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Abstract

This document presents the design of a multi-model system, including the following models: MATCH (from SMHI), MOCAGE (from Météo-France), SILAM (from FMI), and FLEXPART and WRF-Chem (both from ZAMG). Every model has the capacity of data assimilation or of inverse modelling. The system design includes a review of the user requirements, a description of the models and their capacity for data integration, a description of the type of observations that will be integrated, the link to the Early Warning System, and finally the resulting products that are under development as part of the aviation service.

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Executive Summary

Aviation is vulnerable, in different ways, to “airborne” hazards, including volcanic eruptions emitting ash and sulphur clouds, nuclear accidents or explosions, and other high-density aerosol plumes such as generated by sand storms and forest fires. While several observation networks and satellites provide a large amount of data that are relevant for the monitoring of such events, their integration into numerical models for the provision of services relevant to aviation is not always achieved or in place. This document presents the design of a multi-model system, including the following models: MATCH (from SMHI), MOCAGE (from Météo-France), SILAM (from FMI) and FLEXPART and WRF-Chem (both from ZAMG). Every model has the capacity of data assimilation or of inverse modelling. The system design includes:

- a review of the user requirements,
- a description of the models and their capacity for data integration,
- a description of the type of observations that will be integrated,
- the link to the Early Warning System (EWS),
- the resulting products that are under development as part of the aviation service.

Special care is taken to define the interfaces with the other work packages of the EUNADICS-AV (European Natural Airborne Disaster Information and Coordination System for Aviation) project. The demonstration of integration of data has already started for a specific test case, and its evaluation will serve as a test-bed for future improvement and development in the coming months.

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1. General requirements and purpose of the integrated system

Aviation is vulnerable, in different way, to “airborne” hazards, including volcanic emissions (ash and sulphur clouds), nuclear accidents or explosions, and other high-density aerosol plumes such as sand storms and forest fires. While several observation networks and satellites provide a large amount of data that are relevant for the monitoring of such events, their integration into numerical models for the provision of services relevant to aviation is not always achieved or in place. This is the main aim of Work Package 6 (WP6) of EUNADICS-AV. Such integration requires the development of a dedicated system that matches the users’ needs in terms of numerical models and observations. Users’ needs collected and reported by WP2 (Lipok et al., 2017, D5 EUNADICS-AV report) are summarised in section 1.

1.1 Hazards and challenges

The hazards that are considered in the EUNADICS-AV project are those that pose a threat to aircrafts and/or passengers. While air pollutants can directly pose safety issues during the flight, they can also cause damages to the airplane that necessitate increased maintenance after flying through areas with high concentrations of air pollutants. The service design should take into account the pollutant specific challenges.

Volcanic ash has been known to damage jet engines, up to total loss of power in some cases (Casadevall, 1994). While mapping the presence of ash in the atmosphere has been the main purpose of ash forecasting since the 1990s, the Eyjafjallajökull eruption in 2010 and the following disruption of air traffic over Europe emphasized the need to provide more detailed information on the concentration of ash. Some engine manufacturers (Clarkson, 2017) already consider that an engine can tolerate some exposure dose (i.e., the concentration multiplied by the time of exposure) along a flight track without the risk of total loss of power, although inspection and maintenance may be required. These considerations should motivate monitoring of ash concentrations and the computation of the exposure dose along flight tracks. Sulphur emissions from volcanoes (Schmidt et al., 2014) pose a threat to health of the passengers and crew, and may damage the aircraft due to the high acidity of sulphuric acid.

In numerical models, volcanic emissions (ash and SO_2) are represented by a vertical profile at the vent location versus time. This is called the “source term” throughout this document. The source term depends on the type of volcano, the type of eruption, the location (e.g. whether the volcano is under an ice cap or not), and on the atmospheric conditions. The emission and dispersion of plumes can be monitored by remote-sensing (either satellite or ground-based) and by in-situ observations. Even though scientific understanding of the volcanic emissions has improved over the last decades, each eruption is unique and the source term needs to be assessed using the information available in near-real-time (NRT).

The emissions of radioactive compounds, either coming from the explosion of a nuclear plant or a nuclear bomb pose a direct threat to the health of human beings. The contamination of an aircraft after being exposed to radionuclides may as well be an issue, that requires the assessment of the exposure of the aircraft. The nuclear emissions are considered as point sources with some vertical profile structure. The source term for such nuclear events, in terms of activity, radionuclides and vertical distribution, are subject to a large uncertainty. In addition, the observations are scarce, other than the bulk gamma dose rate measurements, and usually limited to the stack and ground level.

Sandstorms are caused by intense winds in sandy areas, such as the largest deserts in the world. Parametrisations of desert sand emissions have been developed for several years (Marticorena and Bergametti, 1995) and evaluated continuously against satellite and in-situ observations. Most atmospheric composition models today use such well-fitted parametrisations. Sandstorms are monitored regularly by several services that combine both numerical models and observations, among which one can cite the COPERNICUS ATMOSPHERE MONITORING SERVICE (CAMS, www.atmosphere.copernicus.eu) and the WMO SDS-WAS centres (https://sds-was.aemet.es/).

Like sandstorms, forest fires emit pollutants not from a specific point but from a wide area. The detection and quantification of forest fires are usually based on infra-red satellite images. Emission estimates are then obtained through a corresponding parametrisation. However, high uncertainties remain concerning the vertical profile of the emissions and their composition. The Global Fire Assimilation System (GFAS) product (Kaiser et al., 2012) from CAMS provides source term estimates associated with fire events.

EUNADICS-AV/WP6 aims at developing an aviation service from an integrated model system to analyse these hazards from volcanic eruptions, nuclear explosions, sandstorm and forest fires. The design of a system for such high-impact and low-probability hazards, faces some challenges:

- to model the release of pollutants in time, the event has to be detected as early as possible. This is done by the EUNADICS-AV/WP5 Early Warning System (EWS), which sends a notification (Brenot et al., 2018, D28 EUNADICS-AV report),
- In addition, methods to estimate the source term are as well needed, both for wide-spread sources (forest fires and sandstorms) as for point sources (volcanoes and nuclear explosions/accidents). Due to the high uncertainty of the vertical distribution of the emissions and their temporal evolution, the analyses of volcanic and nuclear events can benefit from the source term estimates obtained through source apportionment and inversion methods. However, because it also takes time to compute source term estimates and/or event-tailored approaches, it is challenging to design a fast response system. In order to better understand the impact of the hazards and identify gaps in detection, the integrations of observations into models becomes an essential tool.

