Validation server User Requirements Document

Deliverable title	Validation server User Requirements Document
Deliverable number	D8.1
Revision	02
Status	Final
Planned delivery date	30/04/2012
Date of issue	May 14, 2012
Nature of deliverable	Report
Lead partner	Belgian Institute for Space Aeronomy
Dissemination level	Public

This work has received research funding from the European Community's Seventh Framework Programme ([FP7/2007-2013]) under grant agreement n°284421.

DOCUMENT PROPERTIES

	FUNCTION	NAME	DATE	SIGNATURE
LEAD AUTHORS	Responsible persons at BIRA-IASB for D8.1	B. Langerock M. De Mazière		
CONTRIBUTING AUTHORS	MACC-II partners	K. Lefever S. Chabrillat A. De Rudder		
	MACC-II Val leader	H. Eskes		
	NORS partners	F. Hendrick M. Van Roozendael S. Vandenbussche S. Godin-Beekmann T. Blumenstock J.C. Lambert A. Richter E. Mahieu S. Henne S. Niemeijer L. Breebaart		
REVIEWERS	NORS coordinator WP8 leader	M. De Mazière S. Niemeijer		

Table of Contents

1. Applicable documents

[A] Lambert, J.C., MACC Validation Protocol, EC FP7 Monitoring Atmospheric Composition and Climate (MACC) deliverable D_MAN_3.4, Version 1, 47 p., 11 October 2010.
http://www.gmes-atmosphere.eu/documents/deliverables/man/

[B] QA4EO, A Quality Assurance Framework for Earth Observation. http://qa4eo.org/
QA4EO, The Guide. http://qa4eo.org/docs/QA4EO_guide.pdf
QA4EO Principles, January 14, 2010. http://qa4eo.org/docs/QA4EO_Principles_v4.0.pdf

2. Reference documents

[1] De Rudder, A. et al., Product Specifications, External Interfaces and Validation Means, deliverable MACC D_MAN_3.7 http://www.gmes-atmosphere.eu/documents/deliverables/man/

[2] Eskes H., et al., Skill scores and evaluation methodology for the MACC II project. MACC-II VAL D_85.2 http://www.gmes-atmosphere.eu/documents/maccii/deliverables/val/

[3] Eskes, H., et al., Validation report of the MACC near-real time global atmospheric composition service System evolution and performance statistics until November 2011, February 2012. MACC-II VAL D_82.1 http://www.gmes-atmosphere.eu/services/gac/nrt/.

[4] The MACC global verification web page, http://www.gmes-atmosphere.eu/services/gac/global_verification/

[5] Calisesi, Y., Soebijanta, V. T. and van Oss, R., Regridding of remote soundings: Formulation and application to ozone profile comparison, J. Geophys. Res., 110, D23306, doi:10.1029/2005JD006122, 2005.

[6] Lambert, J.-C., De Clercq, C., and von Clarmann, T., Comparing and merging water vapour observations: A multi-dimensional perspective on smoothing and sampling issues, Chapter 9 (p. 177-199) of book "Monitoring Atmospheric Water Vapour: Ground-Based Remote Sensing and In-situ Methods", N. Kämpfer et al. (Eds.), International Space Science Institute (ISSI) Scientific Report Series, Vol. 10, Edition 1, ISBN: 978-1-4614-3908-0, Springer New York © 2012 (in press).

[7] Rodgers, D., Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing Company, 2000.

3. Introduction

The NORS project will support the development and generation of fit-for-purpose GAS data products and services by providing quality information based on validation results. In NORS the validation will be carried out using NORS data products which are essentially ground-based remote sensing data from the Network for the Detection of Atmospheric Composition Change (NDACC), optimized for the needs of the GAS validation.
The validation processes to be carried out in NORS must comply with best practices as defined by the international community, and all validation results must include traceability information. The validation support by NORS will be delivered as a web-based application that generates default validation reports in an operational way, but which can also be used for the generation of dedicated user-driven validation reports on demand.

(1) A first important remark is that NORS is a demonstration project: it will focus on a limited number of target data products from a limited number of pilot NDACC stations representative of four major atmospheric regimes. The GAS data products will be provided by the FP7 project MACC-II, which is the current GAS prototype of the GMES atmospheric core service.

Nevertheless, the validation service must be built in such a way that it can easily be expanded at a later stage to a larger number of stations and instruments (ideally all NDACC stations/instruments), and to additional GAS data products for which NDACC can provide observational support for validation.

Although the present Validation Server User Requirements Document will focus on the current selection of data products and stations, the possibility of expansion should always be kept in mind. In particular, the current validation service should already be designed such that data from the new potential NDACC stations outside of Western-Europe that are included in the NORS capacity building activity (WP10 of the NORS project) can be included in the validation process (cf (UR3) page 12).

(2) A second important remark is that NORS should not in any sense duplicate what is already being done within the MACC-II project, in particular within the validation (VAL) subproject of MACC-II. VAL has a focus on the reactive gases and aerosol composition on a global scale, which coincides partly with the NORS species list. Duplication is not really an issue because MACC-II VAL is mostly using in-situ data as reference data for the validation of the MACC-II products, and almost not the NDACC remote-sensing data that are the reference data in NORS.
VAL produces 3-monthly validation reports for the near-real time services of MACC-II, and 6-monthly validation reports (updates) for the reanalysis services of MACC-II. NORS and MACC-II VAL will strive for mutual consistency in their validation approach and use of scores for reporting the results. The aim is to achieve an integration between both projects. Therefore, close interaction with VAL is required. This is facilitated by the fact that some NORS partners are also partners in the MACC-II VAL subproject.

(3) Thirdly, in order to comply with current best practices, the validation approach should be compliant with the following principles and guidelines, all peer-reviewed and endorsed by the international community: (i) the general data quality strategy as developed in the context of the Global Earth Observation System of Systems (GEOSS) and applicable among all thematic domains making use of Earth Observation data (Quality Assurance for Earth Observation (QA4EO) guidelines [B]); (ii) the validation roadmap for GMES atmospheric data and services formalised in the MACC Validation Protocol [A]; and (iii) the validation "best practices" published in the scientific literature and in technical notes.

4. Identification of users

According to the background of the users, we can identify four types of users:

- (U1) MACC-II data originators
- (U2) MACC-II VAL subproject
- (U3) NORS (NDACC) data providers
- (U4) MACC-II users

(U1) **MACC-II data originators:** The first objective of the NORS project is to deliver quality information about the MACC-II data products to the MACC-II data originators, in order to enable them to monitor the performance of the data production chain, to identify the strengths and weaknesses of their products and to improve them.

(U2) **MACC-II VAL subproject:** As indicated in Section 3, the VAL subproject is dedicated to issuing validation reports regarding various MACC Services/Products. It has been agreed that the VAL subproject will make use of the default validation reports issued by NORS for integration in the VAL 3-monthly reports (these are deliverables of MACC-II). Therefore, the default NORS validation reports should include the same basic skill scores as the ones defined in the VAL scoring document [2]. Feedback received from NORS on the scoring approach will be integrated in the VAL scoring document.

(U3) **NORS (NDACC) data providers:** Validation always involves two parties, of which one is generally identified as the reference data provider, providing data of documented quality, and the other one is identified as the provider of the data of unknown or less well known quality. Nevertheless, the reference data provider is also interested in getting some feedback concerning the use of his/her data and in the comparison of his/her data to other datasets. In the present context, the NORS (NDACC) data are considered the reference data.

