ESA project

Impact of Spaceborne Observations on Tropospheric Composition Analysis and Forecast (ISOTROP)

Executive Summary

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Impact of Spaceborne Observations on Tropospheric Composition Analysis and Forecast (ISOTROP)

Executive Summary

The ISOTROP project was a response to the ESA ITT "Impact of Spaceborne Observations on Tropospheric Composition Analysis and Forecast", AO/1-6845/11/NL/AF. The general aim is to assess the benefit of the LEO+GEO satellite system for the understanding of local to regional scale tropospheric composition with a focus on Europe. The ISOTROP consortium involved researchers from the European institutes CNRS-GAME, TNO, NILU, FMI, and was led by KNMI. The study focussed on Sentinel 5-P (S5P) and Sentinel 4 (S4) observations, with a sensitivity study for the Sentinel 5, which will have a different overpass time than Sentinel 5-P. The study focussed on four chemical species: NO_2, HCHO, CO and O_3.

Within ISOTROP a comprehensive series of Observing System Simulation Experiments (OSSEs) were performed. Two European air quality modelling and assimilation systems, MOCAGE from France and LOTOS-EUROS from the Netherlands, were used for this.

ISOTROP has followed the steps of a well constructed OSSE study, which are detailed below:

- **Nature Runs** were produced for 3 summer months and 3 winter months with both modelling systems. The resolution is 7x7 km, and runs are available over a large European domain. These simulations were compared with surface observations to investigate the realism of these runs.
- **Synthetic observations** for NO_2, HCHO, CO and O_3 were produced for Sentinel 4 and Sentinel 5-P separately, based on the Nature Run, and for a period of 6 months. The synthetic observation generation follows the DOAS approach for NO_2, HCHO and optimal estimation for CO and O_3. Detailed error estimates are produced, and averaging kernels are provided in the product for individual pixels. Synthetic retrievals of the effective cloud fraction and top pressure are produced from the ECMWF meteorological analyses. The synthetic observations account for the geometry of individual pixels, and the corresponding cloud properties and albedo. Synthetic surface observations were also produced.
- **Reference runs** are produced by both models. Where relevant, this is based on an assimilation of surface observations.
- **S4 and S5P CO and ozone OSSEs** were performed with the MOCAGE system based on synthetic observations computed from the LOTOS-EUROS Nature runs, extended into the stratosphere by simulations with the TM5 model.
- **S4 and S5P NO_2 and HCHO** OSSEs were performed with the LOTOS-EUROS system based on synthetic observations computed from the MOCAGE Nature runs. An Ensemble Kalman filter approach is used which adjusts emissions to optimise the trace gas concentrations.

The main results of ISOTROP may be summarised for each of the four species separately:

Carbon monoxide: The CO observations from S5P / S5 are expected to be of high quality. The observations in the SWIR band show nearly constant averaging kernel profiles with high sensitivity at the surface over land. Typical estimated uncertainties are of the order 2-10%. Based on these synthetic observations the OSSE runs conducted demonstrate a very good skill to reproduce the Nature Run results over mainland Europe, and are able to capture phenomena such as the forest fires that occurred in Portugal during summer 2003. Closer to the coast the results are more influenced by air masses coming from the ocean, less constrained by the observations which are much more uncertain over water. Cloud-covered observations over the ocean help to constrain the concentrations around coastal regions.

Nitrogen dioxide: Compared to present-day capabilities the nitrogen dioxide observations from S4, S5P and S5 bring considerable advances, namely 1) a much improved resolution of about 7 km; 2) hourly observations in the case of S4 providing full diurnal sampling; and 3) foreseen improved uncertainties (to about 15-30% for individual observations) due to advances in the characterisation of aspects like clouds, albedo, aerosol effects. Despite the decrease of the NO_2 sensitivity towards the surface, the EnKF system is strongly adjusting also concentrations close to the surface by adjusting the emissions. Note that this analysis system is less flexible at remote locations with small emission fluxes. In the case of S4, many of the nature run features could be reconstructed throughout the entire day. For S5P or S5 a good impact was observed up to 3-6 hours after the overpass. With the increased observations resolution of 7 km we are able to provide constraints on source sectors such as road traffic.

