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# A quasi chemistry-transport model mode for EMAC

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## Abstract

A quasi chemistry-transport model mode (QCTM) is presented for the numerical chemistry-climate simulation system ECHAM/MESSy Atmospheric Chemistry (EMAC). It allows for a quantification of chemical signals through suppression of any feedback between chemistry and dynamics. Noise would otherwise interfere too strongly. The signal follows from the difference of two QCTM simulations, reference and sensitivity. These are fed with offline chemical fields as a substitute of the feedbacks between chemistry and dynamics: offline mixing ratios of radiatively active substances enter the radiation scheme (a), offline mixing ratios of nitric acid enter the scheme for re-partitioning and sedimentation from polar stratospheric clouds (b). Offline methane oxidation is the exclusive source of chemical water-vapor tendencies (c). Any set of offline fields suffices to suppress the feedbacks, though may be inconsistent with the simulation setup. An adequate set of offline climatologies can be produced from a non-QCTM simulation of the reference setup. Test simulations reveal the particular importance of adequate offline fields associated with (a). Inconsistencies from (b) are negligible when using adequate fields of nitric acid. Acceptably small inconsistencies come from (c), but should vanish for an adequate prescription of water vapor tendencies. Toggling between QCTM and non-QCTM is done via namelist switches and does not require a source code re-compilation.

## 1 Introduction

The recognition of feedback processes in the Earth system is essential to the understanding of past and future changes in the atmospheric chemical composition and climate. Global chemistry-climate models (CCMs) are well suited to investigate such feedbacks, since these models account for the non-linear coupling between atmospheric dynamics, chemistry, radiation, and other processes. However, the presence of feedbacks can hamper the identification of climate effects from,

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for instance, altered emissions of short-lived anthropogenic substances. This is the case if natural variability, here referred to as noise, disguises the expected signal.

For example, the objective of quantifying the expected impact from changes in nitrogen oxides ( $\text{NO}_x = \text{NO} + \text{NO}_2$ ) emissions requires a comparison of at least two model simulations: a reference simulation with reference sources of  $\text{NO}_x$  and a sensitivity simulation with sources that differ from the reference setup slightly. If the simulations include any feedback between dynamics and chemistry, then the meteorology of the two simulations will diverge despite binary identical initialization due to the inherent chaos in the system, a property commonly referred to as butterfly effect. Such behavior is inevitable, even for the smallest chemically triggered perturbation of the meteorological state. After a few time steps with perturbed conditions, the two simulations will differ completely in their meteorological patterns, communicating the meteorological variability to mixing ratios of chemical compounds such as  $\text{NO}_x$  (e.g. Unger et al., 2008).

Note that statistical expectation values of dynamical variables are hardly affected, but that the sequence of meteorological weather patterns can be completely different among the two simulations. Hence, day-to-day mixing ratio differences in the two simulations will be governed by noise (Fig. 1a), and estimation of statistical expectation values of chemical quantities require long and computationally expensive integrations. The problem is particularly strong when focusing on the quantification of effects from small perturbations of multiple emission sources such as road traffic, shipping, and aviation (e.g. Hoor et al., 2009; Unger et al., 2008).

Feedback processes between atmospheric chemistry and dynamics are manifold. Every chemically and radiatively active compound causes such feedback. Typical examples are ozone ( $\text{O}_3$ ), methane ( $\text{CH}_4$ ), chloroflourocarbons (CFCs), and nitrous oxide ( $\text{N}_2\text{O}$ ). A special species is water vapor ( $\text{H}_2\text{O}$ ) as it plays an important role not only in the radiation budget, but also in cloud physics and atmospheric chemistry; latter, for example, as a source of hydroxyl-radical (OH) formation, or, as a product of stratospheric  $\text{CH}_4$  degradation.

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Also, there are substances which are not radiatively active, but which affect dynamical processes such as properties of clouds. The formation of polar stratospheric clouds (PSCs), for example, depends on species such as H<sub>2</sub>O and nitric acid (HNO<sub>3</sub>). Any minor change in HNO<sub>3</sub> mixing ratios will alter PSC formation, and, through the associated H<sub>2</sub>O changes, causes a feedback between chemistry and dynamics.

Yet, chemically-triggered changes to the feedback processes themselves are often small enough to be neglected. It is hence feasible to account for the feedbacks between chemistry and dynamics with prescribed climatologies. With this restriction, chemical perturbations will not affect the meteorological patterns, breaking the feedback between chemistry and dynamics. In either of the two example simulations mentioned above, the patterns of atmospheric dynamics are then binary identical and any difference in chemical mixing ratios is directly attributable to the discrepancy in NO<sub>x</sub> emission rates among the two (Fig. 1b). As a result, the differences in chemical mixing ratios have a much higher signal-to-noise ratio.

We say a CCM is run in quasi chemistry-transport model mode (QCTM) when any impact from the model chemistry on the dynamics is switched off. The opposite case with active feedbacks between chemistry and dynamics is referred to as coupled mode, or coupled simulation. The term “quasi” serves to distinguish from pure chemistry-transport models which do not integrate the prognostic dynamical equations. The model “setup” determines also other model characteristics such as resolution, boundary conditions, and the selection of active submodels. Offline chemical characteristics are imposed on a simulation from outside, whereas online chemical characteristics are part of the simulation’s chemistry integration.

This documentation presents a QCTM implemented into the CCM ECHAM/MESSy Atmospheric Chemistry (EMAC), version 1.10. Section 2 introduces the model system EMAC, and Sect. 3 gives specific information on those submodels of EMAC which are important to the QCTM. Section 4 evaluates the QCTM. Following the conclusions of Sect. 5, the Appendix A informs on how to use the QCTM.

## 2 Model system EMAC

EMAC is a numerical chemistry and climate simulation system that includes sub-models describing tropospheric and middle atmosphere processes and their interaction with oceans, land, and human influences (Jöckel et al., 2006). It uses the first version of the Modular Earth Sub-model System (MESSy1) to link multi-institutional computer codes. The core atmospheric model is the 5th generation European Centre Hamburg general circulation model ECHAM5 (Roeckner et al., 2006). More detailed information, including references, about the model system is available from <http://www.messy-interface.org>. Currently, in EMAC version 1.10, 32 different submodels are available.

The core model of EMAC, ECHAM5, solves the atmospheric primitive equations horizontally via a spectral transform technique. In the vertical it uses the method of finite differences and for time integration a semi-implicit leap-frog scheme with time filter.

Most of the EMAC sub-models act on a Gaussian transform grid and, e.g., handle parameterized physics, transport of atmospheric constituents, and atmospheric chemistry. Depending on the complexity of the chemistry setup, the chemical calculations usually consume a large portion of the total CPU time. Chemistry is dealt with by the sub-model MECCA1 (Sander et al., 2005), which is based on the kinetic pre-processor (KPP) software (Damian et al., 2002) and considers the combined chemical reactions as a stiff system of ordinary differential equations. The system is solved via a Rosenbrock sparse-matrix technique with adaptive time step.

The parallelization is implemented based on the distributed memory concept with different approaches for the spectral and the grid-point representation, and a specific representation for the tracer advection algorithm, respectively. In spectral representation, variables are decomposed into their spherical harmonics, and in Gaussian representation the global domain is decomposed into blocks in latitudinal and longitudinal direction. For the advection an additional vertical decomposition is

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applied. For each variable in Gaussian representation two blocks in North-South direction are combined for an improved load balancing with respect to the distribution of day and night grid-boxes. These combined blocks are further re-arranged into vectors of selectable length to optimally exploit vector registers on vector architectures and cache sizes on scalar architectures.

