ATMO ACCESS
Access to Atmospheric Research Facilities

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Introduction

The objective of the footprint Virtual Research Environment is to provide users with a service shared between ACTRIS, ICOS and IAGOS that provides air mass origin information to analyse atmospheric in situ ground-based observations from fixed and mobile observation platforms. It gives access to state-of-the-art Lagrangian Particle Dispersion Models (LPDM) through cloud computing facilities driven by high resolution meteorological data archives.

Users get access to already computed footprint data and can in case of greenhouse gases and aerosols define through a user-friendly interface the 3D coordinates (with time) of the receptor points and can refine in detail the configuration of the model run. Existing and ready footprint data can be downloaded for use in an analysis. The footprint VRE will show all available footprint data through an attractive GUI.

The on-demand model run(s) are orchestrated to virtual machines in the cloud and the user is informed of the result when complete.

Existing and new model output will be accessible from the respective repository through open access and the dataset will be minted a persistent identifier for later reference or citation.

The model runs are based on a ERA5 and operational ECMWF or GSF data. Where a time resolved emission inventory is available the data can be combined with that emission inventory to derive a forward analysis of concentrations and if available comparison with (NRT) observation data from the data centres. For this the atmospheric footprints are be convolved with state-of- the-art emission inventory data (e.g., EDGAR-Emission Database for Global Atmospheric Research), dependent on the component.

1. Service connected to observation of greenhouse gases, in first instance using the CO -STILT (Stochastic Time-Inverted Lagrangian Transport) model and in a later stage when adequate user demand arises FLEXPART (FLEXible PARTicle dispersion model); The first version will be provide CO_2 predictions, later (in second half of the project) CH_4 will be added, also when enough user demand arises, N_2O and CO will be considered (required background data for these compounds are not readily available).

2. Service connected to observation of aerosol components and products for interpretation of the observations, including vertical information of aerosol distribution – based on the FLEXPART model.

3. Service connected to observation of flight vertical profiles of CO at airports – based on the FLEXPART model.

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Users identify themselves through the AERIS authentication service and get access to the VA services through the central ATMO ACCESS VA Services switchboard. The actual services run on the individual RI platforms. All modules provide data usage statistics to the central VA service through a dedicated API.

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Implementation

The Virtual Access Portal

The ATMO ACCESS virtual access portal can be reached at https://www.atmo-access.eu/virtual-access:

Figure 1 The ATMO ACCESS Virtual Access portal entry pagel (status of 15 June 2023)

After login through the AERIS SSO environment, that allows identification using EduGAIN, ORCID or AERIS/DataTerra accounts, users land at the Virtual Access Portal switchboard page that presents all available online services.

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Figure 2 The ATMO ACCESS Virtual Access Portal switch board page

Here the user can select the Trajectory and footprint analysis button, after which the footprint selection page opens that allows the user to choose between footprint data for greenhouse gases, aerosols, and vertical profiles. This selection is needed because requirements for the model runs, and the parameters needed are very different for these three types of footprint.

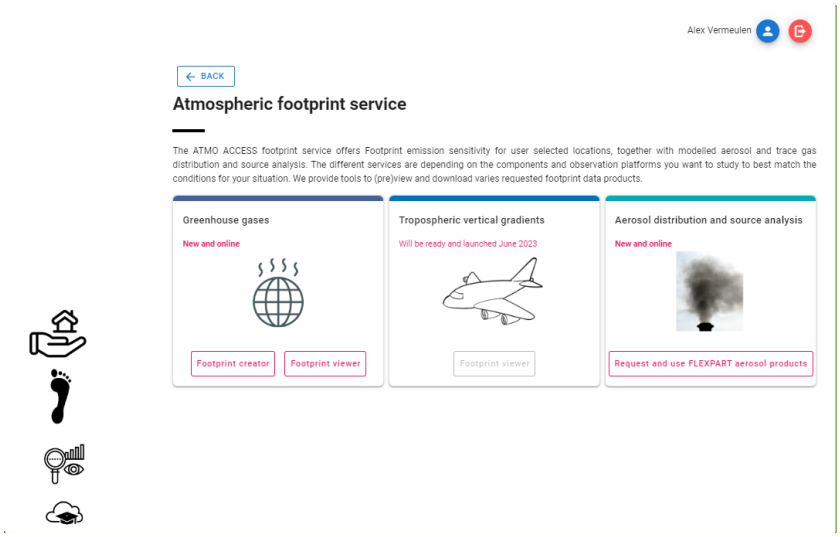

Figure 3 The ATMO ACCESS Virtual Access footprint selector menu

Commenté [BD1]: the page is updated. IAGOS service is now accessible

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Greenhouse gas (GHG) footprint tools

