Coupling global CTMs to ECMWF integrated forecasts system for forecast and data assimilation within GEMS

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Abstract

The paper presents the implementation of a coupled forecast and assimilation system developed within the subproject on Global Reactive Gases (GRG) of the GEMS-project (Global and regional Earth-system (Atmosphere) Monitoring using Satellite and in-situ data, FP6).

One of the main objectives of the GEMS project is to utilise ECMWFs 4D-VAR data assimilation system to assimilate satellite observations of atmospheric composition at the global scale. The GRG subproject focuses on the assimilation of the following gases: carbon monoxide (CO), ozone (O_3), nitrogen oxides ($NO_x = NO + NO_2$), formaldehyde (HCHO) and sulphur dioxide (SO2). These gases play a key role in atmospheric chemistry and are observable from space.

ECMWF's integrated forecast system (IFS) is able to simulate the transport of these tracers but does not contain the modules for the simulation of chemical

conversion, emission and deposition. Instead of directly integrating (in-line coupling) the relevant modules into the IFS, a coupled approach was taken which links the IFS to already established Chemistry transport models (CTM). The coupled approach seemed to be a much smaller development effort, and it offers more flexibility in the choice of the modules for chemical conversion, emission and deposition by coupling different CTMs to the IFS.

The two-way coupled system consists of the IFS and one of the CTMs MOZART3, TM5 and MOCAGE. The coupling software OASIS4 has been implemented to facilitate the data exchange.

In the coupled system, IFS sends meteorological data at high temporal resolution to the CTMs. The CTMs provide concentration tendencies due to emissions and chemical conversion as well as initial tracer conditions to the IFS. The application of external tendencies is required in IFS because its 4DVAR data assimilation needs to account for tracer source and sink terms which are not simulated in the IFS model. Moreover, the tracer transport may benefit from the sophisticated vertical transport schemes of the IFS.

The coupled system has been applied in forecast mode for several months in 2003 in different configurations in terms of vertical transport and coupling synchronisation. Test runs assimilating total columns CO from MOPITT have been successfully carried out for several weeks. Experimental near-real time forecasts with the coupled system have been run since April 2007. This paper focuses on the design of the system.

1 Coupling of earth-system components models

To study the many interactions within the earth-system, numerical models simulating specific aspects of the earth-system can be coupled to each other for an efficient exchange of their results. A coupled model A provides more detailed information about processes which have been treated by simpler assumptions such as explicit or implicit climatologies in model B. If the system is two-way coupled, the response in model B is fed back to model A, leading to different result there, which may again influence model B.

Besides the scientific questions related to the coupling of models, the interaction of the numerical models is a big technical challenge. The transformation of data at different temporal and spatial resolutions as well as computational efficiency, memory consumption, data storage capacity, meta-data communication and code management are issues which have to be addressed.

The most common type of coupling is two-dimensional in space, i.e. the coupled models cover separate three-dimensional domains, such as atmosphere and ocean, which are connected to each other by a two-dimensional interface. Less common is three-dimensional coupling in which both models cover the same or an overlapping spatial domain, e.g. the atmosphere, but consider different aspects of it as in the case of weather forecasts models and chemical transport models (CTM). The amount of data to be exchanged is bigger in three-dimensional coupling and there are further consistency issues if both models simulate the same processes such as transport but in a different way (see section 2.4).

There are various options for the technical implementation of the coupling, which differ in the following aspects:

- Whether or not a dedicated coupling software is used to facilitate the coupling
- Whether or not the coupled models stay independent as executables
- Whether or not the models or modules run concurrent or step-wise sequential.

The tightest way of coupling, often called "in-line", "on-line" or "integrated" coupling, is the exchange by argument passing from subroutines simulating different components and aspects of the earth-system. These "integrated" models tends to have less consistency problems because the integrated modules have been aligned to the general model structure, in particular to model geometry and to decomposition for parallelisation. The integration may require a large coding effort, depending on the code structure of the modules, as well as substantial scientific testing to ensure the scientific integrity of the new modules in the existing model. Further, the integrated approach is less flexible in the choice of the coupled model

and also requires continuous code management in order to benefit from further development of the included models.

For these reasons many coupled systems try to keep some sort of independence of the component models, and the coupling is facilitated by a specific couplingsoftware. Ford and Riley, 2002, give an overview of coupler software developed in North-America and Europe.

