D. Pernigotti, Performance criteria to evaluate air quality modeling applications, Atmospheric Environment, 59, 2012, 476-482.
12. P. Thunis, E. Georgieva, A. Pederzoli, A tool to evaluate air quality model performances in regulatory applications, Environmental Modelling & Software, 38, 2012, 220-230.