

Preface

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Since its start in 2008, the Air Quality Model Evaluation International Initiative (AQMEII), coordinated by the European-Commission Joint Research Center (JRC) and the US- Environmental Protection Agency (EPA) has had as its primary goal the collaboration of the European and North American regional scale air quality modeling communities on the fundamental issue of model evaluation. The key elements driving the AQMEII process are regular dedicated workshops, the organization of international model evaluation studies, and the dissemination of findings from these studies in the peer-reviewed literature.

In the first phase of AQMEII (2010-2012) chemical transport models, used by different groups and applied for the full year of 2006 over the North American and European continents, have been extensively evaluated as described in “AQMEII: An International Initiative for the Evaluation of Regional-Scale Air Quality Models - Phase 1”, (Atmos. Environ., 53, 2012) employing the comprehensive model evaluation framework presented by Dennis et al. (2007). This framework promotes a gradual and fit-for-purpose multi-stage evaluation process that includes operational, diagnostic, dynamic and probabilistic evaluation. These stages are defined as assessing: i) the difference between model results and observations (operational evaluation), ii) the capacity to adequately model specific processes and their role in determining any deviation from observed values (diagnostic evaluation), iii) the response capacity of models with respect to changes in input parameters such as emissions (dynamic evaluation), and iv) the ways in which uncertainty could be estimated and model results generalized in probabilistic ways (probabilistic evaluation). While all these model evaluation modes were employed in Phase 1, most of the contributions focused on operational and probabilistic evaluation as noted in Schere et al. (2012) who reflected on lessons learned from that activity.

The model evaluation framework also forms the basis for the work under AQMEII Phase 2 that is presented in this special issue, and the various contributions cover a fuller range of this framework, most notably a larger number of contributions focused on diagnostic evaluation as well as several contributions covering dynamic and probabilistic evaluation aspects. The key difference between the design of Phase 1 and Phase 2 is that the models participating in Phase 1 were “stand-alone” or “offline” chemistry transport models (CTM) that required meteorology produced by meteorological models (MetM) as input, while the models participating in Phase 2 were on-line coupled or integrated CTMs and MetMs. *On-line coupled or integrated* have distinct meanings as defined in Baklanov et al. (2014): *On-line* identifies the property of the model to generate the meteorology that drives the transport within the model itself, therefore solving equations for momentum, radiation and heat at the same time as transport and chemical transformation of chemically active species. This modeling approach leads to a higher level of complexity in model development, application and evaluation but at the same time also yields intrinsic consistency in the model results which is produced by the solution of a coherent set of equations and numerical methodologies. It is well known that atmospheric dynamics and composition are interconnected, that

variations in heat distribution affect atmospheric flows and physics, and that atmospheric optical and heat properties depend on atmospheric composition. An *online coupled model* is a model in which all these feedback loops are partially or completely closed. Therefore, the evaluation strategy for on-line, coupled models has to consider issues such as:

- Identify the processes which may give rise to feedback loops, and how the feedback processes should be represented as model parameterizations.
- Identify the potential effect of errors in one part of the chain of processes making up a feedback loop on the overall model predictions.
- Identify existing measurement data which may be used for evaluation of coupled models, requirements for observational systems for such purposes and create strategies to evaluate not just the model predictions, but also the parameterizations used to incorporate feedback mechanisms.

These issues present new challenges to the diagnostic evaluation aspect of the model evaluation framework. In uncoupled models the transport, radiation and energy budgets are pre-determined input elements to the chemistry portion of the models, while in coupled models these elements can vary in time and space in response to the atmosphere's chemical composition.

