VAST document on dynamic inversion concept and feasibility analysis

Technical report

Authors: D. Arnold, N.I. Kristiansen, C. Maurer and G. Wotawa
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1. Introduction

One of the objectives of the ESA-funded project VAST was to improve volcanic ash forecasts based on atmospheric dispersion and transport models by a seamless integration of inverse modelling and ensemble prediction approaches. Inverse modelling, through combination of EO data and atmospheric transport model calculations, serves to make estimates of the source term (strength and time) both for ash and SO2. Given that the uncertainty of the source term is largely affecting the accuracy of the forecasts, the possibility of frequent updates of the source term estimates via inverse modelling is desired. Nevertheless, this is not a straight forward task. Although inverse modelling has been applied in numerous case studies of volcanic source terms (e.g. Eckhardt et al. 2008[1],Stohl et al. 2011[2], Moxnes et al. 2014[3]), these have always been done in hindcast, with several months to perform calculations and sensitivity evaluations to adjust the inverse modelling system to particular eruption characteristics. Performing such calculations in real time during an eruption requires a different system.

Within VAST, a first step has been made to automatize the so-called **"ad-hoc" inverse modelling system** used in hindcast based on Eckhardt et al. 2008[1] and further developed by Stohl et al. 2011[2]. The system automatically performs and links all components required to perform the inversion, i.e. running so-called unit-model simulations needed for the source term calculations, matches these with pre-processed satellite data, and calculates an a priori emission estimate. The system allows the user to specify which processes to be run, or to run all processes sequentially. The output of the system is a constrained source term with estimates of: eruption onset and end time, the mass eruption rate, eruption column height and initial vertical distribution. The ad-hoc inversion has been included as a stand-alone component in the current system (Figure 1) but not included in the operational procedures.

The second step in VAST is to make a **dynamic inverse modelling system** capable of being run in real-time, a so-called "dynamic inversion". This dynamic inversion system requires a different approach than that of the ad-hoc inversion in that the calculations need to be re-run as the eruption continues. As more satellite data become available, and also as more meteorological data become available for the model simulations, the source term needs to be re-calculated and updated. This document describes the concepts of the dynamic inverse modelling system.

[1] Eckhardt, S., et al (2008), Estimation of the vertical profile of sulfur dioxide injection into the atmosphere by a volcanic eruption using satellite column measurements and inverse transport modeling, Atmos. Chem. Phys., 8, 3881–3897, doi:10.5194/acp-8-3881-2008.

[2] Stohl, A., A. J. Prata, S. Eckhardt, L. Clarisse, A. Durant, S. Henne, N. I. Kristiansen, A. Minikin, U. Schumann, P. Seibert, K. Stebel, H. E. Thomas, T. Thorsteinsson, K. Tørseth, and B. Weinzierl (2011) Determination of time- and height-resolved volcanic ash emissions for quantitative ash dispersion modeling: The 2010 Eyjafjallajokull eruption, Atmos. Chem. Phys., 11, 4333-4351, doi:10.5194/acp-11-4333-2011.

[3] Moxnes, E. D., N. I. Kristiansen, A. Stohl, L. Clarisse, A. Durant, K. Weber, and A. Vogel (2014) Separation of ash and sulfur dioxide during the 2011 Grímsvötn eruption, J. Geophys. Res. Atmos., 119, doi:10.1002/2013JD02112

