

ECMWF Feature article

.....
from Newsletter Number 143 – Spring 2015

METEOROLOGY

.....
**Atmospheric composition
in ECMWF's Integrated
Forecasting System**
.....



tounka25/iStock/Thinkstock

www.ecmwf.int/en/about/news-centre/media-resources

doi:10.21957/famzeuhd

This article appeared in the *Meteorology* section of *ECMWF Newsletter* No. 143 – Spring 2015, pp. 20–25.

Atmospheric composition in ECMWF's Integrated Forecasting System

Vincent-Henri Peuch, Richard Engelen, Johannes Flemming, Vincent Huijnen (KNMI), Antje Inness

Weather conditions can have a strong influence on atmospheric composition, and composition can in turn have a significant impact on weather-related atmospheric processes, such as radiation and microphysics. Integrating atmospheric composition into numerical weather prediction models can thus not only help to produce reliable forecasts of composition but can also improve the skill of weather forecasts. The benefits of considering the interaction between composition and meteorology have been documented in several individual cases (*Baklanov et al.*, 2014).

As part of the EU-funded Monitoring Atmospheric Composition and Climate research and development projects (MACC), ECMWF has devoted significant efforts to integrating a detailed representation of atmospheric composition and associated processes into its Integrated Forecasting System (IFS). The resulting system, C-IFS (Composition-IFS), is presented in this article. The system has been extensively validated both in model-only and data assimilation configurations and replaced the previous system in September 2014, in anticipation of transitioning to the operational phase of the Copernicus Atmosphere Monitoring Service (CAMS). C-IFS is effectively one of the first examples of a new class of global forecasting systems capable of delivering combined weather and environmental services.

Just like the IFS, C-IFS will undergo continuous development, including a resolution upgrade expected for later this year.

From IFS-MOZART to C-IFS

Modules for the simulation of atmospheric chemistry have been implemented in the IFS since 2009 as part of the MACC series of projects. Forecasts and data assimilation of reactive gases were initially produced with a coupled system, comprising the IFS and a chemical transport model, MOZART, which simulates atmospheric chemistry. IFS-MOZART was used for MACC reanalysis and for daily near-real-time forecasts from May 2007 to September 2014. But the coupled approach had limitations, such as the need for interpolation between IFS and MOZART model grids and the duplicate simulation of transport processes.

The drive towards closer integration led to the development of a new model configuration, called Composition-IFS (C-IFS). In C-IFS, the chemistry scheme complements the previously integrated modules for aerosol and greenhouse gases. C-IFS is computationally much more efficient than IFS-MOZART because the chemistry scheme is fully integrated into the IFS. The first version of C-IFS also uses a different chemical mechanism (CB05), which is simpler and only accounts for tropospheric chemical processes.

C-IFS is expected to provide reanalyses, analyses and forecasts at the global scale, covering atmospheric composition comprehensively (aerosols, reactive gases and greenhouse gases). These datasets constitute the 'global' service line of CAMS. In the following, we present a brief overview of evaluation results for certain key reactive gases. More detailed validation results can be found on the MACC/CAMS website in the form of quarterly reports (www.copernicus-atmosphere.eu). For more details on C-IFS, see Box A.

Evaluation of C-IFS

An evaluation exercise covering the year 2008 has been carried out to compare C-IFS and IFS-MOZART regarding their skill in representing tropospheric composition (*Flemming et al.*, 2015). The MACC reanalysis (*Inness et al.*, 2013), based on IFS-MOZART but including the assimilation of chemical satellite retrievals of CO, O₃ and NO₂, has been used as a benchmark. The evaluation showed that C-IFS performed as well as or better than IFS-MOZART and broadly as well as the MACC reanalysis against independent observations.

Compared to IFS-MOZART, C-IFS had smaller biases for:

- CO in the northern hemisphere,
- O₃ in the upper troposphere, and
- Winter-time SO₂ at the surface in Europe.

The main features of C-IFS

A

C-IFS applies the CB05 Carbon Bond chemical mechanism of the chemical transport model TM5. The implementation of CB05 was carried out in close co-operation with the Dutch meteorological service, KNMI. CB05 describes tropospheric chemistry with 55 species and 126 reactions.

