Chapter 1
Global chemistry-climate modelling with EMAC

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Abstract The Institute of Atmospheric Physics of the German Aerospace Center
(DLR) uses the numerical model system ECHAM/MESSy Atmospheric Chemistry (EMAC). The model has a flexible modular structure and allows for coupled
chemistry-climate simulations. Typical fields of application are related to questions
regarding Earth's climate, atmospheric chemical composition, and aerosol characteristics. In its current setup, the performance of EMAC on LRZ/ALTIX allows for
multi-decadal simulations with climatologically significant results. The good performance demonstrates the multi-purpose capabilities of LRZ/ALTIX because EMAC
involves various different numerical concepts and implementations of parallel decomposition. Our EMAC activities on LRZ/ALTIX are devoted to both model development and production simulations. The former comprise a new upper-boundary
representation, a chemistry-transport mode, the inclusion of a mixed-layer ocean,
and full-Lagrangian transport and dynamics. The latter tackle, for instance, questions related to the environmental impact of anthropogenic aerosol and gaseous substances.

1.1 Introduction

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model 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 [8]. 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 [15]. More detailed information, including references, about the model

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system is available from `http://www.messy-interface.org`. Currently 32 different sub-models are available.

The modular structure of EMAC allows its application for a wide variety of scientific tasks. It can be applied in different configurations; for instance as pure atmospheric general circulation model, as atmospheric-chemistry transport model, the latter also as chemistry-climate model with full feedback between atmospheric chemistry and dynamics via the radiation calculations. Optionally, in order to represent the observed meteorological patterns, the model dynamics can be relaxed towards analysis and re-analysis data of the European Centre for Medium-Range Weather Forecasts (ECMWF). This is particularly useful for the evaluation of the model in comparison to observations.

Besides the flexibility in model configuration and setup the resolution is likewise flexible. The core model, ECHAM5, uses a spectral transform technique, the so-called T-value indicating the degree of triangular spectral truncation. T42, for instance, corresponds to a Gaussian grid of approximately 2.8° by 2.8° in longitude and latitude. Vertically, the model resolves the troposphere and lower stratosphere, implemented as model setups L41DLR and L31ECMWF. The top of the model layers are centered at 5 hPa and 10 hPa, respectively. In further versions, L39MA and L90M, the stratosphere and the lower mesosphere are better resolved, with the uppermost model layer centered at hPa and hPa, respectively. The L-value indicates the number of discrete hybrid-pressure levels. MA refers to "middle atmosphere", and DLR and ECMWF denote specific vertical-layer structures associated with these institutions.

EMAC is easily portable to various architectures because it follows some important standards: Fortran95 standard, ISO/IEC-1539-1, Message Passing Interface standard for parallel computation, MPI-2, and Network Common Data Form data format, NetCDF.

This article demonstrates our modelling activities on LRZ/ALTIX with EMAC. Our activities encompass a wide range of tasks in the field of atmospheric science with some being focused on model development. This makes is hard to combine our activities into a coherent text structure. Rather, we start with a brief overview on computational methods and performance of EMAC in standard configuration (Section 1.2) which forms the basis of our modelling work. Some more specific EMAC sub-modules are presented later in Section 1.3 and 1.4. While the former Section presents activities related to model development, the latter presents results from production-oriented simulations. Finally, we draw conclusions in Section 1.5.

1.2 Technical information

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, i.e. in the physical-space domain. Examples are parameterised physics, advection of atmospheric constituents, and atmospheric chemistry. Depending on the complexity of the chemistry setup, the chemical calculations usually consume the largest portion of the total CPU time. Chemistry is dealt with by the sub-model MECCA1 [17], which is based on the kinetic pre-processor software [1] and considers the combined chemical reactions as a stiff system of ordinary differential equations (ODE). The system is solved via a Rosenbrock sparse-matrix technique with adaptive time step.

The parallelisation is implemented based on the distributed memory concept with three 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, in Gaussian representation the global domain is decomposed into blocks in latitudinal and longitudinal direction, for the advection an additional vertical decomposition is 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.

Table 1.1 provides information on the performance of EMAC on LRZ/ALTIX for a typical setup, including chemistry, in two different resolutions. The wall-clock time per model year is in the range of a few days and the corresponding CPU time in the range of 5–12 kilohours. This benchmark allows for multi-decadal simulations, particularly in T42L41DLR, the default resolution applied for production simulations at our institution. In case of T42L41DLR the performance gain decreases significantly from 64 to 128 CPUs and in case of T42L90MA it does so from 128 to 256 CPUs (not shown). Presumably, these breaks in scalability result from two different effects: first, from overhead enhancement associated with communication between the nodes on LRZ/ALTIX, second, from load-imbalance associated with photo-chemistry as the stiffness of the chemical ODE system varies throughout a simulation day by orders of magnitude. Further tests on this are required and will be conducted in near future. The load imbalance issue, which is architecture independent, is already being tackled so that future EMAC versions will have improved scalability characteristics.