(U4) **MACC-II users:** Data users should have at their disposal appropriate information about the quality and limitations of the MACC-II products, in order to ensure proper understanding of the data products and avoid their misuse and /or misinterpretation. This is especially important when the users are policy makers or developers of Downstream Services. At this point, the NORS server will not generate dedicated reports for this user group. It is assumed that they will find more appropriate information in the validation reports generated by MACCII VAL, and in the NORS deliverable D9.2 "Assessment of GAS products" which will at least partly rely on user-driven validation reports generated via the NORS Validation Server but which will probably require some additional human effort.

In the future, the NORS service for user group U4 will be reconsidered.

Individual users belonging to these four user groups may be given different authorization. These authorization levels will coincide with the different use cases discussed in Section 9. We distinguish 4 authorization levels:

- UALL: Users who don't need authentication: they have access to the public areas of the NORS validation server site;
- UINT: Users who, after authentication, are authorized to request dedicated reports from the server (i.e. different from the reports created by default): e.g., time window, skill scores, request underlying and intermediate data, models, species, …
- UVIP: These users are authorized to submit GRIB formatted model files to the server and to request dedicated validation reports for these model data, and/or, to request validation reports using alternative reference data that they submit in the GEOMS HDF format.
- UAD: Admin users are allowed to configure the NORS server

(UR1) Authentication of the users is done by username/password. The users list is maintained by admin users UAD. Users that must provide a valid email (for the delivery of validation data). Users may change their password (the username is the users email address).

5. Description of NORS products

NORS data are available from the NDACC Data Host Facility database, in GEOMS compliant HDF format, and adhering to a template that is specific per type of instrument, accounting for the various parameters deduced from each technique. They further include relevant ancillary parameters needed to thoroughly and precisely describe the measurement conditions and performances. The templates will be defined in the NORS deliverable D4.1 and will be available also from the AVDC Website (see http://avdc.gsfc.nasa.gov/index.php?site=1178067684).
It has been agreed with the NORS data providers and the NDACC database managers that the affiliation with NORS will be mentioned in the rapid delivery data files, in the FILE_ASSOCIATION global attribute, and that the global DATA_QUALITY attribute will be used to document the data quality associated with the rapid delivery data. Updates of the data file (e.g when the data have been consolidated) will be reflected in the file version number and in the DATA_FILE_VERSION and DATA_QUALITY attributes. If the global attribute DATA_QUALITY in the NORS data file is an empty string, the NDACC database should reject it
The file granularity will differ per site and per instrument.

Hereafter, we use the entries from the GEOMS Table Attribute Value file (TAV, http://avdc.gsfc.nasa.gov/PDF/tableattrvalue_04R004_idl.dat) to identify the different NORS products.

The list of sites

The NORS pilot stations are

(L1) Ile de La Réunion (21°S, 55°E, BIRA-IASB, CNRS.LATMOS) LA.REUNION
(L2) Ny-Ålesund (79°N, 12°E, IUP) NY.ALESUND

(L3) Alps, Bern (47°N; 7°E, UBERN) BERN
(L4) Alps, Jungfraujoch (47°N, 8°E, BIRA-IASB, ULG) JUNGFRAUJOCH
(L5) Obs. de Haute-Provence (44°N, 6°E, CNRS.LATMOS) HAUTE.PROVENCE
(L6) Izaña (28°N, 16°W, INTA, FZK). IZANA

The list of instruments

The ground-based remote sensing techniques are

(I1) Differential Optical Absorption Spectroscopy UVVIS.DOAS
(I2) Multi AXis Differential Optical Absorption Spectroscopy UVVIS.DOAS
(I3) Fourier Transform Infrared Spectroscopy FTIR
(I4) Differential absorption O_3 LIDAR LIDAR
(I5) Microwave radiometry O_3 MWR

The list of NORS products

For reasons of consistency, we use the structure of the filenames in the GEOMS format to indicate NORS products. The NORS products are labelled as a.b_c_d(x), in which

- a=instrument
- b=molecule or aerosol extinction (O3, NO2, H2CO, CO, CH4, AEROSOL)
- c=affiliation
- d=site location
- x=the physical quantity contained in the file: P=vertical profile, C=total column, D=total optical depth

E.g. FTIR.O3_BIRA-IASB_LA.REUNION(P) refers to a NORS product that consists of O_3 profiles from an FTIR measurement carried out by BIRA-IASB at La Réunion. In this case P stands for the data variable O3.MIXING.RATIO_ABSORPTION.SOLAR or O3.COLUMN.PARTIAL_ABSORPTION.SOLAR in the GEOMS file.

Notice that in the GEOMS filenames, the affiliation is followed by a number to indicate the individual instrument: this number has been omitted here.

In the list below we explicitly mention the name of the data variables in the GEOMS hdf files containing the profile, column or optical depth information.

The NORS products are:

- O_3 vertical profile in the stratosphere from LIDAR measurements (10-50km)
  P =O3.MIXING.RATIO_DERIVED
  P= O3.COLUMN.PARTIAL_DERIVED
  (P1) LIDAR.O3_CNRS.LATMOS_HAUTE.PROVENCE(P)
  (P2) LIDAR.O3_UREUNION.LPA_LA.REUNION(P)
- O_3 vertical profile in the stratosphere-mesosphere from microwave radiometers (20-70km)
  P=O3.MIXING.RATIO_EMISSION
  (P3) MWR.O3_UBERN_BERN(P)
  (P4) MWR.O3_IUP_NY.ALESUND(P)
- O_3 vertical profile and total column from FTIR solar absorption observations
  P=O3.MIXING.RATIO_ABSORPTION.SOLAR
  P=O3.COLUMN.PARTIAL_ABSORPTION.SOLAR

C=O3.COLUMN_ABSORPTION.SOLAR
(P5) FTIR.O3_BIRA-IASB_LA.REUNION(P,C)
(P6) FTIR.O3_FZK_IZANA(P,C)
(P7) FTIR.O3_IUP_NY.ALESUND(P,C)
(P8) FTIR.O3_ULG_JUNGFRAUJOCH(P,C)

