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Observation operator for lidar- and aircraft-type datasets

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Abstract

Lidar observations can provide detailed information on the altitude, thickness, and concentration of an atmospheric aerosol plume. This report provides details on the lidar observation operator implemented in the atmospheric transport models of the EUNADICS project. The observation operator enables assimilation of lidar observations of the attenuated backscattering coefficient, the extinction coefficient, or the backscattering coefficient.

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Executive Summary

The objective of Task 4.2 was to implement a lidar observation operator in the WP4 models, so that lidar observations of hazardous aerosols can be assimilated, both in actual cases and in the test scenarios as defined in Tasks 4.3, 4.4 and WP6. The MOCAGE model already included a working implementation of such an operator (Sič, 2014) at the start of the project, and as a result of Task 4.2 activities, observation operators based on the MOCAGE example have also been implemented in the MATCH and SILAM models. The main purpose of this operator is to assimilate various lidar observations that are available from the project in terms of different parameters.

The lidar operator offers the possibility to assimilate observations or retrievals of three different physical quantities:

1. Normalized attenuated backscattering coefficient
2. Backscattering coefficient
3. Extinction coefficient

The attenuated backscattering coefficient is provided as a Level 1.5 (L1) product for the satellite-borne CALIOP lidar measurements, with the lidar specific constants factored out. The backscattering and the extinction coefficients are provided as Level 2 (L2) products for CALIOP. Observations or retrievals from ground-based lidars or lidar networks, such as the EARLINET, MPLNET, or E-PROFILE networks, can also be assimilated.

Assimilation of lidar observations or retrievals requires an operator that maps the simulated aerosol concentrations into backscattering and extinction coefficients. The attenuated backscattering coefficient can be calculated based on these two coefficients, but depends non-linearly on the aerosol concentrations. The backscattering and extinction coefficients are calculated based on the Mie scattering theory for spherical particles. The effect of the relative humidity on the size of hydrophilic particles is taken into account. Rayleigh scattering and absorption by atmospheric O_2, O_3, SO_2, NO_2 and CO_2 are also taken into account at the relevant wavelengths.

The selected test scenarios will be used to determine the quantities that are best suitable for assimilation, as well as to determine useful values for the free parameters of the operator and error estimates of the retrievals.

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1. Introduction and objectives

The lidar observation operator is intended for ground-based and in-orbit lidars. The operator maps the concentrations of aerosols of a transport model into simulated lidar signals, attenuated backscattering coefficients, extinction coefficients, or backscattering coefficients. The difference between the simulated and the measured values is called the innovation vector and is used to solve the posterior probability distribution for the assimilated quantities.
Figure 1 presents the impact of assimilating lidar observations within the MOCAGE transport model.

The three coefficients are measured or retrieved as functions of the distance to the lidar. Lidar measurements thus provide more detailed information on the altitude and the vertical distribution of the aerosols compared to radiance measurements. However, the lidar networks and the lidar-carrying CALIPSO satellite provide a much sparser coverage of both Europe and the Earth than most of the other in-orbit instruments.

Of the three coefficients, the attenuated backscattering coefficient can be obtained from the measured lidar signal without significant retrieval assumptions or estimates, whereas obtaining the extinction and the backscattering coefficients for elastic lidars such as CALIOP requires estimation of the ratio between these two, called the lidar ratio. However, the attenuated backscattering coefficient is the most difficult of these to utilize in data assimilation, due to its non-linear and non-local dependence on the aerosol concentrations. Aerosol backscattering and extinction coefficients can be obtained from ground based lidars equipped with Raman or High Spectral capability without lidar ratio assumptions. Such lidars can even provide direct measurements of range-resolved lidar ratio values.

The calculation of the backscattering coefficient has been shown to be quite sensitive both to the refractive index and the shape of the aerosol particles (Geisinger *et al*., 2017). Generally, neither of the two quantities is known in the event of an emergency situation. As the best quantity for assimilation is not unequivocal either, the objective of Task 4.2 is thus to implement working lidar observation operators within the transport models, whereas the test scenarios of Task 4.4 will be needed for determining the optimal formulation of the operators.

