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Review article

Observing System Simulation Experiments for air quality

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HIGHLIGHTS

- We provide a framework for the application of OSSEs for air quality issues.
- We identify the main elements for air quality OSSEs.
- For each element of these OSSEs, we define a set of requirements.
- We present illustrative examples from existing air quality OSSEs.
- We recommend OSSEs for the optimal design of air quality instruments.

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ABSTRACT

This review paper provides a framework for the application of the Observing System Simulation Experiment (OSSE) methodology to satellite observations of atmospheric constituents relevant for air quality. The OSSEs are experiments used to determine the potential benefit of future observing systems using an existing monitoring or forecasting system and by this can help to define optimal characteristics of future instruments. To this end observations from future instruments are simulated from a model representing the realistic state of the atmosphere and an instrument simulator. The added value of the new observations is evaluated through assimilation into another model or model version and comparison with the simulated true state and a control run.

This paper provides an overview of existing air quality OSSEs focusing on ozone, CO and aerosol. Using illustrative examples from these studies we present the main elements of an air quality OSSE and associated requirements based on evaluation of the existing studies and experience within the meteorological community.

The air quality OSSEs performed hitherto provide evidence of their usefulness for evaluation of future observations although most studies published do not meet all the identified requirements. Especially the evaluation of the OSSE set-up requires more attention; the differences between the assimilation model and the simulated truth should approximate differences between models and real observations. Although this evaluation is missing in many studies, it is required to ensure realistic results. Properly executed air quality OSSEs are a valuable and cost effective tool to space agencies and instrument builders when applied at the start of the development stage to ensure future observations provide added value to users of Earth Observation data.

1. Introduction

Air quality is related to the atmospheric composition of trace gases and particulates near the Earth's surface (McNair et al., 1996;

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Brasseur et al., 2003); it is affected by chemistry, transport and emissions. The adverse impact of poor air quality on human health and ecosystems, with high economic costs to society, makes air quality one of the major societal challenges of the 21st Century (Lahoz et al., 2012). Owing to the influence of local, regional and transcontinental processes on air quality, there is a need for global observations of atmospheric composition, to monitor changes in it, and to check the impact of societal actions, including regulations, taken to reduce the impact of adverse air quality. Currently, satellites, typically in Low Earth Orbit (LEOs) or in Geostationary Earth Orbit (GEOs), are the only observational platform (present or planned) that can provide such global coverage (Lahoz et al., 2012; Bowman, 2013) – for GEOs, this is provided by a satellite constellation (CEOS, 2011).

Since the early 1990s, there have been a growing number of satellite observations on atmospheric composition and, specifically, air pollutants. Examples include GOME, SCIAMACHY on the ESA ERS-2 and Envisat platforms, and MODIS, MOPITT, OMI on the NASA EOS-Terra and EOS-Aura platforms (Lahoz, 2010). In the near future new techniques and satellite instruments will result in even more observational atmospheric composition data becoming available, including new products or species, with increased spatial and temporal resolution and improved accuracy. Examples include the ESA Sentinel 4, a GEO satellite, and the ESA Sentinel 5 and its precursor 5P, both LEO satellites (Lahoz, 2010); the NASA TEMPO mission, a GEO satellite (Chance et al., 2013); and the JAXA AQ-Climate mission, a GEO satellite (Akimoto et al., 2008). To justify new expensive instruments on satellite platforms, the added value of the instrument products and their associated requirements (e.g., high spatial or temporal resolution) needs to be demonstrated in an objective way. In the early stages of instrument design, requirements from data users are essential to help design the instruments that provide the products addressing societal and scientific needs.

