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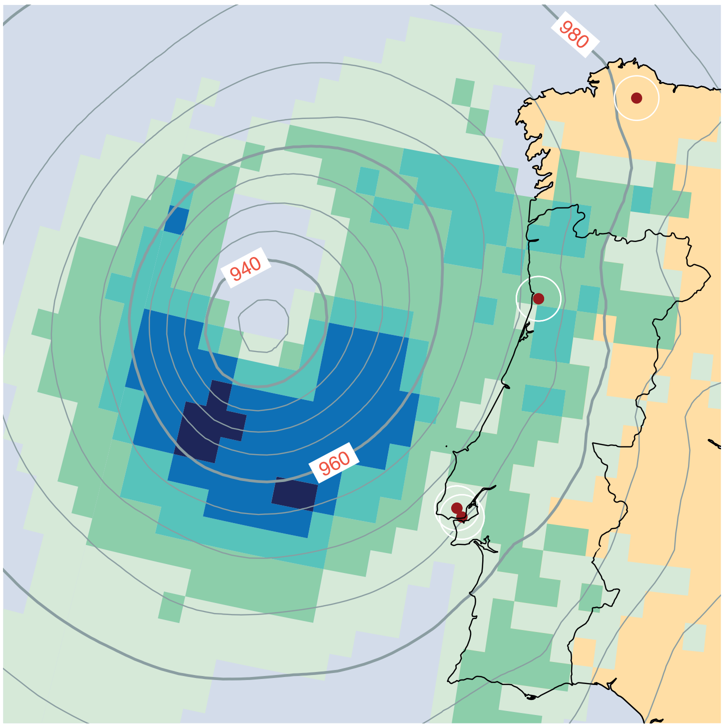
Enhancing OpenIFS by adding atmospheric composition capabilities



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Enhancing OpenIFS by adding atmospheric composition capabilities

Marcus O. Köhler, Adrian A. Hill (both ECMWF), Vincent Huijnen,
Philippe Le Sager (both KNMI)

OpenIFS is a portable version of ECMWF's global weather forecasting model. Over the past decade, its user community has grown continually, and the model is used for research in many areas of atmospheric science. This has been further expanded with the release of the OpenIFS/AC model in 2022. This extension of OpenIFS permits the simulation of atmospheric composition, including trace gases and aerosols and their interaction with other atmospheric processes.

The road to OpenIFS/AC

For more than a decade, the OpenIFS activity has provided supported, portable configurations of the operational ECMWF Integrated Forecasting System (IFS) (Carver, 2022). The broad aims of OpenIFS are to facilitate easier ways for scientists in ECMWF Member and Co-operating States to access the IFS, to enable its external use for research and teaching on numerical weather prediction (NWP), to promote knowledge exchange, and to enhance collaborations between national hydrological & meteorological services, universities and research institutes.

The OpenIFS model is a 3D global forecasting model which consists of the IFS atmospheric model with all the subcomponents for forecast-only simulations, including the fully coupled land surface and ocean surface wave model. Since OpenIFS is designed to be light-weight and for forecast-only applications, the observational data processing system and data assimilation are excluded.

OpenIFS is distributed under a free licence agreement which permits its use for teaching and research. Its user community has grown from year to year, and it now consists of over one hundred licensed institutes, which are mostly located in and around Europe. OpenIFS users engage in a wide spectrum of scientific and technical modelling activities, which cover simulation timescales from short forecasts to climate simulations. The research carried out by OpenIFS users extends over an impressive range of topics that is increasingly reflected in the published literature. OpenIFS is also a useful tool for professional training and for teaching the next generation of atmospheric scientists, both internally at ECMWF and at other institutions. An overview of some of the uses of OpenIFS in training and teaching is shown in Szépszó et al. (2019).