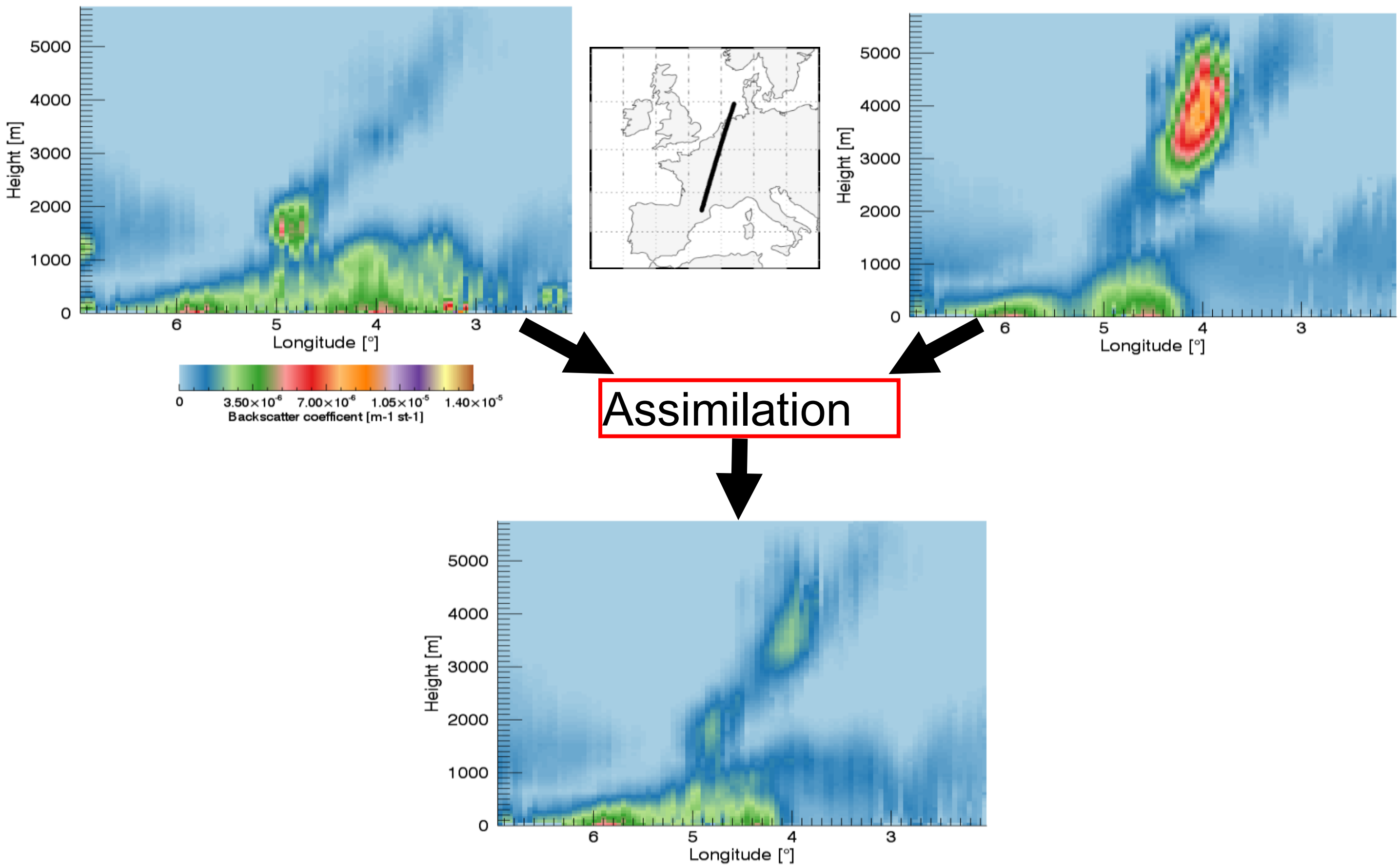

Figure 1: Example of assimilation (lower panel) of CALIOP lidar profile (upper-left panel) in MOCAGE (upper-right panel).