C-IFS benefits from the detailed cloud and precipitation physics of the IFS for the calculation of wet deposition and NO emissions from lightning. Wet deposition modelling accounts for the sub-grid scale distribution of clouds and precipitation. Dry deposition is modelled using

pre-calculated monthly-mean dry deposition velocities with a superimposed diurnal cycle. Surface emissions and dry deposition fluxes are applied as surface boundary conditions in the diffusion scheme. Lightning emissions of NO can be calculated either by cloud height or by convective precipitation. The latter parametrization is used in MACC applications. Anthropogenic emissions are taken from the MACC City inventory and biomass burning emissions from the Global Fire Assimilation System (GFAS).

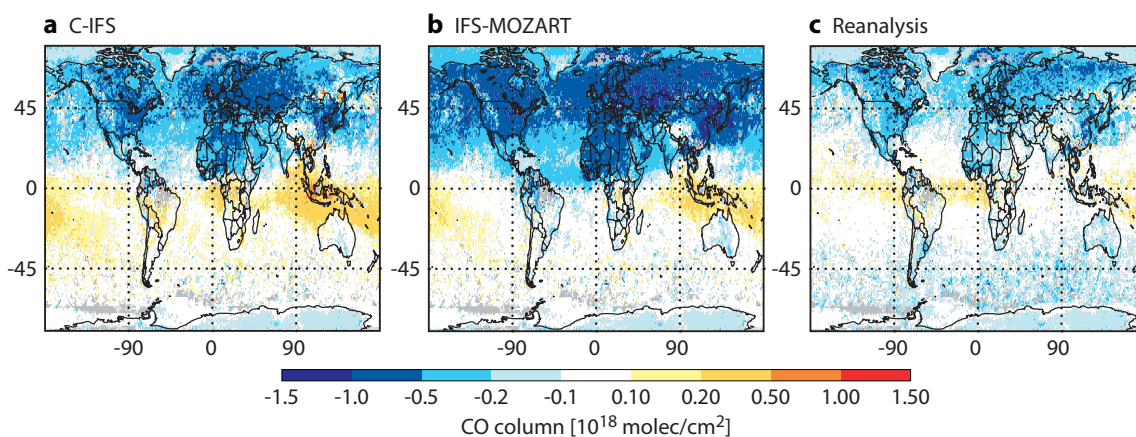


Figure 1 Bias of carbon monoxide (CO) total column with respect to retrieval of MOPITT V6 satellite data for April 2008 of (a) C-IFS, (b) IFS-MOZART and (c) Reanalysis.

As an illustration, Figure 1 shows the bias against MOPITT satellite instrument data for total column CO for April 2008, the month with the highest CO concentrations, of C-IFS, IFS-MOZART and MACC reanalysis. (See Box B for a list of satellite instruments referred to in this article.) Interestingly, the diurnal cycle of surface O₃ also showed greater realism in the C-IFS simulation against independent, spatially representative European air quality observations (not shown). As all configurations used the same emission data, such improvements can partly be explained by differences in the chemical mechanism and the simulation of wet and dry deposition. Further, improvements in SO₂ and the diurnal cycle of O₃ found in C-IFS are most probably caused by the more consistent interplay of diffusion and sink and source processes in the integrated C-IFS compared to the coupled IFS-MOZART system, which by design cannot achieve perfect consistency.

There is still room for improvement of C-IFS. It underestimated surface O₃ over Europe and North America in the spring of 2008 and overestimated it in late summer and autumn. CO was underestimated by C-IFS, in particular in Europe and North America throughout the year and especially in spring and winter, and in the biomass burning season in Southern Africa. Winter-time tropospheric NO₂ over China as retrieved from the GOME-2 instrument was twice as high as the fields modelled by C-IFS, IFS-MOZART and the MACC reanalysis.

Extending the model

Although only one chemical mechanism is used for operational forecasts, C-IFS can apply multiple chemistry schemes. The implementation of the chemistry schemes of the MOCAGE and MOZART chemical transport models (CTMs) has technically been completed, but further optimisation and evaluation is required. Both schemes offer a description of stratospheric chemistry, which is not included in the scheme CB05 currently used in C-IFS. In parallel, work is under way to combine the CB05 mechanism with the stratospheric chemistry mechanism of the BASCOE CTM. In the end, C-IFS is expected to offer several options to represent chemical processes in the troposphere and the stratosphere.