- CO vertical profile and total column from FTIR solar absorption observations
  P=CO.MIXING.RATIO_ABSORPTION.SOLAR
  P=CO.COLUMN.PARTIAL_ABSORPTION.SOLAR
  C=CO.COLUMN_ABSORPTION.SOLAR
  (P9) FTIR.CO_BIRA-IASB_LA.REUNION(P,C)
  (P10) FTIR.CO_FZK_ IZANA(P,C)
  (P11) FTIR.CO_IUP_NY.ALESUND(P,C)
  (P12) FTIR.CO_ULG_JUNGFRAUJOCH(P,C)
- CH_4 vertical profile and total column from FTIR solar absorption observations
  P=CH4.MIXING.RATIO_ABSORPTION.SOLAR
  P=CH4.COLUMN.PARTIAL_ABSORPTION.SOLAR
  C=CH4.COLUMN_ABSORPTION.SOLAR
  (P13) FTIR.CH4_BIRA-IASB_LA.REUNION(P,C)
  (P14) FTIR.CH4_FZK_IZANA(P,C)
  (P15) FTIR.CH4_IUP_NY.ALESUND(P,C)
  (P16) FTIR.CH4_ULG_JUNGFRAUJOCH(P,C)
- O_3 total columns from SAOZ/DOAS and MAXDOAS observations C=O3.COLUMN.STRATOSPHERIC_SCATTER.SOLAR.ZENITH
  (P17) UVVIS.DOAS.O3_BIRA-IASB_JUNGFRAUJOCH(C)
  (P18) UVVIS.DOAS.O3_CNRS.LATMOS_HAUTE.PROVENCE(C)
  (P19) UVVIS.DOAS.O3_CNRS.LATMOS_LA.REUNION(C)
  (P20) UVVIS.DOAS.O3_INTA_IZANA(C)
  (P21) UVVIS.DOAS.O3_IUP_NY.ALESUND(C)
- NO_2 stratospheric columns from SAOZ/DOAS and MAXDOAS observations
  C=NO2. COLUMN.STRATOSPHERIC_SCATTER.SOLAR.ZENITH
  (P22) UVVIS.DOAS.NO2_BIRA-IASB_JUNGFRAUJOCH(C)
  (P23) UVVIS.DOAS.NO2_CNRS.LATMOS_HAUTE.PROVENCE(C)
  (P24) UVVIS.DOAS.NO2_CNRS.LATMOS_LA.REUNION(C)
  (P25) UVVIS.DOAS.NO2_INTA_IZANA(C)
  (P26) UVVIS.DOAS.NO2_IUP_NY.ALESUND(C)
- NO_2 stratospheric profiles from SAOZ/DOAS observations[1]
  P=NO2.MIXING.RATIO_SCATTER.SOLAR.ZENITH
  P=NO2.COLUMN.PARTIAL_SCATTER.SOLAR.ZENITH
  (P27) UVVIS.DOAS.NO2_BIRA-IASB_JUNGFRAUJOCH(P)
- NO_2 tropospheric columns from SAOZ/DOAS observations
  C=NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.ZENITH
  (P28) UVVIS.DOAS.NO2_BIRA-IASB_ JUNGFRAUJOCH(C)
  (P29) UVVIS.DOAS.NO2_CNRS.LATMOS_HAUTE.PROVENCE(C)
  (P30) UVVIS.DOAS.NO2_CNRS.LATMOS_LA.REUNION(C)

[1] The inclusion of this NORS product in the validation server is not decided yet. At this moment it is measured only at Jungfraujoch, and this will most likely not change.

- NO_2 vertical profile and columns in the lower troposphere from MAXDOAS observations
  P=NO2.MIXING.RATIO_SCATTER.SOLAR.OFFAXIS
  P=NO2.COLUMN.PARTIAL_SCATTER.SOLAR.OFFAXIS
  C=NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS
  (P31) UVVIS.DOAS.NO2_BIRA-IASB_JUNGFRAUJOCH(P,C)
  (P32) UVVIS.DOAS.NO2_INTA_IZANA(P,C)
  (P33) UVVIS.DOAS.NO2_IUP_NY.ALESUND(P,C)
- H2CO total column from MAXDOAS observations
  C=H2CO.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS
  (P34) UVVIS.DOAS.H2CO_BIRA-IASB_JUNGFRAUJOCH(C)
  (P35) UVVIS.DOAS.H2CO_INTA_IZANA(C)
  (P36) UVVIS.DOAS.H2CO_IUP_NY.ALESUND(C)
- Aerosol extinction profiles at 360 nm and 470 nm in the lower troposphere from MAXDOAS observations
  P=AEROSOL.EXTINCTION.COEFFICIENT_SCATTER.SOLAR.OFFAXIS
  D=AEROSOL.OPTICAL.DEPTH.TROPOSPERIC_SCATTER.SOLAR.OFFAXIS
  (P37) UVVIS.DOAS.AEROSOL_BIRA-IASB_JUNGFRAUJOCH(P,D)
  (P38) UVVIS.DOAS.AEROSOL_INTA_IZANA(P,D)
  (P39) UVVIS.DOAS.AEROSOL_IUP_NY.ALESUND(P,D)
- O_3 integrated profile data product (vertical profiles from ground to upper stratosphere) developed in the NORS project (WP6).
  (P40) ID to be defined

In some cases, the total columns are not explicitly provided in the data file with the vertical profiles: in these cases, the server computes these derived products from the profile products (cf (UR13) page 16).

Table 1 Overview of NORS products and instruments (NO_2 stratospheric profiles are omitted)

Instruments	Species	Affiliation	Locations
UVVIS.DOAS	O3.C (strato) NO2.C (strato) NO2.C (tropo)	CNRS.LATMOS	HAUTE.PROVENCE
			LA.REUNION
		BIRA-IASB	JUNGFRAUJOCH
UVVIS.DOAS (MAXDOAS)	O3.C (strato) NO2.C (strato) NO2.(P,C) (tropo) H2CO.C AEROSOL.(P,D) (tropo)	BIRA-IASB	JUNGFRAUJOCH
		INTA	IZANA
		IUP	NY.ALESUND
FTIR	O3.(P,C) CO.(P,C) CH4.(P,C)	BIRA-IASB	LA.REUNION
		FZK	IZANA
		IUP	NY.ALESUND
		ULG	JUNGFRAUJOCH
LIDAR	O3.P (strato)	CNRS.LATMOS	HAUTE.PROVENCE
		UREUNION.LPA	LA.REUNION
MWR	O3.P (strato)	UBERN	BERN
		IUP	NY.ALESUND

The NORS products will be uploaded to the NDACC database at the latest one month after data acquisition. The frequency of upload will depend on the site and on the instrument.

(UR2) The global attribute DATA_QUALITY in the NORS data file should mention that the data can be used for validation purposes. If this is not the case, the NORS server should ignore the NORS file[2].

(UR3) The validation server should be designed in such a way new NORS products can be added to the list. The freedom for the admin user UAD to add NORS products is limited to the affiliation and location field: e.g. FTIR.O3_*_*.

6. Description of the MACC-II models

General information about the MACC-II products can be found in the Products portfolio [1]. The MACC-II models include different setups of the coupled models IFS-MOZART and IFS-TM5, with IFS the Integrated Forecasting System of ECMWF (European Centre for Medium Range Weather Forecasting), and MOZART and TM5 two independent chemical transport models. It includes an operational (o-) and an experimental (e-) suite of the IFS-MOZART analysis, a forecast (FC) using the IFS-MOZART and the IFS-TM5 coupled model runs, as well as a long-term reanalysis (REA) by IFS-MOZART, i.e.

(M1) IFS-MOZ AN o-suite (f93i)
(M2) IFS-MOZ AN e-suite (fnyp)
(M3) IFS-MOZ FC (fkya)
(M4) IFS-TM5 FC (fl52)
(M5) IFS-MOZ REA (rean)
(M6) NN (fndl)

In this list, the identifier between parentheses corresponds to the MACC-II model id. This is an internal identifier in the MACC-II project. Only the o-suite and REA will be official MACC products. The e-suite is used for testing of new developments and the two FC (forecast) experiments, which currently still provide output to users, will become less important for users once we are running with an official AN/FC o-suite.

(UR4) The admin user UAD should have a flexible interface to the MARS archive for the MACC-II models, in particular the experimental models.