1.2 Review of user requirements

From a review of the user needs that have been collected and reported by WP2 (Lipok et al., 2017, D5 EUNADICS-AV report), we consider the following relevant aspects in order to design a model service for aviation:

- the concentration of the dispersed pollutants should be made available for different flight layers,
- the target resolution should be 10-km for horizontal layers,
- 5 or more vertical layers are needed in the troposphere,
- the data is expected at hourly step,
- the service should provide analyses (i.e., combination of models and observations) and forecasts,
- a rapid update of the products is needed whenever there was a change, either in the event itself or in the availability of input data,
- multiple scenarios are desirable or a median scenario incorporating upper and lower bounds, and possibly a worst-case scenario,
- the concentration of the pollutants is important information, that is needed to derive exposure dose along the flight tracks, at least for nuclear and ash hazards,
- additional products, such as the arrival time of a plume, are of particular interest.

Different types of users have been interviewed, and they have been divided into three main target groups (Lipok et al., 2017, D5 EUNADICS-AV report):

- Airline operation centres and flight planners, who need tailored and in-depth products.
- Pilots, who need easy to use, precise and condensed information,
- Existing operational centres (such as Volcanic Ash Advisory Centres, VAACs), who make and distribute to end-users the most reliable charts and bulletins from the diverse types of information they have access to (observations, models, etc.).

The user survey showed that the requirements and needs differ significantly between these target groups. The possibility to address the needs depends on the capacities of the models involved and on the resources of the project. So we design in the following a realistic system that addresses the user needs within the model possibilities.

1.3 Way forward to integrate models and observations

In order to address the user needs regarding the target hazards, it is proposed to develop a multi-model system, including the following models: SILAM (from FMI, Sofiev et al., 2015), MATCH (from SMHI, Robertson et al., 1999), MOCAGE (from Météo-France, Guth et al., 2016), FLEXPART (Stohl et al., 2005) and WRF-Chem (Grell et al., 2005), both from ZAMG. Every model of these four models included in EUNADICS-AV has the capacity for data assimilation or inverse modelling using observations from ground-based networks (aerosols, SO_2, radionuclides), satellites (aerosols, ash retrievals, SO_2 columns) and in-situ measurements (aerosols, SO_2, radionuclides). The four models included in EUNADICS-AV and their capacity are described in Section 2.

While numerical models provide a homogeneous, continuous but approximated picture of atmospheric composition, observations are more accurate but fragmented in space and time. That is why both models and observations are complementary to assess efficiently the hazards that are considered in EUNADICS-AV, and integration of observations into models is a critical activity of the project. The observations under consideration are compiled in EUNADICS-AV/WP3 (Graf et al., 2017; Apituley et al., 2017; Papagiannopoulos et al., 2017; Schlager, 2017) and they are as well briefly described in Section 3. The integration of the distributed observational information should provide a harmonized 4-D (space- and time-resolving) quantitative analysis of the crisis situation.

Such an automated multiple scenario fast-response system is of greater interest to some users than others. The aviation service that is designed will provide automated products, without any requirement regarding expertise or action from a human forecaster. Subsequently, the service that integrates models will be designed for the users who have the capacity to handle large datasets and uncertainty, which are:

- flight management, operations centres and automated systems. Furthermore, the service will be designed to **obtain synergies with already existing platforms and channels**,
- operational centres (such as VAACs), in which human forecasters can draw rapid alerts and scenarios from a variety of model outputs. They provide condensed information (such as the most probable or worst-case forecasts) and its uncertainty to pilots and to other decision makers.

The remainder of this document describes the proposed integrated model system, its products and the interfaces with the work packages of the EUNADICS-AV project.

2. Model capacities and design

This section describes the four model systems that are developed, with a special emphasis on their capacity for modelling the hazards under consideration and for the integration of observations.

2.1 SILAM

SILAM is a global-to-meso-scale dispersion model developed for atmospheric composition, air quality, and emergency decision support applications, as well as for inverse dispersion problem solution (Sofiev et al., 2015). The model incorporates both Eulerian and Lagrangian transport routines and multiple chemical-physical transformation modules, including sulphur chemistry, secondary aerosol formation, radioactive decay, and aerosol dynamics in the air. SILAM is run using a user-configurable control file that allows for the selection of the transformation modules, emission terms, meteorological datasets, data-assimilation parameters, as well as an arbitrary horizontal grid and an arbitrary number of vertical levels. SILAM has been actively used for air quality and pollen forecasting since 2006. SILAM forecasts are provided on a daily basis for the Regional CAMS (Marécal et al., 2015). About 90 peer-reviewed scientific publications are based on SILAM results.

SILAM source terms include point- and area- source inventories, sea salt, wind-blown dust, nuclear explosions, and data from the fire information system IS4FIRES. IS4FIRES is built on the basis of active-fire remote-sensing observations following the algorithm described in Sofiev et al., (2009). IS4FIRES utilizes two semi-independent datasets built on the temperature anomaly and fire radiative power. Alternatively, fire emission data from the GFAS product may be used. Emissions of desert dust are included for all desert areas in the world (marked as deserts in the land use map). The modified approach of Zender et al. (2003) is implemented for the saltation mechanism. At present time, no dense plume sulphur chemistry is implemented.

4D-Variational (4DVar), Ensemble Kalman Filter (EnKF) and Ensemble Kalman Smoother (EnKS) approaches are available for inverting source term and for data assimilation. For the EUNADICS-AV test scenarios, the EnKF/EnKS has been applied as the primary data-assimilation method, so that the ensemble may be used to estimate the forecast error. The ensemble of the EnKF and the EnKS is formed through perturbing the time stamp of the meteorological forecast and through perturbing the emission source. An actual meteorological forecast ensemble may also be used if available. The number of ensemble members within the EnKF is freely configurable, and current tests are run with 80 members. A trade-off between the horizontal resolution required and the ensemble size may be considered to allow for a sufficiently quick response.

Source-point inversion for volcanic and nuclear emissions is possible in the model. The volcanic eruption model is currently based on an empirical relationship between the height of the eruption plume and the eruption rate (Mastin et al., 2009). Within the EnKF/EnKS ensemble, the eruption rate is assumed to be log-normally distributed. Compared to a normal distribution, this allows for a significantly larger range of different eruptions to be included within the ensemble, which is essential for the description of the *a priori* probabilities. The eruption model is easily configurable, and for example a source inversion approach where the emission rates in the vertical cells are estimated independently through assimilation can also be used. To avoid a collapse of the ensemble and to take into account temporal changes in the *a priori* probability distribution, the distribution of the emission rates is set to constantly evolve towards a pre-defined distribution within a configurable correlation time, currently set to 24 h.

