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RESEARCH ARTICLE

Improving of local ozone forecasting by integrated models

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Abstract This paper discuss the problem of forecasting the maximum ozone concentrations in urban microlocations, where reliable alerting of the local population when thresholds have been surpassed is necessary. To improve the forecast, the methodology of integrated models is proposed. The model is based on multilayer perceptron neural networks that use as inputs all available information from QualeAria air-quality model, WRF numerical weather prediction model and onsite measurements of meteorology and air pollution. While air-quality and meteorological models cover large geographical 3-dimensional space, their local resolution is often not satisfactory. On the other hand, empirical methods have the advantage of good local forecasts. In this paper, integrated models are used for improved 1-day-ahead forecasting of the maximum hourly value of ozone within each day for representative locations in Slovenia. The WRF meteorological model is used for forecasting meteorological variables and the QualeAria air-quality model for gas concentrations. Their predictions, together with measurements from ground stations, are used as inputs to a neural network. The model validation results show that integrated models noticeably improve ozone forecasts and provide better alert systems.

Keywords Air pollution · Ozone forecast · WRF numerical weather prediction model · Artificial neural networks

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Introduction

Tropospheric ozone is one of the main air pollutants that causes health problems. Consequently, it constitutes an important element of real-time air-quality forecasting. The forecasting of tropospheric ozone is necessary and obligatory due to EU directives that regulate standards of air quality that guarantee the protection of human health as well as the thresholds of ozone for informing and alerting the public when they are violated.

Ozone increases during periods of high temperatures and sunny skies. Beside meteorological variables, various gases in the troposphere also have a documented influence on the formation of ozone. The ozone content changes in the troposphere and the complexity of the processes determining these changes are the reasons why the modelling of the dynamics of atmospheric ozone is the subject of intense research activity.

Air-quality and meteorological models are necessary for accurate forecasts of ozone concentration, which are necessary for informing and alerting the public about exceeded thresholds. These models can be developed using a variety of methods that contain the scientific understanding of the physical processes involved in air quality and meteorology. The alternative to these deterministic models are empirical models, usually obtained with statistical methods, that describe the nonlinear dynamics of air-quality components, formed from available measurement data only. Therefore, there exists a number of methods for the prediction of ozone concentration, based on various modelling techniques.

Deterministic models for air quality and, in particular, ozone forecasting (Im et al. 2015) provide prognostic time- and spatially-resolved concentrations for various scenarios (including atypical ones) and, above all, provide insights into pollutant formation processes (Zhang et al. 2012). Due to their complete spatial coverage, these models also provide forecasts in locations which are not monitored (Žabkar et al. 2015). While air-quality and meteorological models cover large geographical 3-dimensional space, their local resolution is often not satisfactory. This is a disadvantage in the case of topographically complex terrain.

On the other hand, empirical models have the advantage of good local forecasts and they are generally more suitable for modelling the concentrations of air pollutants in complex sites. When these models are developed correctly and well, they provide forecasts of higher accuracy and with better computational efficiency than deterministic models (Zhang et al. 2012). Nevertheless, the physical processes involved in air quality and meteorology cannot be seen transparently in empirical models. Various empirical models are used for air-quality forecasting, ranging from Principal Component Regression to Takagi–Sugeno fuzzy models, e.g., (Al-Alawi et al. 2008; Petelin et al. 2013; Moustris et al. 2012; Mlakar and Božnar 2011; Solaiman et al. 2008). Empirical models can be, as is the case with deterministic models, developed based on various principles each of which has its own properties, something which is stressed in the comparison of Lu and Wang (2014).

The present paper deals with improving the ozone forecasting in micro-locations for the purpose of giving alerts, in Slovenia, which has a complex and geographically diverse terrain (Žabkar et al. 2015). The present paper is part of extensive efforts to develop air-quality forecasting system for Slovenia. The main contribution of the present paper is the integration of deterministic and empirical models for forecasting ozone with the aim of uniting 'the best of both worlds' in modelling, to overcome the problem of the low resolution of deterministic models while retaining their advantages.

The idea of integrating deterministic and empirical models is not a novel one. It is quite common in fields like process engineering, e.g., (Abonyi et al. 2002; Duarte et al. 2004; von Stosch et al. 2014), where it is called hybrid modelling. However, it has rarely been employed in atmospheric science. Applications in (Pelliccioni and Tirabassi 2001; 2006; 2008; Goyal and Kumar 2012) are examples of integrating deterministic and empirical models for the elimination of system errors in diagnostic investigation of the air quality in flat terrain case studies and for so-called tracer experiments using nonreactive gasses.

The novelty of our study is that an integrated model is used for the 1-day-ahead forecast of ozone, as the reactive gas, for improving the deterministic models' insufficient resolution in a real-life situation with a complex terrain, by integrating all available information as input variables. The study is made on 3 years of data for four cities.

The present paper is structured as follows. The problem is described in the next section. The proposed methodology is introduced in "Methodology". "Results and discussion" describes and discusses the results of the experiments to show the feasibility of the proposed methodology. The conclusions are drawn at the end.