The following table indicates which of the above described models deliver MACC II products (e.g. O_3 profiles) on a 3-dimensional global grid (i.e. basically vertical profiles) for the NORS target species:

- O_3 M1-M5
- NO_2 (this still needs to be made available in the MARS archive) M1-M5
- CO M1-M5
- H2CO M1-M5
- AEROSOL M1,2,5
- CH4 M5-M6

(UR5) All MACC-II products in the corresponding models in the above table should be validated

MACC-II data for all models will be retrieved as 6-hourly snapshot files from the ECMWF MARS archive in GRIB-2 format. Data will be retrieved on a regular Gaussian grid, as written by the IFS system. In a later stage, data converted to the HDF file format on a regular

[2] NORS members will provide naming principles for this quality attribute.

lat/lon grid could be provided. The vertical grid corresponds to the 60 ECMWF vertical model levels. A typical 4-species global 6-hourly dataset takes 200 Mb/day, when provided on a regular Gaussian grid (i.e. +/- 75 Gb/year). In the MARS archive a product can be identified by means of a number or a string label (i.e. the O3 profile is identified with number 203.210 and is labelled as GO3). These MARS numbers are required for the data retrieval from the MARS archive[3].

Similar to the NORS products, we indicate here a MACC product in a model using labels: e.g. M1_O3(P) refers to the vertical ozone profile in the first MACC model. The table below shows how MACC and NORS products should be related.

Table 2 MACC-II products and corresponding MARS labels and NORS products

MACC II products	MARS labels: shortname and number		NORS products
*_O3(P)	GO3	203.210	*.O3_*_*(P)
*_NO2(P)	NN	NN	*.NO2_*_*(P)
*_CO(P)	CO	123.210	*.CO_*_*(P)
*_H2CO(P)	HCHO	124.210	*.H2CO_*_*(P)
*_CH4(P)	CH4	62.210	*.CH4_*_*(P)
*_AEROSOL(P)	aergn04	19.210	*.AEROSOL_*_*(P)

A similar correspondence can be set up for total columns or total optical depths. In this case, however, the total columns will not be extracted from the MARS archive directly. The MACC total optical depth or column will be derived from the corresponding MACC profile products, where we take into account the averaging kernels of the measurements (see also Section 7.3 on smoothing and regridding).

7. The Validation Chain

Throughout this section we assume that

1. a time window is fixed
2. a choice of NORS products and MACC-II models has been made

How and by whom these settings will be fixed is described in Sections 8 and 9.

Notice that we will allow alternative model data to be validated, and alternative reference data for the validation, within certain restrictions, as indicated in Section 4 and discussed further in Section 9. For simplicity, we continue to refer to "NORS" data when talking about the reference data, and to "MACC-II" data when talking about the model data to be validated.

7.1. Input of the validation chain: pre-processing

Ingestion, selection, and extraction of data sets

Ingestion of data

[3] a list of these numbers/labels can be found on http://www.ecmwf.int/publications/manuals/d/gribapi/param/filter=grib1/order=paramId/order_type=asc/p=1/table=210

In a first step, the system checks that the NORS data is in GEOMS format and the model data in GRIB format. This format check should only be performed when the data are submitted by the user, not when they come from the NDACC database or from the MARS archive, because then the format check will have been carried out by the managers of the archive.

The server collects all available measurements of the selected NORS product within the given time window. Similarly, it identifies all available MACC-II outputs that lie within the time window.

Selection of temporally co-located data

(UR6) For each NORS product, except the NO_2 stratospheric profiles and total columns[4], a characteristic *n*-hours time interval is defined which is smaller than or equal to the *m*-hours time interval between MACC-II outputs (*m* is typically equal to 6).

The parameter *n* will depend on the temporal/spatial variability of the species in the NORS product. For example, for CH_4, CO and O_3 in the stratosphere, *n* will be chosen equal to *m*, indicating that the maximum time difference between the model and the NORS observation is *m/2* hours. For tropospheric NO_2, *n* might be equal to 1. Therefore *n* determines the temporal colocation between the MACC-II and the NORS data. The exact choice of *n* for each NORS product in the default validation chain will be decided as soon as possible by the NORS partners.

(UR7) UAD should be able to change *n* for each NORS product, and depending on the frequency of the MACC-II model output (*m*).

(UR8) A NORS measurement should only be compared to MACC-II model data within this time interval.

(UR9) No further filtering for quality of the NORS data is required.

Therefore, as a preliminary step in the validation chain, we assume that the server sorts the measurements according to this rule (i.e. NORS measurements outside of the defined time interval are considered too far away in time from the MACC-II model data time and are discarded).

Summarizing:

- the selected NORS products measurements determine a data stream, denoted by B, with indices determined by the measurement times
- for each NORS measurement there is a corresponding MACC-II model data output (which will determine the data stream A as explained further below).

Extraction of secondary data from NORS files[5]

For all gas concentration profiles and total columns *.(O_3,CH_4,H2CO, CO, NO2)_*_*

- The T/P profiles and relative humidity are needed for unit conversions (volume mixing ratio (VMR) to number densities or columns)
- The averaging kernels and a priori profiles and/or columns that are provided in the data files[6]

[4] The pre-processing for the stratospheric NO_2 profiles and total columns is special in the temporal colocation aspect and this is dealt with in Section 7.2

[5] The two lists below may not be complete. This will be updated.

For aerosol extinction profiles *.AEROSOL_*_*

- The T/P profiles and relative humidity are needed for unit conversions
- The averaging kernels and a priori profiles and apriori optical depth that are provided in the data files

Extraction of spatially co-located model data

(UR10) For the spatial co-location, the co-location target associated with each NORS measurement (data point) should be the location of the effective airmass associated with that measurement.

We assume that the location is reduced to a single point in space/time, not an area nor a volume. The approximation will be made that the location of the effective airmass for a column measurement is a point defined by a latitude and longitude, and that the (latitude, longitude) location of a vertical profile is the same at all altitudes in the profile.

For each data product (which is measured off-zenith), the corresponding NDACC working groups will deliver the pseudo-code to calculate the location of the effective airmass corresponding to a measurement (data point), and the appropriate description (e.g., a peer reviewed publication) of the method used to calculate the effective air mass (for the sake of traceability). It must be ensured that all parameters needed in these calculations are available in the NORS data files. In case the working groups cannot (yet) deliver the method to calculate the effective airmass, the server will use the location of the instrument as the co-location target.

(UR11) The design of the server S/W should be such that it is easy for a S/W engineer to implement or update for a given NORS product a code for the calculation of an effective airmass that differs from the location of the instrument, once this code is provided by the NORS consortium. The validation server should then use this calculation for co-locating the MACC-II output.

According to Sections 5 and 6 and the above, every sorted (derived) NORS product data point determines, per MACC-II model (Mi), one associated MACC-II output, and from this output, an associated MACC-II extraction, as follows:

If the data stream B is determined from a NORS product with label

.(O_3, CH_4, HCHO, NO_2)_*_, then the concentration profiles[7] at the four closest grid points in the model output surrounding the effective airmass location should be extracted (i.e. 4 extractions).

.AEROSOL_*_, then the extinction profile and the total optical depth at 532nm, and the total optical depth at the wavelength of the measurement (360nm or/and 469nm) at the four closest grid points in the model data surrounding the sites location should be

[6] for LIDAR.O3 these are not required and therefore are not available in the datafiles – see more in Section 7.3

[7] Even if MACC-II provides column data, we cannot use these because then it is impossible to do the smoothing as requested in Section 7.3. So it doesn't make sense to extract columns from the MACC-II data.7.3

extracted (i.e. 3x4 extractions). If a measurement contains data for different wavelengths, only the measurement at the wavelength closest to 532 nm should be used for validation.