The observation operators that have been developed in SILAM are:

- the concentrations of PM, SO_2, and SO_4 (at arbitrary locations and altitudes),
- column loads, i.e. vertical integrals of concentrations (using an integration kernel if needed),
- altitudes of the centres of mass of the concentrations,
- AOD,
- lidar signal (attenuated backscatter coefficient),
- plume top altitude, observed by, e.g., radar,
- the dose rate of ionizing radiation measured at arbitrary locations and altitudes.

Correlation between the observations and the emission rates or parameters describing the emission allow for estimation of the source term through either 4DVar data-assimilation or the EnKF/EnKS. All observations can be assimilated within a single model run.

2.2 MATCH

MATCH is an Eulerian 3D chemical transport model, capable of data assimilation. It is a so called off-line model thus takes meteorological data as input, in this case from the Integrated Forecast System (IFS) from the European Centre for Medium-Range Weather Forecasts (ECMWF), at regular time intervals, and is normally operating on the same grid definition as the given meteorological data. The model assumes mass conservative transport based on a flux-oriented transport scheme, and semi-implicit vertical diffusion. A number of chemical mechanisms are accounted for like photo chemistry, the formation of secondary organic aerosols (SOA), and radioactive decay chains among others (Robertson et al., 1999, Langner et al., 1998, Bergström et al., 2012). The model is used for chemical forecasting and for national annual surveillance. It is involved in the Regional CAMS (Marécal et al., 2015). It also provides support to national radiation authority for routine nuclear event preparedness (both for nuclear installations and nuclear weapons). The MATCH model is also applicable to volcanic eruptions for modelling both ash and SO_2 dispersion. The part of the model related to nuclear explosions has been extended to include nuclide specific content of the event. Two modules for modelling desert dust are available. Modelling wildfire emissions is possible by importing GFAS satellite retrieved global emission inventory retrieved from ECMWF on a daily basis through the MARS archiving system.

MATCH capacities for integration of observations are made through two different paths with somewhat different purposes. The first one is an online 3DVar analysis scheme mainly applied in chemical forecasting, where the analysis is part of the model forward integration (Kahnert, 2008). The second one is an object-oriented 4DVar system mainly designed for source reconstruction. The system is written with Python, where MATCH is incorporated as an object to be run for the tangent linear model or its adjoint. For applications of nuclide decay the adjoints of the nuclide decay chains are implemented. The observation operators are also processed in the Python framework. The object-oriented approach enables flexible design of assimilation problems, as well as the possibility to test individual parts separately.

The observation operators available are for in-situ measurements, like O_3, SO_2, nuclides etc., and satellite column data, like MODIS, OMI for various L2 species-specific data. Processing aggregated observation information like gamma dose measurements and lidar observations is being implemented, in the framework of the WP4 activities.

2.3 MOCAGE

The MOCAGE 3D multi-scale Chemistry and Transport Model (CTM) has been designed for both research and operational applications in the field of environmental modelling. Since 2000, MOCAGE has covered a wide range of issues, including chemical weather forecasting, tracking and backtracking of accidental point source releases, trans-boundary pollution assessment, assimilation of remote sensing measurements of atmospheric composition, studies of the impact of anthropogenic emissions of pollutants on climate change, with over 80 references in the international refereed literature. Resulting from this, the MOCAGE structure offers flexibility to tailor the model CPU/MEM requirements and parametrisations for the different applications. MOCAGE has been running daily since 2005 for the French operational platform PREV'AIR (Rouil et al., 2009) and also for the Regional CAMS (Marécal et al., 2015) system. MOCAGE can ingest meteorological input from ARPEGE or IFS.
MOCAGE simultaneously considers the troposphere and stratosphere at the planetary scale and over limited-area sub-domains at higher horizontal resolution. The MOCAGE chemistry scheme merges reactions of the RACM scheme (Stockwell et al., 1997) with the reactions relevant to the stratospheric chemistry of REPROBUS (Lefèvre et al., 1994). Aqueous chemistry for the formation of sulphate is represented (Ménegoz et al., 2009). The aerosol module of MOCAGE includes the primary species dusts, black carbon, sea salt, organic carbon (Sic et al., 2015), and the secondary inorganic species sulfate, nitrate and ammonium (Guth et al., 2016). The formation and the multi-phasic equilibrium of inorganic secondary aerosols are modelled by the ISORROPIA-II module. The wildfire emissions from GFAS (Kaier et al., 2012) are included in MOCAGE. The generation of point source volcanic and nuclear emissions are included in MOCAGE. The volcanic emission vertical profile may be represented by the empirical Mastin's law (Mastin et al., 2009) or by the prognostic 1-D model FPLUME (Folch et al., 2016) that accounts for the main microphysical processes in the emission plume.

The MOCAGE-PALM assimilation system has been developed and evaluated during the European ASSET project (Lahoz et al., 2007). This system is particularly versatile, as both the CTM degree of sophistication (for instance, the number of chemical tracers involved, the physical or chemical parametrisations, the horizontal and vertical geometries, etc.) and the data assimilation technique used via PALM can be changed easily. Current available options are 3D-VAR, 3D-FGAT and incremental 4D-VAR methods to assimilate profile and column data for key measured atmospheric constituents, by means of a generic observation operator component. As a first approximation, background error standard deviations are prescribed as proportional to background levels. In order to spread assimilation increments spatially, background error correlations are modelled using a generalized diffusion operator (Weaver and Courtier 2001). Several data assimilation experiments have been published with MOCAGE, both for the stratosphere and troposphere.

The observation operators of MOCAGE enables the assimilation of:

- AOD,
- SO_2 columns (with averaging kernels possible),
- ground-based or satellite-based lidars,
- in-situ PM10 measured at ground stations and with aircrafts.

2.4 FLEXPART and WRF-Chem

At ZAMG two atmospheric transport models are employed. The FLEXible PARTicle dispersion model (FLEXPART, Stohl et al., 2005; 1998) is a Lagrangian model that does not simulate chemical processes except for the reaction with climatological OH concentrations. The Eulerian Weather Research and Forecasting Chemistry online coupled model (WRF-Chem) contains extensive aerosol and chemical process modules. The interaction between the models consists of the following: WRF-Chem can use the source-term produced by FLEXPART, and FLEXPART (in particular. FLEXPART-WRF) can in turn ingest meteorological output from WRF-Chem.

