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# Advances in air quality modeling and forecasting

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ABSTRACT

The importance of and interest to research and investigations of atmospheric composition and its modeling for different applications are substantially increased. Air quality forecast (AQF) and assessment systems help decision makers to improve air quality and public health, mitigate the occurrence of acute air pollution episodes, particularly in urban areas, and reduce the associated impacts on agriculture, ecosystems and climate. Advanced approaches in AQF combine an ensemble of state-of-the-art models, high-resolution emission inventories, satellite observations, and surface measurements of most relevant chemical species to provide hindcasts, analyses, and forecasts from global to regional air pollution and downscaling for selected countries, regions, and urban areas. Based on published reviews and recent analyses, the article discusses main gaps, challenges, applications and advances, main trends and research needs in further advancements of atmospheric composition and air quality modeling and forecasting.



## 1. Implications

Proceeding from global challenges and based on published reviews and recent analyses, the article discusses main gaps, challenges, applications and advances, main trends and research needs in further advancements of atmospheric composition and air quality modeling and forecasting.

## 2. Introduction

Global challenges, such as climate change, environmental degradation, rapid urbanization, or pandemics, require a review of the current understanding and traditional methods of assessing anthropogenic impacts on the environment, and new multi-disciplinary approaches of integrated assessments and methods for sustainable development. The United Nations 17 Sustainable Development Goals (SDGs) and 169 Targets aim to end extreme poverty and create a healthy, sustainable world by the year 2030 [1]. At their core lies the health and well-being of people and our planet. It means air pollution - the deaths and disabilities it causes and its close links to climate change - is a huge threat to delivering on the vision of a better world. Air pollution is specifically mentioned under at least the following four SDGs: Goal 3 focuses on good health and well-being; Goal 7 targets access to clean and affordable energy; Goal 11 focuses on sustainable cities and communities; and Goal 13 tackles climate change. Strategy and actions to improve air quality - such as switching to cleaner energy, green economy, smart cities, cooking and transport solutions - will also address the climate emergency.

During the last decades the importance of and interest to research and investigations of atmospheric composition and its modeling have substantially increased. There are several reasons for these, including increased risks of air pollution for human health, dramatically increased studies of climate change, much better computational capabilities of modern supercomputers and better understanding of physical and chemical processes in the atmosphere. The World Health Organization [2] reported that about 7 million people deaths (1/8 of total annual global deaths) are anticipated due to exposure to outdoor and indoor air pollution (3.7 and 3.3 million, respectively).

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It is important to stress that key air pollutants, particularly black carbon and methane, also have near-term climate impacts that accelerate the pace of global warming. Most of the leading sources of air pollution are among the most significant emitters of longer-lived greenhouse gases, particularly carbon dioxide and nitrous oxide. Therefore, there is a critical need to consider the problem in a complex manner with co-benefits for air quality and climate as well as interactions of climate change and atmospheric pollution.

Additionally to annual average air quality assessments for health impacts, it is also important to realize short-term forecasting of peak pollutants concentrations to prevent health effects from acute episodes. To protect citizens from unhealthy air, many countries have real-time air quality forecasting (AQF) programs in place to forecast the concentrations of pollutants of special health concerns such as ozone ($O_3$), nitrogen dioxide ($NO_2$), particulate matter with diameters less than and equal to 2.5 μm ($PM_{2.5}$, and $PM_{10}$, respectively) e.g., Ref. [3–11]. Such information has been used to issue early air quality alerts that allow government and people to take precautionary measures such as temporarily banning major emission sources, favoring car pooling or taking public transportation to reduce air pollution and minimize their exposures to unhealthy levels of air pollution [12]. Air quality forecasting has been used to schedule and plan numerous field campaigns to effectively track pollutant plume transport and sample pollutant concentrations, which maximizes the usage of expensive instrumented platforms such as airplanes and other limited measurement resources e.g., Ref. [13,14]. Accurate AQF can therefore offer tremendous societal and economic benefits by enabling advanced planning for individuals, organizations, and communities in order to avoid exposure, and reduce pollutant emissions and their adverse health impacts. Driven by crucial regulations, societal and economic needs, scientific advancements, and increasing availability of high performance computing capacity, AQF has evolved from weather forecasting and developed into a new discipline that integrates science and technology from several disciplines including meteorology, atmospheric chemistry/air quality, mathematics, physics, environmental statistics, and computer sciences/engineering.

Two main approaches can be distinguished in AQF: empirical/statistical methods and chemical transport modelling. The empirical/statistical approaches have several common drawbacks for AQF (see review in Refs. [15–17]; and [18]. For example, they cannot predict concentrations during periods of unusual emissions (e.g., substantial emission reductions that have happened during the 2020 lockdown period due to the COVID-19 pandemic) and/or meteorological conditions that deviate significantly from the historical record [19]. These statistical models provide neither the direct linkages between precursor emissions and resultant pollution nor the interrelationships among multiple pollutants (i.e., the interactions among pollutants that may potentially exacerbate one pollution problem while alleviating another problem). Explicit treatments for such linkages and interactions in AQF models are essential to the enhancement of understanding of the physical-chemical system, the improvement of short- and long-term AQF skill, and the development of integrated emission control strategies for multi-pollutants. Therefore chemical transport models (CTMs) are much more commonly used in AQF systems and in this article we will consider mostly chemical transport modelling-based approaches.

There are several comprehensive review papers, e.g., Refs. [7,15,17,20–22,23]; and [18] analyzing current major 3-D global and regional real-time air quality forecasting models and identifying areas of improvement in meteorological forecasts, chemical inputs, and model treatments of atmospheric physical, dynamic, and chemical processes. We will not thus provide a historical overview of existing modeling experience, but based on published reviews and recent analysis, will focus in this article on advances, main trends and research needs in further developments of atmospheric composition and air quality modeling and forecasting.

For example [15], reviewed existing experience and identified several inaccuracies in AQF and their possible causes, including different factors related to:

- meteorology, e.g., inaccurate characterization of the transport and planetary boundary layer (PBL) meteorological processes such as turbulent mechanisms and vertical convection, cloud attenuation of photolysis, local drainage and sea-breeze circulations and PBL heights;
- boundary conditions (BCONs) including inadequate representations of BCONs of $O_3$, $PM_{2.5}$, and $PM_{10}$);
- emissions including uncertainties in anthropogenic emissions of sulfur dioxide ($SO_2$) and volatile organic compounds (VOCs), wildfire emissions, particular matter (PM), dust, pollen and other meteorology-dependent emissions;
- model process treatments, e.g., inaccurate model treatments such as urban processes, gas-phase chemistry, in-cloud oxidation of $SO_2$, secondary organic aerosol (SOA) formation, and dry and wet deposition.

As [24] stressed, to reduce short- and long-term exposure of public to air pollution, especially in developing countries, an internationally coordinated and integrated air quality monitoring, analysis and prediction system must be developed by effectively combining scientific and technological progress in observing capabilities (in situ and space), mathematical models, data analyses, and computer science.

There are the following trends in the development of modern atmospheric composition modelling and AQF systems:

- Seamless prediction of the Earth system approach;
- Online coupling of atmospheric dynamics and chemistry models;
- Multi-scale prediction approach;
- Subseasonal to seasonal forecast;
- Emission modeling for improved emission data;
- Multi-platform observations and data assimilation;
- Data fusion, machine learning methods and bias correction techniques;
- Ensemble approach;
- Fit for purpose approach;
- Impact based forecast.

Given the large scope and many focuses of this field, the paper focuses on selected topics. The advances in several important domains, e.g., in meteorological processes and atmospheric chemical mechanisms for air quality (AQ) modeling, as well as emission modeling for improved emission data are discussed in other recent publications: by Refs. [25–27] and by Ref. [28]. Therefore we will not touch these issues in this article and will concentrate on the following: (i) Seamless prediction of the Earth system, including online coupled chemistry-meteorology modelling, multi-scale prediction systems and seasonal forecasts; (ii) utilizing modern observational data in models, including data assimilation and data fusion algorithms, machine learning methods, bias correction techniques and ensemble methods; (iii) fit for purpose and impact based forecast approaches.

## 3. Toward seamless prediction of the earth system

### 3.1. Seamless environmental prediction systems

The new generation of integrated atmospheric dynamics and composition models is based on the seamless Earth System Modelling (ESM) approach [29] to evolve from separate model components to seamless meteorology-composition-environment models to address challenges in weather, climate, and atmospheric composition fields whose interests, applications, and challenges are now overlapping. "Seamless" is considered in relation to, at least, two aspects. Firstly, at the process-scale, it refers to, for example, the coupling within a model of meteorology and composition processes to represent the two-way interactions between composition and radiative processes or microphysics, or the consistent treatment of water vapor. Secondly, to be considered in terms of time-space-scales, it refers to the absence of discontinuities in model behavior when used at multiple temporal or spatial resolutions to have, for example, consistent treatment of black carbon for air quality and climate applications or consistent coupling interval between land, ocean and atmosphere.

