ASSIMILATION OF EPS TROPOSPHERIC OZONE FOR AIR QUALITY FORECAST

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ABSTRACT

This paper describes the objectives, proposed methodology and preliminary results of the EPS-MetOp RAO project 3029, which objective is to evaluate the feasibility of using EPS tropospheric ozone information to constrain the forecast of air quality at European scale: data assimilation methodologies will be applied in view of improving the analysis of ozone concentrations in the boundary layer. The project builds on two main methodological steps. First, a feasibility study is based on twin numerical experiments, and aims to assess the interest of assimilating tropospheric ozone columns and profiles, to be provided by IASI, for analysing boundary layer ozone. Second, experiments will be performed to evaluate the improvement brought by assimilating IASI tropospheric ozone information: these experiments will be conducted using simulated data, obtained from the IASI instrument model, and with real IASI data when available. The project expects to demonstrate the feasibility of assimilating IASI tropospheric ozone measurements for boundary layer ozone analysis.

Key words: IASI; tropospheric ozone; data assimilation; regional air quality.

1. INTRODUCTION

Air quality forecast requires predicting the concentrations of pollutants in the lowest layers of the troposphere. This is performed using Chemistry-Transport Models specifically designed for tropospheric studies. The performance of the forecast is strongly dependent on the availability and quality of the input data, many of which are not accessible by measurements: emissions, depositions, boundary conditions, meteorological fields, . . . So far, the only available measurements likely to constrain the forecast are provided by ground based air quality monitoring networks: these data have a very good temporal sampling but are irregularly scattered in the spatial domain and are of variable quality. Space borne measurements of the chemical composition of the troposphere are continuously improving and constitute a novel and potentially powerful data source for improving air quality forecast, by providing a measurement network with uniform spatial sampling and quality. However, space-borne measurements of chemical concentrations in the boundary layer are not expected in a near future. The proposed project aims to assess the feasibility and interest of assimilating space borne measurements of tropospheric ozone, to be provided by IASI on the EPS/MetOp platform, for improving the forecast of boundary layer ozone.

The data assimilation experiments will be performed on the air quality modelling system Polyphemus, developed by the CEREA laboratory of ENPC, France, and described in section 2. The first step of the project consists of a feasibility study, building on twin numerical experiments. This study investigates the potential interest of the information, provided by IASI and assumed representative of free troposphere ozone, for improving the quality of the forecast in the boundary layer, and accordingly define the characteristics of an assimilation system dedicated to space borne tropospheric measurements. It is described in section 3. The second step of the project consists in conducting experiments with realistic IASI data for quantifying their interest with respect to air quality forecast. Before the actual availability of IASI measurements after the launch of EPS/MetOp, the experiments will be conducted by generating IASI radiances using a reference atmosphere model and the IASI instrument model, the radiances being then inverted to yield the ozone columns and profiles. These experiments are described in section 4.

The expected outcome of the project consists of conclusions on the interest of assimilating IASI ozone information within a continental CTM for improving air quality forecast in the boundary layer, and recommandations for the optimal vertical and temporal sampling of future tropospheric missions. The perspectives are discussed in section 5.

2. THE AIR QUALITY MODELLING SYSTEM POLYPHEMUS

Polyphemus [1] is a full modeling system for air quality. It is designed to yield up-to-date simulations in a reliable framework, allowing to deal with many fields: photochemistry, heavy metals, radionuclides, aerosols, etc. It

is able to handle simulation from regional to continental scale. The heart of the system is the CTM Polair3d [2], a 3D Eulerian model responsible for time integration. The CTM is controlled by a set of drivers for specific applications, the simplest being direct forecast, other higher level applications concerning sensitivity studies [3], inverse modelling [4], data assimilation [5], or ensemble forecast [6]. The input data required by the drivers are produced by the AtmoData library [7], responsible for accessing raw data sources in their original format and generating the required physical parameterisations, as for instance computation of vertical diffusion from meteorological fields.

Figure 1 depicts a first example of Polyphemus applications: ozone forecast at European scale, performed using ECMWF meteorological fields and EMEP emission inventory. This application has been extensively validated against ground measurements and will be used in the project to generate reference troposphere descriptions.
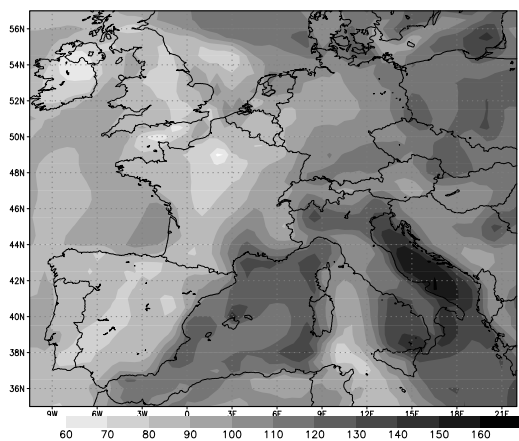

Figure 1. Polyphemus application to ozone forecast at European scale.