The GHG footprint tools already available for ICOS have been extended with dynamic download of the data and integration with the ATMO ACCESS VA portal. This also required integration with the AERIS realm for user authentication and integration of the data usage API.

This also means that users that access the GHG footprint tools through the normal ICOS website menu are presented with an additional entry page, as shown below.

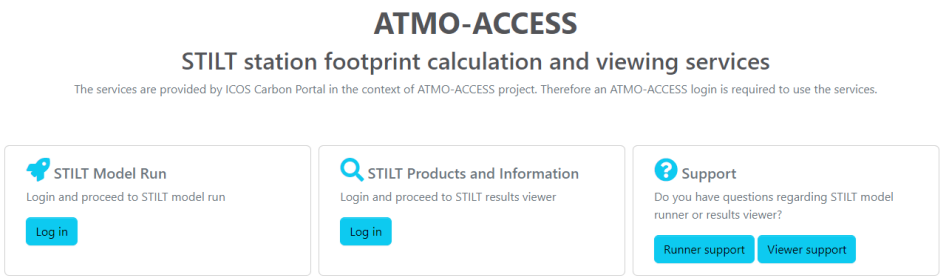

Figure 4 Modified GHG Footprint user entry when starting from the ICOS website. Status of June 2023, later version will have better ATMO ACCESS styling.

From this page users can login with the AERIS SSO and choose one of the services or view the help pages that explain the services. A feedback button will be added later.

The service for the greenhouse gas footprint is divided into three separate services. One service is the so-called worker, that allows the user to specify a new footprint to be calculated. This service is called the job starter, shown below.

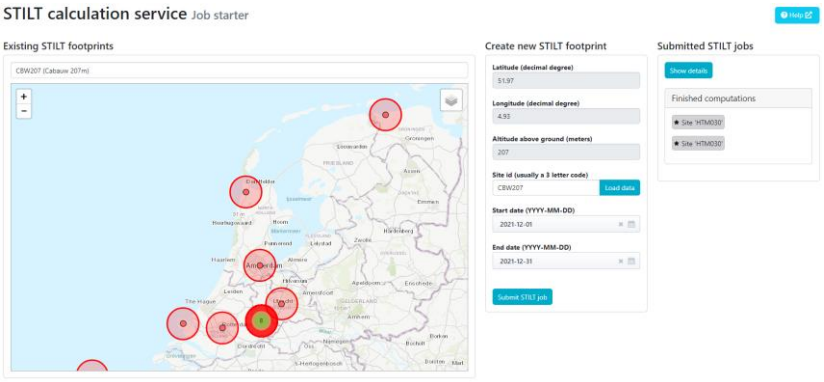

Figure 5 Greenhouse gas Job Starter interface for the Worker to instantiate footprint calculations specified by the user

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After pressing the submit button the calculation is started (or the data from previous runs matching with the request are gathered). The results are displayed in a calculation dashboard when the user selects the Show details button, as shown below.

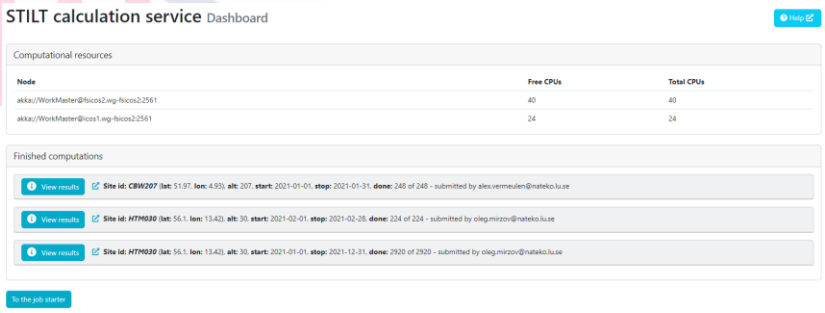

Figure 6 Calculation dashboard

Here the users can see the progress of the ongoing calculations for all users and select the View results button to see the results (thus far) in the so called single-site scoped viewer, as shown below. Calculation will trigger sending of the request metadata to the VA API to log the usage.