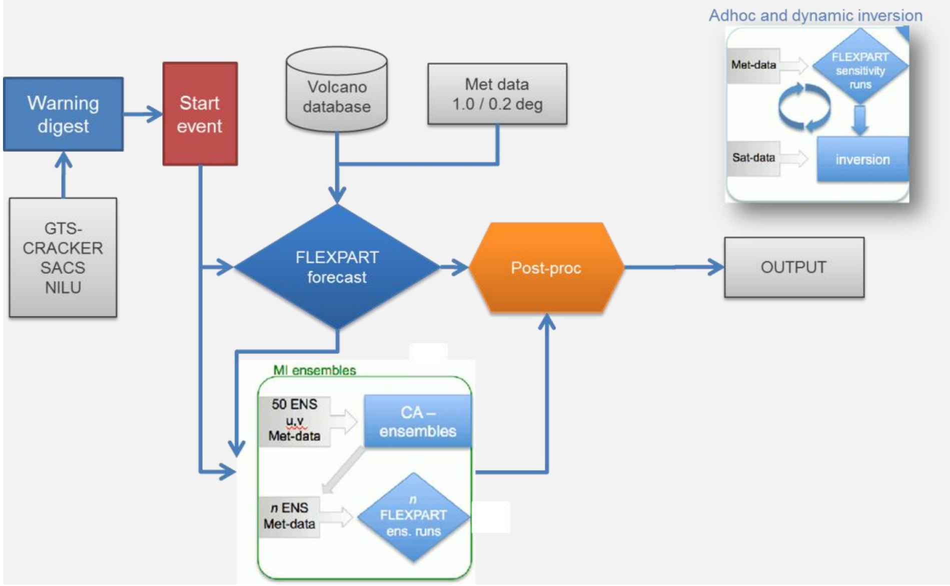


Figure1: Diagram of the operational system and its main components.

2. Dynamic inversion concept

The general concept of a dynamic inversion with GFS data is depicted in Figure 2. The system as represented in this figure needs available satellite data and ECMWF (or GFS) meteorological forecast/analysis data. Satellite data are available quasi real-time, about 15-30 minutes behind real-time. The meteorological analysis data, on the contrary, and depending on organisation access, are available with delays of up to 15 hours compared to real time, depending on the data availability. However, meteorological forecast data, of up to 10 days, are available for modelling at any time and updated twice a day for ECMWF and or four times a day for GFS. This and the frequency of new incoming satellite data determine the frequency of potential updates of the source term. For the inversion first step, FLEXPART runs are started with unit emissions every 3 hours starting from the time of eruption start. The runs are extended as far as satellite data are available. 6 hours later, when new meteorological data is available, all the existing model runs are continued (warm-starts) for another 6 hours, plus two new runs are started. A few hours later, new analysis/forecast meteorological data is available. This data is used to replace forecast data and to redo those sections of the model runs. Eventually, the number of model runs will become larger and larger, so some mechanism to cut off old runs and not include them in the inversion is considered. Improved forecasts for the volcanic emissions are then available 7 to 15 hours after the start of the eruptions and updated every 6 to 12 hours.