### 3 Specific submodels and QCTM implementation

The implementation of the QCTM involves the EMAC submodels H2O, HETCHEM, RAD4ALL, and PSC, which are commented on here. Switching between QCTM and coupled mode does not require a re-compilation of the EMAC source code, so that the same executable can be used for both modes. Instead, it requires the modification of certain switches and adjustments in the respective namelists (see Table A1).

#### 3.1 Submodel H2O

The submodel H2O serves two purposes. First, it defines the gas-phase tracer H<sub>2</sub>O as part of the model chemistry, in contrast to the specific humidity being inherent to the ECHAM5 core model. To clearly separate these two aspects, we will refer to the water vapor fields from the H2O submodel as H<sub>2</sub>O tracer, and to the water vapor field from ECHAM5 as specific humidity. Optionally, the H2O submodel initializes the H<sub>2</sub>O tracer in the stratosphere and mesosphere from satellite data. These domains are notoriously too dry in the basemodel ECHAM5. Second, the H2O submodel controls the feedback between the H<sub>2</sub>O tracer and specific humidity, and the contribution by CH<sub>4</sub> degradation. There are five different options, and these are controlled by the CPL namelist of the H2O submodel:

- *I\_H2O\_TENDENCY* = -2: the H<sub>2</sub>O tracer is defined and initialized with the specific humidity, without correction from satellite data in the stratosphere and the

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mesosphere. No CH<sub>4</sub> oxidation from chemical submodels is taken into account. The H<sub>2</sub>O tracer and the specific humidity are completely detached.

- *I\_H2O\_TENDENCY* = -1: same as above, but the H<sub>2</sub>O tracer is initialized in the stratosphere and the mesosphere from satellite data.
- *I\_H2O\_TENDENCY* = 0: the H<sub>2</sub>O tracer is defined and initialized in the stratosphere and the mesosphere from satellite data. In addition, the tendencies of the H<sub>2</sub>O tracer from all other submodels are synchronized with those of the specific humidity. This option considers the impact from water vapor on the dynamics by online CH<sub>4</sub> oxidation calculated by a full-chemistry submodel.
- *I\_H2O\_TENDENCY* = 1: the H<sub>2</sub>O tracer is defined and initialized in the stratosphere and the mesosphere from satellite data. In addition, a source of H<sub>2</sub>O from climatological offline CH<sub>4</sub> oxidation is added to the overall tendency. The H<sub>2</sub>O tracer and the specific humidity are synchronized to consider the impact on the dynamics by the climatological CH<sub>4</sub> oxidation. This option is implemented for model setups without CH<sub>4</sub> oxidation calculated by a chemistry submodel.
- *I\_H2O\_TENDENCY* = 2: same as for option *I\_H2O\_TENDENCY* = 1, but only the H<sub>2</sub>O-tracer tendency from the climatological offline CH<sub>4</sub> oxidation is used to modify the specific humidity during the synchronization.

For the QCTM, the switch *I\_H2O\_TENDENCY* must be set to 2 as this eliminates the feedback on the dynamics by online chemical tendencies of water vapor. The offline water vapor tendency in options 1 and 2 is calculated based on a satellite climatology of methane mixing ratios and pre-calculated climatological conversion rates. The latter are taken from a coupled simulation. The default involves monthly average conversion rates from a MAECHAM4/CHEM simulation (Steil et al., 2003). These correspond to photolysis and oxidation of CH<sub>4</sub> by OH, O<sub>1</sub>D, and Cl. Alternative input data may be selected through the submodel namelists.

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## 3.2 Submodel HETCHEM

The submodel HETCHEM computes heterogeneous reaction rates for surfaces associated with solid nitric acid trihydrate (NAT), ice, super-cooled ternary solutions, and aerosols. As to the present study, a climatology of  $\text{H}_2\text{SO}_4$  mixing ratios as used by Jöckel et al. (2006) serves as the basis for heterogenous reactions on sulfate aerosol such as  $\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2\text{HNO}_3$ .

Tendencies of the water cycle associated with the re-partitioning of the three phases are neglected in case  $L\_COUPLE\_H2O = 2$  in the HETCHEM-namelist CPL (see also Table A1). This setting prevents water-mediated impact of heterogeneous chemistry on the dynamics.

## 3.3 Submodel RAD4ALL

The submodel RAD4ALL (see Jöckel et al., 2006) is a re-implementation into the MESSY standard of the ECHAM5 radiation code (Roegner et al., 2006). In coupled mode, RAD4ALL relies on online fields for the calculation of radiative transfer. These are with regard to the hydrological cycle: cloud cover, cloud water, cloud ice, prognostic specific humidity; and with regard to the radiatively active chemical species:  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{O}_3$ ,  $\text{N}_2\text{O}$ , CFC-11, CFC-12, depending on the chemical setup.

For the QCTM, the mixing ratios of all radiatively active chemical species, except for the  $\text{H}_2\text{O}$  tracer, must be provided from offline climatologies. The relevant switches are located in the CPL namelist of the RAD4ALL submodel, and the respective offline fields are defined via the REGRID and RGTEVENTS namelists of RAD4ALL (see Table A1). Note the model chemistry still provides online mixing ratios of the radiatively active species, but these are not used by the RAD4ALL submodel if the QCTM is active.

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### 3.4 Submodel PSC

PSCs affect the stratospheric chemistry and chemical composition by heterogeneous reactions occurring on both liquid and solid cloud particles, and by sedimentation of the solid cloud particles. The submodel PSC takes these effects into account within the EMAC framework. It further determines heterogeneous reaction rates. Also, it establishes the vertical redistribution of H<sub>2</sub>O and HNO<sub>3</sub> due to sedimentation of ice, referred to as dehydration, and due to sedimentation of NAT, referred to as denitrification.

The removal of PSC-related feedback is not as intuitive as for the submodels H<sub>2</sub>O, HETCHEM, and RAD4ALL, so that the PSC submodel deserves a somewhat more extensive explanation.

In every time-step, the PSC submodel is initialized with integration results from the previous timestep. Among these are temperature, local pressure, amounts of H<sub>2</sub>O in its three thermodynamic phases, the combined amounts of gaseous and liquid HNO<sub>3</sub>, and the amount of HNO<sub>3</sub> as NAT.

Then, the PSC submodel determines which thermodynamical phases are stable under the current local conditions of temperature, pressure, total-H<sub>2</sub>O content, and amounts of gaseous and liquid as well as NAT. There are three thermodynamic phases: (a) binary or ternary liquid particles only, (b) mixture of solid-NAT and liquid particles, (c) mixture of solid-NAT, ice, and liquid particles. Sulphuric acid tetrahydrate is not accounted for.

The thermodynamic partitioning of H<sub>2</sub>O and HNO<sub>3</sub> is accomplished in two steps. First, the PSC submodel separates the combined gaseous and liquid phases from the solid phase, generating ice in case of (c), and solid NAT in case of (b) and (a). It also determines the size of the solid ice and NAT particles and the user can choose among two different schemes. The simpler one assumes that ice and NAT particles have all the same size (Buchholz, 2005); the more sophisticated one considers a discrete size distribution for the NAT particles (Kirner et al., 2010). As a next step, the submodel

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solves for the amount of super-cooled ternary solution and calculates a composition-dependent size distribution of these liquid particles.

Thereafter, the PSC submodel determines the sedimentation velocities of the solid H<sub>2</sub>O and NAT particles based on temperature, local pressure, and particle size. Liquid particles are regarded as too small for sedimentation. The product of sedimentation velocity and length of the integration time step gives the vertical re-distribution of the solid particles. This, combined with the particle number density, defines the new amounts per model box of ice and solid NAT due to sedimentation. If the particles fall out of the height region where PSCs can occur, then the particle mass is transferred to the corresponding gas phase species.