In a more general sense, the approach considers several dimensions of the seamless coupling, including:

- Time scales: from seconds and nowcasting to decadal and centennial (climate) time-scale;
- Spatial scales: from street-level to global scale (downscaling and upscaling);
- Processes: physical, chemical, biological, social;
- Earth system elements/environments/components: atmosphere, hydrosphere, lithosphere/pedosphere, ecosystems/biosphere;
- Different types of observations and modelling as tools: observations-model fusion, data processing and assimilation, validation and verification;
- Links with health and social consequences, impact, assessment, and services and end-users.

Different aspects of methodology and research needs for realisation of the Seamless Prediction Systems, as a part of WMO research strategy, are presented and discussed in the book "Seamless Prediction of the Earth System: From Minutes to Months" [29].

The ensemble approach integrates modeling results from different models, participants and countries, or at one center with one model, e.g., of the European Center for Medium-Range Weather Forecasts (ECMWF), but with perturbations to initial conditions and physical parameterizations (stochastic physics). This allows information on model process diversity to inform uncertainty in our understanding of Earth system linkages, responses, and impact assessments. It is possible to utilize the full potential of a hierarchy of models: scenario analysis, forward and inverse modeling, modeling based on measurement needs and processes. The models are evaluated and constrained by available in-situ and remote sensing data of various spatial and temporal scales using data assimilation and top-down modeling. The analyses of the anticipated large volumes of data produced by available models and sensors will be supported by a dedicated virtual research platforms developed for these purposes.

Linking between the temporal and spatial scales for modelling and observations is a key aspect of the seamless prediction approach. Both short- and long-term measurements from different observational platforms including field campaigns, laboratory, chamber experiments, satellite, etc. represent valuable contributions to evaluation and verification of different models as well as for studying and modelling of physical-chemical-biological processes at multi-scales and integrated assessment for environment, population, ecosystems, etc. In particular, a hierarchy framework of such modern multi-scale models for different elements of the Earth's system, integrated with the observation system, is being developed within the Pan-Eurasian Experiment (PEEX) multi-disciplinary programme [30,31]. Moreover, the models will inform the development of the in-situ monitoring component of the PEEX Research Infrastructure by providing information on regions, where specific processes or interactions may be important to measure with new observational capability.

### 3.2. Coupled chemistry-meteorology modeling (CCMM)

The use of a coupled meteorology-chemistry model, e.g., WRF-Chem [32] or Enviro-HIRLAM [33], for AQF represents a significant advancement in routine operational AQFs and would greatly enhance understanding of the underlying complex interplay of meteorology, emission, and chemistry. Model evaluation demonstrates that a modeling approach based on CTMs has skills consistent with or better than many statistical forecasting tools [34,35]. Online-coupled meteorology atmospheric chemistry models (CCMM) have greatly evolved in recent decades [36–40]. Although mainly developed by the air quality modeling community, these integrated models are also of interest for numerical weather prediction and climate modeling as they can consider both the effects of meteorology on air quality, and the potentially important effects of atmospheric composition on weather. Migration from offline to online integrated modeling and seamless environmental prediction systems [41] are recommended for consistent treatment of processes and allowance of two-way interactions of physical and chemical components, particularly for AQ and numerical weather prediction (NWP) communities.

Regarding AQF and atmospheric composition modelling, the CCMM approach will certainly improve forecast capabilities as it allows a correct way of jointly and consistently describing meteorological and chemical processes within the same model time steps and grid cells. Applications that may benefit from CCMM are numerous and include [42]: chemical weather forecasting (CWF), numerical weather prediction for precipitation, visibility, thunderstorms, etc., integrated urban meteorology, environment and climate services, sand and dust storm modeling and warning systems, wildfire atmospheric pollution and effects, volcano ash forecasting, warning and effects, high impact weather and disaster risk, effects of short-lived climate forcers, earth system modeling and projections, data assimilation for CWF and NWP, and weather modification and geo-engineering. Online integrated models, however, need harmonized formulations of all processes influencing meteorology and chemistry.

Based on the EuMetChem activities [43], CCMM symposium [41] and further discussions (e.g. Ref. [29,42], the following recommendations for future research have been identified.

For air quality forecasting and atmospheric composition studies the following research needs are stressed:

- Better representation of aerosol processes and their formation (especially in terms of chemical speciation), heterogeneous chemistry and interactions with cloud;
- Experiments that are specifically defined to look at chemistry-cloud-microphysics at different scales;
- More field experimental data to evaluate online coupled models;
- Improved numerical and computational efficiency of the models as the complexity of applications grows (e.g., scales);

- Intercomparisons both at global and regional/urban scale for AQ, NWP, and climate should continue; intercomparisons that are cutting across all 3 fields should be considered.

For meteorological studies and specifically NWP the following research is needed:

- Developing diagnostics and validation methodologies to more explicitly separate different effects of the intertwined feedback processes;
- More collaboration between operational centers and research communities. This needs to be focused on providing schemes with an impact that is proven to be valuable enough to justify the cost of their implementation (even for relatively modest increases in CPU);
- More evaluation of aerosol properties routinely, not only for the indicators PM10 and PM2.5 but also for optical, chemical and microphysical properties;
- The treatment of the indirect effect of aerosols is one of the key uncertainties; ice nucleation processes and parameterizations are less well defined than CCN formation processes and parameterizations;
- Further research is needed to better understand the importance of including more accurate representation of aerosol properties in satellite retrievals;
- Research on the impact of online modeling of aerosols on visibility forecasting, observational constraints on the causes of light extinction and on parameterizations for calculating extinction given model parameters.

For climate research the following main developments in CCMMs are needed:

- Improve our understanding of indirect effects (e.g., BC on clouds);
- Develop CCCMs with prognostic aerosols to assess the tradeoff between a more complex aerosol representation on the one side and model resolution, or the atmosphere-ocean coupling, on the other side;
- Test model performance in terms of relevant physical, chemical, and radiative processes and mechanisms (in contrast to just testing mean performance);
- Test model performance in terms of tropospheric dynamics/meteorology and their effect on composition (and vice-versa).

### 3.3. Multi-scale prediction approach

The AQ monitoring, analysis and forecasting systems should operate at different spatial scales from the global scale to the regional, national, urban and sub-urban scales. In previous decades, AQ models usually were applied only for a specific spatial scale: global, regional, meso-, local, urban or street scales. During last decades research achievements, high-performance computational resources, and real time data access possibilities make it realistic to build a full chain of multi-scale AQ modelling and forecasting.

Zooming or special nesting grid techniques are usually required to transfer model information between the scales. Grid nesting is the most common method, being employed in most CTMs. Many of the currently used CTMs (e.g., WRF-Chem, CAMx [44], CMAQ [45]) allow for grid nesting. Grid nesting is further classified in one-way nesting (sometimes referred to as downscaling), when values of the modelled variables at a coarse resolution are used as boundary conditions for finer (subscale) resolution runs, and two-way nesting, when information from the higher resolution scale is in addition transmitted across the boundaries to the coarser resolution.

For example, the European Copernicus Atmosphere Monitoring Service (CAMS) provides such AQF from global to regional [46,47] and possibly urban scales (FUMAPEX, MEGAPOLI) for European countries [6,48–50]; GURME [51,52], MarcoPolo & PANDA projects [53] developed and tested similar AQF systems for Asian countries (China, India) and selected cities (e.g., Shanghai, New Delhi, etc.).

The development of models dedicated to address urban AQ issues requires also some urbanization of meteorological/NWP models [29] and a good set of data regarding urban structure and many other characteristics. There are important initiatives in that direction providing a more detailed atmospheric dataset, e.g., pollutant fluxes and concentrations, temperature, wind, pressure, and moisture, and also providing important parameters to describe urban features in an aggregate manner that can be introduced into urban scale models with resolutions of 200–2000 m and corresponding physical options in single and multi-layer urban canopy models (Ching et al., 2018).

To forecast street level air quality the downscaling with specific (e.g., obstacle-resolved computational fluid dynamics (CFD) type or parameterized) microscale models is needed. CFD models coupled with mesoscale models can provide this high spatial resolution (up to 1–10 m) because they explicitly resolve the turbulent flow around buildings (see e.g., Refs. [49,54,55]. However, the required computational time increases and it would be difficult, at a reasonable CPU time, to use a direct coupling between mesoscale and CFD models for forecasting purposes. In the near future, CFD models could become an appropriate tool for forecasting due to the increase of computational resources. Nowadays, a database created with CFD simulation of several scenarios represents the best compromise to perform the downscaling of the mesoscale outputs. Another alternative is the use of a parametrized microscale model (e.g., Ref. [56,57]. These models do not resolve explicitly the turbulent flow but use parametrized relations between urban configuration and flow and dispersion variables within the urban canopy. This fact allows a simplified representation of concentrations within the urban canopy in reasonable computational time for forecasting purposes.