There are plans to further improve the link between the physics and chemistry packages in the IFS. For example, detailed information from the IFS surface scheme will be used for the calculation of dry deposition and biogenic emissions during the simulation. A first important step will be to replace the pre-calculated climatological dry deposition velocities with values calculated based on actual weather and surface parameters in the IFS. Once the stratospheric chemistry is fully implemented, the impact of the simulated O₃ fields on the IFS radiation scheme and the corresponding feedback on the temperature fields will be investigated. Another ongoing development is to create closer links between the C-IFS greenhouse gas, aerosol and gas-phase chemistry modules.

Satellite instruments mentioned

B

MOPITT (Measurements of Pollution in The Troposphere) – an instrument carried on the Terra satellite of NASA's Earth Observing System, measuring tropospheric carbon monoxide.

on the MetOp meteorological satellite operated by the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT).

GOME-2 (Global Ozone Monitoring Experiment-2) and IASI (Infrared Atmospheric Sounding Interferometer) – two instruments carried

OMI (Ozone Monitoring Instrument) – instrument carried on the Aura satellite of NASA's Earth Observing System.

Data assimilation

C-IFS has been used since September 2014 to provide daily analyses and 5-day forecasts for MACC and CAMS. To improve the quality of the atmospheric composition forecasts, several of the chemistry variables (O₃, CO, NO₂, SO₂, HCHO) have been included as control variables in the data assimilation part of the IFS. This means that the initial conditions for these fields can be modified by assimilating observations of atmospheric composition.

In this article, we discuss the assimilation of CO, O₃ and NO₂ retrievals from various sensors. This is described here by comparing O₃, CO, and NO₂ fields from an assimilation run for the year 2008 (CIFS-AN) with fields from a control run without data assimilation (CIFS-CTRL) and against independent observations. More details about the setup of these C-IFS data assimilation experiments and the evaluation results can be found in *Inness et al.* (2015), where we also show that C-IFS in data assimilation mode performs similarly well or better than the coupled system used in the MACC reanalysis for CO, O₃ and NO₂, especially in the lower troposphere and at the surface.

MOPITT data for total column CO are assimilated in CIFS-AN. This leads to an improved total column CO field compared to CIFS-CTRL, and also to some improvements in the vertical distribution of CO and CO concentrations in the lower troposphere. The largest impact is found in the northern hemisphere winter, when the CO lifetime is longest (Figure 2a). In the tropics, there is also some improvement in CIFS-AN, compared to CIFS-CTRL, in surface and lower tropospheric CO, particularly during the South African biomass burning season (Figure 2b).

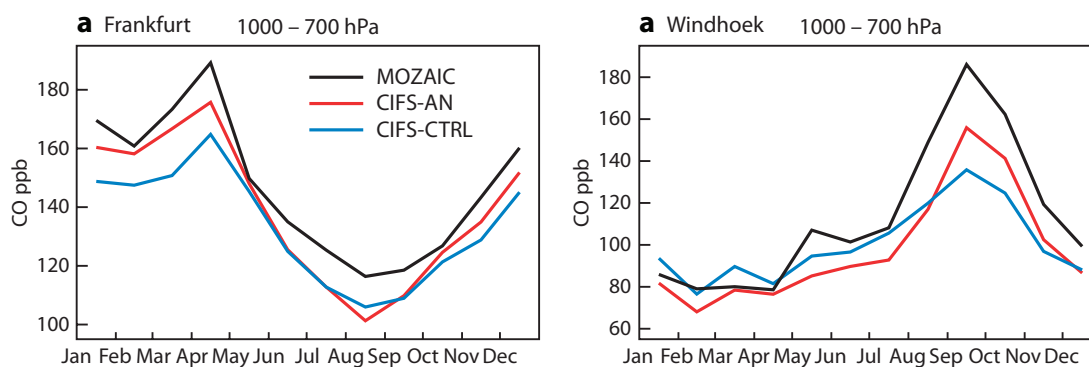


Figure 2 Time series of monthly mean tropospheric carbon monoxide (CO) in ppb over (a) Frankfurt (50°N, 8.6°E, 837 profiles) and (b) Windhoek (22.5°S, 17.5°E, 323 profiles) averaged between 1000–700 hPa from MOZAIC aircraft data, CIFS-AN and CIFS-CTRL in 2008.

