RINGO | Readiness of ICOS

Readiness of ICOS for Necessities of integrated Global Observations

D1.5

Scientific and technical concept for the integration of ground-based greenhouse gas remote sensing into ICOS and resulting costs

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Deliverable Review Checklist

A list of checkpoints has been created to be ticked off by the Task Leader before finalizing the deliverable. These checkpoints are incorporated into the deliverable template where the Task Leader must tick off the list.

- Appearance is generally appealing and according to the RINGO template. Cover page has been updated according to the Deliverable details. √
- The executive summary is provided giving a short and to the point description of the deliverable. √
- All abbreviations are explained in a separate list √
- All references are listed in a concise list. √

The deliverable clearly identifies all contributions from partners and justifies the resources used. ☐

- A full spell check has been executed and is completed. √

DISCLAIMER

1. Executive summary

The goal of this document is to provide the scientific, technical and budget information for an integration into ICOS of the European part of the Total Carbon Column Observing Network (TCCON), a network of ground-based greenhouse gas remote sensing. The document addresses the concept, the requirements and the resources needed to integrate the European part of TCCON into ICOS. In particular, the scientific opportunity, the technical feasibility, and the resources needed are described.

The various components of an atmospheric observing system for greenhouse gases is presented in the general context part, covering in situ measurements (observatories, tall towers and AirCores) and remote sensing observations (ground-based solar absorption measurements, satellite). It shows how each measurement method measures a part of the atmosphere while being complementary and useful to the others. In particular, satellites can be calibrated against TCCON retrievals, and WMO standards can be transferred to satellite retrievals via TCCON measurements. TCCON plays a vital role for the validation of the satellite measurements, resolving spatial biases and/or temporal drifts in the satellite data.

TCCON is a network of 26 stations at the world scale, dedicated to the retrievals of column-averaged dry air mole fractions of CO_2, CH_4, N_2O, HF, CO, H_2O, and HDO. The data processing is currently made by individual groups, and the final QA/QC is performed at Caltech, USA, which maintains also the TCCON data archive. The data become publicly available no later than one year after the measurements are recorded. Europe contributes very significantly to TCCON: 12 out of the 26 TCCON sites are operated by European institutions, but many of the European sites rely on short-term research projects.

TCCON and in situ measurements are complementary. In contrast to the information of in situ measurements the TCCON data are independent of atmospheric vertical transport. As vertical transport is not well constrained in models this can be seen as an advantage to improve source-sink-estimates derived from inverse modelling using column-averaged mole fractions. Moreover, TCCON provides the link between ICOS and the GHG satellite data. TCCON is the reference network for the calibration and validation of GHG satellite retrievals and provides the link between ICOS and the GHG satellite data. TCCON data are also requested by atmospheric modellers, e.g., the ones involved in the Copernicus Atmosphere Monitoring Service (CAMS) to validate their models. In addition, TCCON data are used for the detection and evaluation of long-term trends, which is an important application in the Copernicus Climate Change Service (C3S).

TCCON instrumentation specification and data processing are given in the technical case, and a possible structure for the integration of the Atmosphere Column Thematic Centre (ACTC, i.e. TCCON thematic centre) into ICOS is proposed. The ACTC would extend the list of existing TCs (ATC, ETC and OTC), it would be linked to the ICOS Carbon Portal for data distribution, storage and archiving, while remaining in contact with the global TCCON database maintained by Caltech, USA.

The roles of the ACTC are to centralise key activities currently done by the individual groups and introduce new activities aiming to improve the comparability among the sites. The first task of the ACTC is to maintain the QA/QC services and to offer the central retrieval for European TCCON sites. It includes instrument characterisation with maintenance of gas cells and retrieval of the instrument line shape. The ACTC will also ensure pressure measurements with an accuracy of better than 0.25 hPa, which is needed for the use of XO_2 as an internal standard. The ACTC will also maintain a travelling instrument (EM27/SUN) for comparisons at all sites. The retrieval within the European TCCON will be done at the ACTC with the standardised line-by-line retrieval code GFIT. Final data from European TCCON sites will be available both from the global TCCON database at Caltech and trough the ICOS Carbon Portal. The ACTC will also produce a Rapid Delivery product (RD) which will be available 3-5 days after the measurement. The RD product will be retrieved at the TCCON site, under the PI's responsibility, and it will then be directly delivered to the Carbon Portal. The ACTC will also be in charge of the support to the network (training, knowledge transfer, strategy for instrument deployment, link to WMO scales) and the support of innovation (new technologies, new tools for data providers).

In the resource assessment part, the cost for ACTC and a TCCON site (personal, consumables, other costs, etc. …) are detailed along with a table of depreciation of equipment.

2. General context

The atmospheric observing system for greenhouse gases

In situ measurements

Various available observations of atmospheric CO_2 and CH_4 are shown in Figure 1. Surface in situ observations were started in 1958 at Mauna Loa (Hawaii) by Dave Keeling (Keeling, 1960) and comprise an extended global network today. These in situ measurements are very precise and until recently most of the inverse modelling studies relied on this network to compute optimised surface fluxes of greenhouse gases from atmospheric concentration measurements. The variability of CO_2 and CH_4 atmospheric concentrations near the Earth's surface is produced by a) the sources and sinks (exchange fluxes) of CO_2 and CH_4, which are located at the Earth's surface and b) the vertical transport, which changes depending on solar insolation and atmospheric conditions. Hence the knowledge of the vertical transport in the atmosphere is essential for reliable flux estimates using in situ data. However, the vertical transport is often not well known, which introduces systematic errors in the flux estimates (Denning et al., 1995, Stephens et al. 2007). Moreover, the surface in situ measurements have only a scarce spatial coverage in some regions of the world, especially in the tropics.

In the 1990s at several sites tall tower and aircraft measurements were implemented. The tall towers are up to 350m high and measurements are taken at different levels. These tower measurements are complemented by systematic aircraft profiling throughout the boundary layer and parts of the free troposphere. The towers as well as the aircraft measurements provide information about the vertical transport. However, both are difficult to implement at an extended global network, and therefore only few such sites exist. In addition, aircraft measurements are expensive and provide a low temporal coverage. Since 2010, a novel vertical profiling technique, the AirCore, was introduced (Karion et al. 2010). An AirCore is a tube that is transported to an altitude of up to 30 km by a balloon. On its way up the tube is evacuated due to the dropping atmospheric pressure. When the tube sinks down to the Earth's surface on a parachute, it fills with ambient air according to the surrounding pressure. Hence air from different altitudes is located at different positions in the tube, specifically air from the highest altitudes is at the end of the tube and air from the surface is located at the inlet. Once the tube arrives at the Earth's surface, the air in the tube is analysed. When the analysis is done shortly after the recovery of the AirCore once it has landed, the vertical profile of the atmosphere is preserved in the tube, and therefore the vertical profiles of CO_2 and CH_4 can be established from these measurements.