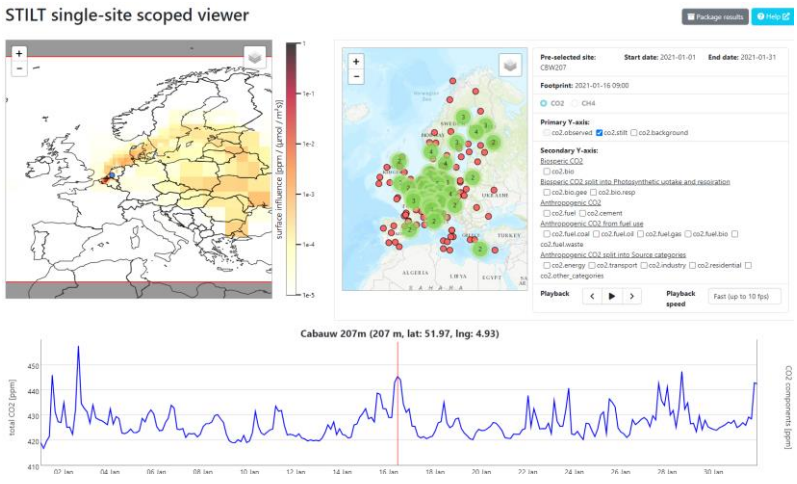

Figure 7 STILT Single site scoped viewer to view user requested data sets with footprint and modeled concentration and contributions from different source categories of the selected compound.

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The viewer is fully interactive, showing animations of the foot print and concentrations and users can zoom in and out for time and concentration range and move the time bar to see corresponding concentrations/contributions with the corresponding footprint.

Through the Package results button the user can request to download the data. Download will trigger sending of the request metadata to the VA API to log the usage.

A final window available to the user is the STILT results viewer that allows to select all available footprint data at the repository. The window is very similar to the single scope viewer, but it allows the user to select any station on the map through the dropdown or by zooming/clicking on the interactive map and then selecting the available time period from the dropdown. From this window the user has the possibility to download the selected data set by pressing the Package results button.

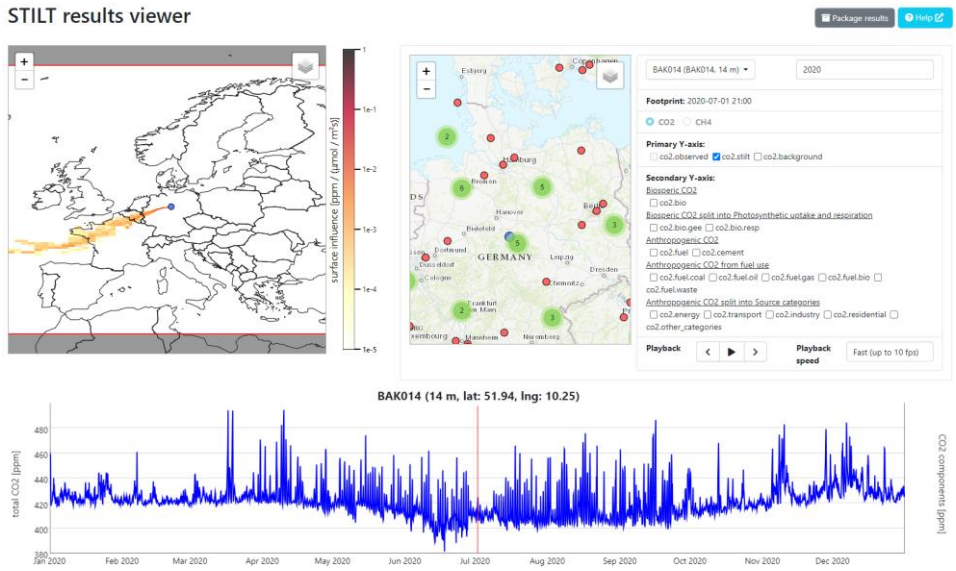

Figure 8 The STILT results viewer where users can select and preview any available footprint.