An expanding area of research is the linkage between air quality, meteorology and associated feedbacks of air quality on weather forecasting. This includes the short-term variability of trace gas and aerosol processes in the atmosphere at a range of spatial scales. When linked to weather forecasts, predicted air quality can contribute to mitigating the public health impacts caused by air pollution. It can also help in the identification of air pollution sources and rapid changes in emissions of primary pollutants or their chemical precursors. Growth in supercomputer performance and improved accuracy in operational forecasting, combined with an improved understanding of atmospheric chemistry and aerosol processes, make it possible to consider full two-way interaction and feedback between chemistry and meteorology in global models.

The standard OpenIFS distribution does not include the scientific or technical capability to simulate composition processes (trace gases and aerosol) alongside meteorology. The OpenIFS – Atmospheric Composition project (OpenIFS/AC) aimed to address this by adding interactive composition functionality. OpenIFS/AC is a collaborative project between ECMWF and Member State scientists in the Netherlands and in Finland, under the leadership of the Royal Netherlands Meteorological Institute (KNMI).
The main aim of OpenIFS/AC is to incorporate atmospheric composition components of the IFS into OpenIFS. These components are used by the EU's Copernicus Atmosphere Monitoring Service (CAMS) implemented by ECMWF. Such a development extends the capability of the OpenIFS model to include additional code that allows the simulation of many processes that affect atmospheric composition coupled to meteorology. This includes both gas-phase chemistry, in the troposphere and in the stratosphere, and aerosol-related processes in the troposphere. This new capability widens the scope of research that can be undertaken by the OpenIFS community, by providing a tool for studying the interactions between atmospheric composition and either NWP or the climate system.

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On the role of atmospheric composition

Understanding and modelling atmospheric composition is fundamental for the prediction of local air quality, which is an important aspect of public health and depends on the ambient concentrations of trace gases and aerosol in the atmosphere. Furthermore, gases and aerosols can interact with Earth's radiative balance, resulting in local heating or cooling, which can influence atmospheric processes in the short term, relevant for NWP, and on longer timescales, relevant for the climate system. On NWP timescales, experimental and modelling studies have shown that many meteorological processes and phenomena, such as cloud and fog formation and lifetime, precipitation, and radiative balance, are influenced by aerosol processes and the chemical composition of the atmosphere (e.g. Miltenberger et al., 2018). So, in future, greater complexity may be justified for global NWP. On longer timescales, atmospheric composition is relevant for studies of the present as well as for past and future climates, reflecting natural variability in the abundance of chemical compounds and their historical change due to human activities. In the context of Earth system modelling, the representation of atmospheric composition and its associated radiative impacts on the climate system have featured prominently in many assessments of the Intergovernmental Panel on Climate Change. In the context of identifying policy measures aimed at improving air quality or mitigating near-term climate change, it is essential to gain an understanding of the processes that govern the presence and the amounts of these constituents and of the factors that affect their variability and temporal evolution.

Many of these constituents are released into the atmosphere through direct natural and anthropogenic emissions. They often form chemical precursor components for complex chemical reaction chains. The distribution of trace gases is partly determined by small-scale processes, such as turbulent mixing, and by large-scale transport processes, such as convection. Physical removal also plays a significant role, either by dry deposition on the Earth's surface or through wet scavenging, involving uptake in cloud droplets and precipitation processes. The largest part of the reactive constituents is, however, controlled through chemical processes, especially photochemistry. This can either occur in the gas phase between trace gases, as seen for instance in summertime ozone smog, or it can involve liquid or solid aerosol particles, for which the processes leading to stratospheric ozone depletion are one of the best-known examples.