A method to objectively determine the added value of future satellite observations and to investigate the impact of different instrument designs is that of Observing System Simulation Experiments (OSSEs). These experiments have been extensively used and shown to be useful in the meteorological community to test the impact of future meteorological observations on the quality of weather forecasts (Nitta, 1975; Atlas, 1997; Lord et al., 1997; Atlas et al., 2003). The OSSEs are increasingly being used by the space agencies to assess the added value of future instruments (e.g., work on ADM-Aeolus; Tan et al., 2007). Although the usefulness of OSSEs is well established, they have limitations, discussed in Masutani et al. (2010) and references therein. A frequent criticism of OSSEs is that they are overoptimistic, largely owing to the difficulties of representing the real Earth System (e.g., the atmosphere), even with state-of-the-art numerical models. Nevertheless, even if overoptimistic, OSSEs provide bounds on the impact of new observing systems, for if additional instruments provide no significant impact within an OSSE, they are unlikely to do so in reality. In Section 2 we provide a description of the OSSE method.

There is a close relationship between OSSEs and Observing System Experiments, OSEs (see e.g., Bouttier and Kelly, 2001 or Masutani et al., 2010). The OSEs assess the value of existing observations for data assimilation. They do so by removing a subset of observations from a data assimilation system to measure the impact of those observations. OSEs can be relatively expensive, as they may need to use a full data assimilation system; however, their expense is significantly lower than the typical cost of a satellite instrument. Meteorological agencies, as well as research institutions, use OSEs and related approaches on a regular basis.

The OSSE technique was first used to test the added value of air quality observations in 2009 (Timmermans et al., 2009a, 2009b; Edwards et al., 2009). Since then several research teams have developed OSSEs for investigating the value of future satellite observations of air pollutants. These studies, presented in Section 3, show that OSSEs are a powerful tool for determining the value of future observations and for defining requirements for specific instruments. However, while meteorological OSSEs are well established within the community, the experience in air quality OSSEs has been hitherto rather limited, and a common approach is still to be developed. The approach in air quality OSSEs also applies to OSSEs for other chemical species with an impact on the environment, an example being the greenhouse gas CO_2.

Air quality OSSEs differ from meteorological OSSEs in a number of ways, the main differences arising from the different characteristics of the meteorological and atmospheric composition elements of the Global Observing System (GOS). The OSSEs should evaluate the added value of new instruments to the current observing system. However, there are less atmospheric composition observations than meteorological observations. As a result, air quality OSSEs tend to compare observation networks including single observation types, instead of multiple observation types. For example, an air quality OSSE often compares the relative impact of two different single satellite platforms proposed as additions to the GOS. As for meteorological OSSEs, comparison of this impact is typically against the performance of a free model run without assimilation of the proposed observing platforms.

Further differences between meteorological and air quality OSSEs occur because the observational errors in the latter are generally less well-characterized, and because data assimilation systems for the latter are relatively less developed, often leading to simpler approaches being implemented for air quality OSSEs. Another difference influencing the OSSE and its set-up is the forcing that drives the model and the divergence or convergence of the model after a prescribed amount of time. Whereas initial conditions generally drive meteorological models, emissions generally drive chemical transport models (CTMs). Meteorological models generally diverge, whereas CTMs generally converge, the latter owing to the constant driving force provided by emissions. This difference is reflected in the design of the OSSE, especially in the choice of models, assimilation system and evaluation indicators. Note, however, that both meteorological and air quality OSSEs need to address the issue of model and/or data assimilation system bias. Ménard (2010) discusses methods to address bias in a data assimilation system.

The goal of this review paper is to provide a framework for OSSEs applied to those observations of atmospheric composition that impact air quality – hence we speak of air quality OSSEs. In Section 2 we introduce the OSSE methodology. In Section 3 an overview of air quality OSSEs performed hitherto is given. In Section 4 we describe the main requirements for air quality OSSEs based on illustrative examples and from critical examination of existing air quality OSSEs. Section 5 provides conclusions. Finally, by showing the potential of air quality OSSEs with respect to observations of atmospheric composition, we wish to encourage their incorporation in the early stages of instrument development for monitoring air quality, e.g., by the space agencies. This should help ensure the usefulness of products from new instruments, as the OSSEs will provide guidance on whether observations can meet the requirements from end users such as the meteorological agencies, the environmental agencies, and the broader scientific community interested in Earth Observation data.

2. The OSSE method

OSSEs are experiments used to determine the potential impact of future observing systems in an existing monitoring or forecasting