Result packages consist of a single zip file that contains three files:

- The footprint as cf-compliant netcdf datafile with all (hourly or 3-hourly) footprints with time as dimension
- The calculated mole fractions of the compound and the contributions of the different source/sink categories and background as csv file

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- A summary json metadata file describing the STILT run including the URL to order another result package for the same parameters

All GHG footprint service pages have a Help button that shows a basic explanatory text to help 1st time users to execute a first model run or result download.

CO vertical profile footprint tool

The IAGOS viewer of FLEXPART footprints and modelled SOFT-IO CO contributions has been launched on 15th of June 2023 and is accessible from the VA portal. The viewer allows a user to explore tropospheric vertical profiles of carbon monoxide mixing ratios (measured by IAGOS) in conjunction with source attribution data (calculated using the SOFT-IO model). The profiles are over airports visited by commercial aircraft equipped with IAGOS' instruments. The SOFT-IO model is based on the coupling of FLEXPART backward footprint (with the receptor points located along the profile) with emission inventory databases:

- GFAS v1.2 (for biomass burning emissions);
- CEDS v2 (for anthropogenic emissions).

(See [1] for details).

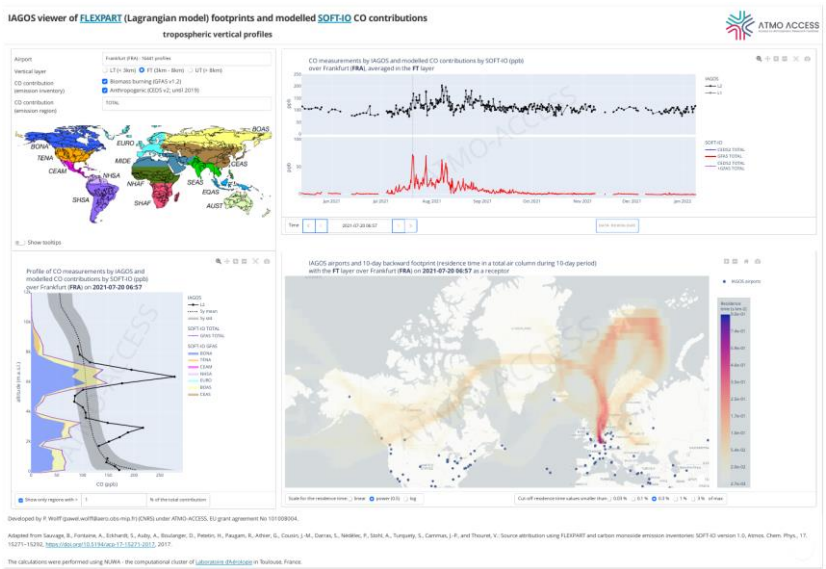

Figure 9 The IAGOS footprint viewer - Selection, visualization and download of CO vertical profile footprint.

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The service provides a visualisation of the above-mentioned data via a simple, attractive user interface. More specifically, the user chooses:

(a) an airport (from a dropdown list or clicking on the map);
(b) a vertical layer: lower troposphere (< 3 km), free troposphere (3-8 km) or upper troposphere (> 8 km);
(c) emission inventory database used by SOFT-IO (GFAS, CEDS or both);
(d) either one of 14 emission regions (as defined by GFED), or the total of all regions;
(e) time (with the granularity of 1 day) of CO measurements, accompanying SOFT-IO model data and the origin of the corresponding footprint
(f) a particular profile (as observed by an aircraft departing from or arriving at the given airport), identified by an exact time.

(In what follows, the letters (a)-(f) refer to the user's choice of the corresponding parameter).

The visualisation consists of three plots:

- The time-series with daily means of:
  - the carbon monoxide mixing ratios over an airport (a) averaged within the vertical layer (b);
  - the modelled amount of CO contribution from emissions (c) coming from a region (d) to the receptor located over the airport (a) within the vertical layer (b).
- The 10-day backward footprint with an origin at the receptor whose location is determined by (a)-(b), and time is defined by (e)-(f).
- The profile over the airport (a) at the time defined by (e)-(f) of CO measurements and CO contributions (from all regions) modelled using the emission inventory (c).