For each NORS product in data stream B, the associated MACC-II profile/column to compare with is then obtained via bilinear interpolation of the 4 associated nearest neighbour points in the MACC-II output.

Align compared parameters

In this step the necessary unit conversions on the modeled data is performed, i.e. during the next phase of WP8 and before the start of the test-phase of the server, the NORS members will provide

- a default unit per NORS product (and conversion methods if user are allowed to choose between different units in the output)
- provide pseudo-code to compute the derived products (profile → total column/total AOD)
- a default vertical unit (pressure/height) and pseudo-code for the conversion between pressure or height as a vertical coordinate.

(UR12) The server allows an easy interface for UAD to change the default units for the different products and height coordinate in the default output (cf. Section 8).

(UR13) If derived products (like total column of total optical depth) are not available in the NORS data or MACC-II data, then the server is responsible for calculating these derived quantities if profile information is available from the NORS data or MACC-II data, respectively.

How to align aerosol extinction data for different wavelengths is described in Section 7.3

Final status after pre-processing

As such, at the end of the pre-processing chain, for each NORS product and each MACC-II model, we end up with a data stream A (MACC-II) and a data stream B (NORS), with an identical number of spatially and temporally co-located data points in each stream, identified via a time index corresponding to the measurement time of the NORS products in data stream B.

7.2. Temporal alignment

For O3, CH4,CO, H2CO, and tropospheric NO2 concentration profiles and total columns
.(O3,CH4, CO, H2CO, NO2 (tropo))_*_

For each NORS measurement technique[8], all NORS data points in the *n*-hours interval are compared with the corresponding MACC-II data point without accounting for the individual time difference between the NORS and the MACC-II data point. In other words, every data

[8] At present, there is only one NORS measurement technique for each product, except for O_3 which is provided by several techniques – see Table 1.

point in data stream A is compared as such with every corresponding (same index) data point in stream B.[9]

For stratospheric NO_2 concentration profiles and columns and total columns

.NO_2 (strato)_*_

In the case of stratospheric NO_2 columns, the diurnal variation is important and it is not appropriate to compare the MACC-II output with all the NORS data points in a characteristic time interval, without accounting for the time difference between the NORS data point and the MACC-II data point. But the diurnal variation is sufficiently well known that one can correct the MACC-II data for their time difference with respect to the NORS measurements. Therefore, in the case of stratospheric NO_2 vertical profiles and stratospheric or total columns, NORS morning (evening) measurements will be compared to the closest MACC-II output in the future (past) of the measurement, and the time correction will be carried out as follows.
For DOAS NO_2 total columns and stratospheric profiles, the photochemical conversion from the MACC-II time to the time of the observation (NORS measurements local time), will be done using a climatology of stratospheric NO_2 vertical profile diurnal variations calculated using the BIRA-IASB stacked box photochemical model PSCBOX initialized with SLIMCAT 3D-CTM meteorological (pressure and temperature) and chemical fields. The conversion of MACC-II stratospheric NO_2 vertical profiles and columns to NORS measurements local time is done as follows:

$$x_M(t_m) = x_M(t_m + \Delta)\left(\frac{x_{LUT}(t_m)}{x_{LUT}(t_m + \Delta)}\right)$$

- with t_m the time of the measurement (for a DOAS observation this is either sunrise or sunset), $t_m + \Delta$ is the closest time for which MACC-II model data is available (note: for morning measurement: $n > \Delta \geq 0$, for evening measurement: $-n < \Delta \leq 0$). n is a characteristic time (we take $n = m/2$, i.e. if MACC data is retrieved at 6h intervals, $n = 3$h,
- x is a NO_2 vertical column density or concentration [NO_2] at altitude z,
- $\left(\frac{x_{LUT}(t_m)}{x_{LUT}(t_m + \Delta)}\right)$ is the scaling factor needed for the conversion and calculated from the modeled stratospheric NO_2 vertical profile diurnal variations. This scaling factor will be determined from the LUT's (Look Up Tables).

Model calculations of NO_2 diurnal variations are performed for the following scenarios: altitude (24 levels between ~8 and 60 km), latitude (18 values covering 85°N→85°S by 10° step), longitude set to 0, months 1-12 (for each month, the initial chemical fields and pressure and temperature profiles are the SLIMCAT data corresponding to the middle of the month averaged over a period of 10 years (2000-2009)). The stratospheric NO_2 diurnal variation will be in ASCII format. An interpolation routine will be created in Fortran 77 in order to extract MACC-II to NORS scaling factor for a given station, MACC-II local time $t_m + \Delta$, and NORS DOAS measurement local time t_m. The scaling factor extractor will be implemented

[9] The case for upper strato/mesospheric O3 needs to be discussed.

in the automatic validation chain. For polar regions in late fall, winter, early spring, sensitivity tests have shown that additional LUTs are needed for denoxification conditions: the use of mean chemical fields and temperature profiles instead of daily data to initialize the photochemical model can lead to an overestimation by up to 20% of the scaling factor. The choice of LUTs will be based on the measured NO_2 columns: below a threshold value depending on the station, the LUTs corresponding to denoxification conditions will be selected in the extraction routine.

(UR14) The NORS validation server should be designed such that it is an easy task for a S/W engineer to update the system when new instruments/products are added to the NORS database. For example, when FTIR stratospheric NO_2 data become available, a procedure similar to the one described above for the DOAS stratospheric NO_2 data will be applied.

For Aerosol extinction profiles *.AEROSOL_*_*

For now, the co-location target is the location of the instrument. It is assumed also that MAX-DOAS observations in an *n*-hours time interval centred around the MACC-II output time will be compared to the MACC-II model output, with *n* to be defined by the MAXDOAS partners.

7.3. Vertical regridding and smoothing

For further details we refer to [7]. Whenever averaging kernels are mentioned, we always refer to vertical averaging kernels.
The concept and application of averaging kernels is typical of passive remote sensing instruments. For active remote sensing instruments like the O_3 LIDAR, averaging kernels are not relevant. Therefore in LIDAR.O3_*_* no averaging kernel is available and smoothing should not be performed.

- Total column comparisons[10]: *.(O_3, CH_4, CO, H2CO, NO2)_*_*(C)
  If the target is a total column, with an associated total column averaging kernel, then the corresponding MACC-II profile (corresponding to the effective location of the NORS column) should (1) first be regridded to the vertical grid of the NORS profile, and (2) be smoothed according to the formula $C_s = C_a + A_C^T(x - x_a)$ in which C_a and x_a are the a priori column and profile of the reference NORS data, respectively, x is the MACC-II vertical profile and A_C^T is the NORS product's averaging kernel vector in column units. The smoothed MACC-II total column C_s is the one to be compared to the NORS column as this procedure reduces discrepancies due to the difference in vertical smoothing and resolution between the model output and the measurement. The situation where the NORS data does not provide apriori information (e.g. in UVVIS.DOAS measurements), the server will determine the apriori profile and column[11].

[10] Some users (including MACC-II data providers in some cases) are most interested in having information about the quality of the total column output.
[11] The description of how the server determines this apriori information will be provided by the NORS members.