When considering NWP spatial and temporal resolutions, these processes have historically been simulated with considerable detail through Chemical Transport Models (CTMs). CTMs are driven by external meteorological fields, such as operational forecasts or global reanalyses. Importantly, they cannot give direct feedback on the meteorological fields. This dependence on meteorological inputs without any feedback represents a limitation in the sense that the full loop of interactions between constituents and physical processes is not closed. An alternative to CTMs are weather forecasting models in which the explicit treatment of atmospheric composition is coupled to the meteorology. An overview of such models is shown in Baklanov et al. (2014). One of these is the IFS in CAMS configuration, which is an extended version of the IFS used to simulate trace gases and aerosol in the atmosphere in an operational context and to provide reanalyses that contain assimilated observations of atmospheric composition. Such interactive coupling between composition and meteorology generates additional computational costs when they both use the same model grid. The increase in the performance of high-performance computing facilities in recent years enables the inclusion of explicit and detailed chemistry in global weather forecasting models, such as OpenIFS. OpenIFS/AC is a research tool that offers some of the capabilities of the operational IFS as used in CAMS, by permitting the full interaction between meteorology, its impacts on atmospheric composition, and related radiative feedbacks.

Creating OpenIFS/AC

Version 1 of OpenIFS/AC, which was released in 2022, includes the implementation of a chemistry and aerosol scheme in the model. This has been achieved by porting modules developed for the IFS as part of CAMS activities. The tropospheric chemistry module originates from the TM5 CTM, as developed and updated at KNMI (Flemming et al., 2015), and the reactions are based on a modified version of the Carbon Bond 2005 (CB05) chemical mechanism, originally developed for the US Environmental Protection Agency. Additionally, a stratospheric chemistry module can be enabled, which is based on the Belgian Assimilation System for Chemical ObsErvations (BASCOE) (Huijnen et al., 2016). The AER bulk bin aerosol scheme to represent tropospheric aerosol (Rémy et al., 2019) has also been included. The OpenIFS/AC model can therefore be used in various configurations, either with tropospheric chemistry (CB05), additional stratospheric chemistry (CB05+BASCOE) and optionally with the AER tropospheric aerosol code enabled. In the current release of OpenIFS/AC, the tropospheric chemistry and aerosol schemes are closely aligned with those used for the CAMS reanalysis. Note that in the stratosphere the tropospheric chemistry version uses a linearised ozone parametrization. A more complete technical description of the OpenIFS/AC model is available in Huijnen et al. (2022). Examples for results from atmospheric composition modelling are given in Figures 1 to 3, showcasing the ability of OpenIFS/AC to simulate stratospheric ozone, enhanced aerosol due to anthropogenic and fire emissions, and tropospheric NO_2, which is a marker of various pollution sources and plays an important role in tropospheric ozone production.

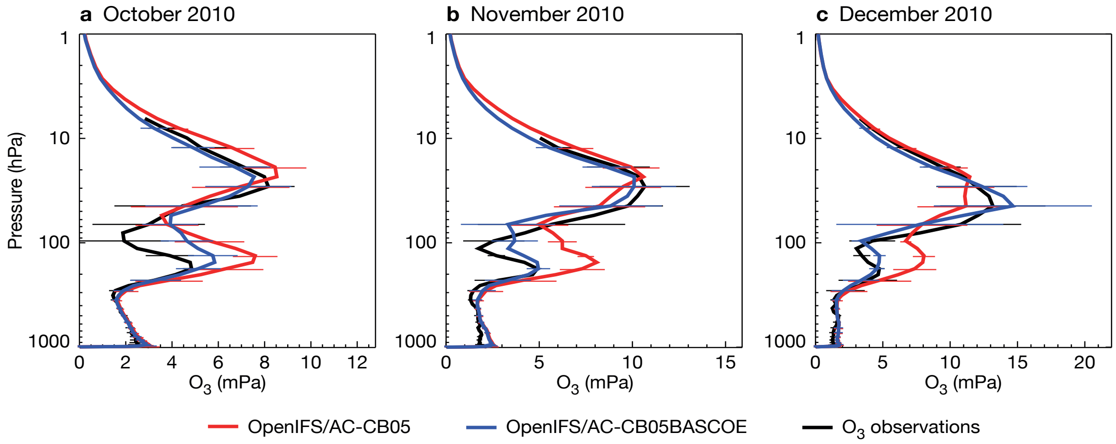

Figure 1 Evaluation of OpenIFS/AC stratospheric ozone against sondes (black lines) during (a) October 2010, (b) November 2010, and (c) December 2010 at Neumayer station (Antarctica) showing the performance of OpenIFS/AC-CB05 (red lines) and the OpenIFS/AC-CB05BASCOE (blue lines) configurations to simulate stratospheric ozone depletion.