Furthermore, the service allows a download (in netCDF format) of the timeseries with daily means of CO measurements and CO contributions for the airport (a).

[1] Sauvage et al.: Source attribution using FLEXPART and carbon monoxide emission inventories: SOFT-IO version 1.0, Atmos. Chem. Phys., 17, 15271-15292, https://doi.org/10.5194/acp-17-15271-2017, 2017.

Aerosol and Black carbon footprint tool

This tool is available by redirect at https://flexpart-request.nilu.no/. It has been launched on May 15th, 2023 and can also be accessed from the VA portal as shown earlier. The footprints for aerosol and black carbon can be viewed and requested through the virtual-access entry and tool. The products are generated for surface concentration, but also height information

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on different vertical level, which is necessary for aerosol profiles (lidar data) can be viewed. In addition there is the option to get support for existing products or to get help when ordering them, and to understand the use and outcome in relation to the observations.

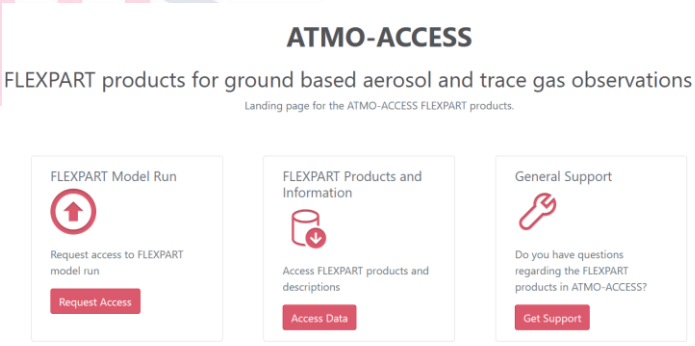

Fig 10: Landing page viewing model results, requesting new products or getting support.

There is a map and list provided, which shows the simulations and analysis already available, these can be accessed via a map or the table, where the years and stations are visualized.

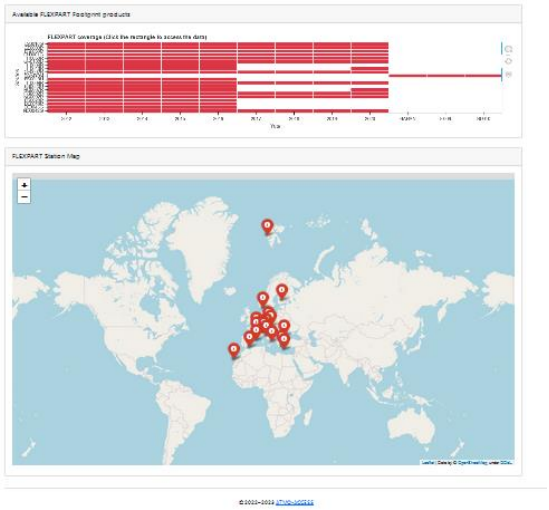

Fig 11: Selection possibilities for the FLEXPART aerosol products, on the upper panel selection by time and station, the lower panel shows a map with selectable station locations.

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Following options are selectable for browsing through the FLEXPART products for the webpage, which looks like:

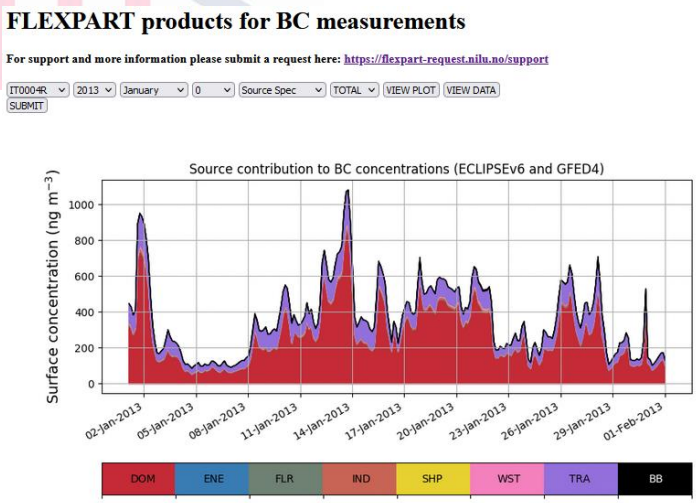

Fig 12: Monthly product for modelled black carbon split by the different sources, here the domestic burning emissions and the transport sector are the main sources for BC concentration on that station. The buttons on top can be used to navigate through the different products.