The coupling-software mainly consists of two interconnected entities:

- A mechanism to let the coupled models runs together and enable them to exchange data
- An infrastructure to process mete-data needed for the communication of the models

The model developer who wants to couple the models (i) has to include couplerspecific interfaces in the models, and (ii) has to provide the model and coupling meta-data according to standards of the coupling software. Both tasks can be time consuming, and the gain of interoperability has to be balanced against the costs of the implementation.

There are two basic design concepts for the coupling software: "Concurrent coupling" means that independent model executables or modules run at the same time on different computer resources. An additional coupler/driver executable controls the data exchange between the models. "Sequential coupling" relies on a "superstructure" which calls the components models sequentially for each coupling-time step using the same system resources. Sequential couplers can be considered as a partly automated procedure for the "manual" integration of component models as subroutines in one unified model code. Figure 1 shows the schematic of a concurrently coupled system (the GRG system) and integrated / sequential - coupled system. Sequential coupling tends to have less latency problems than concurrent coupling if the two components differ in their computation time. OASIS4 (Valcke and Redler, 2006) and OASIS3 (Valcke, 2006) are examples of concurrent couplers. ESMF (www.esmf.ucar.edu) is an example for "sequential" coupling.

2 The GEMS GRG coupled system at ECMWF

As part of the GEMS subproject on global reactive gases (GRG), a system coupling ECMWFs integrated forecast system (IFS) with chemical transport models (CTM) has been developed. The coupler software OASIS4, which is being developed as part of the prism project and the prism support initiative (http://www.prism.enes.org/), is used to couple the two components in concurrent fashion. The OASIS4 interfaces in the IFS, and the run and configuration environment for the coupled experiments can easily be adapted to couple other earth system model to IFS.

The main motivation for the development of the GRG coupled system was the need to account for sink and source processes, namely chemical conversion, in the assimilation of satellite observation of chemical tracers within the 4D-VAR data assimilation of the IFS. Since it seemed to be costly to integrate complex chemical mechanisms in the IFS, tendencies describing sink and source processes should be provided by well established CTMs, being coupled to the IFS. The three candidate CTMs for the GRG coupled system are MOCAGE (Josse et al., 2004), MOZART (Horowitz et al., 2003), and TM5 (Krol et al., 2005).

A clear benefit of the coupled approach, in contrast to integration, is the flexibility in the choice of different coupled chemical schemes represented by the different CTMs. However, the required three-dimensional coupling is less consistent than an integrated system because of feedback delay and dislocation due different transport representations (see section 2.4) in the IFS and the CTM.

2.1 Configuration of the GRG coupled system

The GRG coupled system is a three-dimensional two-way coupled system: IFS provides atmospheric fields at high temporal resolution to drive the CTMs, and the IFS receives tracer concentration fields and tracer tendencies due to source and sink processes from the CTM. A further coupling option is the feedback of concentration fields from IFS to the CTM.

Depending on which tendency data is exchanged, the GRG coupled system can be run in three modes:

- CTM forecast mode
- IFS tracer forecast mode
- IFS tracer data assimilation mode

The CTM forecast mode is a one-way coupling in which IFS provides the meteorological data on-line to the CTM. The main difference to CTM off-line runs is the high temporal resolution at which the CTM gets the atmospheric data. Typical frequency for the coupling is one hour whereas the temporal frequency in off-line runs is six hours.

In IFS tracer forecast mode the CTM provides initial condition for the chemical tracers (NO_x , NO_2 , SO_2 , CO, HCHO and O_3) and 3D fields of tracer tendencies due to emissions, deposition and chemical conversion to IFS. The IFS simulates the horizontal and vertical transport of these tracers and applies the CTM tendency data in order to account for the source and sink processes not simulated in the IFS. The CTM itself runs as in CTM forecast mode. The feedback option enables replacing the CTM concentration fields, in particular the initial conditions, with the tracer fields of the IFS.

In IFS tracer data assimilation mode, the IFS tracer forecast mode is applied in the outer loops of ECMWF data assimilation system, i.e. the calculation of the trajectories runs of the "complete" model of the 4D VAR (Mahfouf, J. F. and F. Rabier, 2000) The inner loops used in the minimisation step with the tangent linear and adjoint model are currently run uncoupled, i.e. without the application of the source and sink tendencies from the CTM.

