Interactive comment on

"Variational assimilation of IASI SO 2 plume height and total-column retrievals in the 2010 eruption of Eyjafjallajökull using the SILAM v5.3 chemistry transport model"

by Julius Vira *et al.*, Geosci. Model Dev., doi:10.5194/gmd-2016-200

Overview

This paper describes the development of an observation operator for the simultaneous assimilation of the OMI retrievals of total SO2 columns and "plume height" (or more correctly, height of centre of mass) associated with volcanic eruptions; the implementation of this observation operator into an existing variational assimilation system; its testing and set-up using synthetic observations; and its application to the Eyjafjallajökull eruption 1-20 May 2010.

As explained by the first reviewer already, this research is timely and of high interest. While a large amount of work was invested in the development of the observation operator, the improvement due to plume height assimilation seems marginal and requires much more thorough evaluation. I will not focus on the inversion results for the real-life case and the corresponding discussion, first because this was already addressed in the first review and second because I have serious concerns about the assimilation approach itself. These concerns may be due to misunderstandings on my side, reflecting a lack of clarity and completeness in the manuscript. In such a case the manuscript requires major revisions in sections 3 and 4. If on the other side the concerns raised here can not be alleviated, the assimilation approach is wrong (which could explain the limited success to improve the estimation of plume height) and I would recommend a serious re-examination of the assimilation algorithm before re-running all the inversion experiments - i.e. most probably a withdrawal of the current manuscript.

Absence of a priori term in the cost function

I believe that the authors used a deeply flawed implementation of the variational assimilation method. Canonical expressions of the cost function (see e.g. Talagrand, 1997) decompose it into a first term $\frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b)$ measuring the distance between the a priori (i.e. background) and optimized model state, and a second term measuring the mismatch between model state and observations. The success of this approach relies on a proper estimation and balance between the corresponding background error covariance matrix (**B**) and observations error covariance matrix (**R**). Even though systematic model errors (biases) are often neglected in such variational assimilation systems, the a priori errors can not be ignored.

As best as I can guess, the authors decided that the cost of the a priori information could be neglected because the optimized parameter **f** is taken as zero during the first forward model integration (although this is not clearly stated in section 3). The authors probably chose as initial background model state $\mathbf{x}_0^b$ (i.e. initial condition for the first iteration) the output at the end of the previous assimilation window (note this too should have been clearly stated in section 3). The corresponding first guess is thus that the volcanic eruption suddenly ended at the beginning of the current assimilation window, with SO_2 abundance simply dissipating due to advection and decreasing due to photochemistry. Such a priori information is quite far from the truth during the eruption, and the associated background error must be quite large. In any case, the background term $\frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b)$ can clearly not be zero – except during the first iteration of the first assimilation window.

I suspect that the addition of a regularization term (section 3.4) was considered as an attempt to make up for the absence of a background term. I note that the regularization term is fundamentally different because it depends directly on the model parameter while the background term depends on the model parameter through the model state. In any case the regularization is abandoned in favour of a truncated iteration, which I only see as a way to prevent the system from wandering too far from its first guess despite the absence of the corresponding term in the cost function.

There are two clues that the absence of an a priori term in the cost function prevented the system from behaving correctly:

- The authors had to supplement the observation error with a model error (line 209: $\mathbf{R} = \mathbf{R}_{obs} + \mathbf{R}_{model}$). This makes no sense because model error should be considered in model (gridded) space and be applied to the model state. Its dimension excepted, this matrix $\mathbf{R}_{model}$ is exactly the first estimation which one could use to account for the impact of model errors on a priori error and evaluate **B**. Indeed the background error covariance matrix is often approximated as diagonal, with values set arbitrarily from educated guesses of the model error (Errera and Ménard, 2012).

- The blue lines on the right plots in figures 3 and 4 shows that after an "optimal" number of iterations, the RMS error using synthetic observations increases again with the iteration number. One would expect from a well-behaved iterative assimilation system that once it has reached convergence, the number of iterations does not change the error of its output.