Remote sensing measurements

Ground-based solar absorption measurements in the near-infrared (IR) spectral region prior to 2002 were limited to a few years at Kitt Peak. Using these spectra Yang et al. (2002) and Washenfelder et al. (2003) demonstrated that CO_2 and CH_4 can be retrieved with high precision. In Europe the first time series of ground-based solar absorption measurements in the near-IR started in 2002 at Ny Ålesund (Spitsbergen) (Warneke et al., 2005) where it is still continued. In 2004 the Total Carbon Column Observing Network (TCCON), a ground-based solar absorption network for near-IR measurements, was founded providing the framework for highly standardised measurements and retrievals (Wunch et al., 2011). The first satellite instrument providing useful CO_2 and CH_4 data with high sensitivity to the ground became available in 2002 with SCIAMACHY onboard the Envisat mission (Buchwitz et al., 2007). The remote sensing measurements, from satellite as well as from the ground, provide the column-averaged dry air mole fraction (denoted by prefix 'X'), which is a different information compared to the in situ measurements. This column-averaged mole fraction is almost insensitive to vertical transport. In addition, the satellites provide global coverage, overcoming the limitation of sparse spatial coverage of the in situ network. However, the remote sensing measurements are less precise than the in situ measurements, are not easy to calibrate against the WMO standards and can be subject to systematic errors. Over the last 17 years the precision of the remote sensing measurements has increased and a better understanding of systematic error sources improved the retrieval. For the calibration against WMO standards the following approach has been taken: High altitude vertical in situ profiles (aircraft and/or AirCore) are taken above TCCON sites. These in situ profiles are calibrated against the WMO standards and by comparison with the TCCON retrievals the TCCON data are tied to the WMO reference scale. The calibration can then be transferred to the satellite measurements by comparison with TCCON. Besides the calibration, TCCON plays a vital role for the validation of the satellite measurements, resolving spatial biases and/or temporal drifts in the satellite data. An example is the following: For the S-5P mission the TCCON data played a significant role in the validation of the CH4 and CO products, resulting in a recommendation to ESA for the public release of these two products (Fig 2-3). Remote sensing measurements have continuously improved and it can be expected that the precision and relative accuracy will continue to improve.

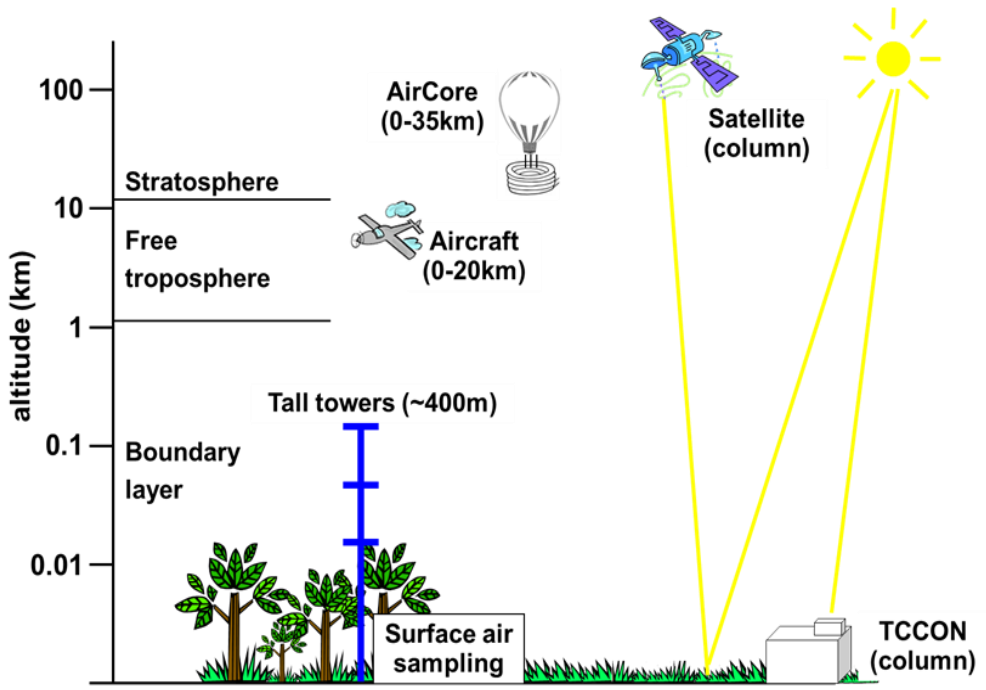

Figure 1: Observations of atmospheric greenhouse gases

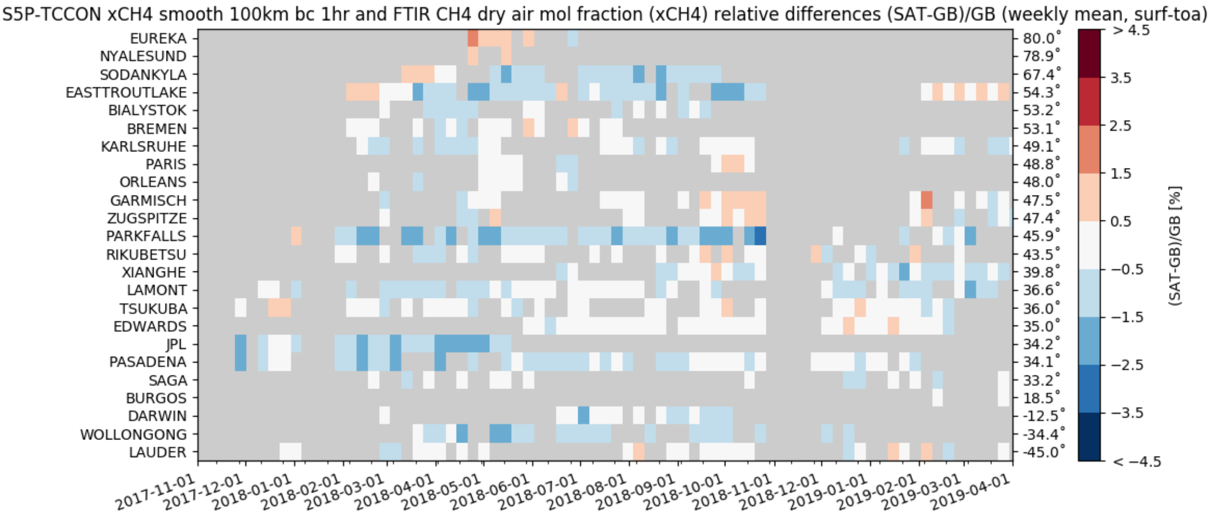

Figure 2: Weekly mean bias of the S-5P XCH4 compared to the TCCON for each site since the start of the mission until 1st of April 2019 (Sha et al., in preparation).