In the coupled system the IFS runs in a T159 spectral resolution and the grid point space is represented in the reduced Gaussian grid (Hortal and Simmons, 1991). The vertical coordinate system is given by 60 hybrid sigma-pressure levels. In order to avoid difficulties in the vertical interpolation by the coupler, the CTM use the same 60 vertical levels. The coupler only has to perform horizontal interpolations for which the bi-linear mode is applied. The resolution of the CTM is lower (~T63) as the IFS resolution because of the high computational cost of the CTMs (see table 1). The IFS is run on a higher horizontal resolution would limit the acceptance

of high resolution observations within data assimilation. The coupling frequency is 3600 s which is the largest acceptable time step for the IFS at a T159 resolution, and also the time step of some of the CTMs. The exchange of data can be either provided via a master-process only or via a direct exchange via all processes involved in the simulations.

The following variables are covered by the OASIS4 interfaces in the IFS and the CTMs:

- IFS to CTM
 - o T, Q, U, V (3D grid point)
 - o O₃, NOx, SO₂, CO, HCHO concentration (3D grid point)
 - o ps, taux, tauy, shflx, qflx (2D grid point)
 - Vorticity, Divergence, ps (3D/2D spectral fields)
 - Wavenumber-info (3D/2D spectral fields)
- CTM to IFS (3D grid point)
 - O₃, NOx, SO₂, CO and HCHO tendencies due to chemistry, wet deposition and atmospheric emissions
 - O₃, NO_x, SO₂, CO and HCHO tendencies due to surface fluxes (emission, dry deposition)
 - $\circ~O_3$, NOx, SO₂, CO and HCHO concentration

2.2 Initial condition handling within coupled experiments and feedback

The coupled long-term simulation and data assimilation runs are structured as a sequence of coupled runs (6 h in data assimilation, 24 h in forecast mode) because the IFS needs a re-start from a meteorological analysis as often as possible. The CTM provides the tracer initial conditions of the IFS for the first forecasts. There are three modes of how the initial conditions for the GRG-tracers are obtained in the subsequent forecasts (see Figure 2).

In the "CTM constrained" mode, the IFS gets the initial tracer conditions from the CTM at the start of each forecast. The CTM gets the whole set of initial conditions from the previous CTM run.

In the "free running" mode, this exchange of initial conditions happens only at the first forecasts. Both the IFS and the CTM use initial tracer conditions from their previous runs in all following coupled forecasts.

In "feedback" mode, the CTM will use the tracer initial conditions provided by IFS after the first model run. The IFS tracer fields may now contain information from observations (analysis mode) or may be different from the CTM fields because of different vertical transport simulation in IFS.

2.3 Computational performance of the GRG coupled system:

The main factor for the computational performance of the coupled GRG-system is the individual run time of the IFS and the CTMs at ECMWF high performance computing facility (IBM power5). The computational cost of the CTMs is clearly higher than the one of the IFS in forecast mode (see table 1). The good scalability of the MOZART-3 model at ECMWFs computer led to acceptable run time within the coupled system. However, the MOZART-3 run time is still three times longer than the one of the IFS using only 25% of the CPUs. Further improvements in the run time of TM5 and MOCAGE are required to achieve acceptable run time within the coupled system.

The overhead because of the coupling can be attributed to the couplers set-up phase (only once per run) and the time of the data transfer and interpolation at every coupling time step. In the given setup the overhead is below about 3 % of the IFS stand-alone run time and about 1 % of the overall run time with coupled system IFS-MOZART-3.

A further constrained is the memory consumption of the component models and the OASIS4 coupler. The memory consumption of the coupler occurs only temporarily during the exchange events but can reach up to 60 % of the IFS memory consumption, 15 % of the MOZART-3 consumption and 12 % of the total consumption. Figure 3 shows the memory consumption for each mpi-process of the coupled system IFS-MOZART-3

2.4 Dislocation and feed-back delay

In the case of the GRG coupled system, both the IFS and the CTM simulate both atmospheric transport processes. Different advections scheme or spatial and temporal resolutions may lead to different concentrations fields in the IFS and the CTM. Thus, the applied CTM tendencies can be inconsistent with the concentration fields in the IFS. The worst case scenario would be negative concentration values in the IFS, due to un-balanced loss processes.