FLEXPART simulates the transport, mixing, gravitational settling, dry and wet deposition, radioactive decay, as well as simple chemical reactions (e.g. OH-reaction in case of SO_2) of trace gases and aerosols. It is typically applied to study air pollution, both in research and operational environments, but is also used for other problems requiring the quantification of atmospheric transports, such as the global water cycle or the exchange between the stratosphere and the troposphere; see Stohl et al. (2005). It can be run in either forward or backward mode. The forward mode is typically used to determine the downwind concentration or mixing ratio of pollutants. The backward mode can be used to estimate footprint areas, i.e. to determine the origin of observed emissions. The open-source code version 8.2.3, and more recently version 10, is quasi-operationally used for volcanic and nuclear plume dispersion at ZAMG. Analysis and forecast data from ECMWF and National Center for Environmental Prediction (NCEP) in different spatial resolutions are used as meteorological input. WRF-Chem output fields can also be used to drive the WRF version of FLEXPART, FLEXPART-WRF. Nesting of, both the meteorological driving data, as well as the output data is possible. The meteorological input defines the maximum 3D domain in which computational particles can be tracked.

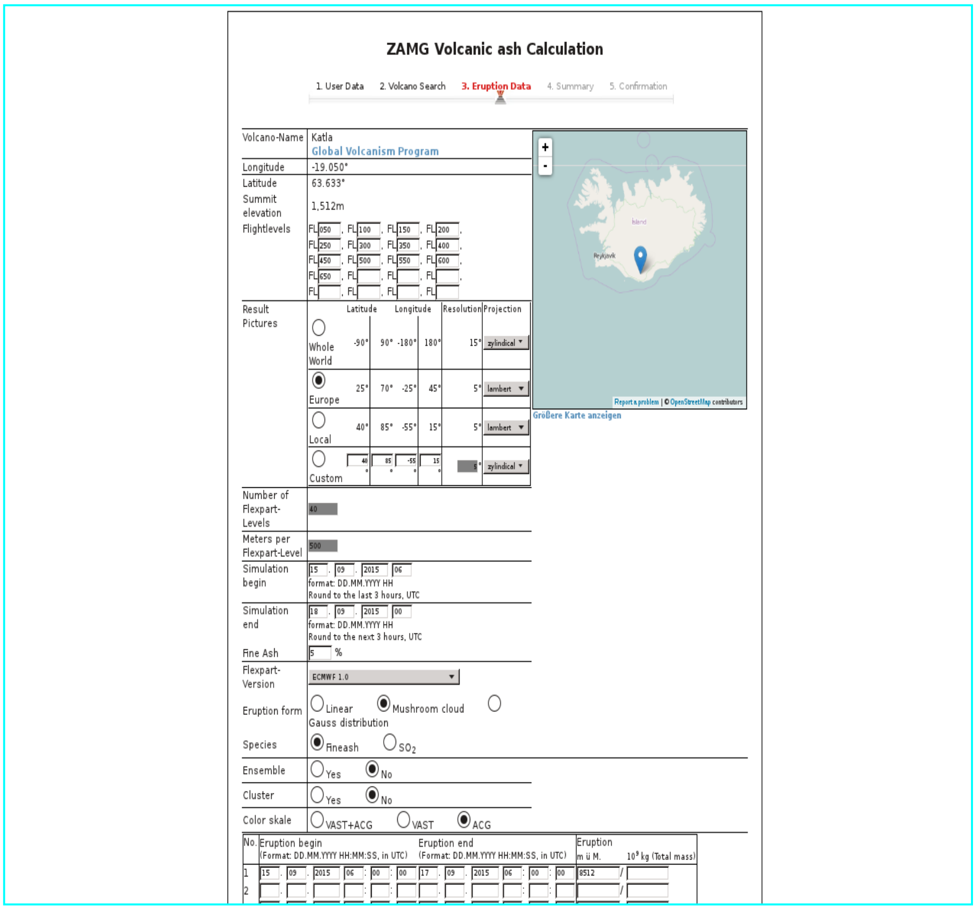

Figure 1: Specification of run parameters in FLEXPART for a selected volcano.

Currently, the integrated modelling system at ZAMG is accessible by a dedicated web-interface (see Figure 1), that handles then internally the whole procedure of atmospheric transport modelling and related post-processing. This was produced during the previous project: Volcanic Ash Strategic Initiative Team (http://vast.nilu.no/). The procedure consists of running FLEXPART with an *a priori* source term, created with parameters from a database (containing volcanic ash emissions typical for the specified volcano: total ash mass as a function of typical release duration and a typical eruption height as well as the default fine ash fraction) for approximately 1500 volcanos worldwide, based on the work of Mastin et al. (2009). During EUNADICS-AV, two processes will be added, namely the inverse modelling that creates an *a posteriori* source term and the running of FLEXPART with this *a posteriori* source term. Apart from fine ash, SO_2 can also be modelled with a default mass of 1 Teragram (within EUNADICS-AV a scaling procedure based on observations will be implemented).

Default emissions in case of nuclear power plant accidents follow International Atomic Energy Agency (IAEA) assumptions for containment/non-containment failure. Radionuclides currently considered are Cs-137, I-131 (both gas phase and particulates) and Xe-133. For both volcanic eruptions and nuclear accidents release quantities can be also entered manually. Nuclear surface and air burst emissions are based on information from the Radiation and Nuclear Safety Authority in Finland STUK (radionuclide inventory) and Harvey et al. (1993,

geometry as well as activity distribution as a function of particle size and altitude). Due to the multitude of nuclides considered summed output is given for aerosol-bound species on one side and noble gases on the other. The modules needed to simulate sand and forest fire emissions have not yet been implemented.
Model variables are available at individual model levels (around 500 m resolution) which allows the computation of derived parameters such as average concentrations between model levels, between flight levels (FL), total columns, column maxima, averaged concentrations over multiple layers as well as vertical concentration-time cross sections at airport locations. In case of radionuclides qualitative levels of equivalent doses are also provided.

An ensemble option for high-altitude volcanic eruption dispersion modelling allows using five representative ECMWF-EPS (Ensemble Prediction System) members from the total of 50 ensemble members, to be used for a multi-input ensemble. This option yields maximum concentrations as well as probability of exceedance plots.