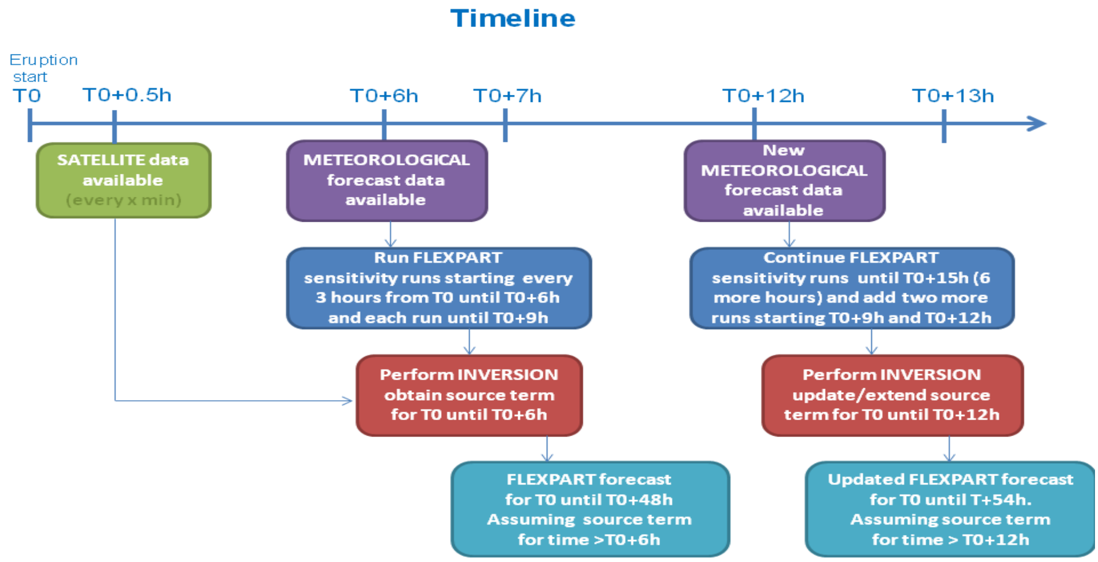
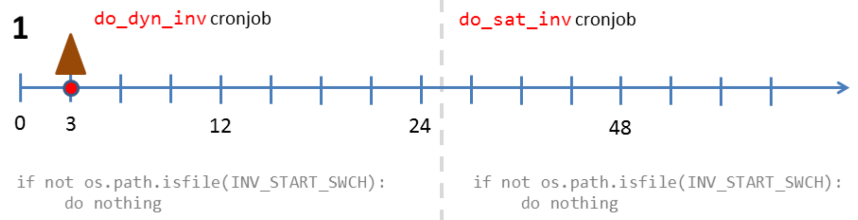


Figure2: Diagram of the updates in the source term estimates as new GFS meteorological incoming data is available to the system, with, in this case, two source term estimates per day.

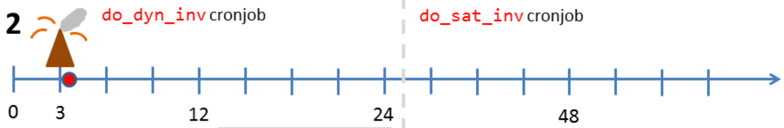
It is clear from the initial concept above that updated source term estimates with new incoming meteorological data (both forecast and analysis) are less frequent than the potential updates due to new satellite data. Table 1 shows a more detailed set-up of the dynamic inversion, with the two parallel processes that need to be run in the background to a) calculate all the extended and new unit runs and b) to account for the new incoming satellite data and perform the inversions. One of the processes is in charge of organising the FLEXPART unit model runs whenever new meteorological data becomes available. In Table 1, it is represented on the left side as **do_dyn_inv**. This requires not only new runs, but extension (warm-starts) of already existing runs. The right column of Table 1, shows the process that controls the new incoming satellite data and, **do_sat_inv**, and, together with do_dyn_inv, it generates periodic updates of the source terms, both when new satellite data is available and also when new or extended FLEXPART model runs exist.

Table 1: table with an example of 8 consecutive steps for dynamic inversions with incoming satellite and ECMWF meteorological data with updates every 12 hours.

Inversion with new meteo fields	Inversion with new satellite data



2 do_dyn_inv cronjob | do_sat_inv cronjob



From the volcano tool:
CONTROL.inv
INV_START_SWCH

From the volcano tool developed in VAST

```
0101-06=_ 1725 -
17.336
64.415
2011052112
```

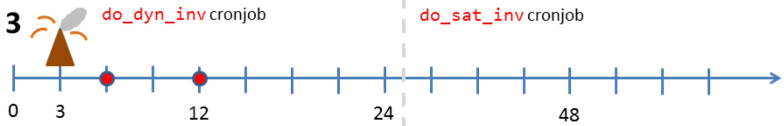
If not os.path.isfile INV_RUN_SWCH:
  start of all procedure!
  RUNNING
  generate tree for unit runs and summed runs

```
if os.path.isfile(INV_START_SWCH):
    if os.path.isfile (RUNNING):
        do nothing
```

unit runs ready and sumings ongoing, no data ready to use

FLEXPART unit runs, three hourly, 24/48/72 hours FC
Make the summing
SUMMED_DATES
CYCLE_TRACK (1 in this case)
Erase RUNNING file