The entire numerical scheme presented above is restricted to those atmospheric regions where PSCs are allowed to exist. The user prescribes an equatorward latitude limit as well as upper and lower pressure bounds to avoid PSCs where observations do not support their existence. Inside these pre-defined regions, the PSC submodel performs any PSC-related calculation only where the current local equilibrium temperature of ice is smaller than that of NAT. Here it is assumed that NAT nucleates on ice and that the ice forms in case of supersaturation.

The PSC submodel causes feedback between dynamics and chemistry through the following processes:

1. It defines heterogeneous chemical reactions via the HETCHEM submodel. These, in turn, alter the distribution of radiatively active substances through the chemistry submodel MECCA1. The RAD4ALL radiation submodel then communicates the chemical perturbation to the dynamics. In case of water vapor, the hydrological cycle represents an additional communication path.
2. Sedimentation-caused mixing ratio changes of H<sub>2</sub>O depend on HNO<sub>3</sub> through ice particle size and partitioning. Again, hydrological cycle and radiation close the feedback towards the model dynamics.
3. The amount of HNO<sub>3</sub> determines which thermodynamic phases are stable and thus impacts on the PSC-relevant regions (see above). For these regions,

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the CLOUD submodel suppresses the occurrence of any cirrus clouds, hence generating feedback. Additionally, the PSC-relevant regions re-enter the PSC submodel in the next time-step.

A removal of the PSC-related feedbacks by avoiding PSCs at all would be trivial to do. However, PSCs are important to the Earth system, e.g., through their impact on stratospheric ozone mixing ratios and dynamics, and should be accounted for. Rather than having no PSCs at all, it is hence better to remove only the PSC-related feedbacks.

The QCTM settings in the submodels HETCHEM and H2O (see Sects. 3.2, 3.1, and Table A1) remove any feedback associated with item 1 in the above list. Items 2 and 3 represent feedback through non-chemical mechanisms which involve HNO<sub>3</sub>. Figure 2 illustrates how the feedback removal is implemented in this case. The main idea is to replace online total-HNO<sub>3</sub> mixing ratios by an offline climatology where necessary in the code, while affecting PSC-related effects such as sedimentation as little as possible.

Partitioning within PSCs is therefore evaluated twice:

1. Using an offline total-HNO<sub>3</sub> climatology in order to make the following quantities and characteristics independent of the KPP-solved chemistry: water vapor tendencies, particle radii, and thermodynamic phase. The water vapor tendencies and particle radii go into the sedimentation scheme. In a similar way, the thermodynamic phase goes into the cirrus-related computations by the CLOUD submodel.
2. Using online total-HNO<sub>3</sub> fields from the KPP chemistry solver. As an important consequence of the double calculation, PSC-related partitioning/sedimentation induces KPP-dependent HNO<sub>3</sub> tendencies, which remain in the chemistry domain and do not affect the dynamics. Yet, the water vapor tendencies remain unaffected by KPP as these would otherwise establish a feedback between dynamics and chemistry.

Table A1 informs about the namelists which make the partitioning QCTM conform.

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## 4 Evaluation of EMAC in QCTM

This Section presents and discusses EMAC simulations in QCTM and coupled mode. Section 4.1 demonstrates that the QCTM has been successfully implemented into EMAC. It gives an example where sensitivity and reference simulations in coupled mode fail to provide meaningful results due to a low signal-to-noise ratio. Based on this exemplary situation, the QCTM is shown to perform and to tackle the underlying scientific problem.

Section 4.2 evaluates the QCTM-related effects on dynamical and chemical characteristics of the atmosphere. This is accomplished through a comparison of simulation pairs that differ only by the settings required to switch between QCTM and coupled mode.

### 4.1 Demonstration of performance

Figure 3 shows the per-cental difference in  $O_3$  mixing ratios between a sensitivity and its reference in QCTM (a and c) and fully coupled mode (b and d). The sensitivity differs from the reference by 5% stronger emissions from biomass burning of CO, non-methane volatile organic compounds (NMVOCs), and  $NO_x$ . In the presence of  $NO_x$  and sunlight, oxidation of CO and NMVOCs produces  $O_3$  in a complicated nonlinear way (Unger et al., 2008). The chemical scheme which has been evaluated by Jöckel et al. (2006) and which we adopted in our simulations accounts for the nonlinear ozone production. The nonlinearity implies considerable complexity of the impact on tropospheric chemical composition by altered  $NO_x$ , CO, and NMVOC emissions. Yet, the perturbation between sensitivity and reference is small (5%), and applied to CO, NMVOC, and  $NO_x$  simultaneously. It is hence reasonable to assume throughout the following discussion that their tropospheric mixing ratios, together with those of  $O_3$ , in general should be higher for the sensitivity simulation with its stronger emissions.

In the QCTM simulation, there is a clear positive anomaly in the troposphere of  $O_3$  (Fig. 3a and c),  $NO_x$  (Fig. 4), CO, and the NMVOCs (not shown).

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The anomaly is solely due to the chemistry as the dynamical states of sensitivity and reference are binary identical (not shown). It is emphasized that the amplitude of the mixing ratio anomaly is similar for snapshot (Fig. 3a) and monthly average (Fig. 3c). The reason is that the sensitivity, compared to the reference, has biomass burning emission rates which are enhanced by a constant factor (5%) and which include no day-to-day variability. However, the anomaly pattern is spatially less variable for the monthly mean, due to the smoothing of the day-to-day tracer transport variability. Note in this context that the spatio-temporal transport variability is binary identical for sensitivity and reference in QCTM, in contrast to that in coupled mode. Finally, the  $O_3$  response is consistent with the general situation. Enhanced African biomass burning causes higher near-surface mixing ratios of  $NO_x$  (Fig. 4), CO, and NMVOC (not shown) just north of the Equator. The enhanced mixing ratios are transported upwards by convection, and southward by the Hadley circulation, increasing the  $O_3$  mixing ratios on their way.

The coupled mode, in contrast, does not give a consistent result (Fig. 3b and d). Instead of a widespread positive pattern, there are noisy patches of both positive and negative anomalies, which also applies to  $NO_x$ , CO, and the NMVOCs (not shown). Such behavior indicates transport-related interference with the chemical signal as the dynamical states have diverged between the two simulations despite binary identical initialization, as sketched in Fig. 1a. This is due to the feedback between chemistry and dynamics (see Sect. 1). Also, the anomalies are weaker and tend to spread farther for the monthly averaging (Fig. 3d) than for the instantaneous snapshot (Fig. 3b). Such behavior is likely to result from the averaging which acts as a low-pass filter on the spectrum of atmospheric dynamics, and hence on tracer mixing ratios. Applying statistical analysis to quantify, or even identify, a chemical signal would be a fruitless endeavor due to the overwhelming noise (compare Fig. 3c and d taking into account the different scaling).

## 4.2 Impact on simulation climatologies

The removal of chemistry-climate feedbacks from EMAC represents an interference with the model chemistry and dynamics and it is important to evaluate the associated side effects. In this context, we compare simulations in coupled mode against a simulation in QCTM. The setup is identical for each simulation. We assume that such a comparison also serves to check whether the side effects cause significant inconsistencies for the QCTM simulation itself.

Figure 5a reveals significant discrepancies in temperature between two simulations, one in fully coupled mode and one in QCTM (see Table 1). The largest discrepancies occur above the 1 hPa level, culminating near the uppermost model layer in a +30 K temperature difference, a +50% difference in relative humidity, and a -60% difference in ozone mixing ratios. A further distinct feature is a widespread pattern of opposite sign showing negative temperature differences in the height region between 1 hPa and 100 hPa.