Problem description

The problem considered in this paper is to improve ozone forecasting and consequently to increase the reliability of alerts for cities in the orographically and meteorologically diverse area of Slovenia. The solution shall circumvent a real-life problem that is caused by the low resolution of the meteorological and air-quality models, something which becomes problematic at microlocations in complex terrain. The selected locations for which the reliability of alerts is to be increased are shown in Fig. 1 and listed in Table 1. All locations are urban locations, where exceeding the threshold limits affect quite large part of population, and these are the kind of locations where alerts based on EU directives are necessary.

The online forecasting model is aimed at predictions of the daily maximum ozone concentrations 1-day ahead of the target day. The daily maximum value is, in our case, defined as the maximum value of the hourly average ozone concentrations obtained between 1 and 24 h on a particular day. The predictions of the model for the target day are made at 07:30 UTC of that day.

Methodology

Our goal is to develop an integrated ozone-forecasting model, composed of deterministic and empirical models. Such a model allows us to use the advantages of both and produce more accurate forecasts. Two deterministic models are used in our study: one for air-quality predictions and another to predict the meteorological variables. Besides those, we use a database with various historical meteorological and air-quality values measured in specific locations for the training of empirical models.

Fig. 1 Geographical locations of the selected locations showing the topographical diversity (Wikimedia 2016)

Four sets of ozone-concentration predictions will be developed for each of the selected locations:

1. Predictions based on deterministic air-quality and meteorological models, together denoted by Model 1.
2. Predictions based on an empirical model, viz., a neural network model that has been developed based on air-quality and meteorological measurements for the target day. This model is highly accurate for the microlocation from where the measurements have been sampled. However, it is unrealistic, because in reality, the meteorological regressors for the time of prediction can be based on meteorological forecasts only. Nevertheless, the predictions of such a model are in our case used for comparison with the other model's accuracy, and the model will be referred to as the idealistic neural-network model and denoted by Model 2.
3. Predictions based on an empirical model, viz., a neural-network model that has been developed based on meteorological forecasts and the history of air-quality and meteorological measurements—this is the realistic scenario. Air-quality predictions are not taken as an input in this case. This model will be referred to as the realistic neural-network model and denoted by Model 3.
4. Predictions based on an integrated model for each of the selected microlocations, which will integrate all available information, i.e., the history of air-quality and meteorological measurements from that specific location, and air-quality and meteorological forecasts from the deterministic models available for that region.

   The aim of the integrated model, denoted by Model 4, is to attain the prediction quality of the idealistic neural-network model and at the same time retain the transparency of the deterministic model.

Two deterministic models are used in our study: one to predict air quality (QualeAria) and the other for meteorological forecasts (WRF model). Note that any other available models to predict air quality and meteorological parameters can be used.

The air-quality model—QualeAria

Air quality predictions for selected locations are obtained with the QualeAria forecasting system. QualeAria implements three-dimensional state-of-the-art models to describe the emission, dispersion and transformation of pollutants in the atmosphere. It is based on the Flexible Air quality

Table 1 Air quality monitoring sites describing type of area/influence (EU-Commission 2011) and topographical features expressed with hlTc index, that explains the height and length of topographic complexity (Božnar et al. 2012)

Monitoring Site	Abbreviation	Type of area	Type of influence	Altitude [m]	hlTc [m]
Nova Gorica	NG	Urban	Traffic	113	500,3000
Koper	KP	Urban	Background	72	180,3000
Ljubljana	LJ	Urban	Background	299	200,2500
Celje	CE	Urban	Background	240	100,2000

Regional Model—FARM, a 3D Eulerian model simulating the dispersion and chemical reactions of atmospheric pollutants (Kukkonen et al. 2012). The model is operationally run by the ARIANET company and is coupled with the meteorological model called the Regional Atmospheric Model System—RAMS, Srl and ENEA (2016). It is part of the MINNI Italian national modelling system (Zanini et al. 2005) and is based on the same meteorological and air-quality models.

The QualeAria system is currently configured on two nested computational grids (see Fig. 2), the wider one covering Europe at a horizontal resolution of 48 km, and the smaller one covering Italy and its near neighbourhood at 12 km resolution. Slovenia is placed in the inner part of the second modelling domain, far enough from the domain's border so that the results for Slovene territory are not heavily affected by the boundary conditions. QualeAria produces air pollution forecasts for Slovenia for up to 2 days in advance at 1-h time resolution and also at 12 km spatial resolution. The first day predictions are utilised for the modelling. The predictions of the main pollutants from this configuration are validated in Božnar et al. (2014) and are available online on a daily basis on the KOoreg website (MEIS d.o.o. 2016).