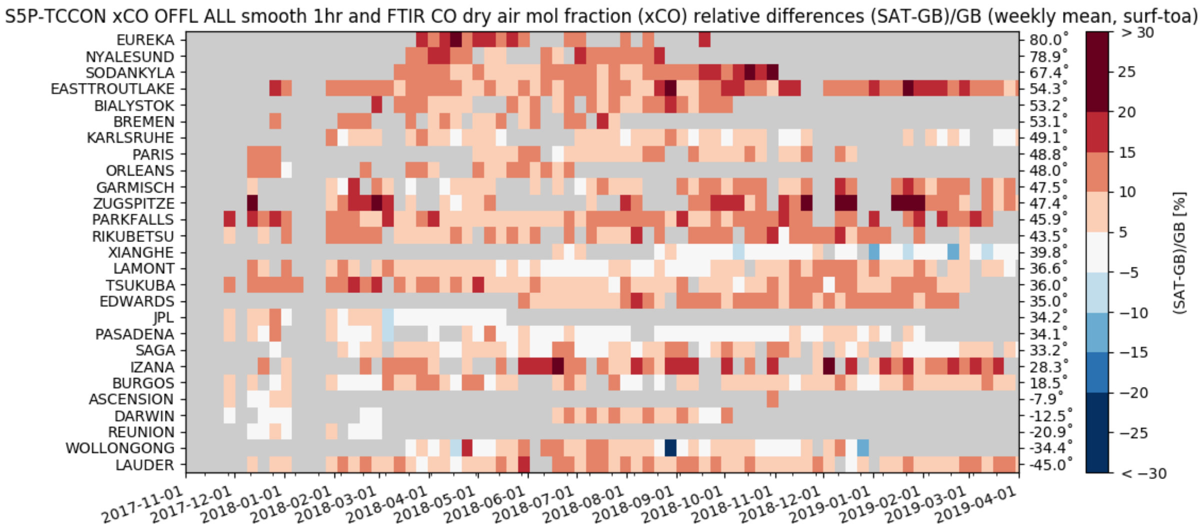

Figure 3: Weekly mean biases of the S-5P XCO compared to the TCCON XCO for each site since the start of the mission until 1st of April 2019 (Sha et al., in preparation).

ICOS RI

The Integrated Carbon Observation System Research Infrastructure (ICOS RI) is a Pan-European research infrastructure that was first conceived of in 2006 by researchers in the European Sixth Framework Program (FP6) projects, particularly the CarboEurope and CarboOcean projects. It subsequently entered the European Strategy Forum on Research Infrastructures (ESFRI) roadmap and started a preparation phase that lasted from 2008 to 2013. In 2015 ICOS was established as a European Research Infrastructure Consortium (ERIC). ICOS' mission is 'to enable research to understand the greenhouse gas (GHG) budgets and perturbations'. This mission statement is embedded in the organisation's structure and defines its activities, such as the promotion of research, education and innovation in the field of environmental and most notably climate studies. Its main purpose is to provide long-term observations required to describe the present and future behaviour of the global carbon cycle and anthropogenic GHG emissions. The mission statement is guided by two main objectives:

- ICOS is to provide effective access to a single and coherent data set to facilitate research into multi-scale analysis of GHG emissions, sinks and the processes that determine them.
- ICOS provides '…information, which is profound for research and understanding of regional budgets of greenhouse gas sources and sinks, their human and natural drivers and the controlling mechanisms.'

The aims of ICOS RI are defined hereafter:

- Long time series of data to investigate historic trends and make reliable extrapolations
- Uniform data collection methods with
  - standardised measurement instruments
  - standardised reference samples
  - well- known and preferably uniform instrument specifications
- Linked measurements of ocean, atmosphere and land-based GHG balances
- Consistent metadata that describes the dataset and makes uncertainties explicit, so the data are more easily shared across communities
- An accessible repository for climate scientists world-wide according to the FAIR principles: Findable, Accessible, Interoperable, Reusable of ICOS RI.

TCCON

A map of the TCCON in 2018 is shown in Figure 4. The sites which are operated by European institutions and are therefore relevant for ICOS are listed in Table 1.

The TCCON data products are column-averaged dry air mole fractions (XGas) of CO_2, CH_4, N_2O, HF, CO, H_2O, and HDO. These data are provided together with the corresponding a priori profiles and averaging kernels. The retrieval is currently done by the individual groups performing the measurements using a standardised code (Wunch et al., 2011, 2015). The processed data are delivered to Caltech, USA, where a final QA/QC is performed before uploading the data to the TCCON data archive. User guides, documentation describing the methods and evaluation are provided, along with appropriate information necessary for using the data to evaluate models and other measurements (e.g. averaging kernels, a priori profiles, error description, etc.). The format of the data is NetCDF. The data become publicly available no later than one year after the measurements are recorded. Several sites choose to release their data sooner. Within validation projects it has been shown that the final data can be made available 3 months after the measurement. The doi for the description of the current TCCON data are available from 10.14291/TCCON.GGG2014.DOCUMENTATION.R0/1221662.

The TCCON community and governance

The TCCON charter (https://tccon-wiki.caltech.edu/Network_Policy/TCCON_Charter) states: "TCCON is a partnership of the individual sites that comprise the network. TCCON participants agree to adhere to a common set of standards for instrumentation, data acquisition, calibration, and analysis as determined by the TCCON

Steering Committee. The TCCON Steering Committee, comprising one representative from each site, is charged with making policy for the network. The committee can invite further members onto the Steering Committee. This committee is also responsible for admission of new sites into the network and for setting data quality standards. The Steering Committee is led by a chair and co-chairs elected by the members to a three-year term. Policy changes to the Charter and/or Protocol are made on a 2/3 vote of the Steering Committee with one vote per site."

Information exchange is facilitated by a) a wiki (https://tccon-wiki.caltech.edu), b) an email list, c) bimonthly teleconferences and d) an annual face-to-face meeting. Europe contributes very significantly to the TCCON: 12 out of the 26 TCCON sites are operated by European institutions. Many of these European sites rely on short-term research projects.

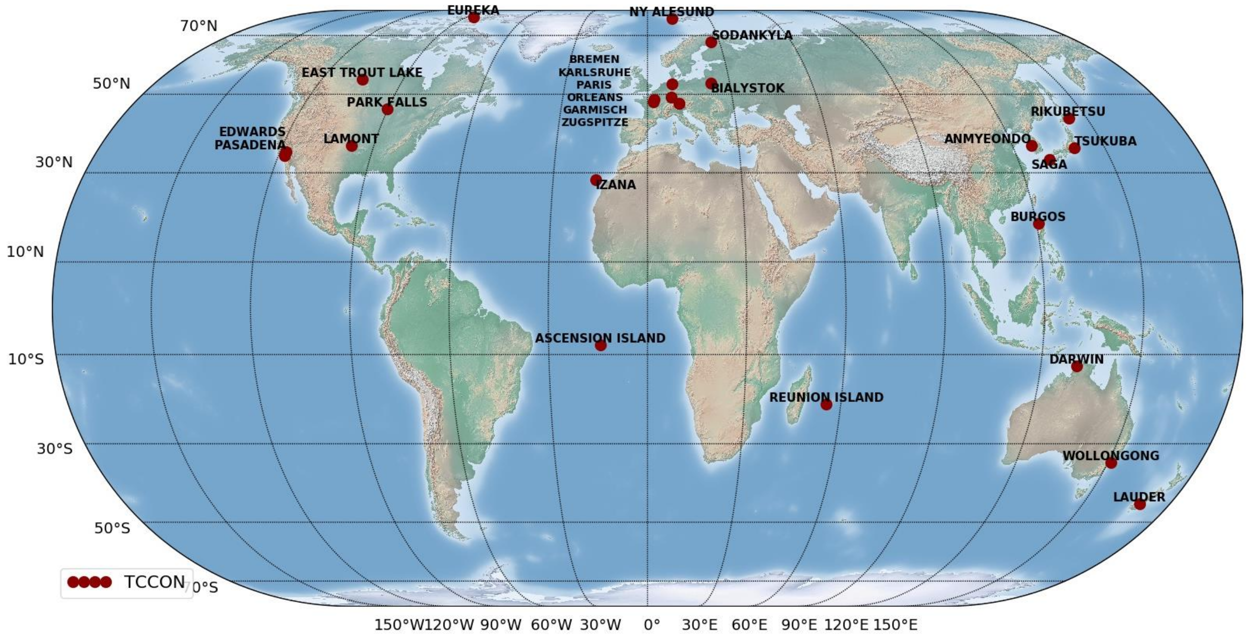

Figure 4: Map of operational TCCON sites in 2018.