The simple stratospheric ozone photochemical parametrization used by the standalone C-IFS (CB05) system to model the stratospheric ozone field is designed to be used in a data assimilation context and leads to a biased stratospheric and total column ozone field in CIFS-CTRL. In CIFS-AN, a combination of ozone total column and stratospheric profile retrievals are assimilated, which greatly improves the total column, the stratospheric ozone field and the upper tropospheric ozone field compared to CIFS-CTRL.

Because no tropospheric O_3 data as such are assimilated, the differences between CIFS-CTRL and CIFS-AN in tropospheric O_3 come from the residual of total column O_3 and the stratospheric profile data and are smaller in the mid- and lower troposphere than in the upper troposphere, as characteristics of the chemistry scheme become more important. For example, a large positive bias in lower tropospheric ozone over East Asia is not reduced by the analysis, and there is little difference in lower tropospheric ozone over Europe and North America during the summer (Figure 3). Nevertheless, there is some improvement in CIFS-AN in the troposphere compared to CIFS-CTRL: the positive ozone bias seen in CIFS-CTRL over Europe and North America during winter and spring in the lower troposphere is reduced.

Testing is under way for the assimilation of O_3 profile retrievals from the GOME-2 and IASI instruments. This will hopefully provide a better constraint on both the stratospheric ozone profiles and the tropospheric ozone burden.

Tropospheric NO_2 column data from the OMI instrument are assimilated in CIFS-AN. As shown in Figure 4, their impact is small because of the short lifetime of NO_2 . Compared to NO_2 retrievals from the GOME-2 instrument, C-IFS with or without assimilation of OMI NO_2 data severely underestimates wintertime NO_2 over East Asia (Figure 4b) and overestimates NO_2 over Southern Africa during the biomass burning season. At other times and over Europe, the agreement is better (Figure 4a).

Even though the assimilation leads to large NO_2 analysis increments, this information is not retained by the model, and most of the impact of the data assimilation is lost from one analysis cycle to the next. It might be possible to improve this slightly by using a shorter assimilation window, e.g. 6-hour 4D-Var, and by using NO_2 retrievals from more than one satellite with different overpass times, but ideally the NO_2 data should be used to adjust the emissions in addition to the initial conditions.