- Profile comparisons: *.(O_3, CH_4, CO, H2CO, NO2)_*_*(P)
  If the target is a vertical profile, then (1) the MACC-II profile x must be regridded to the vertical grid of the NORS profile, and (2) smoothed with the NORS profile averaging kernel matrix A, according to the equation $x_s = x_a + A(x - x_a)$.

- Partial column comparisons: *.(O_3,CH_4,CO, H2CO,NO2)_*_*(P)
  When the number of degrees of freedom for signal (DOF, obtained as the trace of A) of the NORS reference profile is relatively small (≤5), it doesn't make sense to compare the profiles gridpoint-wise. In such cases, one defines partial column boundaries, in between which there is about one DOF, and one compares the partial columns between these boundaries.
  For each NORS product Pn, the partial column boundaries will be fixed by the PI. The same settings will apply to all instances of that product. The partial columns are obtained by integrating the (smoothed) profile (in partial column units)) between the boundaries.

(UR15) UAD must be able to set/change the partial column boundaries to be used in the default use case, for each NORS product (Pj); the settings will apply to all instances of (Pj).

- Comparison of aerosol extinction profiles: *.AEROSOL_*_*(P)
  The first step is to convert to a common extinction wavelength between the two datasets to be compared. This is done by scaling the MACC profile at 532nm to the wavelength of the measurement. The scaling factor is determined as the ratio of the MACC total optical depth at 532nm and the MACC total optical depth closest to the measurement wavelength (these wavelengths are extracted from the models: 360nm or 470nm). The UVVIS NDACC working group will decide on the vertical grid that should be used to compare extinction profiles. The smoothing of the profiles is performed using the averaging kernel and the apriori profile from the NORS data as before.

(UR16) UAD must be able to set/change the vertical grid for the comparison of aerosol extinction profiles

- Regridding to a common vertical grid
  In practice, every instrument/site will report data on its own vertical grid. Following the above procedure, we end up with comparison pairs on different vertical grids. As soon as the number of instruments/sites grows, it becomes interesting to make some statistics and to draw more general conclusions. For example, one may want to consider all comparisons for a given target species within some given latitude band and draw statistically valid conclusions for that latitude band. This requires having all data on a common vertical grid.
  To this end, it is useful to define a common grid, e.g. a grid equidistant in pressure and to convert the (possibly smoothed) MACC-II data and the NORS data to this common grid.

(UR17) UAD must be able to set/change the common vertical grid for enabling more extensive statistical evaluations

- Error propagation
  Concerning the measurement data, error propagation should be considered when the measurement is smoothed and or re-gridded to the standardized grid (or a customized grid). The procedures hereto will be delivered by the NORS partners.

8. Description of the output of the validation server

The validation server generates validation output either of default nature or upon request by a user of type UINT. In this section we describe the possible outputs the validation server should be able to generate. The actual output may differ per use case (see Section 9)

Recall that the data stream for a specific NORS product is denoted by a capital letter B, i.e. B^{P23} is the data stream for NORS product (P23) and carries an index representing the measurement time. If we do not wish to mention explicitly the NORS product, we simply write B. Data stream B might also be a quantity derived from a NORS product (e.g. the total O_3 column derived from an O_3 profile). The validation server will compare the datastream B^{P23} with extracted and modified/aligned/smoothed data from a MACC-II model data stream denoted by $A^{(M1,P23)}$. The creation of the latter data stream is described in Section 7. The data stream A carries the same index as data stream B. I.e., the extracted MACC-II model data points in data stream A have the same indices as the corresponding data points from data stream B with which they are compared. So for example, if the characteristic interval for comparison of the CH_4 FTIR data product is a 6-hours interval, then for each FTIR data point in that window, the time index of the FTIR data B_i is also attached to the associated MACC-II model data, for ease of identification of the correspondences.

The description below assumes that the validation covers a certain time window (e.g., 3 months), i.e. for each NORS product data stream B_i, i=1,…,N, the number N represents the number of measurements incident within the given time window.

8.1. Outputs

8.1.1. Statistics over the given time interval

(UR18) The MACC-II VAL scoring ([2],[3]) contains all statistical quantities that should be implemented.

(S1) Mean bias
(S2) Root mean square error
(S3) Modified normalized mean bias
(S4) Fractional gross error
(S5) Correlation coefficient (only if $N \geq 10$)
(S6) Spearman rank correlation coefficient (only if $N \geq 10$)
(S7) Relative mean bias

The notations used in the scoring document should be mapped onto our notations as follows: $f = A^{(M1,P2)}$ and $o = B^{P2}$. Such a relation is applicable to any MACC-II model and NORS product.

Statistics must be made per NORS product (species/instrument/site, cf. Section 5) and MACC-II model (cf. Section 6).

8.1.2. Plots

(UR19) In addition to the statistical quantities, the system creates plots. All plots allow colours. Apart from plotting w.r.t measurement time, the server also allows plots for which a finest time unit is given (e.g., seasons DJF, MAM, JJA, SON within a validation plot over a total time interval of one year cf. [3], p20). The data plotted is then the average over the finest unit (i.e. the average of all biases for all measurements in a season).

For scalar NORS products (and derivations)

- (S8) A plot of the individual data streams, i.e. the NORS product or the MACC product (or derivatives) vs. measurement time/index;
- (S9) A combination of plots of (S8) for different models
- (S10) Bias vs measurement time, i.e. a plot of $(i, f_i - o_i)$
- (S11) Relative bias vs measurement time, i.e. . a plot of $\left(i, {2(f_i - o_i)}/{(f_i + o_i)}\right)$
- (S12) Plots containing several plots of type (S10) or (S11), i.e. combinations of bias plots for different models. E.g. plots of (S11) for product (P5) FTIR O_3 profile at LA.REUNION validated against all models (M1,2,3,4,5) for which O_3 is available.
- (S13) Modified normalized mean bias vs measurement time
- (S14) Plots containing several plots of type (S13), i.e. combinations of modified normalized bias plots for different models.
- (S15) Taylor diagram where one model is compared with different sites for a given species cf. [3], p22.

For profile NORS products

- (S16) Plot of the mean model profile with the RMS vector indicated as error bars on it (see also [3], p18:fig 5.1.2)
- (S17) Combination of plots of type (S16) for different models in which the NORS product appears
- (S18) Mosaic plots of the model or measurement profile, time vs altitude, where the vmr's or concentration values are indicated by a colour code.

(UR20) All plots should contain
- a clear indication of the physical quantity that is plotted with its unit,
- the identification of the NORS products (species, instrument, location, data provider) and the MACC-II models, including the data file version for both,
- a corresponding legend in the case of multiple plots in one figure.

8.1.3. Data

(UR21) The server produces for every validation process

- (D1) All the datastreams B^{P1} and associated model data streams $A^{(M1,P1)}$ used in the validation process (after smoothing/interpolations/regridding)
- (D2) When applied in the validation process, the averaging kernels and apriori profiles

8.1.4. Traceability output

(UR22) The server produces for every validation process

- (T1) The filenames of the NORS data used
- (T2) The MACC-II models experiment id's and that part of the changelog files of the MACC-II models that covers the time interval under consideration
- (T3) A detailed overview of the different steps executed in the validation process (i.e. including the toolset command lines used for the data manipulations)

8.2. Output formats

(UR23) The ouput format of the data produced by the server is described in the following list.