A total of 20 groups took part in this project by submitting their model results. These groups are, in alphabetical order:

- Air Quality Research Section, Atmospheric Science and Technology Directorate, Environment Canada, Toronto, Canada
- Atmospheric Modeling and Analysis Division/NERL/ORD/US-EPA, Research Triangle Park, NC, USA
- Center of Excellence SPACE-SI, Ljubljana, Slovenia
- Centre for Atmospheric & Instrumentation Research, University of Hertfordshire, Hatfield, United Kingdom
- Department of Marine, Earth and Atmospheric Sciences, North Carolina State University, Raleigh, USA
- Department of Physical and Chemical Sciences, Center of Excellence for the Forecast of Severe Weather (CETEMPS), University of L'Aquila, L'Aquila, Italy
- Earth Sciences Department, Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain
- ECMWF, Shinfield Park, Reading, United Kingdom
- Environmental Software and Modelling Group, Computer Science School, Technical University of Madrid (UPM), Campus de Montegancedo, Boadilla del Monte, Madrid, Spain
- Karlsruher Institut für Technologie (KIT), Institut für Meteorologie und Klimaforschung, Atmosphärische Umweltforschung (IMK-IFU), Garmisch-Partenkirchen, Germany
- Laboratory for Air Pollution and Environmental Technology, Empa, Duebendorf, Switzerland
- Leibniz Institute for Tropospheric Research, Leipzig, Germany
- Met Office, FitzRoy Road, Exeter, United Kingdom
- National Center for Atmospheric Research, Boulder, Colorado, USA

- National Institute of Meteorology and Hydrology, Bulgarian Academy of Sciences, Sofia, Bulgaria
- Netherlands Organization for Applied Scientific Research (TNO), Utrecht, The Netherlands
- Ricerca sul Sistema Energetico (RSE SpA), Milano, Italy
- Section Environmental Meteorology, Division Customer Service, ZAMG - Zentralanstalt für Meteorologie und Geodynamik, Wien, Austria
- University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia.
- University of Murcia, Department of Physics, Physics of the Earth, Campus de Espinardo, Murcia, Spain

These groups operated a total of eight different models built around six different meteorological cores, and some models were run in multiple different configurations.

The primary focus of Phase 2 was on simulating the year 2010, but updated inputs were also prepared for 2006 for North America to enable direct comparisons to Phase 1 results as well as facilitate dynamic evaluation studies. As in Phase 1, the coordination of the NA activities was led by US-EPA while the coordination of the EU activities led by the Joint Research Centre. The Joint Research Center acted also as center of collection of measurement data and modeling data through the ENSEMBLE facility (Galmarini, et al. 2012) and center for the collective analysis of the results. The coincidence in scopes of the AQMEII phase 2 and a European COST funded project stimulated a direct collaboration between the two activities. The COST Action ES1004: European framework for online integrated air quality and meteorology modelling (EuMetChem) promotes and coordinates European activities in the area of online coupled modelling (see: <http://www.eumetchem.info/>). It is focusing on a new generation of online integrated atmospheric chemical transport and meteorology (numerical weather prediction and climate) modelling with two-way interactions between different atmospheric processes including chemistry (both gases and aerosols), clouds, radiation, boundary layer, emissions, meteorology and climate. COST 1004 encouraged their modelling community to contribute to the AQMEII phase 2 activity which became a unique opportunity for benchmarking the current state of a range of new model systems that have been developed only recently.

US-EPA and TNO (NL) prepared emission inventories for 2006 and 2010 for NA and 2010 for Europe respectively, with inputs and assistance from other organizations including the Finnish Meteorological Institute for fire emissions and Environment Canada for updating specific portions of the inventories. Chemical boundary conditions were provided by ECMWF for the modelling domains in the two continents based on the MACC-II global atmospheric chemical composition modeling (Inness et al., 2013).

All modeling groups were requested to follow the protocol illustrated in Figure 1 for their simulations. In this protocol, meteorological analyses were used to initialize the model simulations. Following twelve to twenty-four hours of spin-up in the absence of coupling, forecasts of duration forty-eight hours were carried out, the final chemical states of which were used to provide chemical initial conditions for the subsequent overlapping forty-eight hour simulations. These consecutive forty-eight hour forecasts were carried out in either coupled or uncoupled mode, and in each case formed a continuous time series of model outputs which could then be compared to observations. The model performance analyses

undertaken here should thus be considered in the context of synoptic time-scale meteorological and air-quality forecasting, as opposed to free-running or climatological prediction.