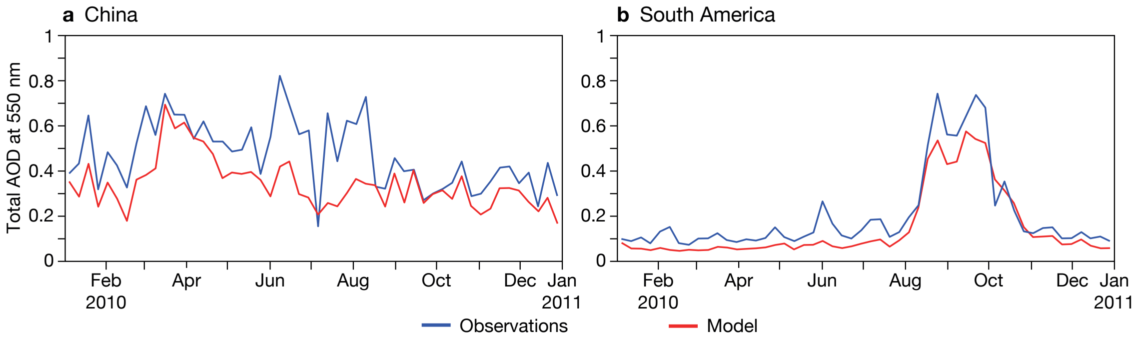

Figure 2 Evaluation of total aerosol optical depth (AOD) at 550 nm from OpenIFS/AC (red) against observations from the AERONET network of ground-based sun photometers (blue) between January 2010 and January 2011 for stations in (a) China, and (b) South America, representative of pollution due to anthropogenic and biomass burning sources.

The chemistry schemes have been designed to represent essential chemical processes on a global scale, suitable for a global forecast model in an NWP framework. It is, however, possible to adapt these schemes to different purposes. Complexity can be added or removed for specific applications or to provide various constraints to the model to simulate certain time periods. This can be achieved by providing relevant input parameters for the initial conditions and composition surface fluxes at the start of the run. Different ways to constrain meteorology and surface fluxes throughout the run can also be used. One feasible way to achieve this is by running the model in 'nudged mode', relaxing various meteorological variables either globally or regionally towards provided input fields. The nudging method is particularly suitable to constrain the model towards specific atmospheric conditions that occurred during a given period in the past.

The computational requirements for the simulation of complex atmospheric chemistry are high. The reason is, firstly, the introduction of additional model fields for atmospheric composition data, including calculations related to their transport and associated diagnostics. Secondly, additional calculations required for chemical reactions and physical loss processes also make a big contribution. Huijnen et al. (2022) estimate that activating the tropospheric chemistry scheme increases computational

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costs between a factor of three to four compared to an OpenIFS experiment without chemistry. As a result, a compromise between model resolution and the complexity of chemistry needs to be found to reduce the computational overhead. Because atmospheric composition uses the same grid as the other model processes, global model experiments with atmospheric composition often use grid resolutions that are significantly coarser compared to those used in NWP. Also, for longer simulation time periods, alternative chemical mechanisms with reduced complexity are used. To make simulating atmospheric composition computationally affordable, a range of chemistry and aerosol schemes with varying complexity need to be employed depending on the science goals.