The meteorological model—WRF

Meteorological predictions for selected locations are obtained with the Weather Research & Forecast—WRF model (Skamarock et al. 2008). The WRF model is a numerical weather prediction system that is used for operational forecasting and for atmospheric research. The WRF model was developed cooperatively by the US institutions National Centers for Environmental Prediction (NCEP), National Center for Atmospheric Research (NCAR), and the meteorological research community. There are two dynamics solvers in the WRF software framework: the Advanced Research WRF (ARW) and the Nonhydrostatic Mesoscale Model (NNM) solver. For this study, the ARW solver, primarily developed and maintained by NCAR, is used. The

Fig. 2 Larger and smaller geographical domains used in WRF (areas with circles in corners) and QualeAria (areas with crosses in corners) model (Google 2016).

configuration of the ARW model, which runs permanently on daily basis at the MEIS company, is as follows:

- two geographical domains,
- a larger domain (central Europe): 101 by 101 cells in a resolution of 12 km per 3 hours (see Fig. 2),
- a smaller domain (Slovenia with surroundings): 76 by 76 cells in a resolution of 4 km per 30 min (see Fig. 2),
- the horizon of prediction: two days and three hours,
- The simulation of the model is finished approximately at 5:30 UTC using the data from Global Forecasting Model (GFS) at 00:00 UTC. Our simulation runs for one hour and a half, and it is repeated and finished again at 17:30 UTC. Each run's predictions overwrite the previous prediction in the overlapping time horizon in the database. This way the weather forecast is enhanced because we are using as regressors the present day forecasts.

The model with a given configuration running over the terrain of Slovenia is validated in Božnar et al. (2012). Vertical grid consists of 44 points distributed in the vertical domain of pressure from 1013 hPa (surface) to 50 hPa (top) and following topography by ETA coordinates. Used physical features (Skamarock et al. 2008):

- Cumulus parameterization proposed by Kain-Fritsch scheme (Kain 2004) in the 1st domain and none in 2nd,
- Microphysics scheme proposed by Lin et al. (1983),

Table 2 Available variables' measurements: ozone concentration (O_3), solid particles ($PM10$), nitrogen oxides concentration (NO_x), nitrogen dioxide concentration (NO_2), carbon monoxide (CO), air temperature ($AirTemp$), relative humidity ($RelHum$), global solar radiation ($GlSolRad$), wind speed ($WindSpd$), wind direction ($WindDir$), air pressure ($Pressure$) and precipitation ($Precip$)

Nova Gorica	Koper	Ljubljana	Celje
$O3$	$O3$	$O3$	$O3$
$GlSolRad$	$GlSolRad$	$GlSolRad$	$GlSolRad$
$AirTemp$	$AirTemp$	$AirTemp$	$AirTemp$
$RelHum$	$RelHum$	$RelHum$	$RelHum$
$WindSpd$	$WindSpd$	$WindSpd$	/
$WindDir$	$WindDir$	$WindDir$	/
NOx	NOx	NOx	NOx
$NO2$	$NO2$	$NO2$	$NO2$
/	/	$SO2$	$SO2$
$PM10$	$PM10$	$PM10$	$PM10$
$Precip$	$Precip$	$Precip$	$Precip$
$Pressure$	$Pressure$	/	/
/	/	CO	/

Table 3 The selected regressors for the empirical models. $k+i, i = 0, 1$ denotes consecutive time instants

	Daily maximum of hourly values
1	$O3(k)$
2	$GlSolRad(k+1)$
3	$AirTemp(k+1)$
4	$AirTemp(k)$
5	$GlSolRad(k)$
6	$RelHum(k+1)$
7	$NOx(k+1)$
8	$Pressure(k+1)$
9	$Pressure(k)$

- Planetary Boundary Layer by Yonsei University scheme (Hong et al. 2006),
- for long wave radiation it uses the Rapid Radiative Transfer Model (Mlawer et al. 1997) and
- for short wave radiation it uses the Dudhia scheme (Dudhia 1989).

The initial and boundary conditions were provided by Global Forecasting Model (GFS).

The neural network model

Statistical models are widely used for representing and predicting the dynamic state of environmental systems. They outperform the deterministic ones where localised on-line prediction is needed. Neural network (NN) models have been widely used for gas concentration forecasting since the early 1990s (Božnar et al. 1993; Dutot et al. 2007; Ibarra-Berastegi et al. 2008).

Multilayer feed-forward NN models can be understood as a nonlinear mapping from inputs to outputs (Ibarra-Berastegi et al. 2008). The mapping function is established during a training phase, where after making a previous choice of the network architecture, the NN learns to correctly associate inputs and outputs. Defining a certain type of architecture involves choosing the number of layers, the number of nodes per layer, and the number of connections.

Table 4 Performance measures in relative units (Appendix A) for different locations for predictions of daily maximum O_3 concentrations: QualeAria predictions (Model 1)

Performance measure	RMSE [$\mu g/m^3$]	SMSE	PCC	MFB	FAC2
NG	25.848	0.46	0.857	0.116	0.946
KP	25.561	0.643	0.859	0.234	0.972
LJ	21.466	0.369	0.834	0.029	0.924
CE	22.711	0.451	0.803	0.064	0.93

Table 5 Performance measures for different locations for predictions of daily maximum O_3 concentrations: idealistic NN model using measured data only (Model 2)

Performance measure	RMSE [$\mu g/m^3$]	SMSE	PCC	MFB	FAC2
NG	16.104	0.18	0.911	-0.077	0.96
KP	13.395	0.18	0.909	-0.004	0.988
LJ	13.999	0.16	0.921	-0.057	0.93
CE	15.608	0.21	0.894	-0.025	0.94

Once the network architecture is defined, the final values of the weights corresponding to the mapping function will be obtained after a fitting process which generally starts with random values of the optimisation parameters to estimate.