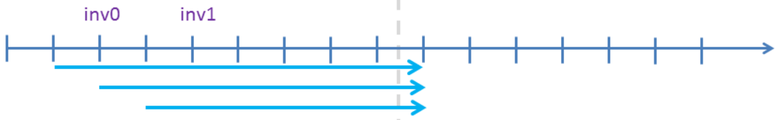
3 do_dyn_inv cronjob | do_sat_inv cronjob



It is now, 12 UTC, is there new meteo data? Maybe 00. Is it worth? No, i keep the same FCs

INV_START_SWCH
INV_RUN_SWCH
SUMMED_DATES (it includes paths, SOURCEDATES file)

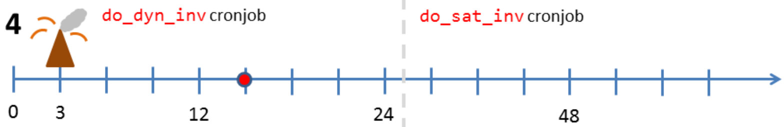
  Get a list of the satellite data (OBSDATES)
  Make inv1 tree structure
  Match the observations with the summed runs
  Make the inversion
  Make a forward run



FLEXPART unit runs, three hourly, 24/48/72 hours FC
Make the summing
SUMMED_DATES
CYCLE_TRACK (1 in this case)
Erase RUNNING file

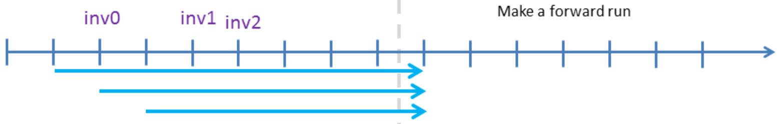
How often do we get analysis? Every 8 hours!

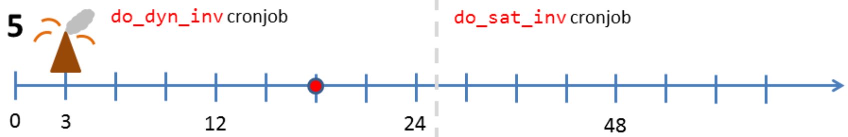
4 do_dyn_inv cronjob | do_sat_inv cronjob



It is now, 15 UTC. No new meteorological data. No new FLEXPART runs or extensions are needed

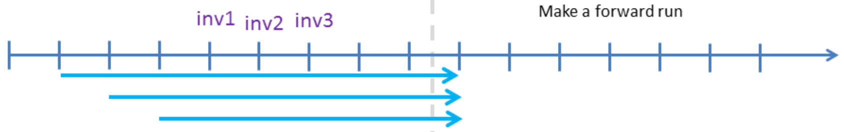
INV_START_SWCH
INV_RUN_SWCH
SUMMED_DATES (it includes paths, SOURCEDATES file)
  if os.is.file (OBSDATES):
    make a newOBSDATES
    if newOBSDATES .ne. OBSDATES: ! New data!
      Make inv2 tree structure
      Match the observations with the summed runs
      Make the inversion
      Make a forward run

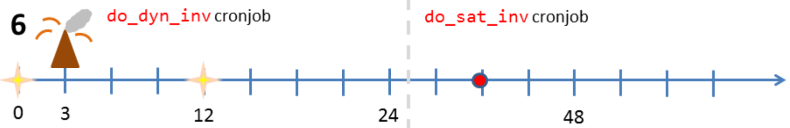




It is now, 15 UTC… do we have new meteo? Then do nothing

INV_START_SWCH
INV_RUN_SWCH
SUMMED_DATES (it includes paths, SOURCEDATES file)
if os.is.file (OBSDATES):
make a newOBSDATES
if newOBSDATES .ne. OBSDATES: ! New data!
Make inv3 tree structure
Match the observations with the summed runs
Make the inversion
Make a forward run