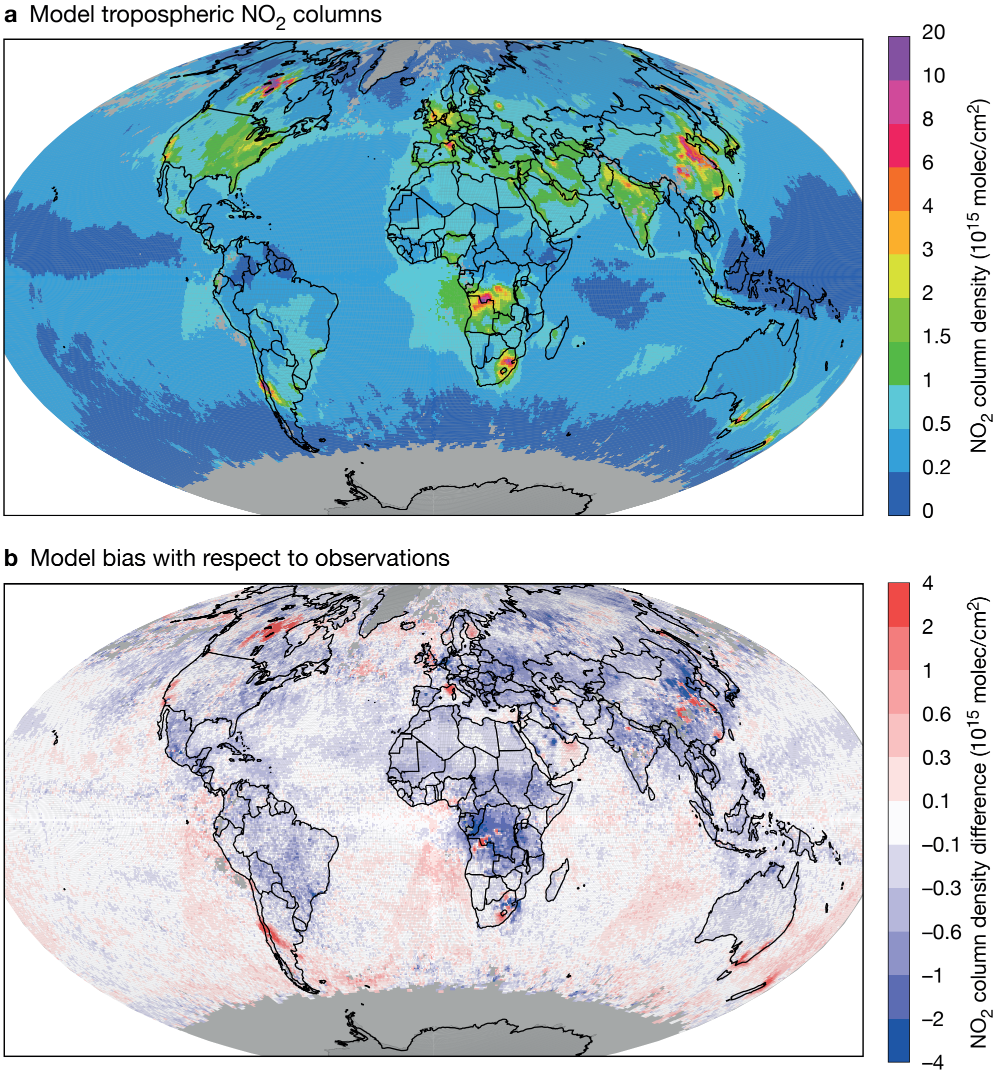

Figure 3 Evaluation of OpenIFS/AC-CB05 tropospheric NO_2 columns against Ozone Monitoring Instrument (OMI) satellite observations, averaged for July 2010, showing (a) model tropospheric NO_2 columns, and (b) model bias with respect to the observations. The hotspots in the biases are mainly driven by emissions.

While OpenIFS can be used with a wide range of horizontal model grids and a varying number of vertical levels, equivalent to those available for the IFS, using this flexibility for OpenIFS/AC would require providing input data at all grid resolutions. Currently the input data for the model chemistry is only made available for one model grid configuration, a linear reduced Gaussian grid of TL255, corresponding to approximately 80 km grid point spacing, and for 91 vertical model levels. This grid resolution was selected as a compromise between computational costs and expected usefulness for a range of model applications. Input data for other model grid resolutions will become available in the future.