2. Implementation of the lidar observation operator

The single-scattering lidar equation is defined as:

$$P(H) = \frac{P_0 K O(H)}{H^2}\left(\beta_{mol}(H) + \beta_{aer}(H)\right) \exp\left[-2\int_{H_0}^{H}\left(\alpha_{mol}(h) + \alpha_{aer}(h)\right)dh\right]. \quad (1)$$

It gives the received power P of a laser pulse that is scattered back from altitude H to the lidar instrument located at altitude H_0 and emitting power P_0. K is an instrumental constant and $O(H)$ is the instrument-specific overlap function. $\alpha(h)$ is the extinction coefficient and $\beta(h)$ the backscattering coefficient at altitude h. The coefficients refer to the effect of gas molecules (*mol*) and of aerosols (*aer*).

The optical depth of the layer [H_0, H] is defined as:

$$\tau(H) = \int_{H_0}^{H} \left(\alpha_{mol}(h) + \alpha_{aer}(h)\right)dh, \tag{2}$$

whereas the transmission from H_0 to H equals to the negative exponent of the optical depth (the factor of two in the lidar equation comes from the fact that the laser pulse needs to traverse twice through this area). When the known functions and constants of the lidar equation are factored out, we are left with the attenuated backscattering coefficient, defined as:

$$\lambda(H) = \left(\beta_{mol}(H) + \beta_{aer}(H)\right) \exp\left[-2\int_{H_0}^{H} \left(\alpha_{mol}(h) + \alpha_{aer}(h)\right)dh\right]. \tag{3}$$

The observation operator for the attenuated backscattering coefficient thus requires the computation of both $\alpha(H)$ and $\beta(H)$ from the aerosol and gas concentrations of the model, as well as an estimation of the contribution of the atmospheric gases that are not simulated.

For the aerosols, the extinction and backscattering coefficients are solved based on the Mie approximation, which is valid when the particle diameter is at least of the same order of magnitude as the wavelength of the lidar. The effect of the relative humidity on the diameter of hydrophilic particles is taken into account through a particle growth factor. After the deliquescence point has been reached, the particles are taken to be water droplets in the Mie calculations. For a given particle diameter, the extinction and backscattering coefficients are directly proportional to the concentration of particles of that diameter, the proportionality constants being called the extinction and backscattering efficiencies.

There are several code packages for computing the extinction and backscattering efficiencies. Both the Mie solver by Wiscombe (1980) and the one by Bohren and Huffman (1983) have been applied. The Mie computations require knowledge of the effective refractive index of the particles, which is generally not known, especially not in the case of an emergency situation. For volcanic ash, the refractive indices of, for example, basalt, andesite, or rhyolite can be used, whereas for desert dust, the refractive index can be based on the Global Aerosol Data Set (Koepke *et al.*, 1997).

The aerosol extinction and backscattering coefficients are obtained from the efficiencies by integrating the particle concentrations (as a function of diameter) weighted by the corresponding efficiencies over the entire range of particle diameters. Alternatively, the backscattering coefficient can be directly obtained from the extinction coefficient by multiplying it with an inverse lidar ratio estimated for each aerosol type (either as a constant or as a function of particle diameter). This approximation is justified as the backscattering coefficient of a perfectly spherical particle fluctuates strongly as a function of the diameter, and as it is also generally very sensitive to particle shape and refractive index (Geisinger *et* *al*., 2017). However, it is to be determined whether directly assimilating a retrieved extinction coefficient in such a case would be beneficial instead.

For the O_3, NO_2, and SO_2 gases, the extinction coefficients are computed by multiplying the gas number concentrations with tabulated values of the temperature and wavelength dependent molecular absorption cross sections. The gas number concentrations can be based on either modeled values or on climatological data of volume mixing ratios.

At infrared wavelengths, extinction by O_2 and CO_2 is also relevant. The corresponding optical depths are computed using the narrow-band Goody (Ellingson and Gillis, 1978) or Malkmus (Rodgers, 1968) models, with the variations of temperature and pressure along the path of the light being taken into account through the Curtis-Godson approximation (Ellingson and Gillis, 1978).