JRC and Environment Canada collected, compiled and harmonized a massive amount of monitoring and observation data for model evaluation. As was the case in Phase 1, these data were contributed by a large number of research and operational monitoring networks in the two continents. For 2010, for the two continents this included one year of surface monitoring at roughly 4,000 stations for gas phase species, 3,000 stations for particulate matter, 3,000 stations for meteorology and 150 stations for aerosol optical depth. In addition, there were vertical profiles of ozone and meteorology at roughly 15 ozone sonde stations and three airports. The large variety of sources of information led to a substantial effort in data harmonization and screening. All data were transferred to the JRC-ENSEMBLE (Galmarini et al., 2004, Galmarini et al., 2012) system, georeferenced and coupled with the model data that were also gathered there.

The analysis of models results and comparison with observations was distributed throughout the community of participants, which took the charge of addressing specific research questions. This Atmospheric Environment AQMEII issue has therefore been organized as follows. The first set of papers (Pouliot et al., 2015; Soares et al., 2015; Giordano et al., 2015; Stoeckenius et al. 2015) focuses on setting-up the case study by presenting the common emissions and boundary conditions used by all modeling groups and a comparison of the observed meteorological and air quality conditions in 2006 and 2010 over North America. These model input and overview papers are followed by collective analysis papers describing operational, diagnostic and probabilistic evaluation of participating models (Im et al., 2015(a,b); Brunner et al., 2015; Wang et al., 2015a; Campbell et al., 2015), with some papers specifically focusing on the role of feedback effects on model meteorological and chemical performance (Makar et al, 2015(a,b), Kong et al., 2015, San Jose et al., 2015), the role of assumptions about aerosol optical properties on simulated aerosol optical depth (Curci et al, 2015), and the role of different chemical mechanisms on simulated gas phase concentrations (Knote et al. 2015). These collective analysis papers are followed by a group of papers from groups that used the same modeling system (i.e. WRF-Chem) and coordinated a model-specific activity so that the effects of specific process parameterizations and feedback processes could be intercompared in a systematic manner (Balzarini et al., 2015; Baro et al., 2015; Forkel et al., 2015; San Jose et al., 2015). The remaining papers are individual contributions from participating modeling groups covering various aspects of fully coupled model construction and operational, diagnostic and dynamic evaluation (Badia and Jorba, 2015; Gan et al., 2015; Hogrefe et al., 2015; Gong et al., 2015; Wang et al., 2015b, Yahya et al., 2015).

This body of work contained in this special issue represents a first step in the systematic evaluation of online coupled modeling systems through a multi-model intercomparison approach. The potential scope of research in this new field is broad, and not all issues relating to coupled models could be addressed. However, the papers contained herein provide clear indications on the main issues requiring additional research, and on the modelling strategies needed for a systematic evaluation of coupled models. A key recommendation from several of the contributions that follow is that future work should focus on shorter-duration process-focused sensitivity simulations, in order to better intercompare process representations and model coupling methodologies. Another important finding highlighted in several contributions was

that inter-model variability typically is greater than the feedback effects simulated with a given model. This implies that factors other than feedback effects such as emissions, boundary conditions, and process representations of chemistry and/or transport remain the key determinants for overall model performance. However, within a given model, the feedback effects were shown to be capable of improving both meteorological and chemical forecasts, especially for specific episodes, and hence represent a fruitful direction for future research.

Some of the other highlights of findings from Phase 2 of AQMEII include:

- Results indicated that it is important to include interactions between meteorology and chemistry (especially aerosols and ozone) in online coupled models
- Aerosol indirect and direct effects often counteract each other, direct effects are weaker on the annual scale. The Russian forest fire and Sahara dust case studies have shown significant aerosol direct effects on meteorology (and loop back on chemistry). High levels of PM (such as over the Moscow area during these episodic events) caused significantly reduced downward shortwave radiation and surface temperature and reduced PBL heights as also noted in previous studies (e.g. Wong et al., 2012)
- The aerosol indirect effect (cloud microphysics implementation) is a prime cause of model differences
- The representation of aerosol indirect effects is weak/poor and needs to be further developed and improved in online coupled models.