Figure 2 depicts application to ensemble forecast: a set of ozone profiles generated by varying the physical parameterisation of the model, clearly illustrating the high variability of ozone forecast and the need for better constraining the forecast system.

The project will make extensive use of Polyphemus data assimilation capacities: drivers have been developed or are being developed for sequential (optimal interpolation, rank reduced and ensemble Kalman filter) as well as variational (4DVAR) data assimilation procedures: designing a data assimilation system for IASI mainly requires establishing an observation operator, that links the model state variables (i.e. ozone concentrations) to IASI measurements (ozone columns and profiles), and observation error statistics.
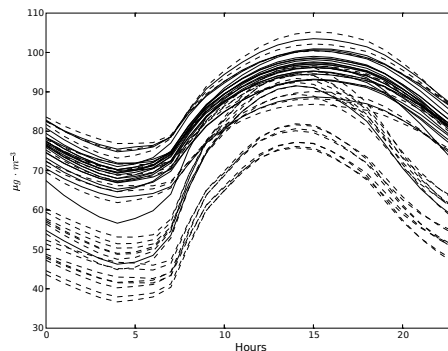

Figure 2. Polyphemus application to ensemble forecast.

3. FEASIBILITY OF ASSIMILATION OF EPS TROPOSPHERIC OZONE

The tropospheric ozone information, to be provided by IASI, is mainly sensitive to the free troposphere, whereas air quality application is mainly concerned with boundary layer concentrations. Therefore, the assimilation of IASI tropospheric ozone within an air quality forecast system requires the prior analysis of its potential impact on forecast results. To this end the following issues have been investigated:

Relative weight of boundary layer ozone in the 0-5km column: this indicates the amount of information on the boundary layer provided by the IASI column, and is performed by analysing a reference situation: Polyphemus have been run to perform ozone analysis during the month of July 2001, and the resulting ground ozone levels validated against ground measurements, proving a good agreement: RMS is 22.6 $\mu g.m^{-3}$ for peak ozone values, correlation between model outputs and ground measurements is 81%. The ozone column is computed from this reference situation up to an altitude of 5km, the upper limit of the modelling domain. Boundary layer ozone represents in average 14% of the 0-5km column, indicating that the IASI tropospheric ozone column carries a significant amount of information on the boundary layer.

Sensitivity of boundary layer ozone to free troposphere ozone: even if boundary layer ozone has a significant weight in the column, the IASI instrument and its inversion scheme produce more errors in the lowest layers of the troposphere, and hence, the provided ozone column is more representative of free troposphere than of boundary layer. The assimilation of the ozone column will be interesting with respect to air quality application if it can be proved that boundary layer ozone is sensitive to a change of concentrations in the free troposphere. This has been performed by the following sensitivity analysis: (1) free troposphere ozone concentra-

tions are arbitrarily perturbed, either at an initial date, or a regular intervals corresponding to MetOp revisit period; (2) Polyphemus is run with these perturbed concentrations; (3) the impact on boundary layers concentrations is analysed. The sensitivity analysis indicates an overall sensitivity of 50%, the maximal perturbation of boundary layer ozone being observed 27h after the perturbation of free troposphere ozone, as illustrated in figure 3. This allows to conclude that bounary layer is ozone is sensitive to corrections applied to free troposphere ozone, thus assimilating IASI columns is likely to improve the analysis of boundary layer ozone.
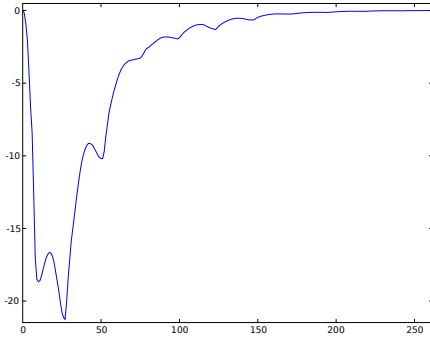

Figure 3. Time vs mean relative difference between rreference and perturbated boundary layer ozone, after an initial perturbation of -50% of free troposphere ozone.

Assimilation of simulated ozone columns: data assimilation experiments have been conducted using twin numerical experiments: (1) from a reference situation, simulated measurements of the tropospheric columns are generated by applying a 5% perturbation of the columns; (2) perturbated Polyphemus runs are generated, either by applying a 20% perturbation of the initial condition (in this case, the forecast converges to the reference situation after a week), or by perturbating the parameterization of vertical diffusion (in this case the perturbed run remains different from the reference); (3) simulated ozone columns are assimilated using an optimal interpolation scheme. The results show that the assimilation significantly improves the forecast: the figure 4 depicts an example of results, where the perturbation has been applied to the initial condition: the figure displays the mean difference (in $\mu g.m^{-3}$) with the reference situation along time (in hours). The solid curve represents the perturbated run without assimilation, which becomes equal to the reference after 140h. The dashed curves represent runs with assimilation, with a prior standard deviation of measurements errors of 2, 1, 0.5 respectively. Assimilation is performed every 24h. One can observe that the runs with assimilation converge quicker to the reference, proving the efficiency of the assimilation. This numerical framework will also make it possible to specify the vertical and temporal sampling of space borne measurements in order to reach a given improvement of air qual-