Two additional test simulations are performed in order to unravel the mechanisms behind these discrepancies. These simulations are identical to the QCTM simulation mentioned above except that in each case a single coupling pathway remains switched on. One simulation includes the coupling due to radiative effects, the other the coupling associated with PSCs (see Table 1).

Obviously, the removal of radiative-feedback effects explains the lion's share of the temperature discrepancies above the 100 hPa level (see Fig. 5b); for the following reason: in coupled mode, the radiation scheme uses online mixing ratios of the radiatively active species whereas it relies on offline mixing ratios in QCTM. For the particular case presented here, the QCTM setup adopts horizontally uniform, height-decreasing, mixing ratios of CFC-12, N<sub>2</sub>O, and CH<sub>4</sub>. Mixing ratios of O<sub>3</sub> are those by Fortuin and Kelder (1998). Note that for both setups the radiation scheme, RAD4ALL, uses the same CO<sub>2</sub> and CFC-11 fields. Also for both setups, the radiation scheme employs the prognostic specific humidity which, in coupled mode, depends on the KPP chemistry solver via the H<sub>2</sub>O tracer, but not in QCTM (see Sect. 3.1).

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in long-wave cooling from  $\text{N}_2\text{O}$ , CFC-12, and  $\text{CH}_4$ . Conversely, the positive deviation in mesospheric  $\text{O}_3$  mixing ratios could also explain the widespread negative deviation in stratospheric temperatures, in the height region between 100 and 1 hPa. The mechanism responsible is that stronger absorption in the mesosphere means less short-wave radiation is available to heat the stratosphere below.

To circumvent the aforementioned discrepancies the radiation scheme of the QCTM simulation has to be driven with appropriate offline climatologies of  $\text{O}_3$ ,  $\text{N}_2\text{O}$ , CFC-12, and  $\text{CH}_4$ . These should be obtained from the same coupled reference simulation that was used to derive the offline climatology of  $\text{HNO}_3$  (see Table 1). However, this is beyond the scope of this documentation.

Figure 5b demonstrates the temperature effect without the radiation-induced contribution by non- $\text{H}_2\text{O}$  species such as  $\text{O}_3$ ,  $\text{N}_2\text{O}$ , CFC-12, and  $\text{CH}_4$ . Hence, the remaining effect is associated with the removal of  $\text{H}_2\text{O}$ -related feedback mechanisms (Sect. 3.4): the substitution of chemical  $\text{H}_2\text{O}$  tendencies by climatological  $\text{CH}_4$  degradation, the omission of heterogeneous-chemical  $\text{H}_2\text{O}$  tendencies, and the PSC-related sedimentation of  $\text{H}_2\text{O}$  made to “see” climatological  $\text{HNO}_3$  offline mixing ratios.

There are two obvious structures of temperature deviation. The tropical/subtropical mesosphere displays a deviation of  $-0.6\text{ K}$ , and the entire troposphere a deviation of about  $-1\text{ K}$ . Both structures appear to result from deviations of  $\text{H}_2\text{O}$  and  $\text{O}_3$  (Fig. 6a and b): in the mesosphere, the positive  $\text{H}_2\text{O}$  deviation increases long-wave radiative cooling, and the negative  $\text{O}_3$  deviation decreases short-wave radiative heating. The  $\text{H}_2\text{O}$  deviation by itself results mainly from the substitution of the online chemical  $\text{H}_2\text{O}$  tendencies by climatological  $\text{CH}_4$  degradation, and the  $\text{O}_3$  deviation occurs as an effect to this. In the troposphere, a negative  $\text{H}_2\text{O}$  deviation is known to reduce the long-wave heating, producing the negative temperature deviation in Fig. 5b. The tropospheric  $\text{H}_2\text{O}$  deviation by itself is likely to arise from the omission of heterogeneous-chemical  $\text{H}_2\text{O}$  tendencies as  $\text{CH}_4$  degradation plays a minor role there. Finally, the removal of non- $\text{H}_2\text{O}$  radiative feedback artificially compensates for the tropospheric deviation in temperature (Fig. 5a) and  $\text{H}_2\text{O}$  (not shown).

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Again, a remedy for these H<sub>2</sub>O-related discrepancies would be to feed the QCTM simulation with appropriate climatological offline tendencies of H<sub>2</sub>O. These should originate from the coupled reference simulation (see Table 1) and describe the tendencies of H<sub>2</sub>O from CH<sub>4</sub> oxidation.

Figure 8a depicts the temperature deviation due to removal of feedback from PSC-related H<sub>2</sub>O sedimentation. The pattern of statistical significance is typical for type I random errors from multiple testing in the presence of spatial auto-correlation (von Storch and Zwiers, 1999). Hence, the deviations are not considered as robust, particularly for the southern polar lower stratosphere where PSCs most frequently occur. The same holds for mixing ratios of total HNO<sub>3</sub> (Fig. 8b) and radiatively active substances such as H<sub>2</sub>O and O<sub>3</sub> (not shown). The lack of deviation in temperature and tracer mixing ratios demonstrates that the QCTM approach is reliable.

## 5 Conclusions

A quasi chemistry-transport mode, QCTM, has been implemented into the EMAC chemistry-climate model system. The QCTM is demonstrated to eliminate any feedback between chemistry and dynamics, which is a pre-requisite for meaningful sensitivity studies on the impact from small chemical perturbations. Such studies have been hampered by the feedback-triggered noise from the chaotic climate system.

Specifically, the elimination of radiation-induced feedbacks is achieved by feeding offline mixing ratios of radiatively active substances to the radiation scheme. An equivalent approach is not applicable in case of H<sub>2</sub>O as it feeds back on the model dynamics not only via the radiative transfer, but also via the hydrological cycle and other, PSC related, processes. In this case, the tendencies of H<sub>2</sub>O are disconnected from the KPP chemistry solver.

1. H<sub>2</sub>O tendencies from homogeneous chemistry are limited to climatological CH<sub>4</sub> oxidation.

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2. H<sub>2</sub>O tendencies due to thermodynamic re-partitioning are neglected.
3. H<sub>2</sub>O tendencies from PSC-related sedimentation are calculated using prescribed mixing ratios of HNO<sub>3</sub>.

Activation of the QCTM is accomplished by adjustment of certain namelist switches (see Table A1).

It is also required to feed the radiation scheme with appropriate offline fields of the radiatively active species, except H<sub>2</sub>O, and the PSC scheme with appropriate offline fields of total HNO<sub>3</sub>. These fields should be compatible with the general chemical and dynamical characteristics of the QCTM simulation. Specifically, it is highly recommended to perform a coupled simulation with similar setup, derive mixing ratio climatologies of the relevant substances, and feed these into the associated QCTM simulation.

The two simulations in different mode, yet similar setup, are designed to yield consistent results. Hence, a comparison of the two simulations serves to evaluate the QCTM:

1. The offline fields of radiatively active species dominate the QCTM climatology. Associated inconsistencies can be large, especially in the mesosphere and the stratosphere, so that a prescription of adequate offline fields is important.
2. The removal of PSC-related feedback is consistent.
3. Acceptably small inconsistencies are associated with the disconnection of the H<sub>2</sub>O tendencies from online chemistry.

Elimination of the inconsistencies under item three would require a prescription of the offline H<sub>2</sub>O tendencies from the coupled reference simulation. These should climatologically represent the H<sub>2</sub>O tendencies from homogenous chemistry and thermodynamic re-partitioning.