Seamless unified modelling system that allows a single platform to operate over the full scale (i.e., across-scale) will represent a substantial advancement in both the science and the computational efficiency. The Model for Prediction Across Scales for Atmosphere (MPAS-A) being developed by the U.S. National Center for Atmospheric Research is a good example of such a modelling system (mpas-dev.github.io; [58]. MPAS-A uses the unstructured Voronoi meshes (hexagons) and C-grid discretization. The former allows for smoothly-varying mesh transitions and local refinement. The latter solves for normal velocities on cell edges and is well-suited for higher-resolution, mesoscale atmosphere and ocean simulations. Two other examples of recently developed community-based, coupled, comprehensive multi-scale Earth modeling systems are the MUlti-Scale Infrastructure for Chemistry and Aerosols – MUSICA [59] and the Unified Forecast System [60] to support the Weather Enterprise and to be the source system for NOAA's operational numerical weather prediction applications including the atmospheric composition.

Major challenges include globalization/downscaling with consistent model physics and two-way nesting with mass conservation and consistency. Such a unified global-to-urban scale modelling systems will provide a new scientific capability for studying important problems that require a consideration of multi-scale feedbacks.

### 3.4. Subseasonal to seasonal forecast

Significant progress has been made in recent decades on medium-range weather forecasts and seasonal climate predictions. Because of a difficult time range that is not as well defined as weather and seasonal forecasting, subseasonal forecasting has not received as much attention as weather or seasonal forecasting. Advancements in real-time weather and air quality forecasting models and the data analysis techniques have made reasonably accurate predictions and data analytics for extended timeframes possible. Seasonal and subseasonal forecasts are generated at monthly intervals out to 7 months and weekly intervals out to 5 weeks, respectively. The subseasonal to seasonal forecast will bridge the gap between weather and climate and bring the weather and climate communities together to tackle the intervening time range, harnessing shared and complementary experience and expertise in forecasting, research and applications, toward more seamless weather/climate prediction systems and more integrated weather and climate services [61,62]. Seasonal and subseasonal forecasts deliver easy-to-use, predictive analysis that anticipates market behavior and potential risks for scientific communities, government, and many sectors such as agriculture, aviation, media, energy, and insurance. For example, they can be used for market shifts that may affect profitability in the 3- to 5-week, 1- to 4-month, and 5- to 7-month timeframes. In particular seasonal forecast for wildfires and smog pollution is underdeveloped within the VFSP-WAS [63].

Subseasonal weather and air quality forecasts have been identified as research and operation priorities by WMO [62,64] and several countries such as the U.S [65,66]. Subseasonal forecasts will have large societal benefits, as many market behaviors and management decisions in agriculture and food security, water, risk reduction of weather disaster and hazards (e.g., drought, wildfire, heatwave, cold wave) and health fall into the subseasonal to seasonal time range.

## 4. Improvements by utilizing modern observation data and ensembles

One of the key modern trends to improve AQF systems is developing new methods of utilizing modern observational data in models, including data assimilation and data fusion algorithms, machine learning methods and bias correction techniques.

### 4.1. Multi-platform observations and data assimilation

During last decades the techniques and possibilities of multi-platform (in-situ, ground, aircraft and satellite remote sensing) observations of air pollution and atmospheric parameters, as well as their near real time (NRT) or real time (RT) availabilities and citizen science opportunities [67], are dramatically improved and increased. This leads to a revision of concepts of AQF and importance of data assimilation (both chemical and meteorological measurements) in AQF systems [23,68] and measurement-model fusion for air quality and deposition assessments [69].

In particular, the new generation of geostationary satellites, consisting of GEMS (Asia), Sentinel-4 (Europe) and TEMPO (USA), expects to provide an unprecedented view of air quality from space [70–72]. Given these planned missions, it is even more imperative to develop effective data assimilation systems for AQF that optimally incorporate satellite information.

Correspondingly, experience in the assimilation of chemical and aerosol observations from ground-based and satellite instruments into AQF and CCMM has grown significantly [23,29,73–75]. Optimal interpolation, variational approaches, Ensemble Kalman filter (EnKF) or hybrid techniques combining the advantages of both variational and EnKF techniques are all applicable in CTMs [76]. Other methodologies such as inverse modelling of emission fields appear as a promising technique to improve the skill of AQF and may have a stronger impact for short-lived pollutants than chemical data assimilation (CDA) has on initial conditions. CDA has been implemented in many operational AQF and some CCMM models, such as the ECMWF/Copernicus Integrated Forecast System (IFS-CTM) [47], the Weather Research and Forecasting Model coupled with chemistry (WRF-Chem) [77], and the Goddard Earth Observing System Model, version 5 (GEOS-5) [78]. CDA is used to initialize air quality forecasts and for retrospective analysis of atmospheric composition. It has been shown that corrections to emissions as part of the CDA procedure can help to improve the impact of the observations on the predictions.

A main challenge of CDA is the limited information content of the atmospheric composition observations [41]. More routine evaluation of aerosol properties, not only for the indicators $PM_{2.5}$ and $PM_{10}$, but also for optical, chemical, and microphysical properties, are needed. Spatial and temporal coverage of important parameters such as aerosol composition is limited because of network design, viewing geometry, or cloud cover masking [29]. Also, vertically integrated observations, such as aerosol optical depth or total column, have to be distributed to model levels. Furthermore, biases between different observing systems (e.g., satellite data, lidars, ceilometers, ground observations) should be removed before the assimilation [23].

Although the importance of assimilating atmospheric composition data into CCMM to get realistic chemical fields has been demonstrated, there is little experience in assimilation of both meteorological and chemical observations into CCMM. Further research is needed to better understand the importance of including more accurate representation of aerosol properties in satellite retrievals.

### 4.2. Measurement-model fusion, machine learning and bias correction techniques

Tremendously growing number and different types of observations became available during the last decade, require and give a strong impulse for development of new methods for measurement-model fusion to improve AQF [69]. We have considered in previous sections first of all most applicable 3D numerical atmospheric transport models and classical data assimilation methods, however other types of data fusion algorithms, such as the statistical methods, optimal interpolation, objective analysis, bias correction, as well as relatively new artificial intelligence, neural network, machine learning and hybrid methods, were also actively developed during last decades. Several recent publications considered such methods and analysed their applicability (e.g., Ref. [16,18,69]. Statistical methods are simple, but require a large amount of historical data and highly depend on them. Artificial intelligence, neural network, and machine learning methods have better performance, but can be unstable and also depend on data. Hybrid or combined methods have a better quality. Such methods can also improve AQF utilizing additional observational data. For example [79], applied machine learning methods for ozone ensemble forecast, they performed sequential aggregation based on ensemble simulations and past observations. Further development of machine learning methods provides a potential way to bridge the resolution gap between global, low-resolution model output and local, high-resolution information requested by end users. However, further research is needed to identify applications where machine learning may have particular advantages.

Another broadly used approach to improve the AQF model performance is bias correction techniques. They have been proven to be effective in improving the forecasting accuracy and applied to the routine $O_3$ and $PM_{2.5}$ forecasting in many forecasting models such as the U.S. NOAA's operational forecasting model, the National Air Quality Forecast Capability (NAQFC) [80–84]. Several bias correction methods have been implemented in air quality forecasting models, e.g., for wildfire plumes. The simplest and also most commonly-used method is the mean subtraction method, in which the mean bias is subtracted from the forecasted values at each monitoring site. This method, however, does not always guarantee a positive value. The second approach is the multiplicative ratio adjustment method, in which the forecasted value is multiplied by the mean ratio of the sum of the observed value to the sum of the forecasted value at each monitoring site. This alternative correction guarantees that the concentrations will remain positive and increases forecasting skill, but the ratio-adjustment method provides additional improvement over the mean subtraction method for models with the highest biases. The third method is to force the zero differences between observed and simulated seasonal means by using an empirical linear fit between forecasted and bias corrected values. More advanced bias correction methods have also been developed and applied for improvement of AQF, e.g., the Kalman Filter (KF) bias correction [85,80–82,86,87]. KF has been combined with the Kolmogorov-Zurbenko (KZ) filter to correct biases in air quality forecasting [80]. KZ filter can be used to separate observed and simulated time series data into the short-term and baseline components to discern major systematic model errors [11,88–90]. The former is influenced by prevailing weather conditions and the latter is influenced mainly by emissions, boundary conditions, and other slow-varying processes. The KF bias correction technique can be applied to the baseline component of the time series at a monitoring location, which can significantly improve the forecasting accuracies. The KF or the coupled KF-KZ bias correction method can be potentially extended to locations where no monitor information is available for these methods to generate bias-corrected spatial maps of forecast products.

The performance of bias-corrected forecast depends on the performance of the raw model forecast to which the bias-correction method is applied. While bias correction methods have shown obvious short-term benefits, the improvements of model inputs such as emissions and boundary conditions and model representations of key chemical and physical processes such as secondary organic aerosol formation are necessary to address the mechanistic deficiencies of the AQF models for long-term benefits.