The NN model used in this study is the nonlinear autoregressive model with exogenous inputs (NARX). In particular, it is the MultiLayer Perceptron (MLP) network (Božnar et al. 1993). The weights of the MLP are adjustable optimisation parameters, the model inputs are exogenous variables, and the model output is the variable to be predicted. MLP can feature any smooth functional relationship between one or more inputs and variables to be predicted. This can be achieved with one hidden layer of neurons, as it is in our case.

This regression problem can be presented as a static single-output process with an n-input matrix $\mathbf{X}$ and an output vector $\mathbf{y}$. So, the estimated model can be represented by:

$$\hat{\mathbf{y}} = f(\mathbf{X}, \mathbf{w}) + \varepsilon, \quad (1)$$

where f is the nonlinear mapping realised with basis functions that are represented with activation functions and $\mathbf{w}$ are weights, i.e., the optimisation parameters of the neural regression to be estimated. ε is a zero-mean random variable. In this study, we train the NN model with 20 neurons, tangent sigmoid activation functions in the hidden layer and a linear activation function in the output layer. The weights are trained by gradient descent with a momentum optimisation algorithm (*Learning rate* = 0.1, *Momentum* = 0.1) (Božnar et al. 2012). All the NN models in our study share the same structure.

Validation methodology

The proposed integrated model (Model 4) will be compared to (i) the existing QualeAria system (Model 1), (ii) the idealistic NN model trained with inputs based on measurements only (Model 2) and (iii) the realistic NN model trained with measurements from previous days and forecasts for the target day for input meteorological variables from the WRF model (Model 3).

To make it more reliable, the methodology is validated in four different locations in Slovenia with different properties. Nova Gorica has a Mediterranean climate, with its air quality strongly influenced by the river Po and the industrial Friuli region in Italy. Koper is an industrial and port town on the Adriatic coast with a Mediterranean climate and is influenced by the same factors as Nova Gorica. Ljubljana is the biggest city in Slovenia and has an unfavourable geographical location in a wider basin with a continental climate, where industrial air pollution is combined with the air pollution from traffic and domestic heating. Similar characteristics apply to the Celje region.

All the empirical models, including the integrated models, have been trained on measurements from a period of 1 year and tested on measurements from the period of the two subsequent years. This was done for the purpose of demonstrating the performance of the forecasting models for a longer period.

Results and discussion

Measurements

The meteorological and air-quality variables at the selected locations were measured and then elaborated on an hourly basis. The measured data in this study were acquired for all the available variables, as listed in Table 2, for each location, for a period of 3 years (from the beginning of 2012 to the end of 2014).

Table 6 Performance measures for different locations for predictions of daily maximum O_3 concentrations: NN using measured data and WRF meteorological predictions (Model 3)

Performance measure	RMSE [$\mu g/m^3$]	SMSE	PCC	MFB	FAC2
NG	17.601	0.213	0.892	-0.065	0.937
KP	14.513	0.207	0.891	-0.03	0.987
LJ	16.288	0.212	0.89	-0.053	0.919
CE	17.134	0.257	0.87	-0.054	0.93

Besides the measurements, 1-day ahead predictions of meteorological variables obtained from the WRF modelling system, and air-quality variables forecast by the QualeAria system for the same period of time are available.

Regressor selection

To gain a credible ozone forecast, the model needs input data of all influential variables. However, with the number of available variables and their lagged values, the size of the regression vector or input features and, consequently, of the model, increases noticeably. For this reason, it is necessary to select only the regressors that add the most information to the prediction. Various methods for the selection of the regressors or features are available.

In this paper, we use the methodology of input variable selection presented in Kocijan et al. (2016). This methodology combines various regressor-selection algorithms, where the rankings achieved are first averaged for every location and these are later grouped to obtain the final sequence of regressors, ordered in terms of their importance. In the second stage, we determine how many of regressors should be used in order to produce the best prediction, using 10-fold cross-validation. The first nine regressors from the final selection give the best results on average on all locations and measures and are given in Table 3. Note that the integrated model uses one additional regressor: the value of ozone from the QualeAria system for the target day ($O3(k+1)$). As prediction for NO_x needed in integrated model is not available from QualeAria model, NO_2 is used instead which is a reasonable substitute for NO_x. In the case that there are no measurements for some regressors, the training and prediction are performed without that time interval. All listed regressors have been used for the empirical as well as for the integrated models, but forecasts are used instead of measurements when necessary according to the type of model. Note that the NO_x regressor is not used in the realistic NN model because the measurement for the target day is not available.