- (O1) (Dj) is in HDF format. The metadata should indicate
  - the units
  - the physical/mathematical quantity,
  - the data provider (both for NORS and MACC data),
  - the data creator (e.g., NORS validation server v1)
- (O2) (Sj<7) in text format
- (O3) (Sj>7) in pdf and png format.
- (O4) (Tj) in text format.

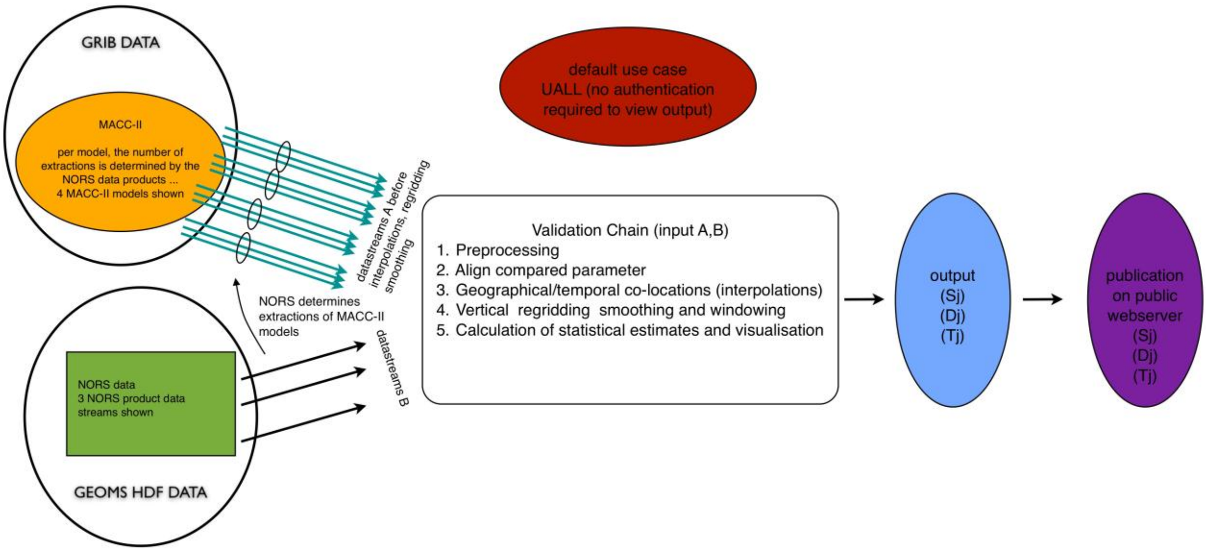
9. Description of use cases

In this section we describe the different use cases. The structure of each use case is:

1. Definition of the users group (and the corresponding authorization)
2. Description of the output
3. Description of the user interface on the web server
4. Description of data management

Each use case is presented with a schematic overview.

9.1. The default use case



9.1.1. User group: UALL

9.1.2. Output

Time windows for the default use case are:

Seasonal and monthly time windows

(UR24) For each scalar NORS product and MACC-II model in which the NORS product appears:
(S10) Bias vs measurement time (finest time unit=days)
(S11) Relative bias vs measurement time (finest time unit=days)
(S13) Modified normalized mean bias vs measurement time (finest time unit=days)
E.g. a plot of product (P5) FTIR O3 at LA.REUNION compared against (M1)

(UR25) For each profile NORS product and MACC-II model: (S16) Mean model profile plot and (S18) Mosaic plots

(UR26) For each MACC-II model: (S15) Taylor diagram

(UR27) Overlay plots of type (S12) for (S10) and (S11) (finest time unit=days)
Overlay plots of type (S14) for (S13) (finest time unit=days)
Overlay plots of type (S17) for (S16)
A fixed colour coding is used to distinguish between the models (cf [3]).

A moving time window of 3 months

(UR28) For each scalar NORS product and MACC-II model in which the NORS product appears:
(S10) Bias vs measurement time (finest time unit=days)
(S11) Relative bias vs measurement time (finest time unit=days)
(S13) Modified normalized mean bias vs measurement time (finest time unit=days)

(UR29) For each profile NORS product and MACC-II model: (S16) Mean model profile plot and (S18) Mosaic plots

(UR30) For each MACC-II model: (S15) Taylor diagram

(UR31) Overlay plots of type (S12) for (S10) and (S11) (finest time unit=days)
Overlay plots of type (S14) for (S13) (finest time unit=days)
Overlay plots of type (S17) for (S16)
A fixed colour coding is used to distinguish between the models (cf [3]).

9.1.3. User interface

(UR32) The user may choose among the different time windows, the different NORS products (determined by instrument/molecule/locations/affiliations), the MACC-II models. The web interface is interactive: if a user chooses an instrument/molecule/locations/affiliations and a MACC-II model, the web content adapts and shows all plots/results that fit the user’s choice. The user can select the final validation product and automatically downloads a zip file containing the statistics/plots along with the underlying data (Dj) and the traceability report (Tj).

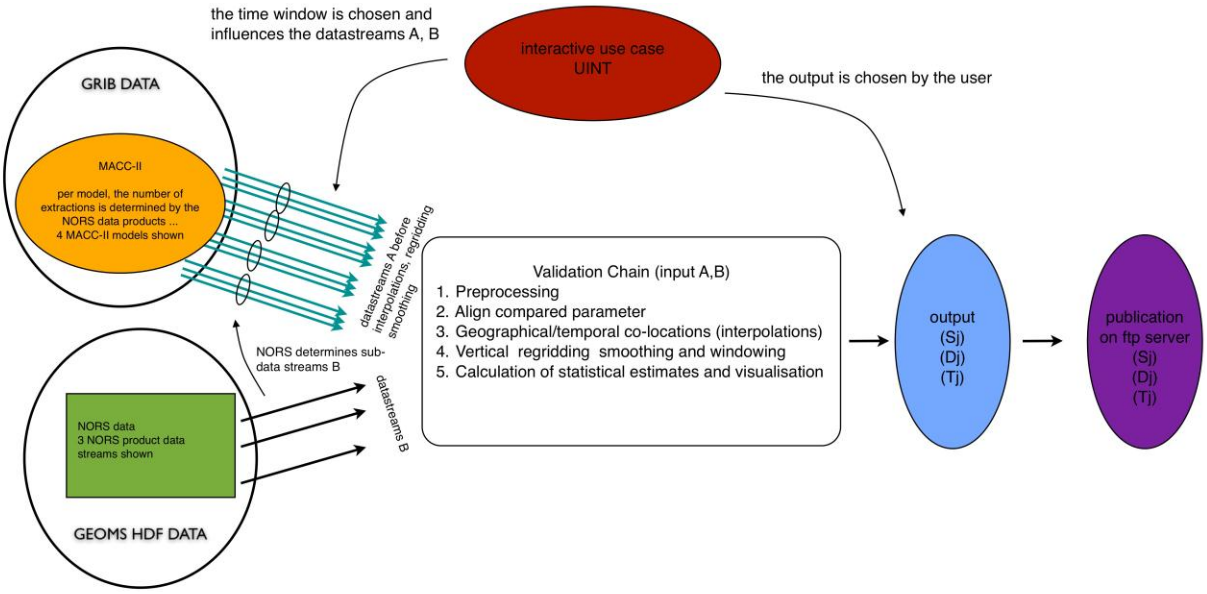
9.1.4. Data management

(UR33) All seasonal and monthly data should be stored permanently. The moving time window is updated daily and previous results are not stored.