### *4.3. Ensemble approach*

Ensemble forecasting is a numerical prediction method that is used to produce a representative sample of the possible future states of a model system. Ensemble forecasting can be implemented using multiple models or one model but with different inputs (e.g., varying meteorological input forcings, emission scenarios, chemical initial conditions) or different process parameters (e.g., varying chemical reaction rates) or different model configurations (e.g., varying grid spacings) or different models. Ensemble forecasting has shown significant statistical improvements for both $O_3$ (e.g. Ref. [86,91–93], and $PM_{2.5}$ forecasts over any individual forecast [94]. Multi-model ensemble air quality forecasting has been emerging for AQF on global scale and regional scales (e.g., over Europe, U.S. and China) (e.g., Ref. [86,87,91–96]; Solazzo et al., 2012; Monteiro et al., 2013; Žabkar et al., 2013; Im et al., 2015; [53,97]. For example, Delle Monache et al. (2004) performed one of the first multi-model real-time $O_3$ forecasts over the U.S. The regional air quality production of the Copernicus Atmosphere Monitoring Service (CAMS) is based on ensemble of seven state-of-the-art numerical air quality models developed in Europe. Under the MarcoPolo-PANDA EU FP7 Projects (http://www.marcopolo-panda.eu/), nine different models were used for multi-model ensemble over China [53,97]. The most recent International Cooperative for Aerosol Prediction (ICAP) multi model ensemble (ICAP MME) consists of nine global models [98]. Multi-model ensemble results provide a range and an indication of the robustness of the forecasts and help to improve the accuracy of chemical weather and air quality forecasting.

The ensemble forecast is usually a weighted linear combination of the individual ensemble members, in which the weight factors may be equal or unequal for individual members. As such, it is subject to the inherent limitations of individual ensemble members and is sensitive to the selected weighting factors. More advanced ensemble forecast approaches have been developed. One such method is the ensemble forecast of analyses (EFA) of [79]. EFA couples an ensemble forecasting approach (i.e., sequential aggregation) with CDA techniques to forecast an analysis from data assimilation, instead of observations.

## 5. Fit for purpose approach and impact based forecast

The Earth system modelling approach provides a broad AQF platform for different applications, but the modelling system should fit for purposes and be optimized for specific tasks. For example, for smog pollution from wildfires the problem is more complex than for AQF with fixed anthropogenic emission sources and includes first of all the forecasting of fire danger and sources of wildfire emission, including detection of sources, mass of emitted species, plume rise, fire behaviour, etc. Research challenges facing fire and smoke prediction were evaluated by the Interdisciplinary Biomass Burning Initiative (IBBI) [23,63,99].

As mentioned, there are also several user communities (e.g., NWP, climate) and specialized applications of AQF system developments for long-term prediction and specific episodes of atmospheric harmful contamination, affecting not only health but many other sectors of economics. In particular, sand and dust storms pose a major challenge to sustainable development in arid and semi-arid regions of the planet. Airborne dust presents serious risks for human health [100]. Sand and dust storms are also detrimental for ecosystems and diverse socio-economic sectors. Surface dust deposits are a source of micro-nutrients for both continental and maritime ecosystems. Although dust can work as fertilizer, it has many negative impacts on agriculture, including reducing crop yields by burying seedlings, causing loss of plant tissue, reducing photosynthetic activity, and increasing soil erosion. Reductions in visibility due to airborne dust also have an impact on air and land transport. Poor visibility conditions are a hazard during aircraft landing and taking off operations – flights landings may be diverted and departures may be delayed. Dust can also scour aircraft surfaces and damage engines. Reduced radiation at the surface has an impact on the output from solar power plants, especially those that rely on direct solar radiation. Dust deposits on solar panels are a main concern of plants operators. Volcanic eruptions contribute to natural aerosols directly via emissions of ash and other particulates, or indirectly through the release of sulfur gases that subsequently condense to form sulfate aerosols. Volcanic aerosols are particularly important for aviation safety and climate modelling, as was witness by the eruption of the Icelandic Volcano Eyjafjallajökull, that paralyzed for several days air traffic throughout Europe.

Society is impacted by both long-term and short-term changes to atmospheric composition. Volcanic ash, desert dust, natural and anthropogenic gas emissions are good examples demonstrating both immediate impacts, for example, on aviation and human health – and longer-term, including climate forcing and impacts from the changing atmospheric composition. While both present a range of challenges, the former places considerable additional demands in terms of data timeliness and temporal and spatial resolutions. This near-real-time need for observations is indeed a common requirement across a range of impacts, but one that is not always conducive to the significant processing involved in producing fully assured atmospheric composition data. However, timely data can be produced and has the potential to be of considerable use for a wide range of applications. In recognition of this, the WMO Global Atmosphere Watch Programme [101] has identified the need for increased support for the development and expanded use of services and research activities concerning the forecasting of atmospheric composition and its induced environmental phenomena.

So, the AQF should not be limited only to the concentrations of air pollutants but should also consider their impacts on different sectors (e.g., health, agriculture, land transport, aviation, energy, etc.) and provide warning and recommendations proceeding from different thresholds, risks, and cost functions (Fig. 1). Such impact-based forecast and assessment systems will help stakeholders and responsible agencies to improve air quality and public health, mitigate the occurrence of acute harmful air pollution episodes. The suggested approach combines state-of-the-art models, high-resolution emission inventories, space observations and surface measurements of most relevant chemical species to provide hindcasts, analyses, and forecasts of regional air pollution in a specific region (using boundary and initial conditions from global AQF system such as the CAMS) and downscaling for selected countries and urban areas.

The still unsolved challenge to make the produced AQF information available to end users in a simple way fitting for purpose. So, such a common platform for air quality forecasts would increase the usability of these systems and make it much easier to integrate them into decision-making processes.

## 6. Summary and perspectives

Further improvements to AQF and modeling systems will likely follow several directions:

– Online coupling of atmospheric dynamics and chemistry models,
– Better representation of aerosol processes and feedbacks, their interactions with clouds and radiation,
– Improved data assimilation and fusion, machine learning, and artificial intelligent methods
– Toward seamless Earth system modelling,
– Multi-scale prediction approach,
- Subseasonal to seasonal forecasting,
- Impact based forecast and fit for purposes systems.

Air quality forecast and assessment systems help decision makers to improve air quality and public health, mitigate the occurrence of acute air pollution episodes, particularly in urban areas, and reduce the associated impacts on agriculture, transport, economy, ecosystems and climate.

Seamless modelling is a prospective way for future single-atmosphere modelling systems with advantages for applications at all space- and timescales for multi applications not only for air quality, but also for NWP, climate and other atmospheric composition models.

The advance approach combines an ensemble of state-of-the-art models, high-resolution emission inventories, space observations, and surface measurements of most relevant chemical species (coarse and fine PM, ozone, reduced and oxidized nitrogen, etc.) to provide hindcasts, analyses and forecasts of from global to regional air pollution and downscaling for selected countries and urban areas.

Dramatically increasing possibilities of multi-platform (in-situ, ground, aircraft and satellite remote sensing) observations in real or near-real time, as well as citizen science opportunities, lead to a revision of concepts of AQF, increase importance of data assimilation techniques. New measurement-model data fusion, machine learning and artificial intelligence methods have a good potential to bridge the resolution gap between global, low-resolution model output and local, high-resolution information required by users.

Improved data assimilation, both in terms of techniques and choice of aerosol variables to be assimilated. Key questions for the future are whether there is a benefit to move from assimilating AOD to assimilating clear-sky radiances in the shortwave spectrum and how to make the best possible use of vertical profiles from lidar observations.

Although we did not focus deeply on emission modelling methods in this paper, it is important to highlight the importance of emission data and models as one of the key uncertainties in AQF. In particular, dramatic changes of emissions from COVID-19

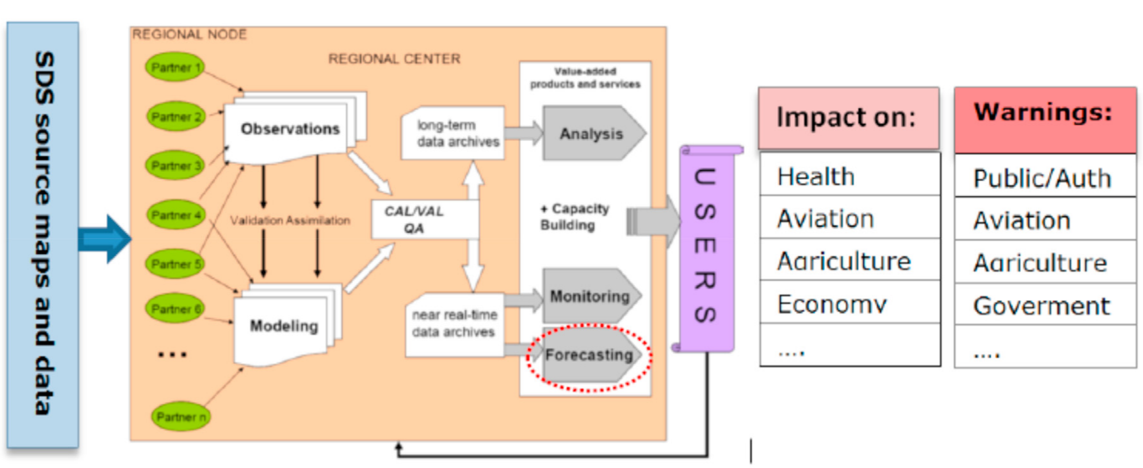


Fig. 1. Example of impact-based forecast and assessment systems for the WMO Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) (after [102].

lockdown-related reduced activities, as well challenges with meteorology-dependent emissions (e.g., wildfires, dust storms, pollen, VOC, secondary aerosols and climate forcers), required further research efforts in online monitoring and assessments of emissions using remote sensing observations, crowdsourcing data, modern inverse models, and machine learning and artificial intelligent methods.