Table 1.1 Performance of EMAC on LRZ/ALTIX. The model configuration includes detailed atmospheric physics and complex atmospheric chemistry but neglects detailed aerosol effects.

resolution	number of CPUs	CPU time (10^3 h/model year)	wall-time (days/model year)
T42L41DLR	64	5.4	3.5
T42L41DLR	128	7.9	2.6
T42L90MA	64	12.0	7.9
T42L90MA	128	12.1	4.0

1.3 Model development

Much of our modelling activity on LRZ/ALTIX is related to indispensable model development which represents a prerequisite for many of our planned production simulations. At the same time, these activities are absolutely necessary to keep pace with scientific questions becoming more complex and to push the state of the art of global chemistry-climate modelling. Our activities are focused on

- establishing a new upper-boundary parameterisation for our 41-layer setup of EMAC (Section 1.3.1),
- creating a chemistry-transport mode for EMAC where dynamics and chemistry are completely decoupled (Section 1.3.2),
- coupling a mixed layer ocean to EMAC atmospheric dynamics and chemistry (Section 1.3.3),
- creating a Lagrangian base model for EMAC as an alternative to ECHAM5 (Section 1.3.4).

1.3.1 Upper-boundary parameterisation

A high spatial resolution of our global chemistry-climate model is desirable to resolve all relevant physical and chemical processes. It is limited however, by the available resources: CPU time, memory, and storage. Our standard spectral horizontal resolution for production simulations is T42, corresponding to $2.8° \times 2.8°$ in longitude and latitude. The highest vertical resolution available is 90 layers between surface and top of the atmosphere (L90).

One focus of atmospheric research at the DLR is to study the effects of transport emissions on climate. Aircrafts usually fly at levels between 200-350 hPa and all other anthropogenic emissions occur in the surface boundary layer. Therefore, we do not rely on a high vertical resolution at altitudes above 100 hPa and, hence, can benefit from the advantage associated with fewer vertical layers. We use a 41 layer setup (L41) instead of L90. L41 has a higher vertical resolution between surface and 100 hPa, and simulations are about 2.4 times faster and have less than half the storage requirements than L90. A speed-up by 2.4 is important as a typical 30-year simulation with L90 and comprehensive chemistry would require about 360 kCPUh (see Table 1.1).

On the downside, the vertical resolution of L41 decreases above 100 hPa. The atmosphere above 10 hPa is represented by 36 model layers in L90, but by just one layer in L41. A single layer is not sufficient to describe the chemical processes involving Br, N2O, CH4, and CFCs, in that altitude range correctly. Reaction rates are calculated for the 5 hPa centre level and assumed to be vertically constant throughout the whole uppermost layer in L41 which ranges from 10 to 0 hPa. However, real reaction rates depend on altitude non-linearly. Therefore, the 5 hPa rates are un-

likely to represent the bulk rates for the 10 to 0 hPa layer. This affects 13 different multi-component gas phase reactions and 10 different photolytic reactions.

We developed a technique to account for the drawbacks associated with L41. Artificial reservoir species are introduced, which are not transported and exist in the uppermost layer only. The products from the degradation reactions of N2O, CFCs, CH$_4$ and Br- compounds go into their respective reservoirs, with rate coefficients modified in order to approximate the L90 rates in L41. Reservoir species are then transformed into reactive species with a turn-around time of five years, taking into account stratospheric transport this way.

Currently, we are basing the correction factors on the inter-comparison of two simulations; on the cumulative losses in the upper 36 layers of a L90 simulation and on the losses in the uppermost layer of a L41 simulation. Both simulations had two years of spin-up and there are three years for evaluation. This is relatively short for climatological averaging, but the noise is reasonably low due to slow stratospheric dynamics and fixed boundary conditions controlling photolysis reactions. It is desirable to start future simulations from a steady state with non-empty reservoirs. Also, strong alterations of the chemical configuration may represent a problem since the upper boundary parameterisation is currently based on only two simulations with a specific setup. Finally, a comparison with observations will be the ultimate test of our parameterisation.