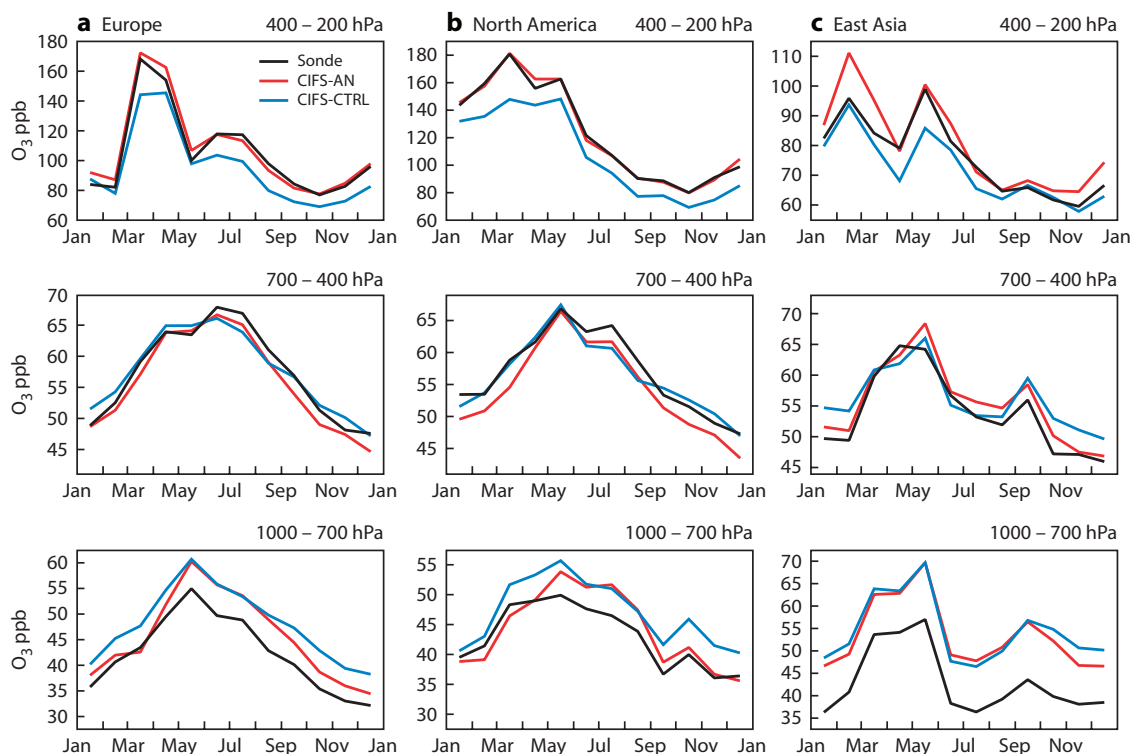


Figure 3 Time series of monthly mean tropospheric ozone (O_3) in ppb over (a) 11 sites in Europe, (b) 11 sites in North America and (c) 4 sites in East Asia averaged in the pressure bands 1000–700 hPa (bottom), 700–400 hPa (middle) and 400–200 hPa (top) from ozone sondes, CIFS-AN and CIFS-CTRL in 2008.

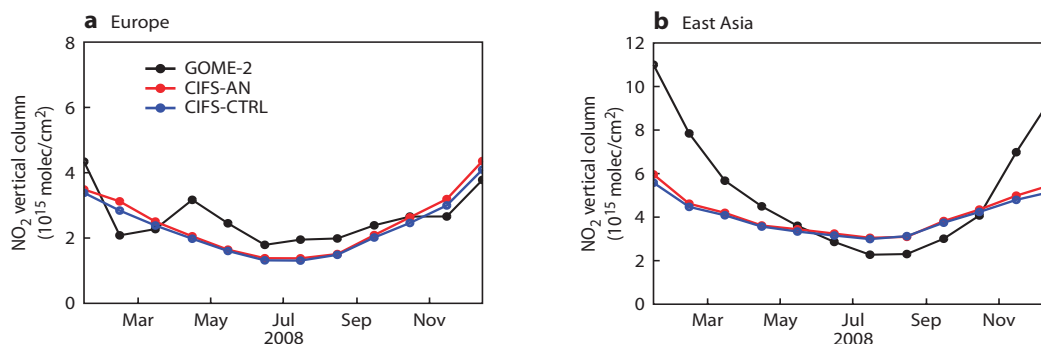


Figure 4 Time series of area-averaged tropospheric nitrogen dioxide (NO_2) columns in 10^{15} molecules/ cm^2 from GOME-2 retrievals, CIFS-AN and CIFS-CTRL for (a) Europe and (b) East Asia. (Figure provided by A.-M. Blechschmidt, University of Bremen.)

Towards a higher resolution

C-IFS currently runs at a horizontal resolution of approximately 80 km at 60 vertical levels (T255L60). While this is a significantly higher resolution than is typically used in current global chemical transport models, it is far less than is used for numerical weather prediction (NWP), which currently runs at approximately 16 km spacing and 137 levels (T1279L137). Increasing the resolution (in particular in the horizontal) of the MACC system is one of the key user requirements. With the move to CAMS, ECMWF will be in a position to increase the resolution of C-IFS in 2015. We have carried out tests at T511L60 (40 km at 60 levels) with the current C-IFS (CB05) system in data assimilation mode.

Two short data assimilation runs were performed at 40 km resolution (T511L60) from 1 to 5 December 2013 and 1 to 5 June 2014. The results were compared with a reference run at 80 km resolution (T255L60). Figure 5 shows 5-day global forecasts of total column carbon monoxide starting from the analysis of 5 December 2013. The standard-resolution experiment is shown in Figure 5a and the increased-resolution experiment is shown in Figure 5b. At first sight, differences are fairly small, because global CO concentrations are mostly determined by large-scale sources and transport.