## CRediT author statement

The corresponding author is responsible for ensuring that the descriptions are accurate and agreed by both authors.

The role of each of the two authors are almost equal: review of the problem, analysis and writing the manuscript.

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## References

[1] UN SDGs, Sustainable Development Goals. United Nations, 2015, 2015, website: https://sustainabledevelopment.un.org/.

[2] WHO, Burden of Disease from the Joint Effects of Household and Ambient Air Pollution for 2012, World Health Organization, 2014, 25, March 2014, http://www.who.int/phe/health_topics/outdoorair/databases/FINAL_HAP_AAP_BoD_24March2014.pdf?ua=1.

[3] P. Manins, Air Quality Forecasting for Australia's Major Cities: 1st Progress Report, CSIRO Atmospheric Research: Aspendale, Australia, 1999. SB/1/407 25, http://www.dar.csiro.au/publications/Manins_1999a.pdf.

[4] U.S. EPA, Guideline for Developing an Ozone Forecasting Program, U.S. Environmental Protection Agency Rep., 1999. EPA-454/R-99-009, 88 pp. (Available from Office of Air Quality Planning and Standards, EPA, Research Triangle Park, NC 27711.).

[5] J.A. Pudykiewicz, A.S. Koziol, The application of Eulerian models for air quality prediction and the evaluation of emission control strategies in Canada, Int. J. Environ. Pollut. 16 (2001) 425–438.

[6] A. Baklanov, O. Hänninen, L.H. Slordal, J. Kukkonen, N. Bjergene, B. Fay, S. Finardi, S.C. Hoe, M. Jantunen, A. Karppinen, A. Rasmussen, A. Skouloudis, R.S. Sokhi, j.H. Sorensen, V. Ødegaard, Integrated systems for forecasting urban meteorology, air pollution and population exposure, Atmos. Chem. Phys. 7 (2007) 855–874. www.atmos-chem-phys.net/7/855/2007/.

[7] J. Kukkonen, T. Olsson, D.M. Schultz, A. Baklanov, T. Klein, A.I. Miranda, A. Monteiro, M. Hirtl, V. Tarvainen, M. Boy, V.-H. Peuch, A. Poupkou, I. Kioutsioukis, S. Finardi, M. Sofiev, R. Sokhi, K.E.J. Lehtinen, K. Karatzas, R. San José, M. Astitha, G. Kallos, M. Schaap, E. Reimer, H. Jakobs, K. Eben, A review of operational, regional-scale, chemical weather forecasting models in Europe, Atmos. Chem. Phys. 12 (2012) 1–87, https://doi.org/10.5194/acp-12-1-2012.

[8] M.-T. Chuang, Y. Zhang, D.-W. Kang, Application of WRF/Chem-MADRID for real-time air quality forecasting over the southeastern United States, Atmos. Environ. 45 (34) (2011) 6241–6250, https://doi.org/10.1016/j.atmosenv.2011.06.071.

[9] Y. Zhang, C.-P. Hong, K. Yahya, Q. Li, Q. Zhang, K.-B. He, Comprehensive evaluation of multi-year real-time air quality forecasting using an online-coupled meteorology-chemistry model over southeastern United States, Atmos, Environ. Times 138 (2016) 162–182, https://doi.org/10.1016/j.atmosenv.2016.05.006.

[10] P. Lee, J. McQueen, I. Stajner, J. Huang, L. Pan, D. Tong, H. Kim, Y. Tang, S. Kondragunta, M. Ruminski, S. Lu, E. Rogers, R. Saylor, P. Shafran, H.-C. Huang, J. Gorline, S. Upadhayay, R. Artz, NAQFC developmental forecast guidance for fine particulate matter (PM2.5), Weather Forecast. 32 (1) (2017) 343–360, https://doi.org/10.1175/WAF-D-15-0163.1.

[11] S.T. Rao, H. Luo, M. Astitha, C. Hogrefe, R. Mathur, N. Kumar, On regional modeling to support air quality policies, in: C. Mensink, G. Kallos (Eds.), Air Pollution Modeling and its Application XXV. ITM 2016. Springer Proceedings in Complexity, Springer, Cham, 2018, pp. 25–29, https://doi.org/10.1007/978-3-319-57645-9_4.

[12] R.A. Wayland, J.E. White, P.G. Dickerson, T.S. Dye, Communicating real-time and forecasted air quality to the public, Environ. Manag. 28–36 (2002) (December).

[13] A.M. Lee, G.D. Carver, M.P. Chipperfield, J.A. Pyle, Three dimensional chemical forecasting: a methodology, J. Geophys. Res. 102 (1997) 3905–3919.

[14] F. Flatøy, O. Hov, H. Schlager, Chemical forecasts used for measurement flight planning during POLINAT 2, Geophys. Res. Lett. 27 (2000) 951–954.

[15] Y. Zhang, C. Seigneur, M. Bocquet, V. Mallet, A. Baklanov, Real-time air quality forecasting, Part I: history, techniques, and current status, Atmos. Environ. 60 (2012a) 632–655, https://doi.org/10.1016/j.atmosenv.2012.06.031.

[16] Y. Zhang, A. Baklanov (Eds.), Best Practices and Training Materials for Chemical Weather/Air Quality Forecasting, The First Edition ETR-26, World Meteorological Organization (WMO), Geneva, Switzerland, 2020, p. 565.

[17] W.F. Ryan, The air quality forecast rote: recent changes and future challenges, J. Air Waste Manag. Assoc. 66 (6) (2016) 576–596, https://doi.org/10.1080/10962247.2016.115146.

[18] L. Bai, J.-Z. Wang, X.-J. Ma, H.-Y. Lu, Air pollution forecasts: an overview, Int. J. Environ. Res. Publ. Health 15 (2018) 780, https://doi.org/10.3390/ijerph15040780.

[19] W.R. Stockwell, R.S. Artz, J. Meagher, R.A. Petersen, K.L. Schere, G.A. Grell, S.E. Peckham, A.F. Stein, R.V. Pierce, J.M. O'Sullivan, P.Y. Whung, The scientific basis of NOAA's air quality forecast program, Environ. Manager, December 8 (2002) 20–27.

[20] L. Menut, B. Bessagnet, Atmospheric composition forecasting in Europe, Ann. Geophys. 28 (2010) 61–74, 2010.

[21] Y. Zhang, C. Seigneur, M. Bocquet, V. Mallet, A. Baklanov, Real-time air quality forecasting, Part II: state of the science, current research needs, and future prospects, Atmos. Environ. 60 (2012b) 656–676, https://doi.org/10.1016/j.atmosenv.2012.02.041.

[22] A. Baklanov, K.H. Schlünzen, P. Suppan, J. Baldasano, D. Brunner, S. Aksoyoglu, G. Carmichael, J. Douros, J. Flemming, R. Forkel, S. Galmarini, M. Gauss, G. Grell, M. Hirtl, S. Joffre, O. Jorba, E. Kaas, M. Kaasik, G. Kallos, X. Kong, U. Korsholm, A. Kurganskiy, J. Kushta, U. Lohmann, A. Mahura, A. Manders-Groot, A. Maurizi, N. Moussiopoulos, S.T. Rao, N. Savage, C. Seigneur, R.S. Sokhi, E. Solazzo, S. Solomos, B. Sørensen, G. Tsegas, E. Vignati, B. Vogel, Y. Zhang, Online coupled regional meteorology chemistry models in Europe: current status and prospects, Atmos. Chem. Phys. 14 (2014) 317–398, https://doi.org/10.5194/acp-14-317-2014.

[23] A. Benedetti, J.S. Reid, P. Knippertz, J.H. Marsham, F. Di Giuseppe, S. Rémy, S. Basart, O. Boucher, I.M. Brooks, L. Menut, L. Mona, P. Laj, G. Pappalardo, A. Wiedensohler, A. Baklanov, M. Brooks, P.R. Colarco, E. Cuevas, A. da Silva, J. Escribano, J. Flemming, N. Huneeus, O. Jorba, S. Kazadzis, S. Kinne, T. Popp, P.K. Quinn, T.T. Sekiyama, T. Tanaka, E. Terradellas, Status and future of numerical atmospheric aerosol prediction with a focus on data requirements, Atmos. Chem. Phys. 18 (2018) 10615–10643, https://doi.org/10.5194/acp-18-10615-2018.

[24] R. Kumar, V.-H. Peuch, J.H. Crawford, G. Brasseur, Five steps to improve air-quality forecasts, Nature, 6 September 561 (2018) 27–29, 2018.