At the moment, ZAMG uses a pre-defined set of source terms based on Mastin's formulas (Mastin et al., 2009), but other methods are under investigation (including: PLUMERIA, Devenish, 2012). In order to deduce a more realistic source term, Bayesian inverse modelling based on Stohl et al. (2011) for the calculation of an *a posteriori* source term for volcanic ash and SO_2 is employed. For the inverse modelling system, L2/L3 volcanic ash columns are needed; ground-based lidars would probably be used solely for evaluation. L2/L3 SO_2 columns are of use as well and the vertical averaging kernels for them have to be taken into account. For radionuclides, ground-based activity concentrations, aircraft activity measurements and specifically, gamma dose rate measurements, including bulk and spectrometric ones, at ground level are required.

WRF-Chem (Grell et al., 2005) simulates the emission, transport, mixing, and the chemical transformation of trace gases and aerosols simultaneously using the meteorological data. This model, which that is the first community open-code, supported model is operationally used for air quality forecasts in Austria.
Analysis and forecast data from IFS are used to initialize meteorological conditions. Chemical input data comprise emissions from different sources. Anthropogenic emissions are merged from local Austrian inventories, Netherlands Organization for Applied Scientific Research (TNO) (Visschedijk et al., 2007), and the European Monitoring and Evaluation Programme (EMEP) (http://www. ceip.at/ceip). Dust emissions are based on an on-line emission processor (based on land-use and wind) using Global Ozone Chemistry Aerosol Radiation and Transport (GOCART) (Chin et al., 2000) chemistry. Since our modelling domain includes the northern part of Africa, Saharan dust will also be simulated.
To realistically simulate volcanic events, the estimation of source terms for volcanic ash and SO_2 will be based on the FLEXPART source term inversion (see above). The modelling of the volcanic eruption itself follows an improved version of Freitas et al. (2011) and Stuefer et al. (2013). In case of wild fires, emissions data will be provided by FMI. In contrast to FLEXPART, nuclear events will not be investigated with WRF-Chem.

The GOCART scheme is used to model aerosol processes. Gridpoint statistical interpolation (GSI) 3DVAR is used to assimilate AOD measurements from MODIS (Liu et al., 2011; Schwartz et al., 2012) as well as in-situ PM2.5 measurements (Pagowski et al., 2014). WRF-Chem output includes information of black and organic carbon (2 bins), sea salt (4 bins), dust (5 bins), sulfur, dimethyl sulfate (DMS), methanesulfonic acid (MSA), SO_2, and unspecified PM10 and PM2.5.

2.5 Other input data

These four models can be complemented by additional data coming from other sources, such as the operational CAMS service, that provide the concentration of SO2 and of different aerosol types, in a global domain (at 0.5° resolution) and it a European domain (at 0.1° resolution).

3. Observations for integration

Based on WP4 activities, the models have the capacity to assimilate of different kinds of observations in order to address the hazards considered in the project. Data assimilation will be used to compute analyses and source-inversion will be used to compute point source terms.

3.1 Observations

For each type of hazard, different observations can be integrated. A list of them has been defined with WP3 and WP5. Depending on the potential usage of these observations for assimilation, we consider 3 categories of observations:

- routine assimilated observations (B0), which are unspecific to an event. These observations are assimilated in the models on a regular basis, in order to characterize the background of aerosols and SO_2. For instance, total (AOD) fall in this B0 category, as such measurements mix information about all types of aerosols. Access to B0 observations is possible through pre-existing channels, outside of EUNADICS-AV, such as EUMETSAT, EUMETNET, NASA, etc.
- observations (B1) that are specific to an event and that are provided by WP3 or by WP5. These observations are particularly of interest to compute source terms.
- observations (B2) that are specific to an event and that will be developed later on in the project by WP3 or by WP5.

The B1 and B2 observations will be made available from a KNMI server for integration in the four models. Regarding these categories and the different types of hazards, the list of observations to be integrated is presented in Table 1.

	B0 - Routine assimilated observations	B1 - Existing observations that would be assimilated in case of an event	B2 - Future tailored products (from WP3 and WP5) that would be assimilated in case of an event	Other sources of information
Volcanic SO_2	**SO_2** Ground-based measurements	**SO_2** satellite columns (UV, IR) **SO_2** aircraft measurements	**SO_2** satellite plume height **SO_2** profiles from ground-based spectrometers	
Volcanic ash	**AOD** (from satellite and ground-based instruments) **Lidar attenuated backscatter** (from satellite and ground-based instruments) **PM** ground-based measurements	**Ash** plume height (from radars) **Ash** total column and plume-height (from satellite) **PM** aircraft measurements	**Ash** layer altitude from ground-based lidars	
Nuclear hazard	none	Gamma dose measurements	none	
Desert dust	**AOD** (from satellite and ground-based instruments) **Lidar attenuated backscatter** (from satellite and ground-based instruments) **PM** Ground-based measurements	none	Desert dust layer altitude from ground-based lidars	
Forest fires	**AOD** (from satellite and ground-based instruments) **Lidar attenuated backscatter** (from satellite and ground-based instruments) **PM** ground-based measurements	none	none	GFAS emissions (from CAMS)

Table 1: List of observations that are considered for integration in the models, per type of hazard.

3.2 Use of observations in the integrated model system

Observation operators are developed in the project (WP4), to enable the use of these observations, either for the direct assimilation or for the inversion of the point-sources.

Assimilation
The assimilation of observations produces an analysis, accurate model state (i.e., 3D concentrations of the pollutants). This analysis is as close as possible to the assimilated observations, under the assumption of prior information (error statistics).

Point-source term inversion
In EUNADICS-AV, source term inversion is used for the volcanic and nuclear point-sources, although the method could also theoretically be used for area-sources. Observations (remote and in-situ) are used as input for inverse modelling for source term reconstruction, which provides estimates of the strength, height and time-evolution of the point-source emission. The different models involved and the different methods for source term inversion will provide various source terms. In addition, or prior to inversion, additional volcanic ash source terms will be computed from the empirical Mastin's law and from the prognostic model FPLUME.

As a consequence, for each volcanic and nuclear event, a variety of source terms will be computed, and such diversity will be helpful to account for the high uncertainty of these source terms. They will be shared through the repository ftp://ftp.umr-cnrm.fr/SOURCE_TERM/ at Météo-France, using a common format, and they will be integrated in the different models.