However, a closer look at, for instance, the European domain makes the impact of an increased resolution more visible, as shown in Figure 6. In this particular case, there is a significant difference in the area around the Alps and the Rhône and Po valleys. At the 40 km resolution, the mountains and valleys are much better resolved, resulting in lower total column CO values over the Alps (the column is smaller because the mountains are higher), and higher values in the river valleys, possibly also because of stronger blocking by the mountains for the Po valley and stronger confinement to the river valley for the Rhône.

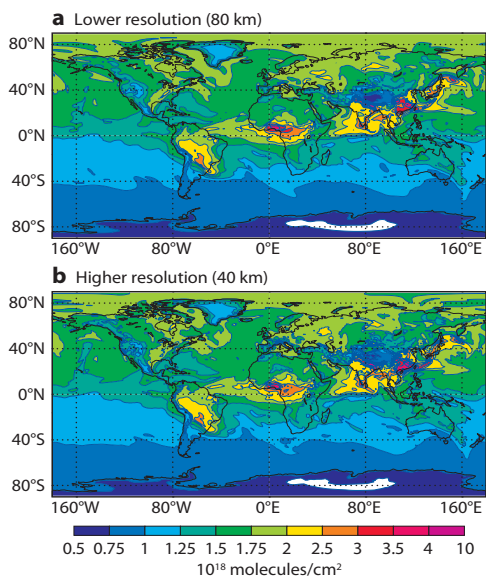


Figure 5 Five-day forecast of total column carbon monoxide (CO) in 10^{18} molecules/ cm^2 starting from 5 December 2013 at (a) T255L60 and (b) T511L60 resolutions.

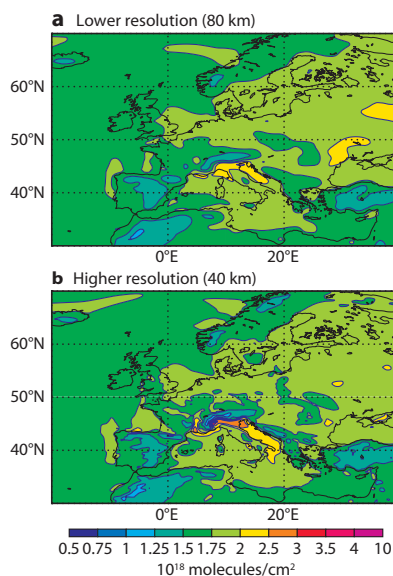


Figure 6 Five-day forecast of total column carbon monoxide (CO) in 10^{18} molecules/ cm^2 for the European domain starting from 5 December 2013 at (a) T255L60 and (b) T511L60 resolutions.

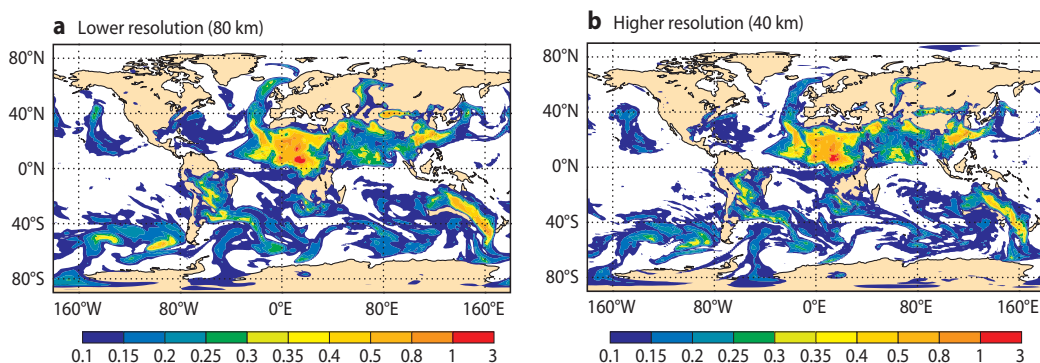


Figure 7 Five-day forecast of aerosol optical depth (AOD) starting from 5 December 2013 at (a) T255L60 and (b) T511L60 resolutions.