[25] R.T. McNider, A. Pour-Biazar, Meteorological modeling relevant to mesoscale and regional air quality applications: a review, J. Air Waste Manag. Assoc. 70 (1) (2020) 2–43, https://doi.org/10.1080/10962247.2019.1694602.

[26] M. Mircea, G. Calori, G. Pirovano, C.A. Belis, European Guide on Air Pollution Source Apportionment for Particulate Matter with Source-Oriented Models and Their Combined Use with Receptor Models, JRC technical report JRC119067, 2020, p. 66, https://doi.org/10.2760/470628.

[27] W.R. Stockwell, E. Saunders, W.S. Goliff, R.M. Fitzgerald, A perspective on the development of gas-phase chemical mechanisms for Eulerian air quality models, J. Air Waste Manag. Assoc. 70 (1) (2020) 44–70, https://doi.org/10.1080/10962247.2019.1694605.

[28] V. Matthias, J.A. Arndt, A. Aulinger, J. Bieser, H.D. van der Gon, R. Kranenburg, J. Kuenen, D. Neumann, G. Pouliot, M. Quante, Modeling emissions for three-dimensional atmospheric chemistry transport models, J. Air Waste Manag. Assoc. 68 (8) (2018) 763–800, https://doi.org/10.1080/10962247.2018.1424057.

[29] WWRP, Seamless Prediction of the Earth System: from Minutes to Months, vol. 1156, WMO-No., 2015, ISBN 978-92-63-11156-2. Available from: http://library.wmo.int/pmb_ged/wmo_1156_en.pdf.

[30] M. Kulmala, H.K. Lappalainen, T. Petäjä, T. Kurten, V.-M. Kerminen, Y. Viisanen, P. Hari, S. Sorvari, J. Bäck, V. Bondur, N. Kasimov, V. Kotlyakov, G. Matvienko, A. Baklanov, H.D. Guo, A. Ding, H.-C. Hansson, S. Zilitinkevich, Introduction: the Pan-Eurasian Experiment (PEEX) – multidisciplinary, multiscale and multicomponent research and capacity-building initiative, Atmos. Chem. Phys. 15 (2015) 13085–13096, https://doi.org/10.5194/acp-15-13085-2015.

[31] M. Kulmala, Build a global Earth observatory, Nature 553 (2018) 21–23, https://doi.org/10.1038/d41586-017-08967-y, 2018.

[32] G.A. Grell, S.E. Peckham, R. Schmitz, et al., Fully coupled "online" chemistry within the WRF model, Atmos. Environ. 39 (2005) 6957–6975.

[33] A. Baklanov, U.S. Korsholm, R. Nuterman, A. Mahura, K.P. Nielsen, B.H. Sass, A. Rasmussen, A. Zakey, E. Kaas, A. Kurganskiy, B. Sørensen, I. González-

Aparicio, The Enviro-HIRLAM online integrated meteorology–chemistry modelling system: strategy, methodology, developments, and applications (v. 7.2), Geosci. Model Dev. (GMD) 10 (2017b) 2971–2999, https://doi.org/10.5194/gmd-10-2971-2017.

[34] J.N. McHenry, W.F. Ryan, N.L. Seaman, C.J. Coats Jr., J. Pudykiewics, S. Arunachalam, J.M. Vukovich, A real-time Eulerian photochemical model forecast system: overview and initial ozone forecast performance in the Northeast U.S. corridor, Bull. Am. Meteorol. Soc. 85 (2004) 525–548.

[35] A.M.M. Manders, M. Schaap, R. Hoogerbrugge, Testing the capability of the chemistry transport model LOTOS-EUROS to forecast PM10 levels in The Netherlands, Atmos, Environ. Times 43 (2009) 4050–4059, https://doi.org/10.1016/j.atmosenv.2009.05.006.

[36] Y. Zhang, Online coupled meteorology and chemistry models: history, current status, and outlook, Atmos. Chem. Phys. 8 (2008) 2895–2932, https://doi.org/10.5194/acp-8-2895-2008.

[37] A. Baklanov, Chemical weather forecasting: a new concept of integrated modelling, Adv. Sci. Res. 4 (2010) 23–27, 2010.

[38] G.A. Grell, A. Baklanov, Integrated modelling for forecasting weather and air quality: a call for fully coupled approaches, Atmos. Environ. 45 (2011) 6845–6851, https://doi.org/10.1016/j.atmosenv.2011.01.017.

[39] K. Alapaty, R. Mathur, J. Pleim, Ch Hogrefe, S.T. Rao, V. Ramaswamy, S. Galmarini, M. Schaap, R. Vautard, P. Makar, A. Baklanov, G. Kallos, B. Vogel, R. Sokhi, New directions: understanding interactions of air quality and climate change at regional scales, Atmos. Environ. 49 (2012) 419–421.

[40] J. Pleim, R. Mathur, S.T. Rao, J. Fast, A. Baklanov, Integrated meteorology and chemistry modeling: evaluation and research needs, Bull. Am. Meteorol. Soc. (2014) ES81–ES84, https://doi.org/10.1175/BAMS-D-13-00107.1.

[41] CCMM, Coupled Chemistry-Meteorology/Climate Modelling (CCMM): Status and Relevance for Numerical Weather Prediction, Atmospheric Pollution and Climate Research (Symposium Materials), WMO GAW Report #226, WMO, Geneva, Switzerland, 2016. March 2016. Available from: https://www.wmo.int/pages/prog/arep/gaw/documents/Final_GAW_226_10_May.pdf.

[42] A. Baklanov, D. Brunner, G. Carmichael, J. Flemming, S. Freitas, M. Gauss, Ø. Hov, R. Mathur, K.H. Schlünzen, C. Seigneur, B. Vogel, Key issues for seamless integrated chemistry–meteorology modeling, Bull. Am. Meteorol. Soc. 98 (2017) 2285–2292, https://doi.org/10.1175/BAMS-D-15-00166.1.

[43] EuMetChem, Coupled chemistry–meteorology modelling: status and relevance for numerical weather prediction, air quality and climate communities, in: A. Baklanov, B. Vogel, S. Freitas (Eds.), Special Issue Jointly Organized between Atmospheric Chemistry and Physics and Geoscientific Model Development, 2016, p. 370. http://www.atmos-chem-phys.net/special_issue370.html.

[44] Ramboll Environ, User's Guide - Comprehensive Air Quality Model with Extensions. Version 6.40, Ramboll Environ, Novato, California, 2016, p. 283.

[45] R. Mathur, J. Xing, R. Gilliam, G. Sarwar, C. Hogrefe, J. Pleim, G. Pouliot, S. Roselle, T.L. Spero, D.C. Wong, J. Young, Extending the Community Multiscale Air Quality (CMAQ) modeling system to hemispheric scales: overview of process considerations and initial applications, Atmos. Chem. Phys. 17 (2017) 12449–12474, https://doi.org/10.5194/acp-17-12449-2017.

[46] A. Hollingsworth, R.J. Engelen, C. Textor, A. Benedetti, O. Boucher, F. Chevallier, A. Dethof, H. Elbern, H. Eskes, J. Flemming, C. Granier, J.W. Kaiser, J.-J. Morcrette, P. Rayner, V.-H. Peuch, L. Rouil, M.G. Schultz, A.J. Simmons, Toward a monitoring and forecasting system for atmospheric composition: the GEMS project, Bull. Am. Meteorol. Soc. 89 (2008) 1147–1164, https://doi.org/10.1175/2008BAMS2355.1.

[47] J. Flemming, A. Inness, H. Flentje, V. Huijnen, P. Moinat, M.G. Schultz, O. Stein, Coupling global chemistry transport models to ECMWF's integrated forecast system, Geosci, Model Dev 2 (2009) 253–265.

[48] A. Baklanov, M. Lawrence, S. Pandis, A. Mahura, S. Finardi, N. Moussiopoulos, M. Beekmann, P. Laj, L. Gomes, J.-L. Jaffrezo, A. Borbon, I. Coll, V. Gros, J. Sciare, J. Kukkonen, S. Galmarini, F. Giorgi, S. Grimmond, I. Esau, A. Stohl, B. Denby, T. Wagner, T. Butler, U. Baltensperger, P. Builtjes, D. van den Hout, H.D. van der Gon, B. Collins, H. Schluenzen, M. Kulmala, S. Zilitinkevich, R. Sokhi, R. Friedrich, J. Theloke, U. Kummer, L. Jalkinen, T. Halenka, A. Wiedensholer, J. Pyle, W.B. Rossow, MEGAPOLI: concept of multi-scale modelling of megacity impact on air quality and climate, Adv. Sci. Res. 4 (2010) 115–120, https://doi.org/10.5194/asr-4-115-2010.

[49] R. Nuterman, B. Amstrup, A. Mahura, A. Baklanov, A. Zakey, D. Banciu, O. Diaconu, S. Tascu, M. Pietrisi, R. Dumitrache, Core-downstream processing chain test cases. Running the full downscaling model systems based on the MACC forecasts, Report D_OINT_2.7.1-2 (2011) 27. October 2011.

