Inverse Modelling of Eruption Source Term Profiles

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First SAVAA Users Workshop
INGV, Rome, 6-7 April 2009

Outline

1. Basic principle
2. Practical application
3. Issues to discuss

Basic principle

Underlying assumptions

- Quasi-instantaneous release at given time ("*plop*") - continuous release will need modified approach
- Initial horizontal spread negligible (just a column – could, however, be set to, e.g., 5×5 km^2 if desired)
- Sequence of column values (of SO_2, ash, ...) available from satellite measurements

Shape and position of the cloud as function of time (known) depend on . . .

- initial vertical distribution unknown
- 4-dim. wind distribution (esp. vertical profile) known
- → an inverse (optimisation) problem

Solution method

1. Discretise source column
2. Calculate transport & dispersion for each source element
3. Bring satellite data and model data on same grid
4. Look for linear combination of source elements whose superposition matches best the observations

1. Discretise source column

E.g. 16 layers, each 150 m thick → 0–24 km column

2. Calculate transport

- Initialise ≈100,000 particles in each source element
- Track particles and evaluate concentrations on output grid, e.g. 0.3°×0.3°×2000 m

Solution method / 2

3. Bring sat data and model data to same grid

- Resample satellite data to horizontal model grid
- Vertically integrate model data to obtain column values
- Possibly subtract modell results obtained with a-priori source from observed sat data

4. Look for optimum linear combination

- Modelled column values $\mathbf{y} = \mathbf{M}\mathbf{x}$
  where $\mathbf{x}$ is the vector of $x_1, \ldots, x_n$ source contributions and
  $\mathbf{M}$ is the $m \times n$ source-receptor matrix (m is #obs values in RoI)
- Observed values $\mathbf{y^o}$
- Minimise cost function $J = J_1 + J_2 + J_3$

$$J_1 = (\mathbf{Mx} - \mathbf{y})^T \mathbf{diag}(\boldsymbol{\sigma}_\mathbf{o}{}^{-2}) (\mathbf{Mx} - \mathbf{y})$$ misfit model–observation

$$J_2 = \mathbf{x}^T \mathbf{diag}(\boldsymbol{\sigma}_\mathbf{x}{}^{-2}) \mathbf{x}$$ deviation from a priori

$$J_3 = \epsilon (\mathbf{Dx})^T \mathbf{Dx}$$ deviation from smoothness

Solution method / 3

4. Look for optimum linear combination / 2

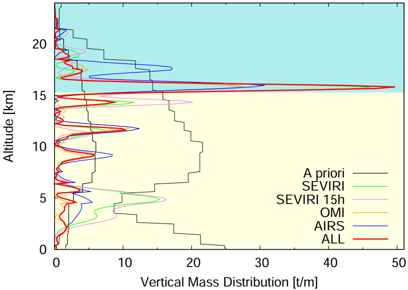
- Minimisation of J leads to linear system of equations of size n, solves very quickly
- Ensuring solution with only positive values by placing penalties on negative values and iteration
- Additional inputs needed:
  - observation weights $\boldsymbol{\sigma}_o$ (were assumed constant for each type of sat data in the Jebel test case)
  - a priori values $\mathbf{x}^a$ and their uncertainties $\boldsymbol{\sigma}_x$ (if desired)
  - value of smoothness parameter ϵ (empirical value)

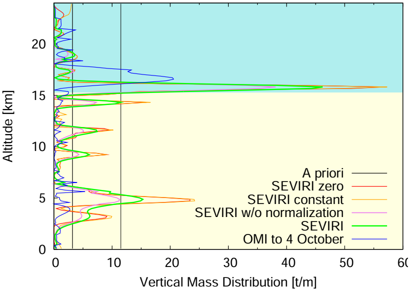
For all the details, read our paper

S. Eckhardt, A. J. Prata, P. Seibert, K. Stebel, and A. Stohl (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
www.atmos-chem-phys.net/8/3881/2008/

Practical application: Jebel at Tair, Sept 2007

Sabine Eckhardt's presentation will include all the details. Here we look only at some methodological aspects.





- was a kind of ideal case (no clouds, nice winds, many satellite data)
- different a priori assumptions
- results are robust, except lower troposphere (weakly constrained)
- even though smoothing condition is applied, realistic layered structure corresponding to atmospheric stability appears

Issues to discuss

List of issues

1. Computation time
2. Specific transport issues of ash and SO_2
3. Uncertain eruption time
4. Partial coverage of the ash cloud meteorological clouds
5. Uncertain retrievals (presence of ice, etc.)
6. Slant viewing path of satellite
7. Overlay of more than one eruption
8. Uncertainty in inversion results
9. Continuous data assimilation

Various issues / 1

Computation time

- Inversion itself is fast
- Satellite data processing – probably not limiting factor
- FLEXPART transport calculation might be a bottleneck
  - proportional to number of particles used
  - very large output grid needs more particles and slows postprocessing
  - more powerful computing environment ("trivial" parallelisation)
  - How often to repeat inversion (suggested 6 h)? When to stop inversion? (cf. data assimilation)

Specific transport issues of ash and SO_2

- For Jebel we looked only at SO_2.
- From which transport time on should one include removal of SO_2 by conversion to SO_4? Ash: gravitational settling to be considered. Particle size from satellite retrieval? Size *spectrum*?
- Are there any other effects that make the substance under consideration behave not like an air tracer?

Various issues / 2

Uncertain eruption time

- It is possible to do the whole procedure for several eruption times (e.g. shifted by 1 hour) and select the one giving the lowest cost function value, if no better information is available

Partial coverage of the ash cloud meteorological clouds

- Satellite algorithm needs to produce the cloud mask, masked pixels not to be used
- Pixels with partial or uncertain cloud influence can be assigned higher uncertainties
- It will be interesting to see in which regions cloud coverage is a seriously limiting factor, and how many valid data we need produce useful results

Uncertain retrievals (presence of ice, etc.)

- Satellite algorithm should assign uncertainty to each pixel, inversion will then make use of it

Various issues / 3

Slant viewing path of satellite

- Could be considered in the aggregation of FLEXPART output to column values, if considered relevant

More than one eruption

- I guess we will not build this into the algorithm (which would be possible in principle), just be aware of the possibility

Uncertainties of inversion

- Formal approach for uncertainty quantification (error propagation) may be implemented in a testbed, to see how much it depends on variable meteorological conditions (variability of the winds)
- Uncertainty of the meteorological input: not expected to be important on 24-48 h transport time scale
- For forecast products, possibility to include ensembles (not foreseen within in SAVAA)

Continuous data assimilation

The problem

After some time, transport modelling errors will cause the model output to deviate from reality even with perfect source profile.

Computation times will grow as more and more data to be considered.

Possible solution

- not foreseen as a product in SAVAA, possibly look into feasibility
- 1D source column to be replaced by a 3D “source” region which is just the ash cloud at the beginning of the assimilation window
- Previous model output will be a very good a-priori
- Vector of unkowns will be larger, but time for FLEXPART simulation shorter, thus total FLEXPART time maybe not too large
- FLEXPART output will be much larger
- Size of inversion problem will be much larger
- Full error propagation (Kálmán filtering) would make the problem more complicated and also computationally larger
- We’ll see . . .

Conclusions

- Inversion method is fast and robust with respect to a priori as well as different types of satellite data
- Robustness with respect to non-ideal settings to be explored in the project
- Quantification of uncertainties both for input to and output of inversion module will need further attention
- Continuous data assimilation – likely a relevant topic for the future