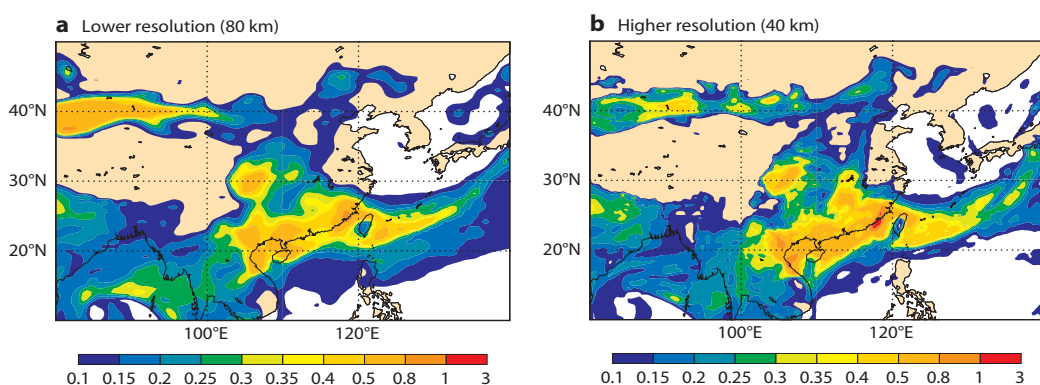


Figure 8 Five-day forecast of aerosol optical depth (AOD) for an Asian domain starting from 5 December 2013 at (a) T255L60 and (b) T511L60 resolutions.

For aerosol the picture is similar. However, as shown in Figure 7, there are larger differences in the global aerosol optical depth (AOD) than in total column CO. This is due to the fact that the amount of sea salt and dust aerosol in the atmosphere is a function of surface wind speeds, which are resolution-dependent, and also because aerosol lifetime is typically of the order of a week (instead of a month for CO), which leaves less time for mixing processes to smooth out high-frequency variability due to emission and transport processes.

This becomes even clearer when we zoom in, this time on South East Asia. Figure 8 shows the AOD distribution for the two runs. The higher-resolution experiment shows more spatial variability, as expected, but also shows much lower values for desert dust over the Gobi desert north of Tibet. The low-resolution run has a smooth field with AOD values between 0.5 and 0.8, while the higher-resolution run has AOD values up to 0.5 with more spatial variability. Validation of longer runs will have to be used to assess which run matches the observed concentrations better.

While the comparisons for CO and AOD are mostly seeing differences due to transport and the meteorological impact on sources, a change in resolution may also be able to improve the modelling of atmospheric chemistry. For example, tropospheric ozone concentrations are determined by highly non-linear chemistry, and a change in resolution will potentially change the extent to which such chemical processes can be captured.

C-IFS has thus been tested successfully in data assimilation mode at a resolution of T511L60 (40 km at 60 levels). While the global distribution of the various species does not change significantly, there are interesting differences at the regional scale. Preliminary results suggest that various factors play a role, such as better-resolved emissions, better-resolved orography, better-resolved transport, the impact of different meteorological conditions on natural surface fluxes, and non-linear chemistry. A thorough investigation is under way to verify these results against independent observations. This should shed further light on the benefits of increasing the resolution of the C-IFS run operationally for CAMS.

Next steps

With MACC-III finishing in mid-2015, CAMS will take over the delivery of services and will progressively transition to operational status. While most CAMS service elements are currently the subjects of Invitations to Tender, global CAMS products will be delivered by ECMWF using C-IFS. Activities are under way between ECMWF's Research, Forecast and Computing Departments in order to organise the transition to operational status. This transition aims to minimise the impact on current users of MACC-III, of whom there are about three thousand now.

In addition to supporting the delivery of CAMS services, C-IFS offers an excellent framework for studying and testing feedbacks between composition and meteorology at the global scale. The coupling between ozone and radiation in the critical region of the upper troposphere and the lower stratosphere is for instance expected to be improved by the explicit treatment of tropospheric ozone. This is expected to improve numerical weather prediction beyond what could be achieved with the linear scheme for stratospheric ozone currently used in the IFS. Aerosol is also a key area for progress. The accurate treatment of highly variable emissions (dust, biomass burning, sea salt, etc.) is expected to capture variability especially in the tropical band. Finally, consideration of atmospheric composition in 4D-Var data assimilation could also bring benefits, in particular because the representation of radiative properties of the atmosphere can be made more realistic for radiance assimilation and because certain species have tracer-like properties that can provide information on atmospheric motions and winds.