One example of the dislocation problem is depicted in Figure 4. O_3 tendency data due to chemical conversion (P&L, green circle) shall be given from a CTM to IFS which does not simulate chemistry. If the O_3 fields in CTM and IFS are dislocated, the tendencies data will be applied in the wrong part of the model domain.

Two-way coupling is required if one wants to study the feedback of processes not included in the models. However, the time scales for the interaction is limited at least by two times the coupling interval. 2-way coupling requires a synchronous run of the two models. Lagged two-coupling, in which one of the component models runs ahead of the other model, is possible if the first model is not sensible to delayed input from the model running behind. Legged two-way coupling can be an option in atmosphere-ocean coupling but is was no option for the GRG-system.

In contrast to one-way coupling or lagged two-way coupling, the information for the next time step is not available in two-way coupling. This makes it impossible to forward-interpolate the external data, e.g. meteorological fields, in time. Instead, they have to be assumed to be constant over the coupling interval.

3 Specific issues of the GRG coupled system

3.1 Formulation of Tendency terms

The exchange of concentration tendencies, rather than concentrations, is a special and perhaps unique feature of the GRG coupled system. The formulation of the tendency terms has to reflect the operator splitting and time stepping in the both the CTMs and the IFS as well as the relation between the tendency and the respective concentration value, and the cost (memory, time) of the exchange. The CTMs use an operator-splitting approach in which chemistry, emission injection, diffusion and deposition are called in sequence and the update of the concentration follows directly within each subroutine.

The total tendency *T* is given by the sum of chemical loss L_C and production P_C , gain due to emissions P_E and loss L_E due to deposition.

 $T = P_C - L_C + P_E - L_D$

Deposition L_D and chemical loss L_C are proportional to the tracer concentration x and a relative formulation L = l x, i.e. a loss rate l, would better link tendency and concentration value and would help to avoid negative concentrations. However, the output arguments of chemical routines provide total tendencies ($P_C + L_C$) for each time step and it would be difficult to distinguish production and loss. The relative formulation of the production is not advisable because it could cause high concentrations values to become even higher. One option would be to link the loss to OH concentrations only.

A disadvantage of separating production and loss, which tend to be much larger in absolute values than the resulting total, seems to be the separate interpolation of these fields. The sum of the interpolated production and loss terms may suffer from inbalances close to strong gradient, in particular if non-linear interpolation is applied.

Emissions are independent of the tracer concentration and can be considered as a surface flux. The injection of the emissions is integral part of the diffusion scheme on MOZART-3, i.e. as lower boundary for the fluxes, whereas TM5 and MOCAGE distribute the injected mass in a fixed ratio over selected layers in the PBL and apply their diffusion operator after the injection. The tendencies of the emissions P_{E_r} , therefore, have to be formulated either as three-dimensional field including the diffusion or as two dimensional flux term. The diffusion in the IFS would have to be switched off if the three-dimension emissions-diffusion tendencies are applied. Air born emissions such as the ones from aircraft would have to be included in the 3D chemistry tendencies, if the surface emissions are expressed as a flux.

Dry deposition occurs at the lowest level and could be expressed both as tendency for the lowest layer or as a flux. Wet deposition would be a three-dimensional tendency field.

The consideration of the arguments discussed above led to the following implementation of tendency extraction within the CTM:

- 1. Process-specific three-dimensional tendencies are determined by calculating the difference of the concentration fields before and after each of the chemistry, emission/diffusion and deposition subroutines.
- 2. The process-specific three-dimensional tendencies are averaged over the coupling interval
- 3. The process-specific tendencies is either added up to **one** three-dimensional total tendency field or added up to **two** three-dimensional tendency fields containing (i) chemistry and wet deposition and (ii) emission and dry deposition.
- 4. The one or two three-dimensional tendency fields are transferred to the IFS

Depending on a control switch, the three-dimensional emission and dry deposition tendencies can be converted into a surface flux by calculating the total column integral within the IFS.

Figure 5 and 6 show profiles of the tendencies due to chemistry and wet deposition as well as emissions including vertical diffusion and convection for NO_x and CO at 12 and 24 UTC. The data are area-averaged over Central Europe (42.0N/-10.0W -55.0N/10.0E) and shown in units of kg/m²s to demonstrate the mass contribution of each model level. Model levels 60-50 cover the PBL, the tropopause is about at level 30. Clearly visible is the day-night difference of chemical loss and production. The emissions are a constant source term but the vertical tendency profiles are shaped by the vertical exchange in the PBL.