This leads us to the most basic question: does this system converge towards a stable solution? A revised paper should show the evolution of *J/n* (cost function divided by number of observations) as a function of the iteration number, for a variety of (synthetic or real) observations and at different dates. This also provides an opportunity to argue for the validity of the current assimilation approach: in the current experiments, compute (a posteriori) the background cost $J_\mathbf{B} = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b)$, using a diagonal **B** with values no smaller than those chosen for $\mathbf{R}_{model}$. Does $J_\mathbf{B}$ remain much smaller than the currently minimized cost $J_\mathbf{R}$ as the number of iterations increase? Does the total cost $J_\mathbf{B} + J_\mathbf{R}$ converge towards a minimum value or does it start increasing after an "optimal" number of iterations?

Other important remarks

The submitted text requires many other clarifications, but it is not worth listing these in detail as long as the fundamental point raised above is not addressed. Yet some points are serious enough to require immediate action in a revised manuscript:

1. There is a systematic confusion between “plume height” and (height of) “centre of mass”. Both quantities seem interchangeable, so I would expect that this was described in a previous paper about the retrieval scheme. This should still be explained with proper references in section 2.2, with much more attention paid to the exact term used throughout the text (including title and abstract). Even if this was published already, consider adding a line plot in section 2.2 to compare the retrieved centre of mass with the plume height observed by radar and cameras (i.e. white dots and barely visible grey dots in figure 7). Note also that such a comparison directly above Eyjafjallajökull would still not be convincing for the downstream plume, where a multi-layered distribution probably happened.

2. What is the width of the Gaussian distribution assumed by the retrieval algorithm? The observation operator does not take into account this Gaussian shape. We are in a case where the vertical resolution leading to the simulated observation is much, much finer than the “vertical resolution” of the observation itself so this looks like a major oversight - especially in a context where Averaging Kernels were not taken into account. In order to simulate the observations correctly, the observation operator should first fit the modelled profile with a Gaussian shape before applying equation (4). Of course this should also be included in the adjoint of the observation operator…

3. The sentence on lines 134-135 is extremely problematic as it seems to show a fundamental misunderstanding about assimilation theory:

   > “Finally, the vector **y** of observations is given by the possibly non-linear observation operator $\mathcal{H}$ as **y**=$\mathcal{H}$ (x)+ε where ε denotes the observation error.”

   $\mathcal{H}$(**x**) is the model state in observation space. **y**-$\mathcal{H}$(x) is the observation departure. Here ε does not denote only the observation error but all possible errors, including the model and representatitvity errors. Most importantly, **y** is not “given” by $\mathcal{H}$, it is simulated by $\mathcal{H}$! This awful confusion continues in equation (3) which does not provide **y** but the (total component of) $\mathcal{H}$(**x**).

4. It appears from lines 307-312 that the assimilation algorithm can use both the algebraic solution with explicit computation of **HM** matrix, and the 4D-Var approach. This should be clearly explained in section 3.1. I assume that Vira and Sofiev (2012) provided all necessary details about this 4D-Var implementation and its adjoint model (e.g., was it generated automatically or manually? Is it as detailed as the forward model? How was it verified?). If that is the case, an additional reference and a few words may suffice. But if that was not the case, or if the 4D-Var implementation changed a lot (beyond the developments described in sections 3.2 and 3.3), then this should be fully described (since appropriate for the GMD journal).

References

Errera, Q. and Ménard, R., Technical Note: Spectral representation of spatial correlations in variational assimilation with grid point models and application to the Belgian Assimilation System for Chemical Observations (BASCOE), Atmos. Chem. Phys., 12, 10015-10031, 2012.

Talagrand, O.: Assimilation of observations, an introduction, J. Meteorol. Soc. Jpn, 277, 191–209, 1997.