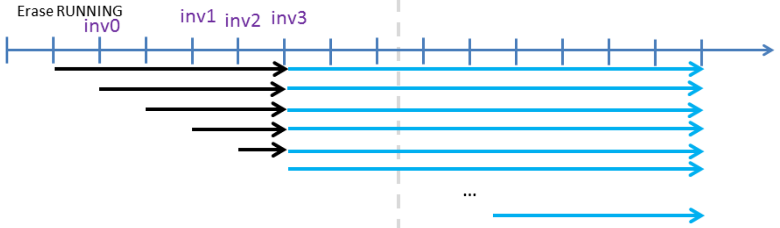


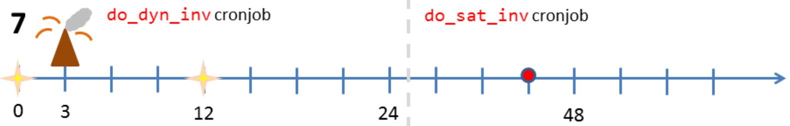
If (current time - startime)/interval >= 2:
we have enough analysis to redo unit runs

Make a new cycle:
RUNNING
start runs from the beginning WITH PARTICLE DUMP
end them half the interval after the last analyses
continue the dumped runs (but keep separated)
produce the remaining forecast runs
summed runs
CYCLE_TRACK (2 in this case)
Erase RUNNING

```
if os.path.isfile(INV_START_SWCH):
    if os.path.isfile (RUNNING):
        do nothing
```

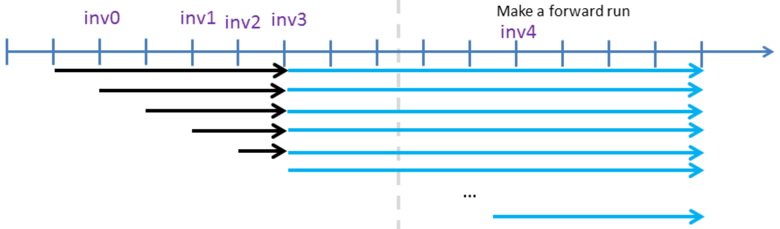
Unit runs ready and sumings ongoing, no new data ready to use

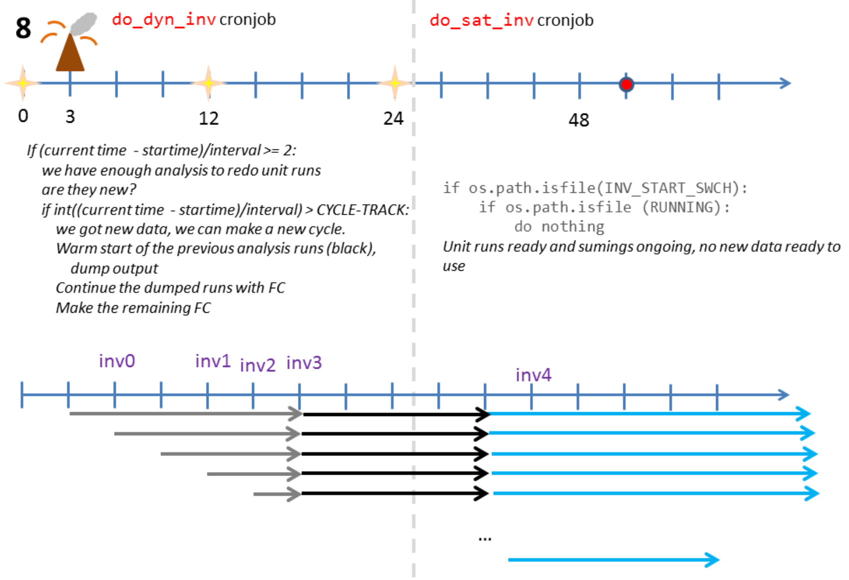




It is now, 36 UTC. No new meteorological data. No new FLEXPART runs or extensions are needed