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## Appendix A

### Use of EMAC in QCTM

This section exemplifies the use of EMAC in quasi chemistry-transport model mode (QCTM), and it is helpful to recapitulate some definitions. EMAC is run in QCTM when any impact from the model chemistry on the dynamics is switched off. The opposite case with active feedbacks between chemistry and dynamics is referred to as coupled mode. The model setup determines other model characteristics such as resolution, boundary conditions, and selection of active submodels. An offline field of chemical characteristics is imposed on a simulation from outside, whereas an online field is part of the simulation's chemistry integration. A reference simulation has a reference chemical setup, from which the chemical setup of a sensitivity simulation differs slightly.

In case of one reference and a single sensitivity it is usually required to perform three different simulations. All simulations should use the same executable. The reference is implemented as two different simulations: once in coupled mode, once in QCTM. The coupled simulation serves to generate climatologies for input into the QCTM reference and sensitivity simulations. Hence, the coupled reference setup and the QCTM reference setup should be as similar as possible, and should usually differ only by the settings required to switch between coupled mode and QCTM (see Table A1). It is up to the user to decide on the length of the coupled simulation and on the details of the climatologies such as base period and temporal resolution.

The coupled simulation is accomplished first. Straightforward summation of the standard output variables  $\text{HNO}_3$  and  $\text{HNO}_3_{\text{nat}}$  serves to establish a climatology of total- $\text{HNO}_3$  mixing ratios. It goes into the QCTM simulations as input variable `pref_HNO3_tot` (see Fig. 2) and removes the PSC-related feedbacks listed in Sect. 3.4 under items 2 and 3.

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Also from the coupled simulation, climatologies of those radiatively-active species should be made which enter the radiative transfer as online fields (see rad4all.nml). This is usually the case for O<sub>3</sub>, N<sub>2</sub>O, CFC-11, CFC-12, and CH<sub>4</sub>. Again, the climatologies are fed into the two QCTM simulations as explained in Table A1. It is emphasized that the measures recommended in this paragraph do not apply to water vapor, which enters the radiative transfer as an online field in both, QCTM and coupled mode.

The QCTM works as well for any arbitrary prescription of O<sub>3</sub>, N<sub>2</sub>O, CFC-11, CFC-12, CH<sub>4</sub>, and predef\_HNO3\_tot. Yet, the offline fields made from an appropriate coupled simulation bring the climatological characteristics of coupled mode and QCTM close together. Even more important, it ensures consistency between the offline fields and the climatological characteristics of the QCTM simulation.

Finally, the desired poor-in-noise response to small chemical perturbations follows from the difference between the two QCTM simulations, reference and sensitivity. In case of more than one sensitivity it is not necessary to make further coupled reference simulations as the one applies to all sensitivities.

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- Buchholz, J.: Simulations of physics and chemistry of polar stratospheric clouds with a general circulation model, Ph.D. thesis, Johannes Gutenberg University Mainz, 2005. 2197
- Clough, S. and Iacono, M.: Line-by-line calculation of atmospheric fluxes and cooling rates  
2. Application to carbon dioxide, ozone, methane, nitrous oxide and the halocarbons, J. Geophys. Res., 100, 16519–16535, 1995. 2203
- Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G.: The kinetic preprocessor KPP – a software environment for solving chemical kinetics, Comput. Chem. Eng., 26, 1567–1579, 2002. 2193
- Fomichev, V. I., Jonsson, A. I., de Grandpré, J., Beagley, S. R., McLandress, C., Semeniuk, K., and Shepherd, T. G.: Response of the middle atmosphere to CO<sub>2</sub> doubling: results from the Canadian Middle Atmosphere Model, J. Climate, 20, 1121–1144, 2007. 2211
- Fortuin, J. and Kelder, H.: An ozone climatology base on ozonesonde and satellite measurements, Clim. Dynam., 103, 31709–31734, 1998. 2202, 2211
- Hoor, P., Borcken-Kleefeld, J., Caro, D., Dessens, O., Endresen, O., Gauss, M., Grewe, V., Hauglustaine, D., Isaksen, I. S. A., Jöckel, P., Lelieveld, J., Myhre, G., Meijer, E., Olivie, D., Prather, M., Schnadt Poberaj, C., Shine, K. P., Staehelin, J., Tang, Q., van Aardenne, J., van Velthoven, P., and Sausen, R.: The impact of traffic emissions on atmospheric ozone and OH: results from QUANTIFY, Atmos. Chem. Phys., 9, 3113–3136, doi:10.5194/acp-9-3113-2009, 2009. 2191
- Jöckel, P.: Technical note: Recursive rediscratisation of geo-scientific data in the Modular Earth Submodel System (MESSy), Atmos. Chem. Phys., 6, 3557–3562, doi:10.5194/acp-6-3557-2006, 2006. 2212
- Jöckel, P., Tost, H., Pozzer, A., Brühl, C., Buchholz, J., Ganzeveld, L., Hoor, P., Kerkweg, A., Lawrence, M. G., Sander, R., Steil, B., Stiller, G., Tanarhte, M., Taraborrelli, D., van Aardenne, J., and Lelieveld, J.: The atmospheric chemistry general circulation model ECHAM5/MESSy1: consistent simulation of ozone from the surface to the mesosphere, Atmos. Chem. Phys., 6, 5067–5104, doi:10.5194/acp-6-5067-2006, 2006. 2193, 2196, 2200, 2211, 2215
- Kerkweg, A., Sander, R., Tost, H., and Jöckel, P.: Technical note: Implementation of prescribed (OFFLEM), calculated (ONLEM), and pseudo-emissions (TNUDGE) of chemical species in the Modular Earth Submodel System (MESSy), Atmos. Chem. Phys., 6, 3603–3609,

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doi:10.5194/acp-6-3603-2006, 2006. 2212

Kirner, O., Ruhnke, R., Buchholz-Dietsch, J., Jöckel, P., Brühl, C., and Steil, B.: Simulation of polar stratospheric clouds in the chemistry-climate-model EMAC via the submodel PSC, *Geosci. Model Dev. Discuss.*, 3, 2071–2108, doi:10.5194/gmdd-3-2071-2010, 2010. 2197

5 Roeckner, E., Brokopf, R., Esch, M., Giorgetta, M., Hagemann, S., Kornblueh, L., Manzini, E., Schlese, U., and Schulzweida, U.: Sensitivity of simulated climate to horizontal and vertical resolution in the ECHAM5 atmosphere model, *J. Climate*, 19, 3771–3791, 2006. 2193, 2196

Sander, R., Kerkweg, A., Jöckel, P., and Lelieveld, J.: Technical note: The new comprehensive atmospheric chemistry module MECCA, *Atmos. Chem. Phys.*, 5, 445–450, doi:10.5194/acp-5-445-2005, 2005. 2193

10 Steil, B., Brühl, C., Manzini, E., Crutzen, P. J., Lelieveld, J., Rasch, P. J., Roeckner, E., and Krüger, K.: A new interactive chemistry-climate model: 1. Present-day climatology and interannual variability of the middle atmosphere using the model and 9 years of HALOE/UARS data, *J. Geophys. Res.*, 108, D4290, doi:10.1029/2002JD002971, 2003. 2195

15 Unger, N., Shindell, D., Koch, D., and Streets, D.: Air pollution radiative forcing from specific emissions sectors at 2030, *J. Geophys. Res.*, 113, D02306, doi:10.1029/2007JD008683, 2008. 2191, 2200

von Storch, H. and Zwiers, F.: *Statistical analysis in climate research*, Cambridge University Press, Cambridge, 1999. 2205