4. Design of the integrated model system

4.1 Model designs

Every model will be run for:

- a European domain, covering a large part of Europe, the Eastern part of North Atlantic and the Mediterranean (see Figure 2) at a horizontal resolution of 0.1° approximately. This domain covers the densest part of the European air space and will be used to address the hazards of European volcanoes (including Iceland and Italy), nuclear power plants of all Europe (including western Russia), strong northernmost Saharan dust storms and forest fires in the Mediterranean area.
- a global domain, at a horizontal resolution of 1° approximately, that will enable the investigation of hazards outside Europe.

Assimilation will be done on both domains. Some hazards that may affect the European air traffic may have their origin outside of the European domain. This is the case, for example, for Saharan desert dust and forest fires (from Siberia, North America, for instance). Because the boundaries of the innermost simulation domain are close to Iceland, under specific wind directions it is also possible that a volcanic plume moves out of the European domain and then re-enters it. To deal properly with such cases, it is required that a global domain, at a coarser resolution, is included.

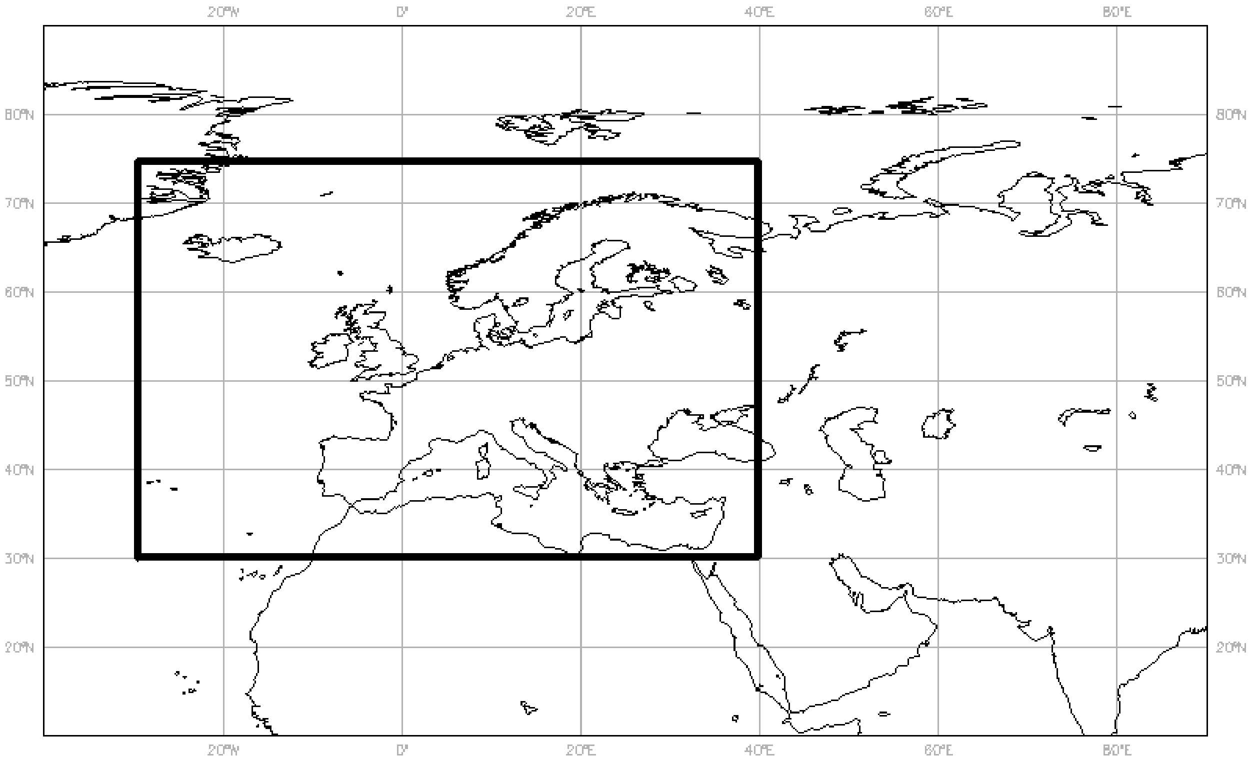

Figure 2: European domain of EUNADICS-AV (bold black rectangle).

The meteorological drivers used by the different models are mostly from the IFS deterministic forecast, or from other models, such as ARPEGE from Météo-France or WRF-Chem. The models that can ingest different meteorological input data will compute several scenarios from them.

From the different models, the diversity of source terms and meteorological input data, it is possible to derive several members. From them, a 4D multi-model ensemble will be computed, that will provide the basis of the model products. The definitive number of members will be defined during the remainder of the project, as it depends on the computational resources and on the assessment of the quality of the ensemble.

4.2 Dataflow and link with early warning system (EWS)

The integrated model system is strongly connected to other work packages of the project: the delivery of observations (WP3), the generation of assimilation and of source terms (WP4) and the Early Warning System (EWS, WP5). The general dataflow is presented in Figure 3. On a regular basis, routine observations (B0 category) are assimilated in the models. Desert dust emissions and forest fire emissions are also included in every model.

One of the objective of the EWS is to detect and to warn against airborne hazards (Brenot et al., 2018, D28 EUNADICS-AV report) utilising the diverse dataset incorporating satellite, ground-based and in-situ measurements that are available. The EWS will produce automated alerts and transfer notifications, that contains information about an event in txt or xml format (date, time, coordinates of measurements, detection type, maximum/mean values detected, number of pixels/coordinates of polygons) and alert data products (images and dataset collection, or link to).

Notifications will be received by WP4 and WP6 teams, by e-mail at least, and they will trigger the following actions:

- computation of source terms (in case of a volcanic or nuclear event), based on the information provided in the notification, and from the observation data available (B1),
- transfer of source terms to the Météo-France platform for sharing source terms,
- use of source terms (in case of a volcanic or nuclear event) and of all available observations (B0 and B1) to calculate several analyses, and provision of the model outputs to the Météo-France platform for sharing model outputs,
- computation of ensemble products from the different model outputs available at Météo-France and delivery to WP7 and WP8.

If an event lasts for a significant duration (more than a few hours), this process chain will be repeated regularly, and updated as soon as new observations are available for assimilation. We can note also that some model outputs, such as total aerosol values and SO_2, will be processed and delivered even when no event is on-going. These products can provide indication to aviation of the present situation and can help for early detection of sandstorms, forest fires or abnormal SO_2 levels.