Extinction through atmospheric Rayleigh scattering is computed through the semi-empirical equation presented by Collis *et al*. (1976). The molecular and Rayleigh extinction coefficients can be converted into corresponding backscattering coefficients through the molecular lidar ratio

$$\frac{\alpha_{mol}(h)}{\beta_{mol}(h)} = \frac{8\pi}{3}, \qquad (4)$$

whose effective value may, however, be weakly instrument-specific, e.g. a value of 8.70 has been suggested for CALIOP instead of $8\pi/3 \sim 8.38$ (Prata *et al*., 2017).

Due to the size of the lidar footprint at large distances, the single-scattering lidar equation is less suitable to be directly implemented for in-orbit lidars compared to air-borne or ground-based systems. Within Task 4.4 activities it may be possible to determine whether a correction factor depending on the thickness of the aerosol plume should be applied, as has been indicated in the literature (Winker *et al*., 2012, Prata *et al*., 2017).

A general list of the advantages and disadvantages of assimilating the various coefficients is presented in Table 1.

Table 1: Advantages and disadvantages of assimilating different datasets.

	Advantages	**Disadvantages**
Signal (L1)	Measurements collected by operation networks (e.g. E-PROFILE)	All the disadvantages of the attenuated backscatter coefficient. Requires knowledge of the instrument-specific constants and the overlap function.
Attenuated backscattering coefficient (L1)	Does not need signal inversion	Needs computation of the full lidar equation. Is non-linear and non-local with respect to the aerosol concentration. The extinction and the backscattering parts have different signs. The backscattering part is sensitive to generally unknown aerosol properties.
Backscattering coefficient (L2)	Can be processed at any chosen level Is linear with respect to the concentration.	Introduces errors due to inversion. Very sensitive to the refractive index and the shape of the aerosol particles.
Extinction coefficient (L2)	Can be processed at any chosen level. Is linear with respect to the concentration. Less sensitive to aerosol particle refractive index and shape than the backscattering coefficient.	Introduces errors due to inversion.

3. Model-specific implementation

This section describes the implementation of the observation operator in all of the platforms. The implemented operators are able to produce profiles at three different wavelengths: at 355 nm, 532 nm, and 1064 nm, which makes them suitable for the assimilation of data from different instruments.

3.1 SILAM

In the SILAM chemical transport model (Sofiev *et al.*, 2015) an optical module has been implemented for computing the extinction and backscattering coefficients. The extinction coefficient is regularly utilized to compute the aerosol optical depth and has been regularly compared against measurement data from the MODIS instrument for several years. The backscattering coefficient can be obtained from either Mie computations or from the extinction coefficient by utilizing an estimated lidar ratio.

In SILAM the Ensemble Kalman Filter is planned to be applied as the primary data-assimilation method for the project and tangent-linear or adjoint observation operators are thus not required.

3.2 MATCH

In the MATCH chemical transport model (Robertson et al., 1999) 4D-Variational data-assimilation is applied for the EUNADICS project, and thus tangent-linear and adjoint observation operators have been implemented for the attenuated backscattering coefficient.

3.3 MOCAGE

In the MOCAGE chemical transport model, the lidar observation operator was developed and tested before the start of the project (Sič, 2014). In MOCAGE variational data-assimilation is applied and tangent-linear and adjoint operators, required for an implementation in such assimilation algorithms, are available. The control variable of the assimilation is the 3D concentration of aerosols. The increments are then distributed into the different MOCAGE aerosol bins.

3.4 WRF-Chem/Flexpart

Assimilation of LIDAR measurements into the fully coupled online Weather Research and Forecasting-Chemistry (WRF-Chem) model (Grell et al., 2005) is performed with 3D-Variational (3D-Var) Gridpoint Statistical Interpolation (GSI, Pagowski et al., 2014). Forward operators, tangent-linear, and adjoint operators for assimilation of lidar measurements at 532 nm and 1064 nm are currently implemented into the Community Radiative Transfer Model (CRTM, Han et al., 2006). Aerosol backscatter and extinction due to aerosols and gases are simulated for space-based nadir-viewing lidar measurements as performed by CALIOP. In the inverse modelling system applied for the FLEXPART model, no sophisticated operators are used and only the total column integrals of the gridded and time-averaged ash concentration with all the corresponding assumptions are utilized.