Table 1: Sites operated by European institutions

Site	**Lat**	**Lon**	**Alt. (km)**	**PI (Country)**	Expected to join ICOS
Ascension Island	7.92 S	14.33 W	0.01	Feist (Germany)	Yes
Nicosia, Cyprus (formerly Bialystok, Poland)	35.14 N	33.38 E	0.18	Petri, Vrekoussis (Germany)	Yes
Bremen, Germany	53.10 N	8.85 E	0.03	Notholt, Warneke (Germany)	Yes
Garmisch, Germany	47.48 N	11.06 E	0.74	Sussmann (Germany)	No
Izana, Tenerife	28.30 N	16.50 W	2.37	Schneider (Germany)	No
Karlsruhe, Germany	49.10 N	8.44 E	0.12	Hase (Germany)	No
Ny Alesund, Spitsbergen	78.90 N	11.90 E	0.02	Notholt, Warneke (Germany)	Yes
Orleans, France	47.97 N	2.11 E	0.13	Warneke, Notholt (Germany)	Yes
Harwell, UK (intents becoming a TCCON site soon)	51.57 N	1.31 W	0.12	Boesch, Weidman (UK)	Yes
Paris, France	48.85 N	2.36 E	0.06	Té, Jeseck (France)	Yes

Reunion Island	20.90 S	55.49 E	0.09	De Mazière (Belgium)	Yes
Sodankyla, Finland	67.37 N	26.63 E	0.19	Kivi (Finland)	Yes
Zugspitze, Germany	47.42 N	10.98 E	2.96	Sussmann (Germany)	No

Figure 5: Map of TCCON sites operated by European institutions in 2018.

3. ICOS-TCCON synergies

- A TCCON-ICOS integration will greatly increase ICOS' visibility, especially towards the satellite community. Currently the ICOS in situ measurements and the remote sensing measurements of GHGs have a poor connection. In the future, there will be an increasing relevance of remote sensing data for carbon cycle research. Remote sensing measurements of GHGs with high sensitivity to the Earth's surface became available about 17 years ago and at the time of the planning/establishment of ICOS these measurements had little relevance for carbon cycle research. The quality of the remote sensing data has dramatically improved and remote sensing data are now an important component in the atmospheric GHG observing system. Advances in spectroscopic data and improvements of retrieval algorithms will almost certainly result in major improvements of the remote sensing data in the future. In addition, the planned GHG satellite missions will result in a higher abundancy of column GHG data. Hence, it is likely that remote sensing column GHG measurements by TCCON and satellite are becoming increasingly important for carbon cycle research. The integration of TCCON into ICOS will establish a concrete link between ICOS and the GHG data from satellites. The integration will benefit both infrastructures on a more technical level with transfer of competence and expertise: ICOS benefits from the TCCON competence in FTIR measurements including EM27/SUN instrumentation, a technology that starts to being used for GHG budget at the scale of cities or industrial sites, a topic of interest for ICOS as well. TCCON on the other hand will benefit from ICOS sustained infrastructure with recognised in high precision instrumental calibration, with a direct link to the SI units. Current GHG satellite missions include GOSAT, GOSAT-2, OCO-2, OCO-3, TANSAT and S-5p and the planned future satellites missions include MicroCarb, MethaneSAT, Sentinel5, GEOCARB, MERLIN, TanSat-2, GOSAT-3, CO2M. All these satellite data will be **essentially useless without careful validation**. Currently all these missions rely on TCCON as the reference network for calibration and validation.

  - "Calibration" of GHG satellite retrievals against WMO standard: Comparison of TCCON with vertically resolved calibrated in situ measurements (AirCore, Aircraft), then comparison of TCCON with satellite.
  - Validation of GHG satellite retrievals (temporal drift, spatial bias)

The integration of TCCON into ICOS will ensure that data are available for the satellite calibration and validation in Europe.

- The integration will increase the data portfolio of ICOS. Satellite and ground in-situ data are complementary and both necessary to correctly address the challenge of monitoring the global GHG cycle. Both are needed to correctly address the data coverage shortage that exists.
- Such an ICOS-TCCON integration will create a larger community with increased scientific production.
- ICOS together with TCCON becomes a stronger player in addressing the challenge of the first global stocktake planned for 2023.
- The integration of European TCCON into ICOS, accompanied with national funding, will secure the European part of TCCON. TCCON is currently a scientific network operated by individual groups that needs to become an operational network. Most European sites rely on short-term funding by research projects. However, TCCON data are used increasingly for monitoring in an operational way by its users (satellite agencies, modellers).
- Timely availability of TCCON data. Currently TCCON guarantees that its data are made available at latest one year after the measurements. Many sites have automated their data processing to such an extent that 3-monthly data delivery is possible in case sufficient personal is available. After an ICOS integration, the central retrieval at the ACTC will guarantee TCCON data availability 3 months after the measurements for all participating sites.
- Availability of rapid delivery (RD) data. Within ICOS an automated retrieval will be implemented at all participating TCCON sites. This data product will not undergo the full quality checks and is similar to the NRT data from the ICOS in situ sites. The availability of this RD data will be 3-5 days after the measurements. TCCON currently does not offer a RD data product.
- Improved network consistency. For most applications (satellite validation, model validation, inverse modelling) it is highly important that no biases between the TCCON sites exist. Within ICOS a novel strategy is planned to ensure this. This involves gas cell and pressure sensor calibrations as well as the deployment

of a travelling reference/standard instrument of the type EM27/SUN performing similar solar absorption measurements as the TCCON.

- Integration of TCCON into ICOS will also facilitate the user experience in terms of centralized access to the data via a coordinated platform that will benefit from the latest FAIR implementation principles notably in terms of interoperability.
- Central data processing. In addition to the guaranteed data delivery 3 months after the measurement, the central processing has the following advantages: a) The spectra from all sites are processed by the same people, which allows an intercomparison of the spectra and an easier and more rapid identification of problems; b) The fast re-processing of all spectra, e.g., with an update of the processing software and/or the spectroscopic linelist. The latter point was a problem within TCCON in the past and likely will be in the future. After developments yielding a more accurate data product had been made, it took a long time (< 1 year) until the data from the individual sites were re-processed. The central processing will ensure that the re-processing will be done within a few weeks for all sites and that the highest quality data product (state of the art retrieval) will be available to the data users.
- Governance structure for involved TCCON sites. Pinty et al. (2019) highlights the importance of secured funding and an improved governance structure for TCCON in view of an operational anthropogenic CO_2 emissions Monitoring & Verification Support (MVS) in Europe. The outlined integration into ICOS will provide an improved governance structure for the involved TCCON sites, including a commitment from ICOS Member States to sustain the infrastructure and operations, and guaranteeing the timely availability of and access to the highest quality data through a centralised data processing and QA/QC facility.
- Access to enhanced information about the vertical distribution of GHGs at ICOS sites. TCCON provides the column-averaged mole fraction of GHGs, a different kind of information than the current ICOS atmospheric in situ measurements (point measurements close to the surface). This information is complementary to the in situ data (e.g. Zhou et al., 2018). In contrast to the information of in situ measurements, the column-averaged mole fraction is independent of vertical transport. Vertical transport is not well constrained in models and therefore the TCCON data will improve source-sink-estimates derived from inverse modelling. This is especially valuable at sites where co-located in situ and TCCON measurements exist.
- A stronger interlocutor with Copernicus. TCCON and ICOS data are requested by atmospheric modellers, e.g., the ones involved in the Copernicus Atmosphere Monitoring Service (CAMS) to validate their models. In addition, TCCON data are used for the detection and evaluation of long-term trends, which is an important application in the Copernicus Climate Change Service (C3S). The integration of TCCON into ICOS will ensure that data from the involved sites will be available for the Copernicus services, in due time, and with the highest state-of-the-art quality.