Formaldehyde: In Europe, mean concentrations of HCHO are relatively low compared to other parts of the World such as the tropics. For individual observations, the noise-dominated uncertainty is expected to be more than 100%, which results in very noisy images for individual orbits. When the data is averaged over a period of a week or longer, the distribution of concentrations starts to emerge from the noise. The LOTOS-EUROS assimilation system has not been specifically optimised to deal with such noisy daily data. Nevertheless, a positive impact from the data could be observed for the fire plumes over Portugal with elevated HCHO columns.

Ozone: For the synthetic observations several choices were made. First, the spectral range was limited to 300-320 nm, discarding the shorter wavelengths, which allows us to retrieve ozone profiles at the full resolution of S4 and S5P (without co-adding). Secondly, we used the ideas of Migliorini to present the information content of the observations in a very efficient way to the (MOCAGE) assimilation system. At the proposal phase it was already clear that we could not expect major impacts in ozone at the surface based on UV ozone profile observations only. From these observations we obtain about one piece of information in the troposphere, with a larger sensitivity in the free troposphere compared to the boundary layer. On the other hand, ozone concentrations are constrained heavily in the boundary layer due to availability of a large number of hourly surface observations. Nevertheless, we could show that good impact from the S4 and S5P observations is found in the middle troposphere. Cloud covered pixels contain similar or maybe even better information than the cloud free scenes.

ISOTROP was an ambitious project, including OSSE studies for 4 compounds for both geostationary and polar platforms. The project has mainly focussed on demonstrating the impact of the observations on the model concentrations and on the degree in which the Nature Run simulations could be recovered based on the synthetic satellite datasets. As such we consider the ISOTROP project as a first step and there is room for complementary studies. The OSSE setups can be further optimised to answer important questions like how much the satellite observations can help to improve our understanding of air pollutant concentrations in the planetary boundary layer, to quantify long-range transport, to improve emission fluxes, and to improve our understanding of chemical composition and processes in the troposphere.

In this context there are a number of recommendations and suggestions for possible follow-up studies:

- **International collaboration.** There is a lot of attention internationally for performing OSSE experiments for atmospheric chemistry. In particular, OSSEs are discussed in the context of CEOS and the global constellation of geostationary platforms for air pollution monitoring. Further international collaboration would be advised and can be sought in this respect. For instance, models, synthetic observations and Nature Runs could be shared with American and Asian teams, and results should be discussed internationally at events such as the OSSE workshop held in Reading, November 2016.
- **Ozone OSSE**. The ISOTROP ozone OSSE was limited to observations derived from the UV. As was shown, this dataset alone is of limited use for air quality and boundary layer composition. A clear recommendation is the combined use of observations from various wavelength ranges, UV, Infrared and possibly the visible part of the spectrum. Several studies have already proved that such combinations will largely increase the information content in the troposphere, and will add information to the lowest few kilometres. An example would be the combination of observations from Sentinel 4 and IRS.
- **Meteorology**: The future satellite monitoring capabilities will have an order of magnitude resolution increases compared to present-day observations. In ISOTROP we decided to focus on 2003 because of the heat wave and fire conditions. A drawback of this approach was that the available meteorological datasets are relatively coarse, and do not reflect the amount of detail resolved by the satellites. For future studies we recommend the use of more modern meteorological analyses at km-scale resolutions, which are achievable today, and corresponding ensemble analyses (uncertainties). This will give a more realistic impression of the impact of the future observations for e.g. emission inversions.
- **Spatial resolution of the clouds and albedo maps**. The ISOTROP synthetic observations are based on relatively coarse resolution albedo maps and coarse resolution model clouds. Furthermore, we find differences between the ISOTROP cloud simulations and observations by OMI, which observes on average larger cloud fractions. Future OSSE studies could improve upon these aspects by using a high-resolution meteorological driver, and by using e.g. albedo maps from MODIS or similar instruments, and by focussing on other years.
- **Treatment of clouds and aerosols in OSSE**. The approach ISOTROP has followed is to compute synthetic satellite observations of cloud cover and height by using the cloud information for the meteorological drivers. Future