20 WMO: *Scientific assessment of ozone depletion: 2006*, vol. 50, in: *Global Ozone Res. Monit. Proj. Rep.*, World Meteorological Organization, Geneva, Switzerland, 2007. 2203

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**Table 1.** Simulations for the QCTM evaluation. All simulations cover the five-year period 1999–2003. Each experiment is conducted with the tropospheric dynamics nudged towards ECMWF re-analysis fields for the period 1999–2003. It forces the simulations to produce a similar sequence of variability, which is necessary due to the presence of feedbacks between chemistry dynamics in the simulations *coup\_full*, *coup\_PSC*, and *coup\_rad*. The nudging reduces the noise in the simulation inter-comparisons and makes these better fulfill the normality assumption inherent to the paired t-test (Fomichev et al., 2007). Mixing ratios of total HNO<sub>3</sub> from *coup\_full* are averaged on a monthly basis before fed into *decoup\_full* and *coup\_rad*. The setup for all simulations is: T42L90MA with EVAL chemistry (Jöckel et al., 2006), submodels CLOUD, CONVECT, CVTRANS, DRYDEP, H2O, HETCHEM, JVAL, LNOX, MECCA1, OFFLEM, ONLEM, PSC, QBO, RAD4ALL, SCAV, TIMEPOS, TNUDGE, and TROPOP.

experiment	description
<i>decoup_full</i>	QCTM input for RAD4ALL (in mol mol <sup>-1</sup> ): CO <sub>2</sub> : 348×10 <sup>-6</sup> , uniform (see Table A1) CH <sub>4</sub> : 1.65×10 <sup>-6</sup> , height decreasing (see Table A1) N <sub>2</sub> O: 306×10 <sup>-9</sup> , " CFC-11: 280×10 <sup>-12</sup> , " CFC-12: 484×10 <sup>-12</sup> , " O <sub>3</sub> : climatology by Fortuin and Kelder (1998) input for PSC: total-HNO <sub>3</sub> from simulation <i>coup_full</i>
<i>coup_full</i>	fully coupled mode
<i>coup_PSC</i>	coupling only due to PSCs, other settings as for <i>decoup_full</i>
<i>coup_rad</i>	coupling only due to radiation, other settings as for <i>decoup_full</i>

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**Table A1.** Namelist settings required to activate the QCTM for EMAC version 1.11 and higher. Regridding is referred to as spatial interpolation of an offline field to the ECHAM5 Gaussian grid (see Jöckel, 2006), triggering as the timed import of the re-gridded field into a running simulation (see Kerkweg et al., 2006).

offline climatologies of radiatively active species	
example for CH <sub>4</sub> (analog for CO <sub>2</sub> , O <sub>3</sub> , N <sub>2</sub> O, CFC-11, CFC-12)	
<b>&amp;CPL</b> in <i>rad4all.nml</i>	
<i>ch4vmr_rad4all = const. value</i>	user-defined mixing ratio for <i>ich4_rad4all = 2</i> or <i>3</i>
<i>ich4_rad4all = 2</i> or	whole atmosphere: mixing ratio set to <i>ch4vmr_rad4all</i>
<i>ich4_rad4all = 3</i> or	troposphere: <i>ch4vmr_rad4all</i> ; decay with elevation above
<i>ich4_rad4all = 4</i>	offline CH <sub>4</sub> climatology (preferred setting if climatology from coupled reference simulation)
<b>&amp;REGRID</b> in <i>rad4all.nml</i>	
<i>var = "CH4_init=CH4"</i>	offline CH <sub>4</sub> climatology: path and regridding
...	"
<b>&amp;RGTEVENTS</b> in <i>rad4all.nml</i>	
<i>RG_TRIG(5) = ...</i>	offline CH <sub>4</sub> climatology: triggering
offline climatology of chemical H <sub>2</sub> O tendencies	
<b>&amp;CPL</b> in <i>h2o.nml</i>	
<i>I_H2O_TENDENCY = 2</i>	offline climatological CH <sub>4</sub> oxidation only
<b>&amp;CPL</b> in <i>hetchem.nml</i>	
<i>L_COUPLE_H2O = F</i>	no H <sub>2</sub> O tendencies from thermodynamic re-partitioning
PSC-related partitioning of H <sub>2</sub> O based on offline climatology of total HNO <sub>3</sub>	
<b>&amp;CPL</b> in <i>psc.nml</i>	
<i>I_feedback = F</i>	H <sub>2</sub> O partitioning based on offline climatology of total HNO <sub>3</sub> (preferably from coupled reference simulation)
<b>&amp;REGRID</b> in <i>offlem/psc_offline.nml</i>	
<i>var = "predef_HNO3=HNO3_tot:INT"</i>	offline total-HNO <sub>3</sub> climatology: path and regridding
...	"
<b>&amp;RGTEVENTS</b> in <i>offlem.nml</i>	
<i>RG_TRIG(40) = ...</i>	offline total-HNO <sub>3</sub> climatology: triggering
<b>&amp;CTRL</b> in <i>psc.nml</i>	
<i>KinPar=F</i>	QCTM not tested for microphysical kinetic NAT scheme

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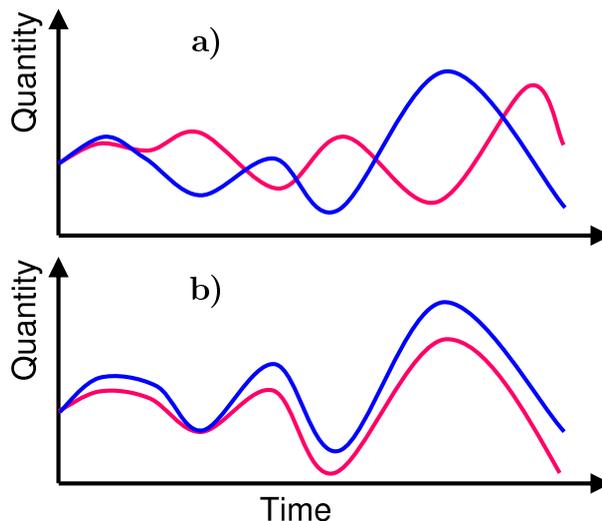


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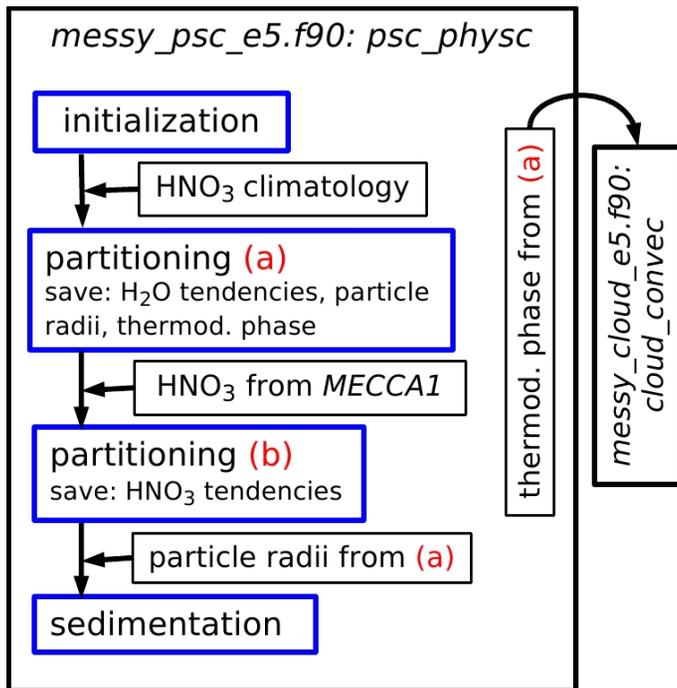
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**Fig. 1.** Mixing ratio  $x$  of an arbitrary chemical tracer from two hypothetical simulations (sketch **a**). The simulation setups differ only by a small chemical perturbation affecting  $x$ , and share identical initialization. Note that the simulations have near-identical statistical expectation values with respect to dynamical quantities such as divergence and vorticity. However, the feedback between chemistry and dynamics causes a completely different sequence of dynamical patterns and associated tracer transport, and hence a low signal-to-noise ratio for the chemistry-related difference  $\Delta x$  among the two simulations. Without feedback between chemistry and dynamics, however,  $\Delta x$  relates directly to the chemical perturbation, and it displays a high signal-to-noise ratio (sketch **b**).