3.2 Implementation of GRG-tracers tendency application in the IFS

The simplified sequence of the simulation of a passive tracer within an IFS timestep is as follows:

- 1. Calculate tendencies due to semi-lagrangian advection scheme
- 2. Calculate tendencies due to "physics"
 - a. Calculate tendencies due to surface flux injection and vertical diffusion within one routine
 - b. Calculate tendencies due to convection
 - c. Calculate tendencies due "other" processes (e.g. chemistry parameterisation)
- 3. Update concentration fields from the start with accumulated tendencies of advection and "physics"

Although the process-specific tendencies are stored for the update in a final step, the processes are not treated in an independent, i.e. parallel way. This is because the diffusion-routine uses the concentrations updated with dynamical tendencies and the convection routine uses the concentration updated with the diffusion (and surface flux) tendencies.

The position of the processes in the time loop is influenced by whether the process is fast or slow in respect to the time scale. More details on the implementation of the IFS physics can be found in Beljaars, 2004. Since the coupling interval (1-3 hours) is larger than the model time step, the processes parameterised by CTM input will appear as slow processes, even if the actual chemical conversion can be rather quick in the CTMs.

In the IFS, emission injection and diffusion are part of one subroutine. Surface emissions, and likewise (dry) deposition, can be treated as surface fluxes. If the applied CTM tendencies already included the effect of diffusion and convection, the respective routine in the IFS physics would have to be switched off for this GRG-tracer.

The application CTM source and sink information can be implemented in two modes:

1. IFS with complete CTM "physics" for tracers: All "physics" tendencies (diffusion, convection, emission, chemical conversion, deposition) come from CTM.

2. IFS with CTM chemistry tendencies (3D) and CTM surface fluxes (emission and dry deposition)

In the first mode, the IFS would only advect the GRG-tracers. The CTM tendency field, consisting of the contributions of all source and sink processes, would be consistent in itself. Dislocation could occur due to different advection in the CTM and the IFS.

In the second mode, a consistent treatment of the emission injection and vertical transport would be achieved. In particular, the adjoint formulation of diffusion and convection in data assimilation would be consistent with the forward model. However, dislocation of the chemistry tendencies is more likely than in case 1 because the IFS concentration fields tend to differ more from the CTM fields.

3.3 A diagnostic NOx inter-conversion operator for fast reaction not captured by the coupled approach

The fast and quickly moving diurnal NO_2 - NO inter-conversion caused by solar radiation in the upper stratosphere could not be handled by the coupled system with a coupling frequency of one hour. Instead of a steady movement of the day-night border, a "carved" stripe-shaped concentrations field were simulated. Therefore it was decided to use NO_x as the model variable since the chemical development of the NO_x fields is not so strongly influenced by solar radiation and the development of the NO_x fields can be simulated by the coupled system.

Since the satellite observations to be assimilated are NO_2 data, a diagnostic NO_x to NO_2 inter-conversion operator *H* was developed. For the application in 4D VAR data assimilation it's tangent linear **H** and adjoint **H**^T had to be coded.

The inter-conversion operator is based on a simple chemical equilibrium between the NO₂ photolysis rate j_{NO2} and the O₃ concentration:

$[NO_2]$	$k_2[O_3]$		
$\left[NO_{x}\right]$	$\int j_{NO_2} + k_2 [O_3]$		

The diagnostic NO₂/NO_x ratio depends on the following variables:

- Solar zenith angle
- O₃ -concentration
- Slant O₃ column above
- Temperature
- Surface albedo

A parameterised approach for the calculation of clear-sky NO₂ - photolysis j_{NO2} rates was used based on the band scheme by Landgraf and Crutzen (1998) in combination with actinic fluxes parameterised following Krol and Van Weele (1997). The diagnostic operator does not reflect the influence of clouds on j_{NO2} , and the adjustments to the equilibrium because of hydro-carbons lower troposphere and abundant O-radical in the higher stratosphere and mesosphere.

The missing cloud influence might be tolerable since the NO₂ observations tend to be restricted to conditions with small cloud cover (Boersma et al. 2004).

The inter-conversion operator links the NO_2 to the O_3 concentration and temperature field in data assimilation. It is the first step towards the consideration of more chemical relationships within the GRG data assimilation system.