1.3.2 Decoupling of dynamics and chemistry

Global chemistry-climate models account for the full non-linear coupling between atmospheric dynamics and chemistry. However, identifying the climate effect of short-lived anthropogenic substances, for instance of nitrogen oxide ($NO_x = NO + NO_2$), requires a comparison of at least two modelling setups: one without a particular NO_x source and one with. This results in long and costly integration times due to noise from atmospheric transport interfering with the NO_x signal [18]. The problem is particularly prominent in case the focus lies on the separate climate impacts by multiple simultaneous NO_x emission sources such as road traffic, shipping, or aviation.

A promising way to deal with such problems is to neglect any feedbacks between atmospheric chemistry and dynamics, i.e., to run the model in chemistry-transport mode. Leaving any coupling processes in the model is not sensible as model dynamics is affected by any slightest disturbance. In chemistry-transport mode, simulations with different NO_x sources display different chemical properties but have binary identical meteorological conditions and transport characteristics. As a result, the integration time needed to detect a given NO_x signal becomes much shorter and in some cases might even be possible solely with this approach. And finally, the approach allows for a quantification of signal feedbacks as it is possible to compare coupled against decoupled simulations.

We have made disengageable any chemistry-climate feedbacks and by far the major hurdle turned out to be feedbacks associated with polar stratospheric clouds (PSCs). PSCs represent an important feature of the global climate system and should not be neglected. Yet, occurrence and characteristics of PSCs depend on the stratospheric chemical composition, for instance on HNO_3 concentrations, and therefore on NO_x emissions. PCSs in turn affect atmospheric water through heterogeneous chemical reactions as well as sedimentation of water-containing particles. Water, finally, transfers the emission signal to atmospheric dynamics via both the hydrological cycle and radiative heating. The result is a chemistry-climate feedback which is not wanted for this purpose.

To resolve the PSC issue, we decided to impose predefined climatological tendencies for liquid water and ice. The tendencies are based on EMAC simulations in chemistry-climate mode. Imposing the tendencies into chemistry-transport simulations must be done water mass preserving. Our approach is to force artificial phase changes, i.e. to create missing ice contents from the model-inherent water vapor concentrations while preserving column-integrated total water. The latter is important because sedimentation redistributes water vertically.

The code has been implemented and tested on LRZ-ALTIX. Clearly, the water mass is preserved and the water tendencies change only little when taken from a chemistry-climate simulation and incorporated into a chemistry-transport simulation. Also, the procedure conserves the overall tendency patterns.

1.3.3 Atmosphere-ocean feedbacks

For studies involving climate feedbacks and climate response it is important to use a chemistry-climate model that includes an ocean module. For our studies EMAC is coupled to a slab ocean model with an oceanic mixed layer of 50 m depth (MLO) [16]. Any heat exchange with the deep ocean is represented by a prescribed climatological annual cycle. A thermodynamic sea-ice model is also integrated in this module [12], enabling albedo feedbacks via changes in ice coverage and ice thickness. An ECHAM5/MLO model configuration has already been used to investigate the importance of physical feedbacks, e.g., cloud feedback, for climate sensitivity. The role of chemical feedbacks, e.g., from ozone, has never been quantified by similar simulations so far.

The MLO module was implemented into the EMAC model system and test simulations were performed on LRZ/ALTIX. Equilibrium climate change simulations driven by external forcings involving both physical and chemical feedbacks have thus become possible [11]. While the slab ocean does not need substantially more CPU time than the pure atmospheric model, equilibrium climate change simulations require 20 spin-up years to adjust the perturbed system to the changes in forcings and feedbacks and at least another 20 simulation years are required in order to study the deviation between the equilibrium climates of the perturbed and the reference simulation. This means that a model system like this has considerable larger de-

mands to computational economy than atmosphere/ocean models without chemistry or chemistry-climate simulations without the ocean component. A specific setup of the chemistry sub-model MECCA1 [17] has been prepared for the intended studies that offers an adequate compromise between chemical complexity and computational resources. We use EMAC with 41 vertical layers, L41DLR, in T42 horizontal resolution (see Section 1.1). Simplifications with regard to chemistry include the omission of reactions involving non-methane hydro carbons and bromine.