4. Technical case

Description of TCCON site

A TCCON instrument is composed of a high-spectral-resolution Fourier transform infrared (FTIR) spectrometer of the type Bruker IFS 125HR operating in the near-infrared spectral region (4000–9000 cm-1), and coupled to a sun tracker, preferably operated automatically or remotely controlled. TCCON agreed on the following observational requirements (https://tccon-wiki.caltech.edu/Network_Policy/Data_Protocol#FTS_Requirements):

- A minimum spectral range of 4000-9000 cm-1.

- Maximum optical path difference (OPD) >= 45 cm with phase resolution (PHR) of at least 1 cm^{-1}.
- Sun tracker pointing with an accuracy of 1 mrad (~0.05°, or 3 arcminutes). This tracker requirement corresponds to an airmass error of 0.2% at 63° SZA, or 0.1% at 45° SZA. The tracking accuracy can and should be routinely monitored in one dimension using the solar-telluric shift (S-G shift).
- Surface pressure measurements accurate to better than 0.3 mbar.
- Surface temperature measurements accurate to better than 1 K.
- Accurate knowledge and reporting of the interferogram zero optical path difference (ZPD) crossing time (within 1 sec).
- Laser sampling errors less than 0.00024 of the sample step. This corresponds to a ghost-parent intensity ratio of 0.0001 for parent frequency 4150 cm-1 (NDACC HF filter) and a ghost-parent ratio of 0.00014 for parent frequency of 5970 cm-1 (TCCON ghost filter). The corresponding bias in XCO_2 is estimated to be 0.02% or less.
- Routine procedures for monitoring instrument line shape (ILS):
  - A line shape monitoring device in the solar beam during all or a continually repeated subset of observations capable of characterising the modulation efficiency (ME).
  - Monthly ILS retrieval from HCl cell spectra acquired with the tungsten lamp source and analysed with LINEFIT code using the TCCON ILS parameterisation. A SNR of ~2500 is recommended for ILS retrieval from cell spectra, and required for manned sites. A relaxed SNR criterion of ~1300 (typically achieved with ~20 scans) is acceptable for container deployments with limited duration lamp operation.
- Criteria for optical alignment, expressed in terms of ME and phase error, to be determined
  - Provisional: The ME shall vary by less than 5% over the 0 to 45 cm optical path difference (OPD), and shall be known to better than 2%.
  - Limit for the phase error (currently not specified, under discussion)

Most of TCCON observations are performed automatically. A weather station coupled to the TCCON instrument is needed to detect atmospheric measurement conditions (cloud-free, no rain). The automation software detects when weather conditions are suitable for doing measurements, opens the cover of the solar tracker and starts the measurements. The data (up to 5 GB/day) are stored locally or transferred via the internet to the institution of the PI of the instrument.

The TCCON data processing

The data processing chain is depicted in Fig. 6. The processing is performed by a common software package maintained at Caltech/NASA JPL (Wunch et al., 2011). The raw data are called interferograms. An interferogram is the measured intensity of the electromagnetic radiation versus the optical path difference of the light coming from the fixed and moving mirror. These interferograms are then processed by a standardised code (I2S), which corrects the interferograms for solar intensity variations, ghosts and phase errors, and then uses a fast Fourier transformation to compute the spectra. The retrieval of the column abundances is done by the column scaling algorithm GFIT. The retrieval package contains the spectral linelist needed for the retrieval. In a post processing routine, the column abundances are converted to column-averaged dry air mole fractions by division by the O_2

column involving airmass corrections and a scaling to account for differences to the WMO reference scale. The final product (L2b data) consists of the corrected column average mole fractions and their uncertainties together with averaging kernels and a prioris.

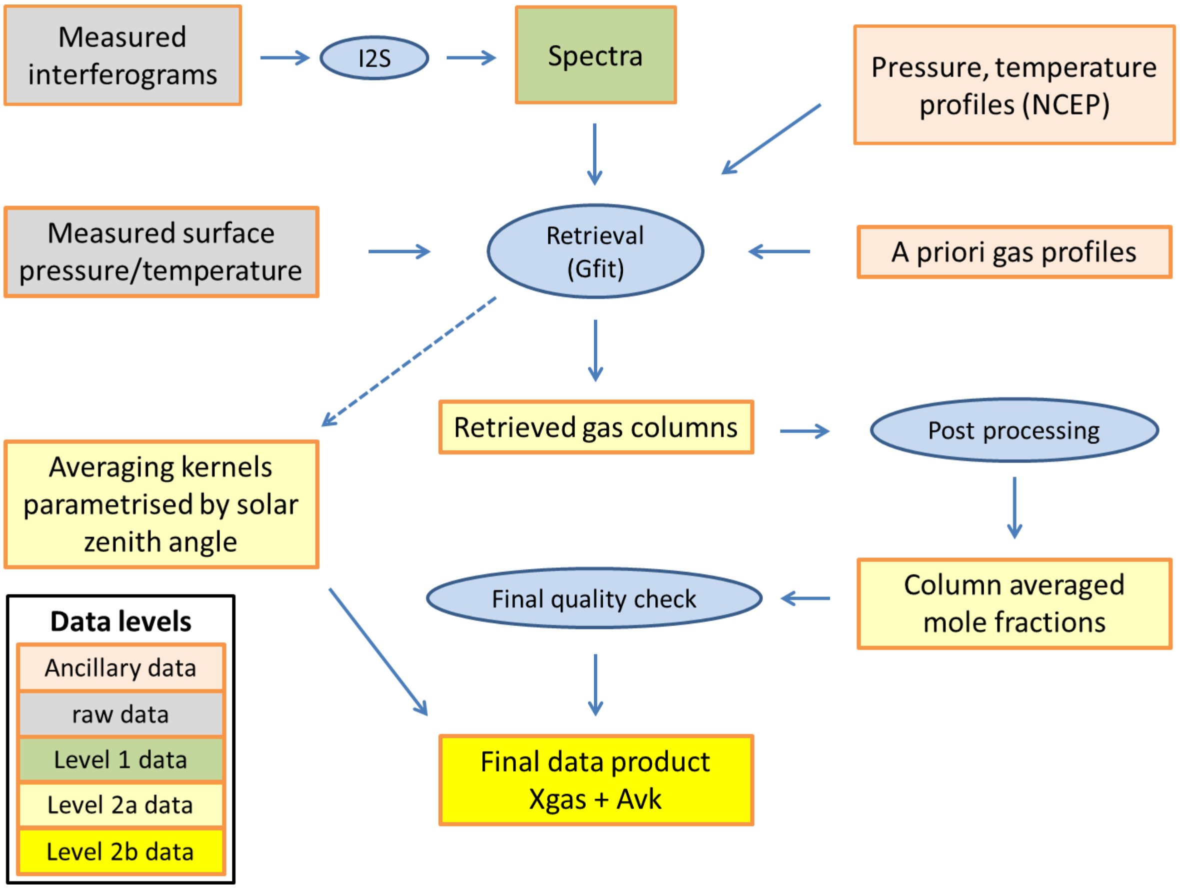

Figure 6: Schematic of the processing chain

Role of the ACTC for ground-based remote sensing measurements

The proposed structure for the integration of the Atmospheric Column Thematic Centre (ACTC) into ICOS is depicted in Figure 7. The ACTC will be strongly linked to the global TCCON network.