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**Fig. 2.** Flowchart of how the QCTM is implemented into the EMAC submodel PSC. The partitioning is calculated twice using (a), offline, and (b), online mixing ratios of HNO<sub>3</sub> (see text for more detailed explanations).

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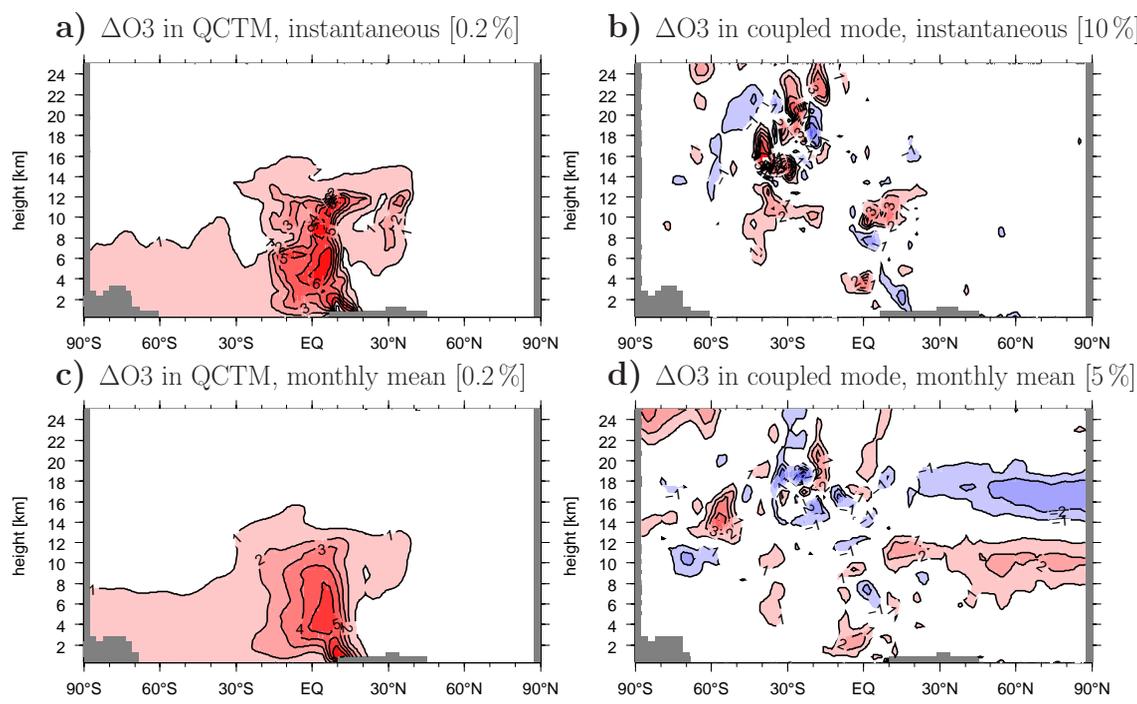
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**Fig. 3.** Latitude-height section of the per-cental difference in  $O_3$  mixing ratios between sensitivity and reference in QCTM (left) and fully coupled mode (right). The sensitivity has 5% stronger emissions from biomass burning of  $NO_x$ , CO, and NMVOC, affecting  $O_3$  mixing ratios chemically (see text). Results are shown for the Greenwich Meridian for a single month under July conditions: 00:00 UTC on 1 July (top), monthly mean (bottom). Isoline intervals are 0.2% in QCTM (left), but 10% (top right) and 5% (bottom right) in coupled mode. Positive values (red) denote higher  $O_3$  mixing ratios for the sensitivity. The model setup is T42L90MA with EVAL chemistry (Jöckel et al., 2006), submodels CLOUD, CONVECT, CVTRANS, DRYDEP, H2O, HETCHEM, JVAL, LNOX, MECCA1, OFFLEM, ONLEM, PSC, QBO, RAD4ALL, SCAV, TNUDGE, and TROPOP.

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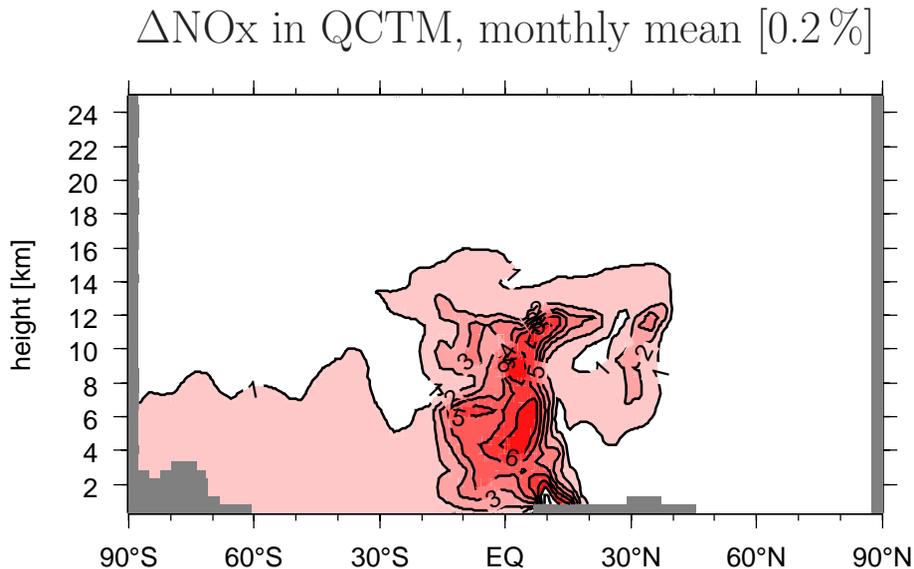
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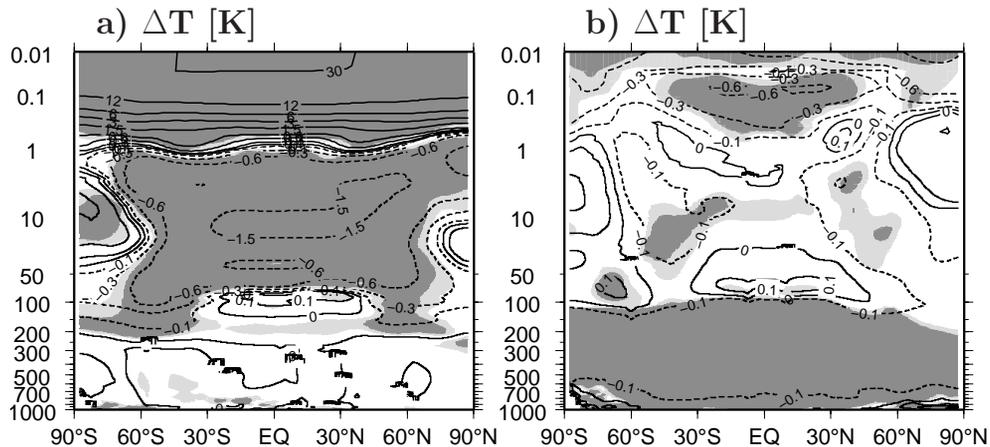




**Fig. 4.** Same as Fig. 3c, but for  $\text{NO}_x$ . Isoline intervals are 0.2%.

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**Fig. 5.** Mean annual-mean temperature deviation (isolines [K]) for the five simulation years 1999–2003. Shading refers to the 99% (dark-gray) and 95% (light-gray) significance levels from a paired t-test with four degrees of freedom. **(a)** Simulation *decoupled\_full* minus *coup\_full*. **(b)** *coup\_rad* minus *coup\_full*. Table 1 presents the simulation setups.