This procedure makes it possible to obtain an averaged set of regressors that encompasses the significant regressors for all the involved locations. The rationale behind the described selection procedure is to obtain a single uniform regression vector for a larger area, in our case the urban parts of Slovenia, and to avoid having to select the regressors every time we include a new location.

Prediction quality

In this section, we compare all four different models used for 1-day-ahead predictions of 1h O_3 daily maxima in four different locations. The predictions are validated with the following performance measures, which are described in the Appendix A: the root mean square error (RMSE), the

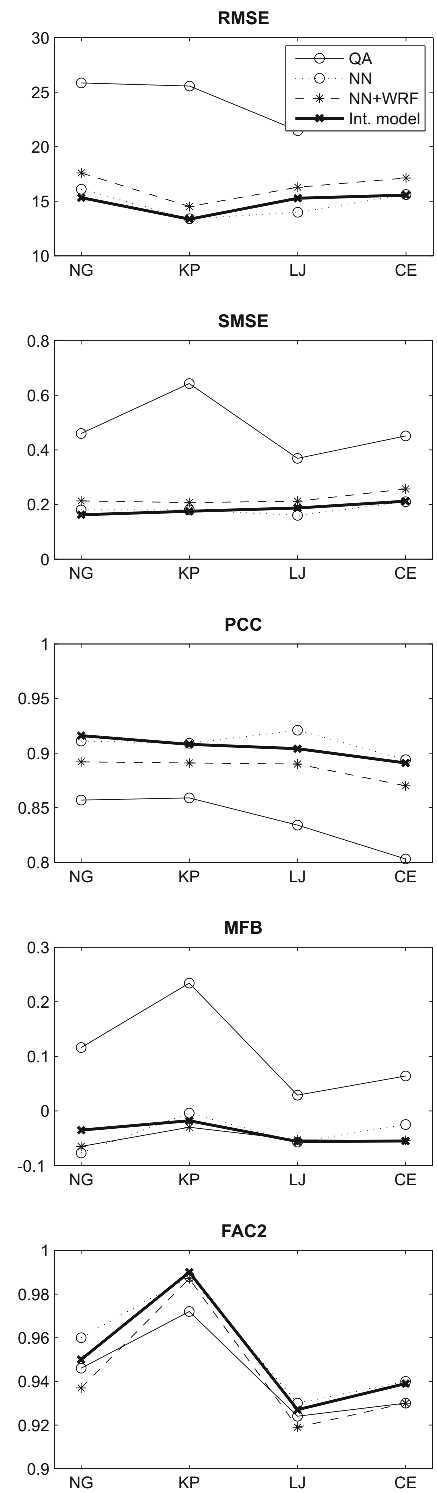

Fig. 3 Site by site comparison: QualeAria predictions (Model 1), NN using measured data (Model 2), NN using measured data and WRF predictions (Model 3) and Integrated model (Model 4)

Table 7 Performance measures for different locations for predictions of daily maximum concentrations: integrated model predictions (Model 4)

Performance measure	RMSE [$\mu g/m^3$]	SMSE	PCC	MFB	FAC2
NG	15.323	0.162	0.916	-0.035	0.95
KP	13.362	0.175	0.908	-0.018	0.99
LJ	15.28	0.187	0.904	-0.056	0.927
CE	15.564	0.212	0.891	-0.055	0.939

standardised mean-squared error (SMSE), Pearson's correlation coefficient (PCC), the mean fractional bias (MFB) and the factor of the modelled values within a factor of two of the observations (FAC2).