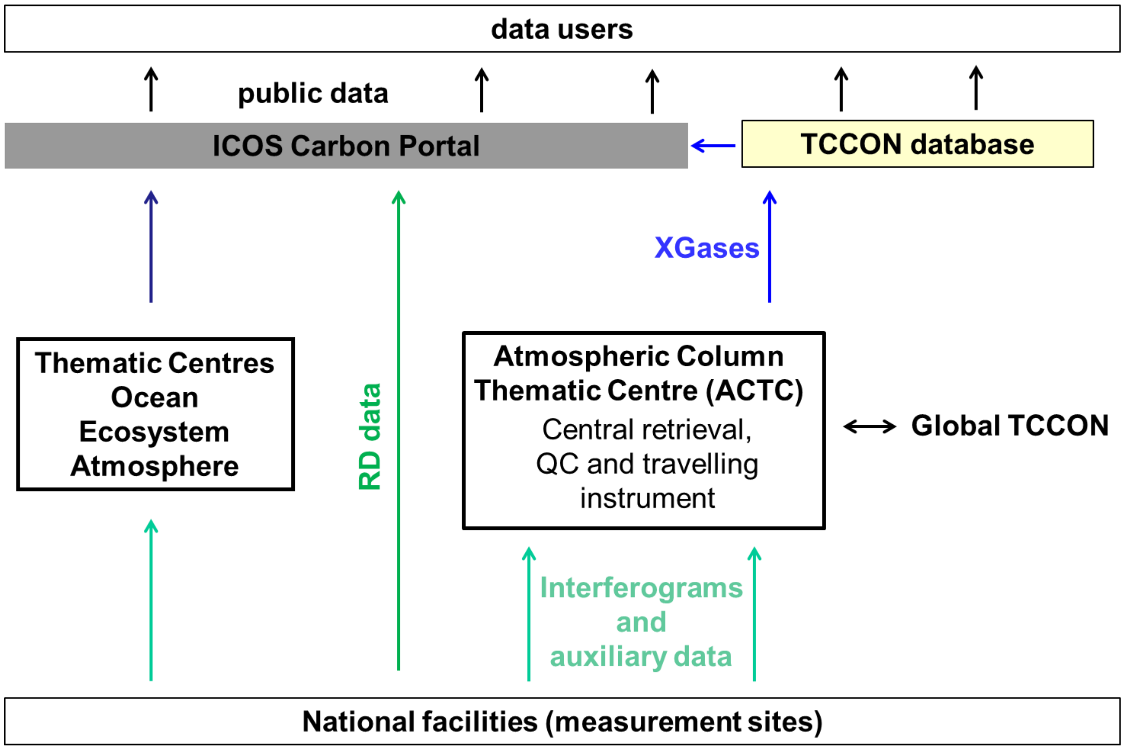

Figure 7: Proposed structure for the implementation of the Atmospheric Column Thematic Centre (ACTC) into ICOS

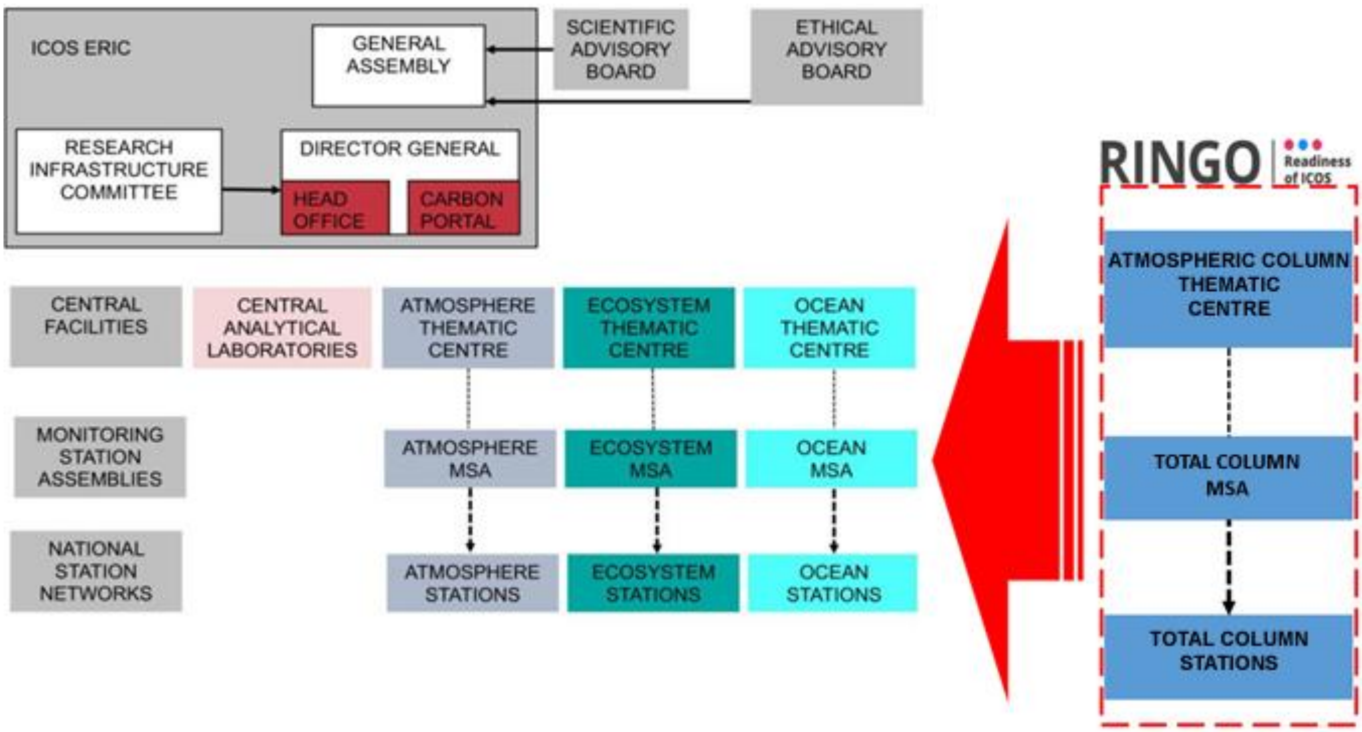

Figure 8: Proposed global structure for the implementation of the Atmospheric Column Thematic Centre (ACTC) in the landscape of the other ICOS Thematic centres.