[50] J. Benavides, M. Snyder, M. Guevara, A. Soret, C. Pérez García-Pando, F. Amato, X. Querol, O. Jorba, CALIOPE-Urban v1.0: coupling R-LINE with a mesoscale air quality modelling system for urban air quality forecasts over Barcelona city (Spain), Geosci, Model Dev 12 (2019) 2811–2835, https://doi.org/10.5194/gmd-12-2811-2019.

[51] X. Tang, Managing disaster risk in a mega-city, WMO Bull 55 (4) (2006). October 2006.

[52] G. Beig, D.M. Chate, S.K. Sahu, N.S. Parkhi, R. Srinivas, A. Kausar, S.D. Ghude, S. Yadav, H.K. Trimbake, System of Air Quality Forecasting and Research (SAFAR – India) vol. 217, WMO GAW Report No., Geneva, 2015, p. 51.

[53] G.P. Brasseur, Y. Xie, A.K. Petersen, I. Bouarar, J. Flemming, M. Gauss, F. Jiang, R. Kouznetsov, R. Kranenburg, B. Mijling, V.-H. Peuch, M. Pommier, A. Segers, M. Sofiev, R. Timmermans, R. van der A, S. Walters, J.-M. Xu, G.-Q. Zhou, Ensemble forecasts of air quality in eastern China – Part 1: model description and implementation of the MarcoPolo–panda prediction system, version 1, geosci, Model Dev 12 (1) (2019) 33–67, https://doi.org/10.5194/gmd-12-33-2019.

[54] K.H. Schlünzen, D. Grawe, S.I. Bohnenstengel, I. Schlüter, R. Koppmann, Joint modelling of obstacle induced and mesoscale changes – current limits and challenges, Journal of Wind Engineering and Industrial AerodynamicsJ. Wind Eng. Ind. Aerodyn. 99 (2011) 217–225, https://doi.org/10.1016/j.jweia.2011.01.009.

[55] J.L. Santiago, R. Borge, F. Martin, D. de la Paz, A. Martilli, J. Lumbreras, B. Sanchez, Evaluation of a CFD-based approach to estimate pollutant distribution within a real urban canopy by means of passive samplers, Sci. Total Environ. 576 (2017) 46–58.

[56] R. Berkowicz, OSPM - a parameterised street pollution model, Environ. Monit. Assess. 65 (2000) 323–331.

[57] Y. Kim, Y. Wu, C. Seigneur, Y. Roustan, Multi-scale modelling of urban air pollution: development and application of a Street-in-Grid model (v1.0) by coupling MUNICH (v1.0) and Polair3D (v1.8.1), Geosci. Model Dev. (GMD) 11 (2018) 611–629.

[58] D. Ahijevych, M. Duda, L. Fowler, S.-Y. Ha, J. Jang, J. Klemp, S.-H. Park, B. Skamarock, W. Wang, M. Wong, C. Zarzycki, MPAS-A: WRF Numerics and Physics with a Height Coordinate on a Centroidal Voronoi Mesh, the 18th WRF Users' Workshop, 2017. Boulder, Colorado, U.S.A., June 12 – 16.

[59] G.G. Pfister, S.D. Eastham, A.F. Arellano, B. Aumont, K.C. Barsanti, M.C. Barth, A. Conley, N.A. Davis, L.K. Emmons, J.D. Fast, et al., A MUlti-scale infrastructure for chemistry and aerosols - MUSICA, Bull. Am. Meteorol. Soc. 101 (10) (2020) E1743–E1760, https://doi.org/10.1175/BAMS-D-19-0331.1.

[60] UFS, The Unified Forecast System (UFS), NOAA-NCAR, 2020. http://ufs-dev.rap.ucar.edu/.

[61] G. Brunet, M. Shapiro, B. Hoskins, M. Moncrieff, R. Dole, G.N. Kiladis, B. Kirtman, A. Lorenc, B. Mills, R.M.S. Polavarapu, D. Rogers, J. Schaake, J. Shukla, Collaboration of the weather and climate communities to advance subseasonal-to-seasonal prediction, Bull. Am. Meteorol. Soc. 91 (2010) 1397–1406, https://doi.org/10.1175/2010BAMS3013.1.

[62] F. Vitart, A.W. Robertson, D.L.T. Anderson, Subseasonal to seasonal prediction project: bridging the gap between weather and climate, World Meteorol. Organ. Bull. 61 (2) (2012) 2012. https://public.wmo.int/en/resources/bulletin/subseasonal-seasonal-prediction-project-bridging-gap-between-weather-and-climate.

[63] WMO, Vegetation Fire and Smoke Pollution Warning and Advisory System (VFSP-WAS): Concept Note and Expert Recommendations, World Meteorological Organization, 2018. GAW Report No235, https://library.wmo.int/doc_num.php?explnum_id=4519.

[64] F. Vitart, C. Ardilouze, A. Bonet, A. Brookshaw, M. Chen, C. Codorean, M. Déqué, L. Ferranti, E. Fucile, M. Fuentes, et al., The subseasonal to seasonal (S2S) prediction project database, Bull. Am. Meteorol. Soc. 98 (2017) 163–173, https://doi.org/10.1175/BAMS-D-16-0017.1.

[65] J. Cortinas, NOAA/OAR Contributions to Subseasonal to Seasonal Research that Will Benefit National Capabilities, Office of Weather & Air Quality NOAA Office of Oceanic and Atmospheric Research (OAR), 2017. January 25, ftp://ftp.oar.noaa.gov/ESPC/Program%20Briefs/AMS%202017/Cortinas%20AMS%20presentation%202_S2S.pdf.

[66] NASEM National Academies of Sciences, Engineering, and Medicine, Thriving on Our Changing Planet: A Decadal Strategy for Earth Observation from Space. Chapter: 7 Weather and Air Quality: Minutes to Subseasonal, The National Academies Press, Washington, DC, 2018, https://doi.org/10.17226/24938.

[67] S. Munir, M. Mayfield, D. Coca, S.A. Jubb, Structuring an integrated air quality monitoring network in large urban areas – discussing the purpose, criteria and deployment strategy, Atmos. Environ. X 2 (2019) 100027, https://doi.org/10.1016/j.aeaoa.2019.100027.

[68] J. Flemming, A. Benedetti, A. Inness, R.J. Engelen, L. Jones, et al., The CAMS interim reanalysis of carbon monoxide, ozone and aerosol for 2003–2015, Atmos. Chem. Phys. 17 (2017) 1945–1983, https://doi.org/10.5194/acp-17-1945-2017.

[69] WMO, Global Atmosphere Watch Expert Meeting on Measurement-Model Fusion for Global Total Atmospheric Deposition (MMF-GTAD) (26-27 February 2019; Geneva, Switzerland), 2020. WMO GAW Report No 250, https://library.wmo.int/index.php?lvl=author_see&id=12920.

[70] J. Kim, U. Jeong, M.H. Ahn, J.H. Kim, R.J. Park, H. Lee, C.H. Song, Y.S. Choi, New era of air quality monitoring from space: geostationary environment monitoring spectrometer (GEMS), Bull. Am. Meteorol. Soc. (2019), https://doi.org/10.1175/BAMS-D-18-0013.1.

[71] P. Ingmann, B. Veihelmann, J. Langen, D. Lamarre, H. Stark, G.B. Courrèges-Lacoste, Requirements for the GMES atmosphere service and ESA's implementation concept: sentinels-4/-5 and–5p, Remote Sens. Environ. 120 (2012) 58–69, https://doi.org/10.1016/j.rse.2012.01.023.

[72] P. Zoogman, X. Liu, R.M. Suleiman, W.F. Pennington, D.E. Flittner, J.A. Al-Saadi, et al., Tropospheric emissions: monitoring of pollution (TEMPO), J. Quant. Spectrosc. Radiat. Transf. 186 (2017) 17–39, https://doi.org/10.1016/j.jqsrt.2016.05.008.