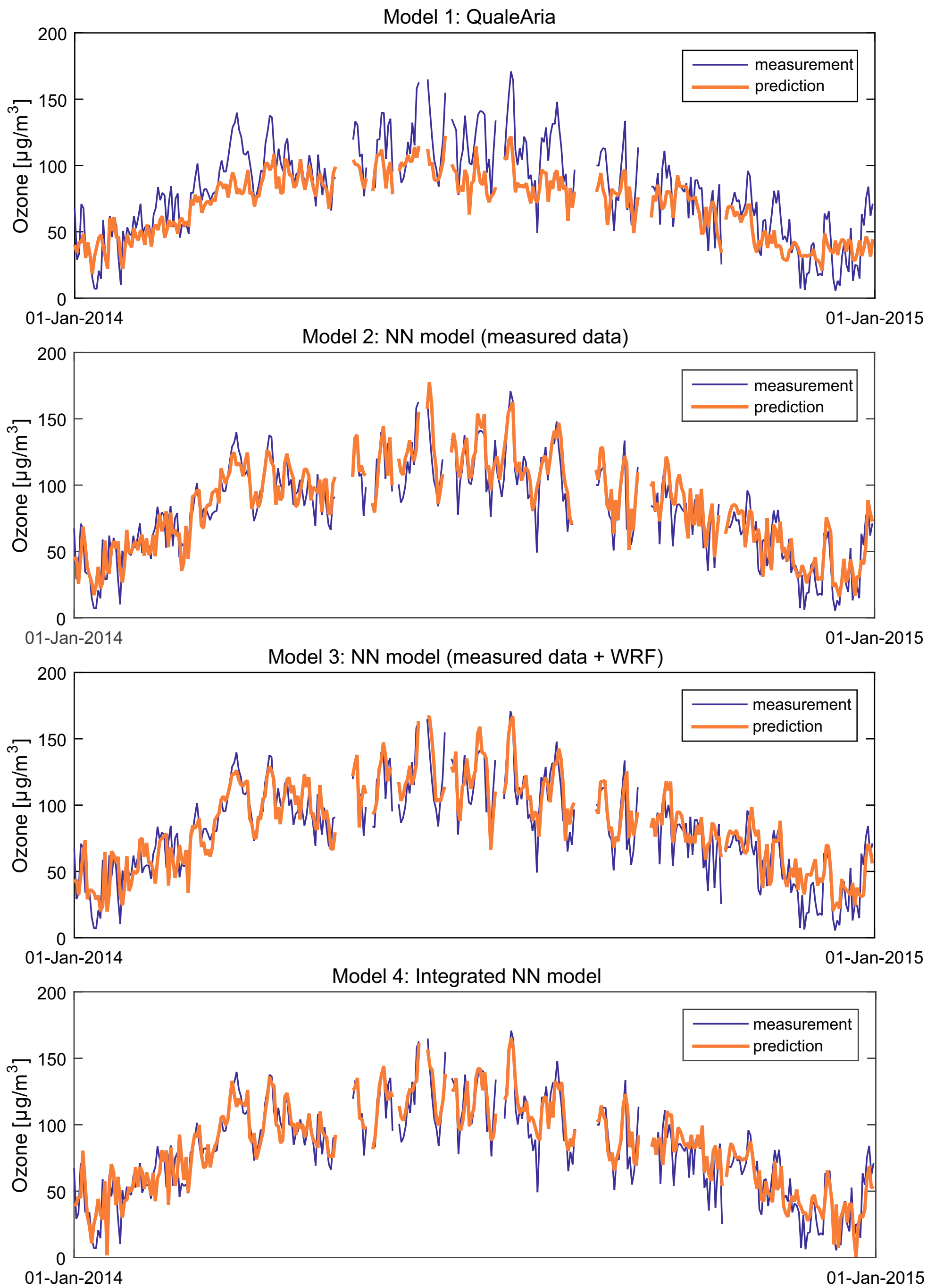

Fig. 4 Time-series plot of predictions for daily maximum ozone concentrations for Nova Gorica: QualeAria predictions (Model 1), NN using measured data (Model 2), NN using measured data and WRF predictions (Model 3) and integrated model (Model 4)

Firstly, we analyse the prediction quality of the QualeAria system. As described in "The air-quality model—QualeAria", its spatial resolution is 12 km. Therefore, we can expect that its predictions are not equally accurate in every location. The problems are related to imperfect emission inventory. For instance, bad inventory for traffic influences the traffic and urban type of stations. Also, the spatial resolution of the inventory and again system itself are not sufficient for the complexity of the terrain (see index hlTc in Table 1). The resulting performance measures for all tested locations are listed in Table 4.

Next, we introduce the idealistic NN model. The regressors from Table 3 are used for training and prediction of the ozone concentration level. In this case, we assume the ideal case, where also the regressors corresponding to the time of prediction (the target day) are taken from the database of measurements as surrogates for a perfect forecast. The rationale is to obtain the best attainable model and predictions that can be used as the reference for other models and their predictions. The evaluation of the model predictions is presented in Table 5. It can be seen from the table that the predictions of the idealistic NN model are much better than those from Table 4. Nevertheless, the idealistic model cannot provide insights into the pollutant formation processes.

In the next type of model, we include the publicly available meteorological forecasts instead of the measurements for the time of prediction. This constitutes a more realistic case study and is a common modelling practice described in the literature. Air quality predictions are not taken as inputs (Model 3).

The evaluations of the NN model's predictions using historical measured data and meteorological predictions from the WRF model are given in Table 6.

The prediction results are, as expected, worse than those of the idealistic NN model, because of the uncertainties of meteorological forecasts. However, the predictions are better than those of the deterministic model, because of their local enhancement.

Finally, we present the evaluation results for the integrated model (Model 4). The idea of the integrated model is to enhance the predictions from the deterministic model with the empirical model. This can be seen as the serial connection of the deterministic model and the empirical model. This way, the addition of the NN to the deterministic model compensates for the model mismatch in microlocations due to resolution inaccuracies.

The integrated model also uses predicted air-quality regressors, including the ozone concentration, provided by the QualeAria forecast system. Consequently, the regressors are combined from the historical measured data of air-quality and meteorological variables, from predicted meteorological regressors obtained from the WRF model, and predicted air-quality regressors for O_3 and NOx from the QualeAria model for the target day.

The evaluation of the integrated model predictions is given in Table 7 and confirms the improvement in the quality of the predictions.