The ACTC is an essential component in the operationalisation of the European TCCON activities and a game changer in improving the data product of the European sites and most probably beyond. For the precision and accuracy of the data products it is important that the observing system as well as the retrieval algorithms satisfy stringent specifications. These specifications are determined and prescribed by the global TCCON. Currently the individual groups are responsible for monitoring the performance of their observing system, checking the quality of the spectra, the retrieval and obtaining funding for comparisons against vertical resolved in situ measurements. This is very time consuming and sufficient resources cannot always be provided in time. The Atmospheric Column Thematic Centre (ACTC) will centralise and standardise these key activities currently done by the individual groups and introduce new activities aiming to improve the comparability among the sites. The tasks of the ACTC are listed and described in the following paragraphs:

Centralising QA/QC and offering central retrieval for European sites

*Instrument characterisation **

This topic includes the maintenance of gas cells and the retrieval of the Instrumental Line Shapes (ILS). One important component in the TCCON observing system is the FTIR spectrometer. Each TCCON spectrometer is equipped with a sealed cell filled with approximately 5 mbar of HCl for monitoring the instrumental line shape (ILS) of the FTIR spectrometer.

A calibration procedure for the HCl cells has been developed at KIT (Hase et al. (2013)). The procedure is able to identify variations of HCl purity between the cells and assigns effective pressure values to each individual cell to account for additional broadening of the HCl lines. This approach improves the consistency of the network by significantly reducing possible station-to-station biases due to inconsistent ILS results from different HCl cells. The cell calibration will be conducted at least once every 24 months. Within the ACTC this “cell calibration” will be made a sustainable, long-term activity.

For the ILS determination dedicated lamp measurements will typically be carried out every 2 weeks by the individual groups and the ILS is retrieved from these gas cell spectra. The retrieval of the ILS from the gas cell spectra is done by the software LINEFIT (Hase et al., 1999), which was developed by KIT. The ACTC will maintain the software LINEFIT and distribute updates to the individual groups and the ACTC. The analysis of the lamp spectra will be done by the site PIs. The results of the LINEFIT retrievals will be transferred to a repository for all QA/QC related parameters at the ACTC.

*Ensuring pressure measurements with an accuracy of better than 0.25 hPa **

The dry air column-averaged mole fractions can be calculated by the use of surface pressure and water or by the use of the retrieved O_2 column. In TCCON the latter approach is used and the XGas is calculated from the column ratio Gas/O_2 multiplied by the O_2 mole fraction in the atmosphere. The advantage of dividing by O_2 is that systematic errors, common to both, O_2 and CO_2, partially cancel out. The underlying assumption that the O_2 mole fraction is constant in the atmosphere is valid since any variation of O_2 in the atmosphere is at least 10 times lower than the TCCON precision.

XO_2 calculated from surface pressure (and retrieved H_2O) also serves as an internal standard within TCCON. Any variation of the XO_2 points to instrumental problems. An additional use of the XO_2 could be the identification of biases within the network. Currently insufficiencies in spectroscopic data prohibit the use of XO_2 to quantify biases between different TCCON sites, but once improved spectroscopic data will become available, this will be possible if accurate pressure measurements exist. The discussion within TCCON about the procedure of the pressure sensor calibration has not been finalised. In ICOS we plan to develop a calibration procedure and circulate a pressure standard for annual comparisons at all sites.

*Maintaining a travelling instrument (EM27/SUN) for comparisons at all sites ***

A vital point for a network like TCCON is the comparability among the sites within the network. This comparability has been demonstrated by a) comparisons to vertical resolved in situ measurements at several sites and b) the calculation of the O_2 mole fraction using the retrieved O_2 column and the surface pressure. The former approach is currently used to infer the overall uncertainty within TCCON and the latter one is used as diagnostic for problems, but the O_2 retrieval is currently not good enough to use the O_2 mole fraction as an internal standard.

The EM27/SUN spectrometers are operated in low spectral resolution but have been demonstrated to be of high stability (Frey et al. (2015,2019)). These spectrometers are able to detect biases between TCCON stations. Within ICOS a travelling EM27/SUN instrument will be employed to conduct comparisons of the TCCON sites. The spectrometer shall visit all the sites involved in ICOS at least every second year. During the site visit of the travel standard, the TCCON spectrometer under investigation will, in addition to the standard TCCON measurements, collect low-resolution, double-sided interferograms applying the same resolution as offered by the travelling standard spectrometer. This results in a perfect match of column sensitivities between the two sensors, allowing for a very sensitive test of any interference on the low-resolution (inner) part of the TCCON interferogram. While the cell QC procedure verifies and characterises the high-resolution performance of the TCCON spectrometer, the travelling standard intercomparison tests for disturbances which essentially leave ILS characteristics intact while still critically affecting the quality of resulting XGas values (non-linearity, double-passing, ghosts, etc) (Sha et al. (2019)).

*Centralised retrieval **

The retrieval within TCCON is done with the standardised line-by-line retrieval code GFIT (Wunch et al. 2015). The code is maintained and distributed by Caltech / NASA (JPL). It is open source and all TCCON partners are welcome to suggest improvements and the code is updated on a regular basis. It is of vital importance that the global TCCON uses a single retrieval code.

Currently the retrieval is done by the individual TCCON PIs. This will change for the TCCON partners participating in ICOS. The ACTC will provide a centralised retrieval. The advantage of a centralised retrieval is that the timeliness of the data is guaranteed and that potential problems in the spectra from one station might be detected earlier since the ACTC has the comparison to the spectra from other stations. In addition, it is easier to implement a centralised quality control as a post-processing step.

All the interferograms of the European TCCON sites participating in the centralised retrieval will be stored at ACTC and centrally processed/reprocessed. The processed L2 data will be available from the TCCON database as well as from the ICOS Carbon Portal 3 months after the measurements. In case of future update of the retrieval software, the central facility will do the re-processing of the data from all the stations.

*Overall QC and submission to the Caltech database **

The final quality control procedure will follow the guideline of TCCON. All the L2 data that passes these quality control procedures will be submitted to Caltech to be uploaded to the TCCON database. The data also includes flags reflecting the information available on repository QA/QC related parameters at the ACTC.

Link between Carbon Portal (CP) and the TCCON database

It is important that the data from the European TCCON sites is available from the TCCON database as well as from the ICOS Carbon Portal (CP) and that the same data only has one DOI. After the quality check at the ACTC, the data will be sent from the ACTC to Caltech for an upload to the TCCON database and the Carbon Portal will point to the data using a persistent digital identifier.

The current data policy of TCCON is more restrictive than the one of ICOS. It has been discussed within TCCON that the TCCON data base will offer two potential data policies during the data upload: the original TCCON data policy and the **Creative Commons Attribution 4.0 international licence** used in ICOS. This ensures that the data from the European TCCON sites participating in ICOS is available from the Carbon Portal and the TCCON database with the same CC-BY-4.0 license.

Rapid delivery data

The standard TCCON data need a thorough quality check and currently the data are available at least one year after the measurement. After the integration into ICOS the standard TCCON data will be available 3 months after the measurement for the sites integrated in ICOS.