(UR34) In case NORS data are updated, all seasonal and monthly plots and traceability reports based on these data should be regenerated. In the case MACC-II data is updated (e.g., if an output time is missing and added at a later stage) the server updates all monthly and seasonal plots and traceability reports based on this data. Only the most up-to-date version is available online.

9.2. The interactive use case

9.2.1. User group: UINT



9.2.2. Output

(UR35) The user may request all types of output data described in Section 8. The time unit in the plots can be chosen among presets: days, weeks, months, seasons.

9.2.3. User interface

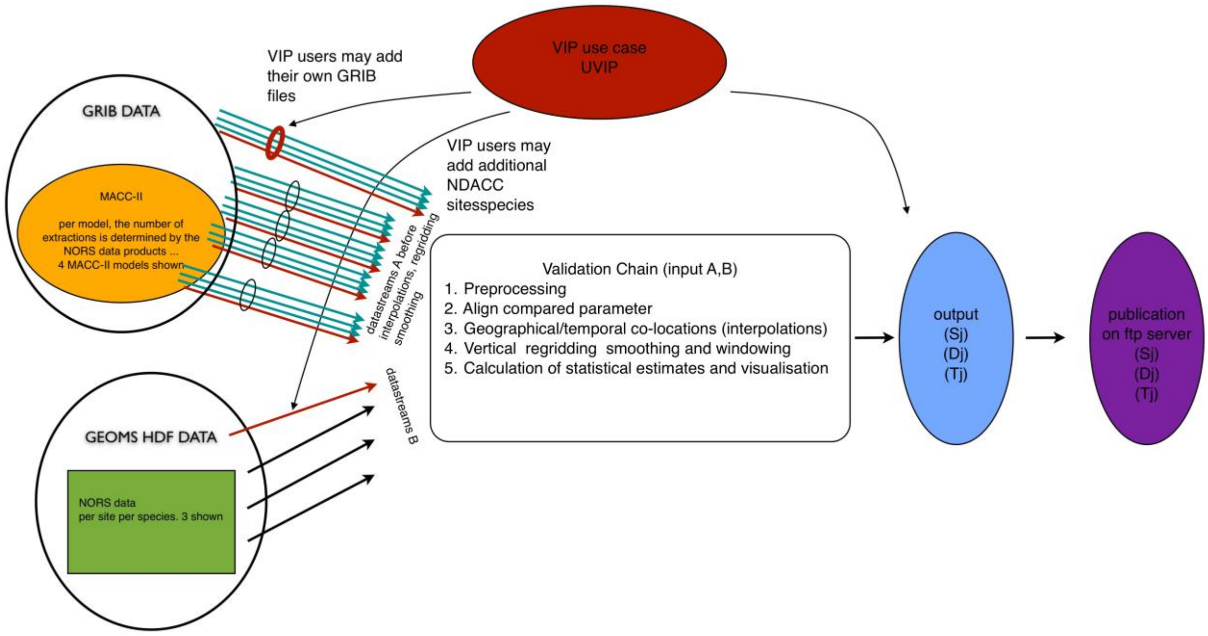
(UR36) After authentication the UINT member is redirected to a webpage on which he/she can chose among the different settings for the specific validation process that will be set up. In particular the user defines the NORS product, the MACC-II model, the desired output. In the definition of the time window, the user may choose the start and end date, or may choose among preset windows per month/seasons. After the validation process finishes, the user will receive a link to a zip file containing the requested data/plots.

(UR37) A scheduling option should be possible where the user requests that this configuration for a validation is performed weekly or monthly.

9.2.4. Data management

The file containing the results should not be stored permanently (i.e. it is available for 2 weeks on the ftp server)

9.3. The VIP use case



9.3.1. User group: UVIP

The UVIP is a subset of UINT.

9.3.2. Output

Same as in interactive use case

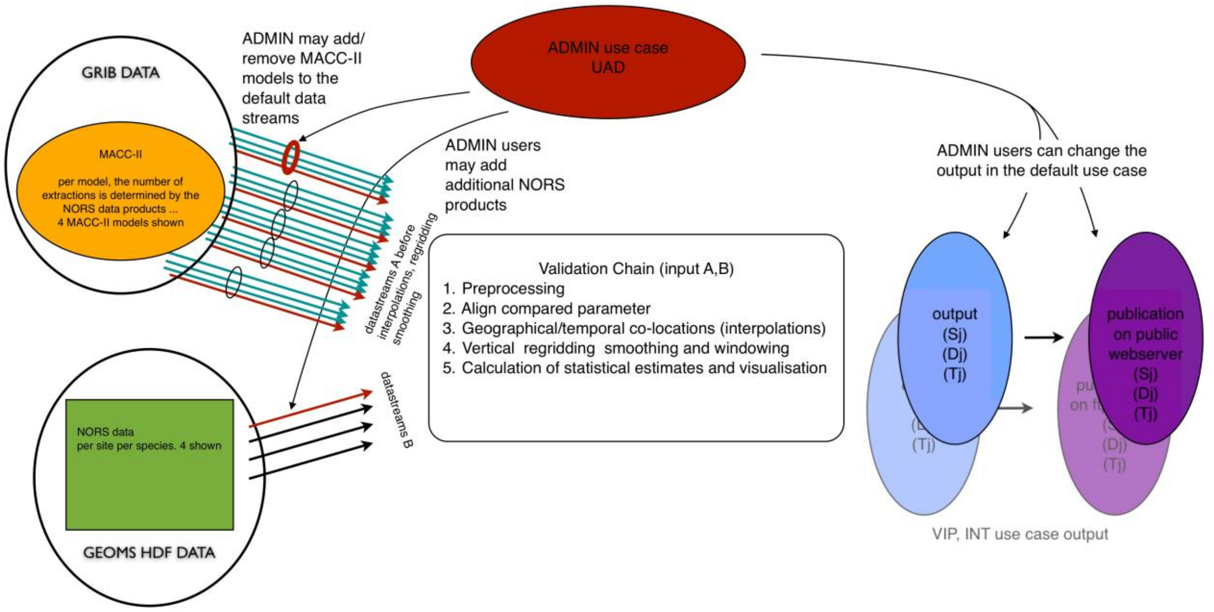
9.3.3. User interface

(UR38) The user interface slightly differs from the interactive case. A user is allowed to upload his own GRIB file(s) or provide the link(s) to an NDACC GEOMS compliant data file. There should be a compatibility check. The species of the NDACC file and the chosen time window should be compatible with the modelled species in the GRIB files. The menu structure should be adapted: the NORS product fields and model fields are enlarged to contain the extra NDACC and GRIB files.

9.3.4. Data management

Idem as 9.2.4

9.4. The administration use case



9.4.1. User group: UAD

9.4.2. Output

Not applicable

9.4.3. User interface

(UR39) He/she is able to adapt existing scripts to add/remove NORS products and MACC-II models.

(UR40) He/she can adapt the web menu structure to add/remove NORS products and MACC-II models.

(UR41) He/she can adapt the colour coding for the MACC-II models and modify the default output template.

9.4.4. Data management

Not applicable