- Upper left box selects station code that the user wants to view.

- On the right of button “Aerosol", the user selects the product that the user wants to view (Source Spec, Footprint, DOM BC, ENE BC, IND BC, FLR BC, SHP BC, WST BC, TRA BC, Fire BC, Continental Spec, Age Spec). These terms are described on the web: FLEXPART Data Portal (nilu.no).

- Final box on the right selects the projection (regional, global).

- Buttons FIRST, -10, PREV, NEXT, +10, LAST navigate between different sampling times.

- Buttons VIEW PLOT and NETCDF (for map products) or VIEW DATA (for spectrum products) switch between plot visualization and links for download the data. Map products (Footprint, DOM BC, ENE BC, IND BC, FLR BC, SHP BC, WST BC, TRA BC, Fire BC) are in gridded arrays and are given in netCDF format, while spectrum products (Source Spec, Continental Spec, Age Spec) are given in ascii format.

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On the webpages it is possible to view footprints of residence times or emission contribution as well as time series of aerosols stemming from different source regions and categories, below is a list of the underlying data and the available categories:

- Footprint: Footprint emissions sensitivity showing the probability of any release occurring in any grid-cell to reach the receptor (station) for 30 days particle tracking.

- DOM BC: Modelled contribution to surface black carbon (BC) from residential and commercial sector plotted on a map (three projections). DOM includes emissions from combustion in heating and cooking stoves and boilers in households and public and commercial buildings (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

- ENE BC: Modelled contribution to surface black carbon (BC) from energy production sector plotted on a map (three projections). ENE includes emissions from combustion processes in power plants and generators (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

- IND BC: Modelled contribution to surface black carbon (BC) from industrial combustion plotted on a map (three projections). IND includes emissions from industrial boilers and industrial production processes (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

- FLR BC: Modelled contribution to surface black carbon (BC) from gas flaring plotted on a map (three projections). FLR includes emissions from oil and gas facilities (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

- SHP BC: Modelled contribution to surface black carbon (BC) from shipping activities in in-land waters plotted on a map (three projections) (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

- WST BC: Modelled contribution to surface black carbon (BC) from waste treatment and disposal sector plotted on a map (three projections). WST resembles emissions from waste incineration and treatment (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

- TRA BC: Modelled contribution to surface black carbon (BC) from transportation sector plotted on a map (three projections). TRA includes emissions from all land-based transport of goods, animals and persons on road networks and off-road activities (ECLIPSEv6, Klimont et al., https://doi.org/10.5194/acp-17-8681-2017).

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- Fire BC: Modelled contribution to surface black carbon (BC) from open biomass burning (excluding agricultural fires) plotted on a map (three projections) (GFEDv4, Giglio et al., https://doi.org/10.1002/jgrg.20042).

- The total modelled BC at the station can be computed from the sum of all 8 BC contributions (not given here but you can do it yourself or see it from the timeseries plots and their ascii files (Continental Spec, Age Spec, Source Spec).

- Source Spec: Timeseries plot of modelled concentrations in 3h resolution showing the contribution of each source (DOM BC, ENE BC, IND BC, FLR BC, SHP BC, WST BC, TRA BC, Fire BC) to surface BC.

- Continent Spec: Timeseries plot of modelled concentrations in 3h resolution showing the continental contribution (OCE: Ocean, GNL: Greenland, SA: South America, CA: Central America, NA: North America, AFR: Africa, EUR: Europe, RUS: Russia, ASI: Asia excluding Russian part, AUS: Australia) to surface BC.

- Age Spec: Timeseries plot of modelled concentrations in 3h resolution showing the age contribution of the plume to surface BC. The latter shows how “fresh” or “old” the air arriving at the receptor is.

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Conclusion

Through the ATMO ACCESS Virtual Access (VA) Portal now the scientific users of atmospheric data from the three participating Research Infrastructures IAGOS, ACTRIS and ICOS have now access to a free and integrated footprint generation and access tool that assists the users in their analyses.

Through the common login, helpdesk, feedback gathering and API of the VA portal the RIs can efficiently gather user responses and activities to further improve and develop the services in the remaining course of the project.

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