Currently, MACC production is run separately from the weather forecasting operation. Research is under way to investigate the merging of production chains by enabling the handling of different simultaneous data grids in the IFS. In addition to providing operational synergies, this will pave the way for next-generation, fully integrated weather and environmental monitoring and forecasting applications.

Further reading

Baklanov, A., K. Schlünzen, P. Suppan, J. Baldasano, D. Brunner, S. Aksoyoglu, G. Carmichael, J. Douros, J. Flemming, R. Forkel, S. Galmarini, M. Gauss, G. Grell, M. Hirtl, S. Joffre, O. Jorba, E. Kaas, M. Kaasik, G. Kallos, X. Kong, U. Korsholm, A. Kurganskiy, J. Kushta, U. Lohmann, A. Mahura, A. Manders-Groot, A. Maurizi, N. Moussiopoulos, S.T. Rao, N. Savage, C. Seigneur, R.S. Sokhi, E. Solazzo, S. Solomos, B. Sørensen, G. Tsegas, E. Vignati, B. Vogel, & Y. Zhang, 2014: Online coupled regional meteorology chemistry models in Europe: current status and prospects, *Atmos. Chem. Phys.*, **14**, 317–398, doi:10.5194/acp-14-317-2014.

Flemming, J., V. Huijnen, J. Arteta, P. Bechtold, A. Beljaars, A.-M. Blechschmidt, B. Josse, M. Diamantakis, R.J. Engelen, A. Gaudel, A. Inness, L. Jones, E. Katragkou, V. Marecal, V.-H. Peuch, A. Richter, M. G. Schultz, O. Stein & A. Tsikerdekis, 2015: Tropospheric chemistry in the Integrated Forecasting System of ECMWF, *Geosci. Model Dev.*, **8**, 975–1003, doi:10.5194/gmdd-8-975-2015.

Inness, A., A.-M. Blechschmidt, I. Bouarar, S. Chabrilat, M. Crepulja, R.J. Engelen, H. Eskes, J. Flemming, A. Gaudel, F. Hendrick, V. Huijnen, L. Jones, J. Kapsomenakis, E. Katragkou, A. Keppens, B. Langerock, M. de Mazière, D. Melas, M. Parrington, V.-H. Peuch, M. Razinger, A. Richter, M.G. Schultz, M. Suttie, V. Thouret, M. Vrekoussis, A. Wagner & C. Zerefos, 2015: Data assimilation of satellite retrieved ozone, carbon monoxide and nitrogen dioxide with ECMWF's Composition-IFS, *Atmos. Chem. Phys. Discuss.*, **15**, 4265–4331, doi:10.5194/acpd-15-4265-2015.

Inness, A., F. Baier, A. Benedetti, I. Bouarar, S. Chabrilat, H. Clark, C. Clerbaux, P. Coheur, R.J. Engelen, Q. Errera, J. Flemming, M. George, C. Granier, J. Hadji-Lazaro, V. Huijnen, D. Hurtmans, L. Jones, J.W. Kaiser, J. Kapsomenakis, K. Lefever, J. Leitão, M. Razinger, A. Richter, M.G. Schultz, A.J. Simmons, M. Suttie, O. Stein, J.-N. Thépaut, V. Thouret, M. Vrekoussis, C. Zerefos, & the MACC team, 2013: The MACC reanalysis: an 8 yr data set of atmospheric composition, *Atmos. Chem. Phys.*, **13**, 4073–4109, doi:10.5194/acp-13-4073-2013.

© Copyright 2016

European Centre for Medium-Range Weather Forecasts, Shinfield Park, Reading, RG2 9AX, England

The content of this Newsletter article is available for use under a Creative Commons Attribution-Non-Commercial-No-Derivatives-4.0-Unported Licence. See the terms at <https://creativecommons.org/licenses/by-nc-nd/4.0/>.

The information within this publication is given in good faith and considered to be true, but ECMWF accepts no liability for error or omission or for loss or damage arising from its use.