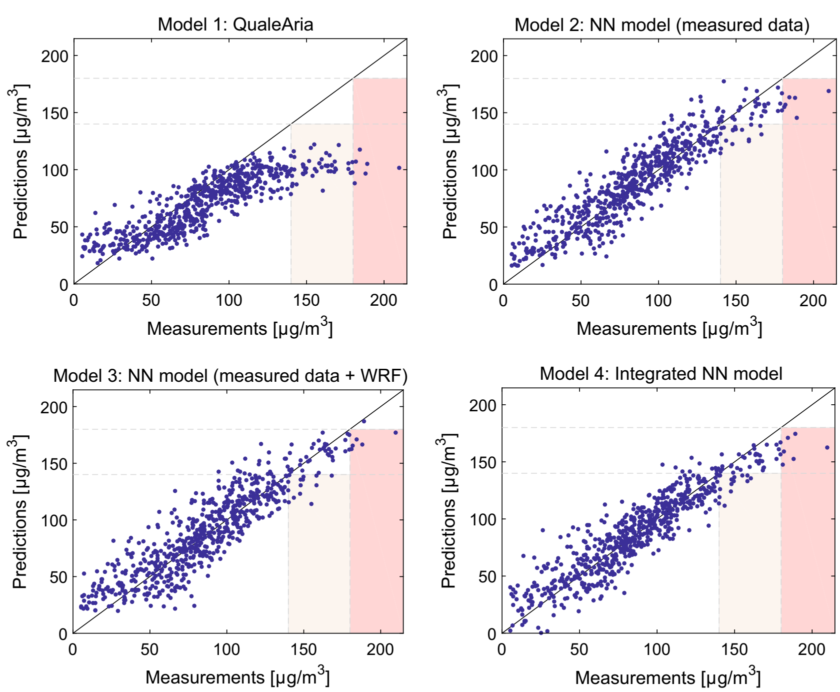

Fig. 5 Predicted values versus observation values for daily maximum ozone concentrations for Nova Gorica: QualeAria predictions (*upper left*), NN using measured data (*upper right*), NN using measured data and WRF predictions (*lower left*), integrated model (*lower right*)

Table 8 No. of threshold violations (Actual alarms/Correct forecasts/False alarms)

	Threshold [$\mu g/m^3$]	QualeAria	NN	NN + WRF	Integrated model
NG	$\geq$ 140	52/0/0	51/36/18	52/40/18	52/39/10
	$\geq$ 180	6/0/0	6/0/0	6/1/0	6/0/0
KP	$\geq$ 140	52/2/0	52/34/14	52/30/17	52/32/10
	$\geq$ 180	5/0/0	5/0/0	5/0/0	5/0/0
LJ	$\geq$ 140	21/0/0	21/16/3	21/13/5	21/13/7
	$\geq$ 180	1/0/0	1/0/0	1/0/0	1/0/0
CE	$\geq$ 140	12/0/0	12/9/6	12/8/0	12/9/3
	$\geq$ 180	0/0/0	0/0/0	0/0/0	0/0/0

The performance measurement statistics compared site-by-site are given in Fig. 3. The improvement of the integrated model prediction results over the realistic NN model and deterministic model can be seen from the presented results.

The results show that in the case of complex terrain, the deterministic air-quality models can be upgraded and their results enhanced with a properly trained empirical model. It is clear that the predictions of the integrated model come sufficiently close to those of the idealistic NN model, but retaining the advantages of the deterministic model.

It is important to note that any suitable deterministic and any properly trained empirical nonlinear model can be used to pursue the proposed modelling and forecasting method for complex terrain. The selection at hand was conditioned by the availability of the data and experience in using artificial neural networks.

Next, a visual comparison of the models' predictions, employing scatter plots and time responses, will be given; due to space constraints, only for one of the considered locations, namely Nova Gorica, where a high ozone level is the most problematic. In Fig. 4, time-series plots of the measured and predicted values for one year (2014) are shown. It can be observed that the predictions by the QualeAria forecasting system are not up to the predictions of the integrated model.

The same prediction results are shown also in scatter plots in Fig. 5. The figures compare the predicted and measured values. It can be seen that the prediction quality for the location of interest improves when NN models are used that use the information gained from measurements at microlocations. The predictions from the idealistic NN model that uses only measured data shall be considered as the reference (see Fig. 5b).

The main purpose of the ozone-concentration forecasting is to predict when concentration values violate the prescribed thresholds. The European Union's Air Quality Directive (EU-Commission 2008) sets four standards to reduce air pollution by ozone and its impacts on health: (i) information threshold: 1-h average ozone concentration of 180 $\mu g/m^3$, (ii) alert threshold: 1-h average ozone concentration of 240 $\mu g/m^3$, (iii) long-term objective: the maximum daily 8-h mean concentration of ozone should not exceed 120 $\mu g/m^3$, (iv) target value: long-term objective (120 $\mu g/m^3$) should not be exceeded on more than 25 days per year, averaged over three years.