[73] M. Bocquet, H. Elbern, H. Eskes, M. Hirtl, R. Žabkar, G.R. Carmichael, J. Flemming, A. Inness, M. Pagowski, J.L. Pérez Camaño, P.E. Saide, R. San Jose, M. Sofiev, J. Vira, A. Baklanov, C. Carnevale, G. Grell, C. Seigneur, Data assimilation in atmospheric chemistry models: current status and future prospects for coupled chemistry meteorology models, Atmos. Chem. Phys. 15

(2015) 5325–5358, https://doi.org/10.5194/acp-15-5325-2015.
[74] D. Tong, L. Pan, W. Chen, L. Lamsal, P. Lee, Y. Tang, H. Kim, S. Kondragunta, I. Stajner, Impact of the 2008 Global Recession on Air Quality over the, 2016.
[75] R.S. Sokhi, A. Baklanov, K.H. Schlünzen (Eds.), Mesoscale Modelling for Meteorological and Air Pollution Applications, Anthem Press, 2018, ISBN 9781783088263, p. 380. November 2018.
[76] G.I. Marchuk. Adjoint Equations and Analysis of Complex Systems, Springer Netherlands, 1995, p. 468p.
[77] G.R. Carmichael, A. Sandu, T. Chai, D. Daescu, E. Constantinescu, Y. Tang, Predicting air quality: improvements through advanced methods to integrate models and measurements, J. Comp. Physiol. 227 (2008) 3540–3571.
[78] J.E. Nielsen, S. Pawson, A. Molod, B. Auer, A.M. da Silva, A.R. Douglass, B.N. Duncan, Q. Liang, M.E. Manyin, L.D. Oman, W.M. Putman, S.E. Strahan, K. Wargan, Chemical mechanisms and their applications in the goddard earth observing system (GEOS) earth system model, J. Adv. Model. Earth Syst. (2017), https://doi.org/10.1002/2017MS001011.
[79] V. Mallet, Ensemble forecast of analyses: coupling data assimilation and sequential aggregation, J. Geophys. Res. 115 (2010) D24303, https://doi.org/10.1029/2010JD014259.
[80] D. Kang, R. Mathur, S.T. Rao, S. Yu, Bias adjustment techniques for improving ozone air quality forecasts, J. Geophys. Res. 113 (2008) D23308, https://doi.org/10.1029/2008JD010151.
[81] D. Kang, R. Mathur, S.T. Rao, Real-time Bias-adjusted $O_3$ and $PM_{2.5}$ air quality index forecasts and their evaluations over the continental United States, Atmos, Environ. Times 44 (2010a) 2203–2212.
[82] D. Kang, R. Mathur, S.T. Rao, Assessment of bias-adjusted $PM_{2.5}$ air quality forecasts over the continental United States during 2007, Geosci, Model Dev 3 (2010b) 309–320.
[83] J. Huang, J. McQueen, J. Wilczak, I. Djalalova, I. Stajner, P. Shafran, D. Allured, P. Lee, P. Li, D. Tong, H.-C. Huang, G. DiMego, S. Upadhayay, L. Monache, Improving NOAA NAQFC $PM_{2.5}$ predictions with a bias correction approach, Weather Forecast. 32 (2017) 407–421, https://doi.org/10.1175/WAF-D-16-0118.1,2017.
[84] I. Stajner, J. McQueen, P. Lee, J. Huang, H.-C. Huang, L. Pan, Y. Tang, D. Tong, A. Stein, J. Wilzak, I. Djalalova, D. Allured, P. Dickerson, J. Tirado, National Air Quality Forecast Capability Prediction Updates: Bias Correction for Ozone, Oral Presentation at the $17^{th}$ Annual CMAS Conference, Chapel Hill, North Carolina, U.S.A, 2018. Oct. 22-24.
[85] L. Delle Monache, J. Wilczak, S. Mckeen, G. Grell, M. Pagowski, S. Peckham, R. Stull, J. Mchenry, J. McQueen, A Kalman filter bias correction method applied to deterministic, ensemble averaged,and probabilistic forecasts of surface ozone, Tellus, Ser. B 60 (2008) 238–249, https://doi.org/10.1111/j.1600-0889.2007.00332.x.
[86] L. Delle Monache, X. Deng, Y. Zhou, R. Stull, Ozone ensemble forecasts: 1. A new ensemble design, J. Geophys. Res. 111 (2006a) D05307, https://doi.org/10.1029/2005JD006310.
[87] L. Delle Monache, T. Nipen, X. Deng, Y. Zhou, R. Stull, Ozone ensemble forecasts: 2. A Kalman filter predictor bias correction, J. Geophys. Res. 111 (2006b) D05308, https://doi.org/10.1029/2005JD006311.
[88] L. Delle Monache, J. Wilczak, S. Mckeen, G. Grell, M. Pagowski, S. Peckham, R. Stull, J. Mchenry, J. McQueen, A Kalman filter bias correction method applied to deterministic, ensemble averaged,and probabilistic forecasts of surface ozone, Tellus, Ser. B 60 (2008) 238–249, https://doi.org/10.1111/j.1600-0889.2007.00332.x.
[89] R.E. Eskridge, J.-Y. Ku, S.T. Rao, P.S. Porter, I.G. Zurbenko, Separating different scales of motion in time series of meteorological variables, Bull. Am. Meteorol. Soc. 78 (1997) 1473–1483, https://doi.org/10.1175/1520-0477.
[90] D. Kang, C. Hogrefe, K. Foley, S. Napelenok, R. Mathur, S.T. Rao, Application of the Kolmogorov-zurbenko filter and the decoupled direct 3D method for the dynamic evaluation of a regional air quality model, Atmos. Environ. 80 (2013) 58–69.
[91] S. McKeen, J. Wilczak, G. Grell, I. Djalova, S. Peckham, E.-Y. Hsie, W. Gong, V. Bouchet, S. Ménard, R. Moffet, J. McHenry, J. McQueen, Y. Tang, G.R. Carmichael, M. Pagowski, A. Chan, t. Dye, G. Frost, P. Lee, R. Mathur, Assessment of an ensemble of seven real-time ozone forecasts over eastern North America during the summer of 2004, J. Geophys. Res. 110 (2005) D21307, https://doi.org/10.1029/2005JD005858.
[92] M. Pagowski, G.A. Grell, S.A. McKeen, D. Dévényi, J.M. Wilczak, V. Bouchet, W. Gong, j. McHenry, S. Peckham, J. McQueen, R. Moffet, Y. Tang, A simple method to improve ensemble −based ozone forecasts, Geophys. Res. Lett. 32 (2005) L07814, https://doi.org/10.1029/2004GL022305.
[93] M. Pagowski, G.A. Grell, D. Devenyi, S.E. Peckham, S.A. McKeen, W. Gong, L. Delle Monache, J.N. McHenry, J. McQueen, P. Lee, Application of dynamic linear regression to improve the skill of ensemble-based deterministic ozone forecasts, Atmos. Environ. 40 (2006) 3240–3250, https://doi.org/10.1016/j.atmosenv.2006.02.006.
[94] S. McKeen, S.H. Chung, J. Wilczak, G. Grell, I. Djalalova, S. Peckham, W. Gong, V. Bouchet, R. Moffet, Y. Tang, G.R. Carmichael, R. Mathur, S. Yu, Evaluation of several PM2.5 forecast models using data collected during the ICARTT/NEAQS 2004 field study, J. Geophys. Res. 112 (2007) D10S20, https://doi.org/10.1029/2006JD007608.
[95] S. Potempski, S. Galmarini, R. Addis, P. Astrup, S. Bader, R. Bellasio, R. Bianconi, et al., Multi-model ensemble analysis of the ETEX-2 experiment, Atmos. Environ. 42 (2008) 7250–7265, https://doi.org/10.1016/j.atmosenv.2008.07.027.
[96] I. Djalalova, Coauthors, Ensemble and bias-correction techniques for air quality model forecasts of surface O3 and PM2.5 during the TEXAQS-II experiment of 2006, Atmos. Environ. 44 (2010) 455–467, https://doi.org/10.1016/j.atmosenv.2009.11.007.
[97] A.K. Petersen, G.P. Brasseur, I. Bouarar, J. Flemming, M. Gauss, F. Jiang, R. Kouznetsov, R. Kranenburg, B. Mijling, V.-H. Peuch, M. Pommier, A. Segers, M. Sofiev, R. Timmermans, R. van der A, S. Walters, Y. Xie, J.-M. Xu, G.-Q. Zhou, Ensemble forecasts of air quality in eastern China – Part 2. Evaluation of the MarcoPolo-panda prediction system, version 1, geosci, Model Dev. Discuss (2019), https://doi.org/10.5194/gmd-2018-234.
[98] W.R. Sessions, J.S. Reid, A. Benedetti, P.R. Colarco, A. da Silva, S. Lu, T. Sekiyama, T.Y. Tanaka, J.M. Baldasano, S. Basart, M.E. Brooks, T.F. Eck, M. Iredell, J.A. Hansen, O.C. Jorba, H.-M.H. Juang, P. Lynch, J.-J. Morcrette, S. Moorthi, J. Mulcahy, Y. Pradhan, M. Razinger, C.B. Sampson, J. Wang, D.L. Westphal, Development towards a global operational aerosol consensus: basic climatological characteristics of the International Cooperative for Aerosol Prediction Multi-Model Ensemble (ICAP-MME), Atmos. Chem. Phys. 15 (2015) 335–362, https://doi.org/10.5194/acp-15-335-2015.
[99] J.W. Kaiser, M. Keywood, Preface for atmospheric environment special issue on IBBI, Atmos. Environ. 121 (2015) 1–3.
[100] A. Tobías, M. Stafoggia, Modeling desert dust exposures in epidemiologic short-term health effects studies, Epidemiology 31 (6) (2020) 788–795, https://doi.org/10.1097/EDE.0000000000001255. November 2020.
[101] GAW, WMO Global Atmosphere Watch (GAW) Implementation Plan: 2016-2023. WMO GAW Report No.228, World Meteorological Organization, Geneva, 2017, p. 81.
[102] S. Nickovic, E. Cuevas Agulló, J.M. Baldasano, E. Terradellas, T. Nakazawa, A. Baklanov, Sand and Dust Storm Warning Advisory and Assessment System, SDS-WAS) Science and Implementation Plan, 2015, pp. 2015–2020.

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