A key finding from AQMEII-2 (as well as previous global model simulations under the Task Force on the Hemispheric Transport of Air Pollution, TF-HTAP, model intercomparison) was that global transport of certain pollutants may exert a significant seasonal influence on simulated regional scale concentrations (Fiore et al., 2009). The influence of global scale background concentrations on regional scale air quality simulations is the primary focus of the *next* phase of AQMEII (Rao et al., 2012) that will contribute to the activities of TF-HTAP. The activity is aimed at applying and comparing modeling techniques to provide policy-relevant information on the impact of long-range transport on regional air quality. The analysis will focus on answering the following questions:

- In which aspects does model performance over North America and Europe differ between global and regional models?
- How do source/receptor linkages differ between global models and regional models linked to the global scale via boundary conditions?

This next phase of AQMEII will continue to involve the North American and European regional scale modeling communities. It is anticipated that both coupled and uncoupled modeling systems will be applied during this phase, and there is also the possibility to apply and compare different modeling techniques such as brute force sensitivity simulations vs. integrated source apportionment approaches in the context of quantifying the impact of long-range transport on air pollution over North America and Europe.

Finally, we would like to note that the monitoring data from all data providers (listed in the acknowledgement hereafter), and that the model results contributed by the various groups for both AQMEII Phase 1 and Phase 2 are available to the broader community for further research and analysis. Interested researchers can contact Stefano Galmarini and Christian Hogrefe for further information.

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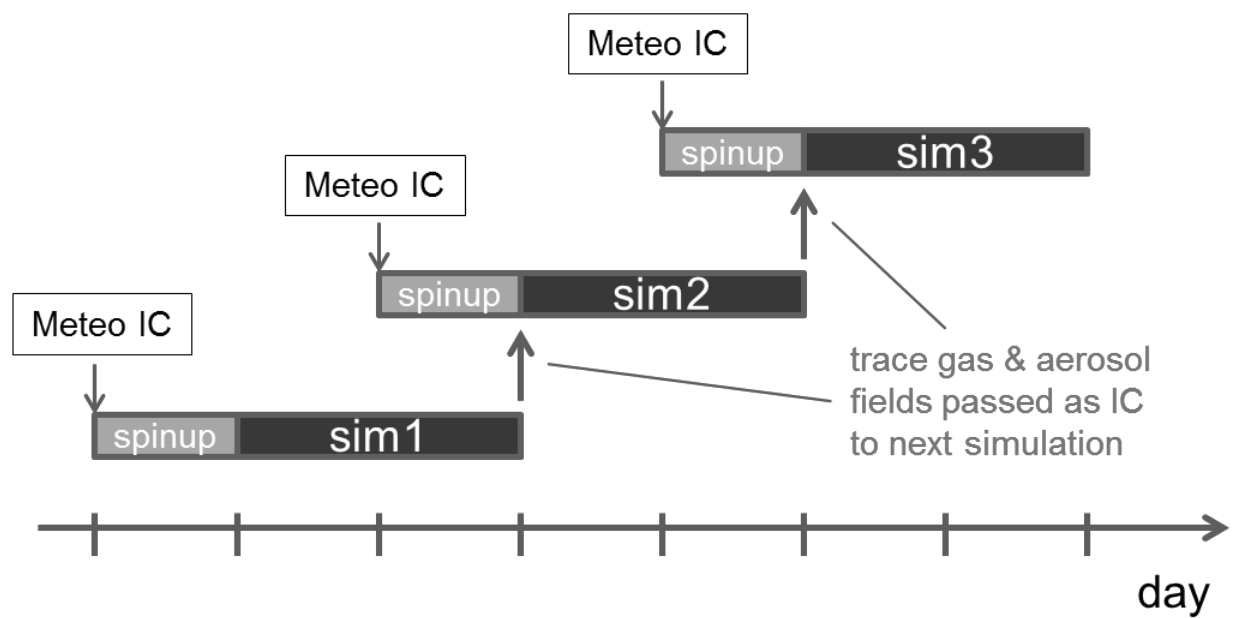


Figure 1. Schematic illustrating the modeling protocol recommended for all AQMEII Phase 2 model simulations.