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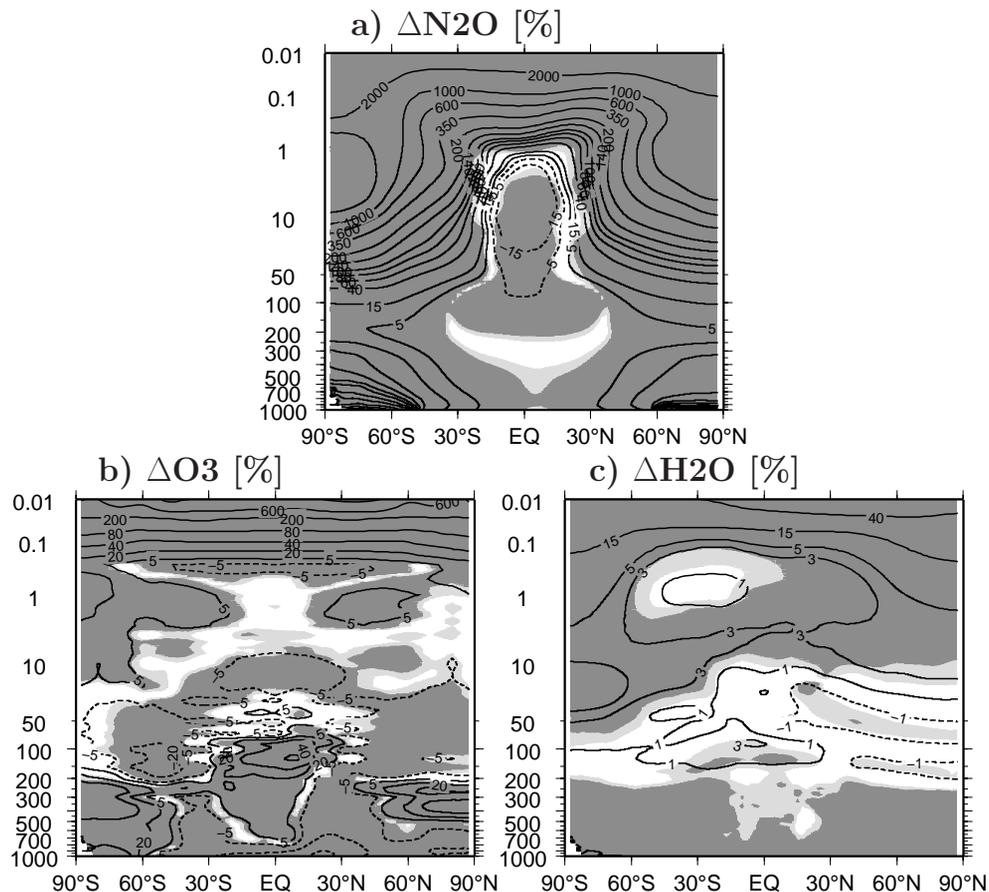
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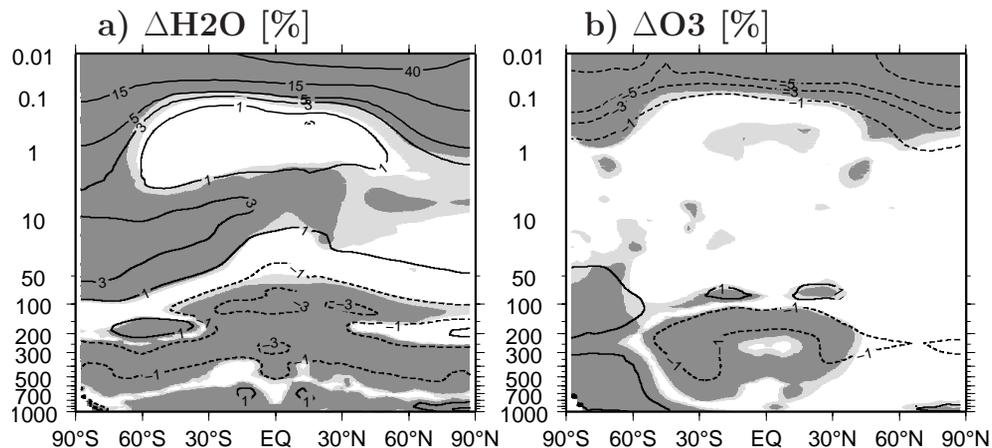


**Fig. 6.** Same as Fig. 5, but for the per-cental deviation of simulation *coup\_rad* versus *coup\_full* (see Table 1). **(a)**  $\Delta H_2O$  [%] (gaseous only), **(b)**  $\Delta O_3$  [%].

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**Fig. 7.** Same as Fig. 5, but for the per-cental deviation of simulation *decoup\_full* versus *coup\_full* (see Table 1). **(a)**  $\Delta\text{N}_2\text{O}$  [%], **(b)**  $\Delta\text{O}_3$  [%], and **(c)**  $\Delta\text{H}_2\text{O}$  [%] (gaseous only). In case of *decoup\_full* there are two different sets of the radiatively active species  $\text{O}_3$ ,  $\text{N}_2\text{O}$ , CFC-12, and  $\text{CH}_4$ . The radiation submodel RAD4ALL relies on their respective offline mixing ratio climatologies, whereas chemistry and transport impact the online mixing ratios.

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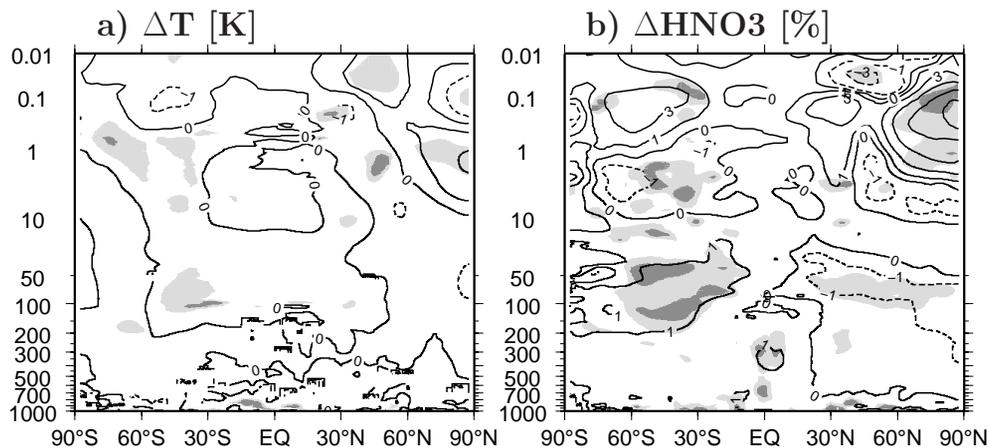
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**Fig. 8.** Same as Fig. 5, but for the deviation of simulation *coup\_psc* versus *coup\_full* (see Table 1). **(a)**  $\Delta T$  [K], **(b)**  $\Delta HNO_3$  [%] (sum of gaseous, liquid, solid).

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