ity forecast: this constitutes an information of interest for the design of the next generation of tropospheric space missions.
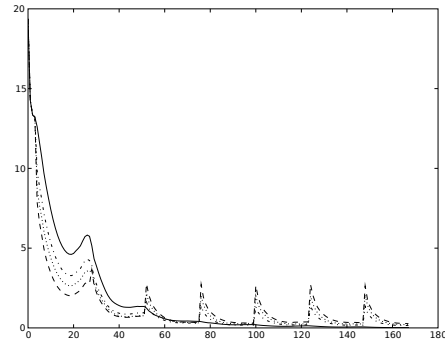

Figure 4. Time vs mean, difference between reference and perturbated runs. Solid: without assimilation; dashed: with assimilation.

4. ASSIMILATION OF EPS TROPOSPHERIC OZONE

Experiments on realistic IASI data will be performed in two steps: first with simulated IASI data, in order to get prepared to the arrival of real data; second, with real data when available. In the following we describe how simulated IASI data have been generated, and what data assimilation experiments will be performed, on both simulated and real IASI data.

The simulation of IASI data buids on:

- An **atmosphere model**, providing profiles of ozone, temperature and pressure in the altitude range 0-60km. In the range 0-5km, the atmosphere model corresponds to the reference atmosphere computed by Polyphemus (i.e. ozone concentrations, ECMWF temperature and pressure). In the range 6-60km, climatologies have been used (mean value from UGAMP for the reference period). In the range 5-6km, profiles are interpolated between Polyphemus outputs and climatologies for ensuring their continuity.
- An **instrument model**, used to generate the IASI radiances from the atmosphere model. It builds on the LBLRTM radiative transfer code on which the IASI instrument model is plugged.
- An **inversion procedure**, used to retrieve ozone columns and profiles from the radiances. We will make use of two different algorithms: the operational SA-NN algorithm [8], a neural network-based algorithm that will be used for the operational retrieval of IASI ozone columns; the Atmosphit model [9], an optimal interpolation algorithm requiring an a priori information on ozone profile: in our case, a priori on ozone is issued from the MOZART model.

The figure 5 depicts a retrieved ozone profile from this procedure together with the associated retrieval error, which as expected is important in the lowest layers of the troposphere.
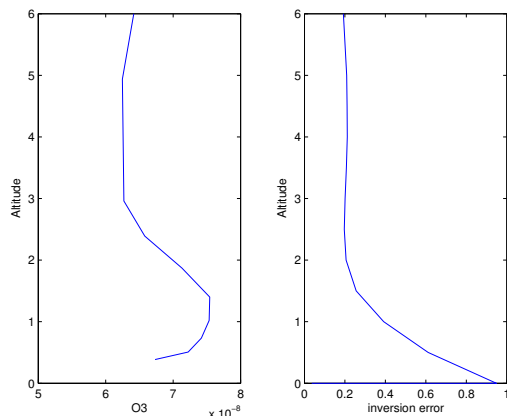

Figure 5. Example of retrieved profile from IASI simulated radiances (left); associated inversion error (right).

Assimilation experiments will first be performed in the framework of twin numerical experiments in order to demonstrate the feasibility: the simulated IASI ozone measurements will be assimilated into a perturbed Polyphemus configuration and compared to the reference run. As compared to the previous twin numerical experiments, the use of simulated IASI ozone measurements allows to properly take into account measurement noise and inversion errors. This experiment will allow to conclude on the feasibility of assimilating IASI ozone measurements for boundary layer ozone analysis. The need for extending the vertical domain of the Polyphemus system will be decided after the results of this experiment: Polyphemus is currently limited to 5km altitude, its extension to the full troposphere requires extending its physical modelling to convection and stratosphere-troposphere exchanges.

Experiments with real data will be then performed and validated by comparing (1) direct runs without assimilation, (2) runs with assimilation of IASI data, and (3) ozone measurements provided by ground based monitoring networks.

5. EXPECTED RESULTS

Improving the forecast of the atmosphere chemical composition in the boundary layer is crucial for air quality applications. It is however not expected that the next generation of satellite sensors are able to provide accurate measurements in the lowest layers of the atmosphere. The proposed project expects to provide objective answers on the potential of IASI ozone measurements to better constrain ozone forecast in the boundary layer. This poten-

tial is analysed through numerical experiments on (1) the sensitivity of boundary layer ozone to free troposphere ozone, and on (2) the feasibility of assimilating ozone 0-6km columns in a continental air quality prediction model. These numerical experiments will also serve to issue recommandations on the required vertical and temporal sampling of future tropospheric missions, in view of improving the analysis of the boundary layer.

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