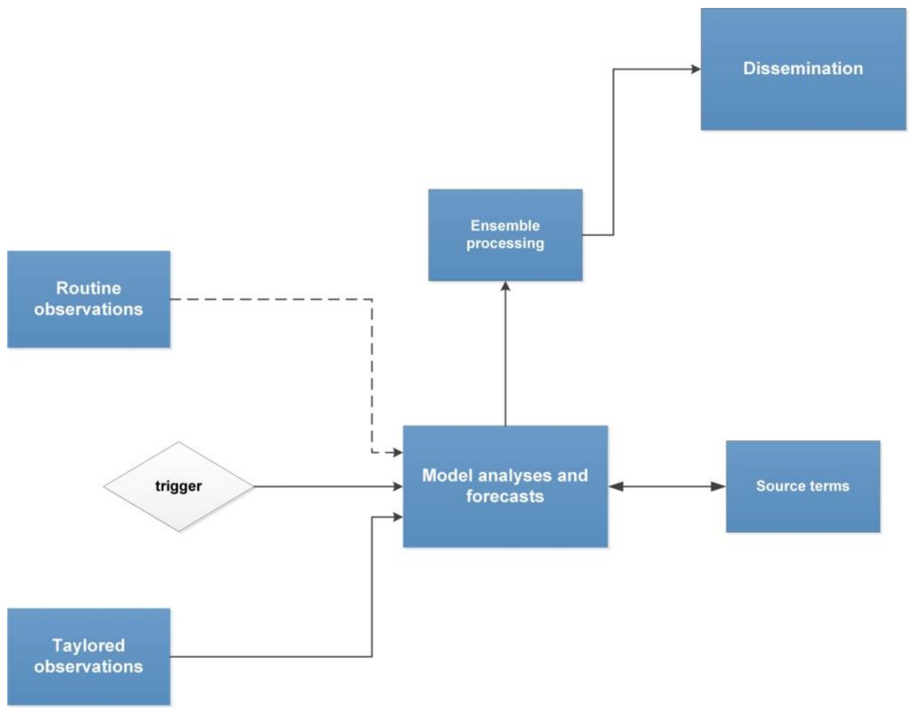

Figure 3: General dataflow of the integrated model system.

The general dataflow of the integrated model system (see Figure 3) goes from the integration of routine (B0) and tailored (B1) observations from WP3 and WP5, the trigger by EWS from WP5), through the computation of source terms, analyses and forecasts (WP4 and WP6), then the calculation of an ensemble (WP6). The output data are finally disseminated (by WP7 and WP8).

5. Products for the aviation service

The collected requirements from end users are twofold: a) products should be comparable, e.g., to already existing VAAC products, and b) model outputs should be provided on high resolution spatial and temporal scales, especially in regards to vertical resolution of the provided concentrations (aerosol and radionuclide). Following these requirements, EUNADICS-AV will produce products/services with different complexities which will be tailored to the requirements of different user groups. The following section describes the first level of the model ensemble output which will be transferred to WP8, where it will be further processed and finally disseminated.
The main products from WP6 are scenario maps of the concentration of SO_2, aerosols and of radioactivity, calculated from a 4D ensemble (see Figure 4). These maps will be made available at specific flight levels (FL).

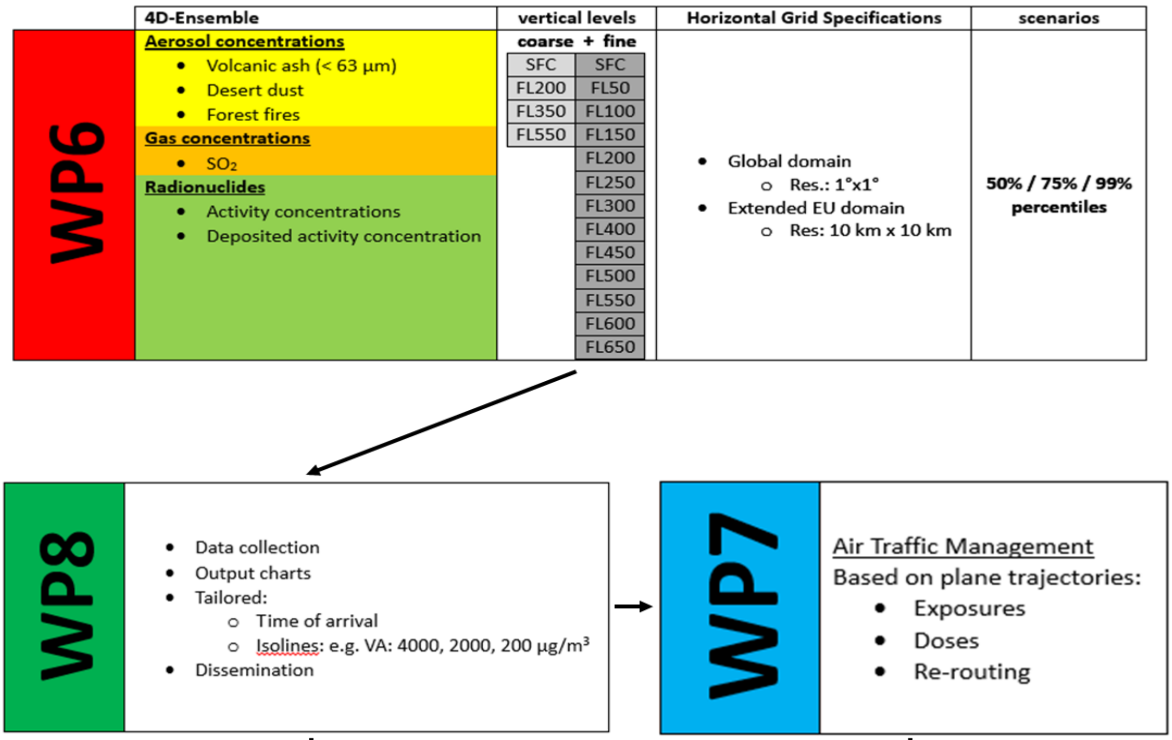

Figure 4: Scheme of the integrated model products and their dissemination to other work package. The dissemination to the final users is handled by WP8 and WP7.

5.1 Product definition and format

Products will be delivered on two grids, one for Europe at 0.1° resolution, and one global grid at 1° resolution (see Section 4.1). The output will be delivered at an hourly time step.