Next steps for OpenIFS/AC

OpenIFS/AC is an ongoing activity. The aim is to continue providing and further expanding the capability of atmospheric composition modelling in future OpenIFS releases. OpenIFS/AC benefits from recent model developments undertaken in CAMS. In addition, new developments and improvements will be included that are currently not available in CAMS. The next release of OpenIFS/AC, Version 2, will be the last to be based on the current OpenIFS 43r3, with subsequent releases using the next available cycle of the OpenIFS model. Version 2 of OpenIFS/AC will include an alternative scheme to represent tropospheric aerosol in the model, together with a parameterized sulphate production scheme, to make it particularly suitable for climate applications.

The main motivation for this effort is that OpenIFS has been adopted as the atmospheric modelling component of the EC-Earth consortium (*https://ec-earth.org*), who develop an Earth system model for climate modelling by its European user community. Earth system climate modelling requires the representation of processes relevant to longer timescales and of compounds relevant to the climate system (such as primarily greenhouse gases and aerosol), many of which are also controlled to a certain degree by atmospheric chemistry. To answer various questions on climate sensitivities, different levels of composition modelling are required. The consortium's latest model, version EC-Earth4, includes the current OpenIFS 43r3 together with its extension for atmospheric composition.

Simulations over longer timescales often benefit from the reduction in computational costs when chemistry schemes with reduced complexity are employed. In Version 2, this will become available through a reduced parametrization focusing on sulphur compounds. The scheme employs monthly climatologies of oxidant fields (e.g. oxides of hydrogen and ozone). For consistency, these oxidant fields have been pre-computed with the full-complexity chemistry scheme, and they provide the necessary inputs for a reduced-complexity sulphate aerosol chemical mechanism. In this case, the explicit simulation of photochemical processes for the short-lived oxidants has been removed. This is an acceptable limitation for studies which extend over long timescales or which have a predominant focus on aerosol processes.

This reduced chemistry can be coupled to a more detailed aerosol code, M7, which will also become available in Version 2. The M7 scheme is a double-moment modal aerosol microphysics scheme, in which aerosol is represented in size modes, with a prognostic mass mixing ratio and number concentration (the number of particles per unit volume of air) for each mode. It accounts for internal mixing of different chemical components within aerosol particles, and it is designed to provide detailed aerosol particle size information. As such, M7 enhances the complexity of aerosol representation compared to the existing AER scheme. AER is a single-moment scheme, wherein aerosol is only represented by mass mixing ratio while the number concentration is assumed. In climate models, double-moment schemes have been shown to improve the description of aerosol optical properties and the representation of important and uncertain aerosol-cloud forcings (e.g. Bellouin et al., 2013), which impact the life cycle of the aerosol particles and their direct and indirect radiative effects. The need for double-moment aerosol schemes in NWP and air quality modelling is an open research question. The inclusion of M7 in OpenIFS/AC creates a flexible system that can tackle this research topic.

Finally, simulating atmospheric composition requires a range of additional model inputs to drive the chemical modules. Initial conditions in the form of global fields for all chemical tracers need to be provided at the start of the experiment, as well as boundary conditions for the duration of the run. These include daily fluxes of emitted chemical species, and information on removal rates by deposition subject to surface type. In the current release of OpenIFS/AC, the emission fluxes from natural biogenic sources, from wildfire emissions, and from a range of anthropogenic sectors are lumped together into a single flux per emitted species. These emission fluxes match those used in the Coupled Model Intercomparison Project (CMIP6). To simplify the input data generation process, we aim to expand the capabilities of the OpenIFS Data Hub in a future release to include initial experiment data for OpenIFS/AC experiments.

Conclusion

The release of OpenIFS/AC in 2022 has provided a first model version of OpenIFS that allows the interactive simulation between atmospheric composition and meteorology, based on code extensions that are used in the CAMS operational model. In forthcoming model releases, we plan to expand this new capability by including alternative codes for composition modelling and by supporting more grid resolutions. We also intend to make the generation of input data more convenient, thus making this new research capability attractive to a wider model user community.

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Further reading

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