INV_START_SWCH
INV_RUN_SWCH
SUMMED_DATES (it includes paths, SOURCEDATES file)
if os.is.file (OBSDATES):
make a newOBSDATES
if newOBSDATES .ne. OBSDATES: ! New data!
Make inv4 tree structure
Match the observations with the summed runs
Make the inversion
Make a forward run





3. Implementation aspects

The ad-hoc inversion and the dynamic inversion software require some minimum software standards. Table 2 gives the minimum specifications for the tool to run.

Table 2: minimum requirements for performing inversions.

Component	Software / modules / programs
FLEXPART unit runs / INVERSION	FLEXPART grib_api/1.11.0 or higher emos/392 or higher Fortran 77 / 90 Jasper
Main structure of the inversion	Python/2.7.5 or higher (**not Python3**)
Post-processing	Python/2.7.5 or higher (**not Python3**) matplotlib
Processing of the satellite data	Python/2.7.5 or higher `Satelliteproc` routines to regrid and time average the satellite data

The system consist of: a set of controlling python routines; a set of python libraries inside the module directory with routines to prepare the FLEXPART unit runs and various controlling and plotting functions; static data required for FLEXPART to run, also inside mods; the FORTRAN source code required to perform the summing and scaling of the unit runs, the matching and the inversion; and, finally, the FLEXPART source code.

```
CONTROL.inv
cycle.track
*.swch
handle_fp_uruns.py
    mods
handle_sat_ing.py
    mods
mods
   *.py
    Staticdata
Src_ftn
   *.f90
   Configuration files
```

Figure 3: Structure of the inversion software.

4. Problems and outlook

The basic technical system for the dynamic inversion is ready but the operational implementation will not be performed until further work has been done to optimize it and ensure feasibility. There are mainly two issues which need to be overcome in order to have the system running fully operationally. These issues were already discussed in the early phase of the VAST project, and include:

1. The availability, quality and uncertainty estimates of the satellite data used for constraining the source term are essential. First, satellite ash retrieval data need to be available on a near-real time basis. In this regard, the SEVIRI geostationary data is key. However, freely available near-real time ash retrieval data is sparse (Pavolonis et al., 2015[4]), and second and more importantly; well-characterized uncertainties related to such data are to date not available. Such uncertainties are needed for the inversion calculations and would preferably come from the satellite retrievals on a gridded basis. This is currently not available, and it is therefore necessary to perform more manual quality control and visual checking of the satellite data that goes in to the inversion system. Third, the post-processing of satellite data needs to be performed. This process, and in particular re-gridding of satellite data on to the model output grid has from previous case-study experiences shown to be a bottle-neck. . Computational demands may be too large to make the process operational. Preferably, satellite data becomes available from the data providers in already time averaged and re-gridded, however, such data are not currently available, particularly not in near-real time. After post-processing such as re-gridding and time-averaging, the data again requires quality control and visual checking.. With new data and retrieval algorithm from future missions, we expect many of these problems to be addressed, and the tool will then be more suitable for an operational implementation.
2. Previous case study experiences (Holuhraun, Kelut and all the cases tested) have shown that the set-up for one particular event does not necessarily provide meaningful results for other events. That means that the inversions require adjustments and expert analysis

[4] https://www.wmo.int/aemp/sites/default/files/P-23_PAVOLONIS.pdf

(mainly through trial and error among some reasonable values). This currently prevents any fully automated operational use of the tool.

The knowledge and experiences gathered during VAST on inverse modelling form a solid basis for further work into this direction when additional data sources are available and additional sensitivity studies are performed. To move forward with a feasible operational implementation, it will be required to reduce the human interaction and to increase the data analysis speed.