4. Conclusions

The lidar observation operators implemented in the atmospheric transport models provide means to map the model aerosol concentrations into more directly observed quantities, i.e. to the attenuated backscattering coefficient, the backscattering coefficient or the extinction coefficient. Moreover, the total optical depth and the aerosol optical depth can also be directly obtained through integrating the extinction coefficients.

Although implemented in the models, the observation operators may need optimization to reach the best performance within the scope of the project. Specifically, one has to decide which one of the three coefficients is best suited for data assimilation, and how to best estimate the errors of the measurements or retrievals. The attenuated backscattering coefficient may pose problems due to its non-linearity and non-locality. For example, within variational data-assimilation, the model layer thicknesses must be small in order for the tangent-linear operator to be reasonably accurate. The non-locality, on the other hand, will cause correlated errors.

The test scenarios selected for the project will provide opportunities to test and tune the observation operators for the best performance. We plan to submit an article covering our most important findings for peer-review later within the project.

References

Bohren, C. F., and Huffman D R.: Absorption and scattering of light by small particles, John Wiley & Sons, 1983.

Collis, R. T. H. *et al.* in Hinkley, E. D. (ed.): Laser Monitoring of the Atmosphere, Springer, 1976.

Ellingson, R. G. and Gille, J. C.: An infrared transfer model. Part I: Model description and comparison of observations with calculations, J. Atmos. Sci., 35, 523–545, 1978.

Geisinger, A., Behrendt, A., Wulfmeyer, V., Strohbach, J., Förstner, J., and Potthast, R.: Development and application of a backscatter lidar forward operator for quantitative validation of aerosol dispersion models and future data assimilation, Atmos. Meas. Tech., 10, 4705-4726, 2017.

Grell, G.A., Peckham, S. E., Schmitz, R., McKeen, S. A., Frost, G., Skamarock, W. C., and Eder, B., Fully coupled "online" chemistry within the WRF model, Atmos. Env. 39, 37, 6957-6975,2005.

Han, Y., van Delst, P., Liu, Q., Weng, F., Yan B., Treadon, R., and Derber, J., JCSDA Community Radiative Transfer Model (CRTM) - Version 1, NOAA Technical Report NESDIS 122, 33 pp., NOAA, Washington D.C, 2006.

Koepke, P., M. Hess, I. Schult, and E.P. Shettle: Global Aerosol Data Set, Report No. 243 of the Max-Planck-Institut für Meteorologie, Hamburg, ISSN 0937-1060, 1997.

Pagowski, M., Liu, Z., Grell, G. A., Hu, M., Lin, H.-C., Schwartz, C. S., Implementation of aerosol assimilation in Gridpoint Statistical Interpolation (v. 3.2) and WRF-Chem (v. 3.4.1), Geosci. Model Dev., 7, 1621-1627, 2014.

Prata, A. T., Young, S. A., Siems, S. T., and Manton, M. J.: Lidar ratios of stratospheric volcanic ash and sulfate aerosols retrieved from CALIOP measurements, Atmos. Chem. Phys., 17, 8599-8618, 2017.

Robertson, L., Langner, J. and Engardt, M., An Eulerian limited-area atmospheric transport model, J. Appl. Met. 38, 190-210, 1999.

Rodgers, C. D.: Some extensions and applications of the new random model for molecular band transmission, Q. J. R. Meteorol. Soc., 94, 99-102, 1968.

Sič, B.: Amélioration de la représentation des aérosols dans un modèle de chimie-transport: Modélisation et assimilation de donnèes, PhD thesis, Université Toulouse, 2014.

Sofiev, M., Vira, J., Kouznetsov, R., Prank, M., Soares, J., and Genikhovich, E., Construction of the SILAM Eulerian atmospheric dispersion model based on the advection algorithm of Michael Galperin, Geosci. Model Dev., 8, 3497–3522, 2015.

Winker, D. M., Liu, Z., Omar, A., Tackett, J., and Fairlie, D.: CALIOP observations of the transport of ash from the Eyjafjallajökull volcano in April 2010, J. Geophys. Res., 117, D00U15, 2012.

Wiscombe, W. J.: Improved Mie scattering algorithms, Appl. Opt. 19, 1505-1509, 1980.