An additional data product, specifically important for Copernicus, will be the rapid delivery (RD) data. This data will be available 3-5 days after the measurement. This data product will not be delivered via the ACTC because the size of the interferograms does not allow to transfer them timely to the ACTC via the internet. Therefore, the RD data will be retrieved directly at the TCCON sites and the transfer will be directly to the Carbon Portal. Since the RD data are currently not part of TCCON it will be only submitted to the Carbon Portal and not to the TCCON database. The retrieval at the site will include and automated quality check, but not the thorough quality check done for the TCCON data. The lag time of 3-5 days mainly arises from the availability of the pressure-temperature profiles.

RD-data processing is currently implemented for the sites Nicosia, Orleans and Reunion. For all other sites the RD data processing has to be implemented, which needs investment in hardware and creation of software. Therefore, the stations that currently do not provide the data product need initial setup costs for the implementation. The maintenance of the rapid delivery data will be provided by the site PI.

Support and support of innovation

*Knowledge transfer and training (e.g. new operators/scientists) ***

The ACTC will contribute to the education of future instrument operators and data providers by providing didactic material and dedicated support (including training) upon request.

*Develop and distribute useful tools for data providers **

Useful tools for data providers shall be developed at the ACTC. These tools will be made freely available and will be distributed via the ACTC but also via the TCCON wiki.

*Make, evaluate and promote new developments, including strategies for developing/improving the European part of the network **, **

New development in the past were done within the standard operation of the network or as part of research projects. It is intended that this will also be the case in the framework of ICOS. These new developments will be evaluated as part of the activities at the ACTC.

Link to WMO scale via comparisons to vertical resolved in situ measurements

TCCON retrievals are linked to a different scale (denoted as “spectroscopic scale” in the following) than the in situ measurements (WMO scale). The link between these scales has been established using vertical resolved in situ measurements and a scaling factor is applied to the TCCON data to account for the difference. It is important to verify the link between the scales and to improve the uncertainty of the scaling factor in the future. Therefore, high quality vertically resolved in situ profiles will be needed at TCCON stations in the future. Ideally, these in situ profiles are established by a combination of AirCore and aircraft measurements, since single vertical in situ profiles with erroneous (too small) errors would have a negative impact on the TCCON calibration. The vertical resolved in situ profiles will not be part of the ACTC. However, the data becoming available will be used within TCCON for establishing the link between the spectroscopic and the WMO scale.

5. ACTC resources assessment

Thematic Centre (annual costs)

The ACTC can be thematically split into activities related to the central retrieval (marked with * in section 4) and activities related to the network/measurement consistency (marked with ** in section 4). Besides the thematic difference, there is another reason for splitting these two sections in the cost estimate below: Belgium shows a high interest in conducting the activities related to central retrieval (*) at the ACTC. This would be synergetic to planned activities of NDACC within ACTRIS. Germany has a high interest in conducting the activities related to the network/measurement consistency (**) at the ACTC. Most of these activities are resulting or have resulted from research activities at KIT.

Cost for the central retrieval at the ACTC

The central retrieval is strongly linked to other activities listed in section 4. All activities included in the cost estimate below are marked with * in section 4.

Personnel

Position	**Fraction of full time position**
Expert manager	0.5
Qualified officer	0.2
Admin assistance	0.5
Expert scientist	1.0
Qualified operator	0.5
Technician	0.1
Total	**2.8**

Other costs

Position	**Cost (EUR)**
ICT costs	12 000
Consumables	1 000
Equipment replacement	2 000
Building maintenance	3 000
Travel	10 000
Total	**28 000**

Cost for the measurement/network consistency activities at the ACTC

All activities included in the cost estimate below are marked with ** in section 4.

Personnel

Position	**Fraction of full time position**
Expert scientist	0.7
Technician	1.0
Total	**1.7**

Other costs

Position	Cost (EUR)
Depreciation of EM27/SUN	10 000
Equipment replacement (damages)	3 000
Pressure calibrations	500
Building maintenance	10 000
Consumables	3 500
Travel	6 000
Total	**33 000**

In addition: The costs for training activities are not continuous. Therefore, we allocate one person-month per year for these training activities and 1500 EUR travel money.

TCCON sites (national facilities)

The cost books for all sites are available. Below ranges are given as indicative costs.

Personnel (per site)

Position	Fraction of full time position
Expert scientist / Qualified operator / Technician	1.0 – 1.5 per site

Other costs (per site, per year)

Position	Cost (EUR)	Example
Consumables	7 000	Solar tracker: mirrors electronics, cables, switches and valves; compressed air system: valves and filter, Vacuum pump: membrane + sealings, desiccant, UPS batteries, IT material, electronics, ...
Shipping cost for EM27/SUN and the pressure standard	400 - 4000	Shipping costs EM27/SUN
Utilities	4 000 – 20 000	Electricity (strongly varying consumption and costs between sites)
Other costs	0 – 7 500	Site rent, internet
Travel	3 000 – 17 000	Site maintenance (cost depend strongly on site location), ICOS-MSA and TCCON meetings.

(The higher costs are arising from the site on Ascension Island. The costs for the individual sites have been compiled and are available upon request.)

Depreciation of equipment (indicative costs, vary with site)

Equipment	Total Cost €	lifetime	Depreciation cost per year €
Bruker 125 HR set-up	€ 371,300	20	€ 18,565
Solar tracker incl cover	€ 90,000	10	€ 9,000
UPS	€ 5,000	5	€ 1,000
Laser	€ 7,000	5	€ 1,400
Computer/IT	€ 8,000	3	€ 2,667
Vacuum pump	€ 6,000	6	€ 1,000
Compressor/air dryer	€ 5,000	4	€ 1,250
Air condition unit	€ 5,000	10	€ 500
meteorological station	€ 9,000	10	€ 900
Special container	€ 90,000	10	€ 9,000
Total Equipment	**€ 596,300**		**€ 45,282**

Costs for the implementation of Rapid Delivery (RD) data

Currently only the stations Bialystok (now Cyprus), Orleans and Reunion have the capabilities to provide rapid delivery data. All other stations need to implement it. For the implementation 3-4 person months and 5000-10000 EUR hardware are needed.

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7. List of abbreviations

ICOS – Integrated Carbon Observation System

TCCON – Total Carbon Column Observing Network

SCIAMACHY – SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY

WMO – World Meteorological Organization

GHG – Greenhouse gas

RI – Research Infrastructure

FAIR – Findable, Accessible, Interoperable, Reusable

QA/QC – Quality Assessment / Quality Check

GOSAT – Greenhouse Gases Observing Satellite

OCO – Orbiting Carbon Observatory

TANSAT – CarbonSat, a Chinese Earth observation satellite

GEOCARB – Geostationary Carbon Cycle Observatory

MERLIN – Methane Remote Sensing Lidar Mission

CAMS – Copernicus Atmosphere Monitoring Service

FTIR – Fourier-Transform InfraRed

ILS – Instrument Line Shape

NDACC – Network for the Detection of Atmospheric Composition Change

SNR – Signal to Noise Ratio

SZA – Solar Zenith Angle

ZPD – Zero Path difference

OPD – Optical Path Difference

ME – Modulation Efficiency

NCEP – National Center for Environmental Predictions

RD – Rapid Delivery

CP – Carbon Portal

PID – Persistent Digital Identifier