OSSEs could investigate other observation-based approaches, for instance by using geostationary cloud observations. In the ISOTROP approach observations are produced for all fractional cloud covers. An alternative approach would be to start with cloud filtering, and to retrieve only the clear-sky observations, accounting more explicitly for aerosols. Such alternative approaches have different error budgets and may result in different impacts on air quality models. Understanding the impacts of such choices is important.

- **Multi-species OSSE**. The LOTOS-EUROS simulations clearly show that observations of one species impact the others. The chemistry of ozone, CO, NO2 and HCHO is tightly linked. In ISOTROP we investigated the impacts of the observations individually. A full impact study of S4/S5/S5P data, however, should assimilate all these observations simultaneously. This is a clear recommendation for future OSSE studies.
- **Formaldehyde.** Formaldehyde observations are special, because of the large uncertainty levels, which is largely of a random noise-like character. The LOTOS-EUROS system is not optimised to deal with such information, and the impact seen is rather small. It is a clear challenge and recommendation to develop other assimilation strategies (e.g. a 4D-Var with a long time window) or pre-processing strategies for the observations (spatial/temporal averaging) to exploit noisy data and to extract the information contained. Because of the large number and high density of observations we are confident that systems will be developed that can deal with the data efficiently.
- **Formaldehyde retrievals.** The synthetic observations for formaldehyde are based on typical slant column errors of 1.2e16 molecules/cm^2. (Source: S5P/TROPOMI HCHO ATBD, 2015) However, more recent results for e.g. OMI suggest that this number is conservative, and 0.8e16 molecules/cm^2 may be achievable/realistic by optimising the DOAS fitting procedure (results obtained in the European QA4ECV project, Isabelle de Smedt private communications). This suggests that a larger impact of the observations may be foreseen than what is found in the ISOTROP HCHO OSSE.
- **CO observations above the ocean**. Carbon monoxide observations above cloud-free ocean are very noisy, due to the very low surface albedo, and do not constrain the OSSE results. However, the cloud-covered oceans have a good signal. It is advised to study such ocean observations in more detail and to better quantify the uncertainties.
- **Sensitivity to OSSE components**. The outcome of the OSSE experiments is a result of all the details of the components of the entire OSSE system: the synthetic observation characteristics and uncertainty estimates, the assimilation approach, treatment of the observations in the assimilation, and modelling details. In general, it is good that OSSE experiments are repeated by other groups to test the robustness of the conclusions and of the OSSE components. In particular, the impact of the assimilation approach chosen is an interesting aspect to study. The Nature Runs in ISOTROP have been assessed, but mainly at the surface. For instance, for the ozone and NO_2 OSSE the realism of the vertical profiles is important and additional studies could be defined accordingly.
- **Emissions:** Improving emissions top-down by assimilating satellite observations is a study by itself. In ISOTROP we have applied the Ensemble Kalman filter, which adjusts emissions to improve the concentrations. We could show that the NO_2 observations were efficiently assimilated, which

adjusted the emissions, which in turn brought the model results in closer agreement with the Nature Run. However, model uncertainties especially concerning chemical processes influence the emission estimates. A multi-species assimilation may be an efficient approach to reduce uncertainties in the model state and processes, and in this way improving the emission estimates. This could be a topic for future OSSEs.

- **Efficient interface to ozone observations:** One of the innovations of ISOTROP is the delivery of the ozone profile information in the form of leading eigenvectors of the radiative transfer code. This represents a very efficient and convenient interface between the retrievals and data assimilation systems. The use of this approach is a clear recommendation for future OSSEs, but also for the delivery of new real-time or reprocessing optimal estimation level-2 datasets of existing and future satellite instruments.