We have analysed how successful our prediction models would be when used to alert about cases of 1-h ozone concentration. It never occurs that the alert threshold (240 $\mu g/m^3$) is violated in the observed years. In Table 8, the number of information threshold violations (180 $\mu g/m^3$) is given, together with the number of violations of additional—lowered—informative threshold (140 $\mu g/m^3$). This threshold is added in order to show the prediction capabilities of our models. In Table 8, all violations detected in 2013–2014 are listed, i.e., actual (correctly/failed forecasts).

The successfulness of the detection of threshold violations for the case of Nova Gorica is illustrated also in Fig. 5. The area marked with lighter colour indicates situations when the model prediction fails to predict violations of the 140 $\mu g/m^3$ threshold, and the area with darker colour indicates failures to predict violations of the 180 $\mu g/m^3$ threshold.

From the presented results, it is clear that the developed integrated model, based on local measured data together with the available predictive meteorological and air-quality values, predicts ozone concentrations better than the currently available QualeAria system at the selected microlocations. Nevertheless, the number of correctly forecast alarms can still be improved, which indicates that the set of regressors is not yet perfect.

Conclusions

An application of an integrated model for improving ozone forecasting at urban micro-locations in the complex terrain of Slovenia is described in the paper. Realistic case studies of four cities, positioned in orographically and meteorologically diverse places, are used for demonstrating air-quality forecasting models that have been developed and validated for the longer time period of 3 years.

The models for these four cities are integrated combinations of the QueleAria air-quality model, the WRF meteorological model and empirical neural network models. The analysis showed that the QualeAria air-quality model cannot forecast ozone accurately enough for the purpose of issuing alerts for microlocations, because its horizontal resolution is too low and it misses a fair amount of details. The ability of the empirical neural-network model to provide higher forecast accuracy as compared to deterministic models has been used to enhance the deterministic models for specific microlocations. This integration enables the combined models to maintain the scientific insights into pollutant formation processes and prognostic abilities for atypical scenarios, but have an improved forecasting ability for these microlocations. Further, the integrated model for forecasting is not much more demanding, computationally, than the air-quality and meteorological models themselves.

Even though this integration has been built from three particular types of models, this methodology can in general be used with any kind of air-quality, meteorological and nonlinear empirical models, provided that these models are developed, validated and implemented correctly.

The analysis shows that the integrated model under realistic conditions provides superior forecasting results than deterministic models and realistic empirical model separately. An effective methodology for the development of a model with an increased reliability of ozone forecasting that can be used for alerting the inhabitants according to regulations has been demonstrated.

Work on improved alerts based on online air-quality model will be continued for other pollutants and other combinations of air-quality forecasting models.

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Appendix A: Performance measures

The following are performance measures used in the study.

– The root-mean-square error – RMSE:

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(E(\hat{y}_i) - y_i)^2}, \tag{2}$$

where y_i and $\hat{y}_i$ are the observation and the prediction in the i-th step, respectively, $E(\cdot)$ denotes the expectation, i.e., the mean value, of the random variable, and N is the number of used observations.

– The standardised mean-squared error – SMSE

$$\mathrm{SMSE} = \frac{1}{N}\frac{\sum_{i=1}^{N}(E(\hat{y}_i) - y_i)^2}{\sigma_y^2}, \tag{3}$$

where σ_y^2 is the variance of the observations.

– The Pearson's correlation coefficient – PCC:

$$\mathrm{PCC} = \frac{\sum_{i=1}^{N}(E(\hat{y}_i) - E(\hat{\mathbf{y}}))(y_i - E(\mathbf{y}))}{N\sigma_y\sigma_{\hat{y}}}, \tag{4}$$

where $E(\hat{\mathbf{y}})$ is the expectation, i.e., the mean value, of the vector of predictions, and $\sigma_y, \sigma_{\hat{y}}$ are the standard deviations of the observations and the predictions, respectively.

– The mean fractional bias – MFB:

$$\mathrm{MFB} = \frac{1}{N}\sum_{i=1}^{N}\frac{E(\hat{y}_i) - y_i}{\frac{1}{2}(E(\hat{y}_i) + y_i)}. \tag{5}$$

– The factor of the modelled values within a factor of two of the observations – FAC2:

$$\mathrm{FAC2} = \frac{1}{N}\sum_{i=1}^{N} n_i \quad \text{with} \quad n_i = \begin{cases} 1 \ \text{for} \ 0.5 \le |\frac{E(\hat{y}_i)}{y_i}| \le 2, \\ 0 \ \text{else.} \end{cases} \tag{6}$$

RMSE and SMSE are frequently used measures for the accuracy of the predictions' mean values, which are 0 in the case of perfect model. SMSE is the standardised measure with values between 0 and 1. PCC is a measure of associativity and is not sensitive to bias. Its value is between -1 and +1, with ideally linearly correlated values resulting in a value 1. MFB is the measure that bounds the maximum bias and gives additional weight to underestimations and less weight to overestimations. Its value is between -2 and $+2$, with the value 0 in the case of a perfect model. FAC2 indicates the fraction of the data that satisfies the condition from Eq. 6. Its value is between 0 and 1, with the perfect model resulting in a value of 1.

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