Two different vertical resolutions are included, covering flight levels:

- a coarse vertical grid: SFC-FL200, FL200-350, FL350-550,
- a finer vertical grid covers: SFC-FL50, FL50-100, FL100-150, FL150-200, FL200-250, FL250-300, FL300-350, FL350-400, FL400-450, FL450-500, FL500-550, FL550-600 and FL600-650.

The following parameters will be delivered, depending on the type of event:

- ✓ Mass concentration of SO_2
- ✓ Mass concentration of volcanic ash (particles with diameter below 63 μm),
- ✓ Mass concentration of desert dust
- ✓ Mass concentration of forest fire smoke
- ✓ Nuclear activity concentration
- ✓ Nuclear deposited activity concentration

The model ensemble output will be provided in specified CF-conformal NetCDF data files comprising the selected parameters on a specified grid and with specified naming conventions. The ensemble will contain the contributions from the different modelling system and also include integrated observational data. The 4D ensemble contains hourly concentration values.

5.2 Usage and dissemination of products

This output of WP6 will be provided for WP8 (dissemination) and partly to WP7 (air traffic management) to produce the final data files and graphics and disseminate them via respective channels.

Based on the multi-model ensemble outputs, different scenarios will be produced and delivered, namely 50%, 75% and 99% percentiles, that correspond to the values of the parameter (concentration or activity) that is exceeded by at least 50%, 75% and 99% of the ensemble members, respectively. These scenarios can be represented directly as maps (of concentrations or activity) and they can be used in diverse ways, depending on the usage of the data. Automated ATM systems may incorporate the probabilities directly to optimize the routes. Operational forecasting centres may analyse the percentiles as a measure of risk assessment, as 50% is a central scenario, 99% the worst-case scenario and 75% an intermediate scenario that can help to characterize the uncertainty around the central scenario.

The computation of potential exposure dose along a flight tracks is possible from the concentration and activity produced. As such computation requires flight tracks as input data, it will be computed in WP7. The concentration and activity concentration scenarios provided by WP6 will be critical input data to assess exposure dose and their uncertainty, which are required for risk assessment.

6. Definition of verification exercises

Verification exercises are required to demonstrate the usability of the designed system as well as providing the basis for verification of the products and meeting of user requirements. For this purpose, demonstration of past events that were hazardous to aviation are considered. The demonstration requires to going through the entire chain of work packages, from the collection of observations (WP3), their assimilation into models (WP4), the definition of EWS (WP5), the integration and the production (WP6), and then the evaluation of the added value for ATM (WP7) and the dissemination (WP8).

The following list of test cases has been defined:

- ✓ Grimsvötn eruption, 21-28 May 2011,
- ✓ Fukushima plant nuclear accident, 11-21 March 2011,
- ✓ Eyjafjöll eruption, 15 April – 23 May 2010,
- ✓ Portuguese wildfires (mixed with Saharan dust), 15-17 October 2017,
- ✓ Etna eruption, 27 October – 5 November 2002,
- ✓ Saharan dust event, 7-11 September 2015.

An agreement was reached that the project initially focuses first on the Grimsvötn 2011 eruption to define products and interfaces (from WP3 to WP8). The demonstration of the integration of data on this case has already started and it will be evaluated in the coming months.

7. Perspectives and conclusions

This document presents a design of a pilot demonstration for the integration and production of services to aviation regarding volcanic eruptions, nuclear explosion, desert dust and forest fires. The design has taken into account the user requirements and the capacities of the models involved. It also incorporates the interfaces with related activities, namely the provision and tailoring of observations, the EWS and the dissemination of products.

The main perspectives of the WP6 for the remainder of the project are to:

- develop and to refine interfaces between the provision of observations and model integration,
- develop data model exchanges inside WP6 and ensemble processing and to assess its quality,
- develop data exchange with WP7 and WP8 for the evaluation in ATM scenarios and for dissemination.

The demonstration of integration of data on a first use case has already started and its evaluation will serve as a test-bed for future improvement and development in the coming months.
Continuous interactions with stakeholders will be sought to improve the prototype.

8. Glossary

AOD: aerosol optical depth
ARPEGE: Action Recherche Petite Echelle Grande Echelle
ASSET: ASSimilation of Envisat daTa
ATM: Air Traffic Management
CAMS: Copernicus Atmosphere Monitoring Service
CTM: Chemistry and Transport Model
DMS: Dimethyl Sulfate
ECMWF: European Centre for Medium-Range Weather Forecasts
ECMWF-EPS: ECMWF-Ensemble Prediction System
EMEP: European Monitoring and Evaluation Programme
EnKF: Ensemble Kalman Filter
EnKS: Ensemble Kalman Smoother
EUMETNET: Network of European Meteorological Services
EUMETSAT: European Organization for the Exploitation of Meteorological Satellites
EUNADICS-AV: European Natural Airborne Disaster Information and Coordination System for Aviation
EWS: Early Warning System
FL: flight levels
FLEXPART: FLEXible PARTicle dispersion model
FMI: Finnish Meteorological Institute
GFAS: Global Fire Assimilation System
GOCART: Global Ozone Chemistry Aerosol Radiation and Transport
GSI: Gridpoint Statistical Interpolation
IAEA: International Atomic Energy Agency
IFS: Integrated Forecasting System
IR: Infra-Red (radiation)
MATCH: Multi-scale Atmospheric Transport and Chemistry
MOCAGE: MOdele de Chimie Atmospherique de Grande Echelle
MODIS: MODerate-resolution Imaging Spectroradiometer
MSA: Methanesulfonic Acid
NASA: National Aeronautics and Space Administration
NCEP: National Center for Environmental Prediction
NRT: near-real time
OMI: Ozone Monitoring Instrument
PALM: Projet d'Assimilation par Logiciel Multimethodes

RACM: Regional Atmospheric Chemistry Mechanism
REPROBUS: REactive Process Ruling the Ozone Budget in the Stratosphere
SDS-WAS: WMO Sand and Dust Storm Warning Advisory and Assessment System
SILAM: System for Integrated modeLling of Atmospheric coMposition
SMHI: Swedish Meteorological and Hydrological Institute
SOA: Secondary Organic Aerosol
STUK: Säteilyturvakeskus (Finland Radiation and Nuclear Safety Authority)
TNO: Netherlands Organization for Applied Scientific Research
UV: Ultra-Violett (radiation)
VAAC: Volcanic Ash Advisory Center
WP: Work Package
WRF-CHEM: Weather Research and Forecasting Chemistry model
ZAMG: Zentralanstalt für Meteorologie und Geodynamik

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