Figure 7 shows a profile of the NO_2/NO_x ratio over Europe at 12 UTC calculated by the diagnostic operator and directly from the MOZART NO and NO_2 fields. An adhock approach of assuming a per-oxy-radical (HO₂ + RO₂) concentration 80 ppt (Kleinman et al. 1995) in the troposphere, multiplied by the cosine of the solar zenith angle to account of the diurnal cycle of the in the per-oxy-radical concentration, improved further the match of the NO_2/NO_x ratio between the diagnostic operator and MOZART.

Photolysis frequencies in MOZART-3 are based on tabulated values of the Tropospheric Ultraviolet and Visible radiation model ((TUV) version 3.0) (Madronich and Flocke, 1998) for clear sky conditions. The adjustment for cloudiness is described in Brasseur et al. (1998).

4 Testing the scientific integrity of the GRG coupled system in forecast mode

The integrity of the coupled system depends on whether the application of external tendency fields accounting for processes not included in IFS (chemistry, emission and deposition) give reasonable results of the forecast length. The objective is that the IFS is able to imitate the CTM concentration developments and does not produce to many negative concentrations due to dislocated loss processes.

We studied area-averaged time series of tracer concentrations and spatial patterns of concentration fields. The following IFS runs are compared with the MOZART concentrations:

- IFS_free: Initial conditions from MOZART, IFS transport
- IFS_tend: Initial conditions from MOZART, IFS advection and CTM sink& source tendencies including vertical transport
- IFS_chem: Initial conditions from MOZART, IFS transport, CTM sink & source tendencies excluding vertical transport

Figure 8 shows examples of time series of the area average over Europe of the GRG species for model level 55 (PBL niveau) of the three IFS runs and the MOZART simulation. If total CTM tendencies (IFS_tend) are applied, the IFS can imitate the CTM upt to a forecast length of 48 h. Differences are obvious if the IFS vertical transport scheme is applied, because the vertical transport schemes differ between MOZART and the IFS. Spurious negative NO_x concentration were detected during the night, when the IFS vertical transport was applied (IFS_chem)

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Compone	Resolutio	Time	Specie	MPI /	Run time 24h
nt	n	step	S	openMP	
IFS	T159, 60L	1800 s	5	8 / 2	3 min (stand
					alone)
MOZART-	T63, 60L	900 s	106	8 / 8	12 min
3					
MOCAGE	2°x2°, 60L	900 s	126	1 / 12	188 min
TM5	2°x3°,60L	1200 s	54	12 / 1	31 min

Table 1 Resources of the IFS and the CTMs MOZART-3, MOCAGE and TM5



Figure 1 Different designs of a coupled system: Concurrent coupling of two independent executables (left) and sequential coupling of model or integration of sub-routine calls (right)



Figure 2 Modes of initial condition handling in a sequence of short simulations.



Figure 3 Memory consumption of the mpi-tasks of the OASIS4 coupled system IFS - MOZART



Figure 4 Dislocation problem: A mismatch in the ozone fields (O3, red) between CTM and IFS causes a mismatch in the application of ozone tendency data (P&L, green) transferred from CTM to IFS.



Figure 5 Profile of the area averaged (Europe 42.0/-10.0 - 55.0/10.0) tendencies in kg/m² per model level due chemistry (green dashed) and emissions including vertical diffusion and convection (blue) for NO_x at 12 and 24 UTC.



Figure 6 Profile of the area averaged (Europe 42.0/-10.0 - 55.0/10.0) tendencies in kg/m² per model level due chemistry (green dashed) and emissions including vertical diffusion and convection (blue) for CO at 12 and 24 UTC.



Figure 7 NO_2 - NO_x ratio profile averaged over Europe on 20020701 12 UTC, taken from MOZART (blue) directly and from the diagnostic inter-conversion operator without (IFS_dia, green, dotted) and with and ad-hoc assumption of tropospheric peroxy-radical concentration (IFS_dia green, dashed).





Figure 8 Time series of area mean over Europe simulated with the MOZART (blue), with IFS using no tendency information (IFS_free, red), with IFS using CTM source and sink tendency information including diffusion and convection (IFS_tend, green) and with IFS using CTM source and sink tendency and IFS vertical transport and emission injection (IFS_chem, black)