1.3.4 Lagrangian modelling

Due to the increasing demand for interactive tracers in climate chemistry simulations it becomes necessary to use global models which meet the needs of a fast and exact tracer transport scheme. Commonly used methods to describe the large-scale transport in a general circulation model of the atmosphere follow the Eulerian method. However, Lagrangian transport schemes offer several advantages with respect to tracer transport: they show no numerical diffusion, they maintain steep gradients and they are efficient in the treatment of a large number of tracers. Therefore, the Lagrangian transport model ATTILA (Atmospheric Tracer Transport in a Lagrangian Model) was developed [13]. It runs in the framework of a general circulation model and advects the centroids of air parcels whose number depends on the selected vertical and horizontal resolution. The latest version was implemented in the EMAC climate model and completed by a Lagrangian convection scheme. This model system is run in T21 and T42 and with 31 or 41 vertical levels. The coarse resolution was used mainly for sensitivity studies related to the resolution of the Lagrangian space with a certain number of Lagrangian air parcels. The computer time increases nearly linearly with the number of Lagrangian air parcels in the T21L19 model resolution requiring about 4 hours/CPU per simulated year for 90000 Lagrangian parcels.

Further research is being done towards the development of a pure Lagrangian dynamical core in the EMAC climate model with the aim of calculating all transport with the same transport scheme. So far, energy and momentum are calculated by the dynamical spectral core of the EMAC model, but tracers are advected by a Eulerian approach to ensure mass conservation. This results in a certain degree of inconsistency, which we plan to overcome. The new Lagrangian dynamical core will be realized with the concept of the Finit-Mass Method [5]. The atmosphere is subdivided into small mass packets each of which is equipped with a finite number of internal degrees of freedom. In ATTILA the Lagrangian air parcel are just mass points without spatial extension. These mass packets move under the influence of internal and external forces and can change their shape to follow the motion. The total mass density results from the superposition of the individual mass packets. The implementation of the Finite Mass Method requires the development of a new sub-model for the temporal integration of the deformation matrix. In a first step we will

analyse the characteristics of the simulated parcel distribution from a set of climate simulations over several years.

1.4 Production-oriented simulations

The sample of scientific results presented here is based on some of our modelling activities on LRZ/ALTIX. Our findings refer to the environmental impact of anthropogenic volatile particles (aerosol), their precursor gases, and other gaseous substances. Section 1.4.1 demonstrates how particle aging changes aerosol characteristics and Section 1.4.2 is devoted to the impact on climate and public health by shipping emissions.

1.4.1 Atmospheric ice nuclei

Black carbon (BC) and mineral dust particles are among the most important atmospheric aerosol types forming ice crystals by heterogeneous nucleation (so called ice nuclei). Anthropogenic changes in the availability of such ice nuclei can have important climate effects. When emitted, most BC and dust particles are externally mixed with other aerosol compounds. Through coagulation with particles, condensation of gases, as well as cloud processing, externally mixed particles gain a liquid coating and are transferred to an internal mixture. These aging processes are essential for the effects of BC and dust particles on climate, since the coating changes the radiative and hygroscopic properties of the particles and, therefore, their cloud activation ability and lifetime. Moreover, laboratory studies have shown that a liquid coating influences the freezing properties of the particles and hence their behavior as ice nuclei [10, 2]. In the upper troposphere and lowermost stratosphere (UTLS) BC is emitted by aircraft engines. With the rapid increase in the amount of air traffic its contribution to the BC concentration is gaining more and more importance [6].

Due to large computational resources required, global climate models mostly parameterise the aging of BC and dust by using estimated turnover times, rather than simulating the aging processes explicitly. The LRZ/ALTIX offers extraordinarily high computational capacities. Hence, we took advantage of this opportunity and further developed a new aerosol model, MADEsoot, which allows for a representation of BC and dust particles and their different states of mixing as well as the relevant aging processes of externally mixed particles. MADEsoot is based on the standard EMAC aerosol module MADE [9]. We implemented MADEsoot in the global chemistry-climate model EMAC [7, 14] and performed a large number of simulations to assess the concentration, size distribution and mixing state of BC and dust particles in the global atmosphere. The mass and number concentration of internally and externally mixed BC and mineral dust particles were simulated separately for particles in two modes; in the Aitken mode, particles smaller than $0.1\,\mu$m,

and in the accumulation mode, particles larger than $0.1\,\mu$m but smaller than $1\,\mu$m. Moreover MADEsoot uses two additional modes for BC and dust free particles and a coarse mode for particles larger than $1\,\mu$m.

Figure 1.1 shows the vertical distribution of the zonal mean of the number concentration of potential ice nuclei (BC and dust particles). The simulation has been performed on LRZ/ALTIX with EMAC-MADEsoot. While at surface the number concentration of potential ice nuclei reaches values between 500 and 1000 particles/cm^3, at the 300 hPa level, which is located at altitudes where cirrus clouds form, it never exceeds 10 particle/cm^3. The highest values are reached over South-West China, which is characterised by very high BC emissions (not shown).

The global aerosol-climate model EMAC-MADEsoot requires about 600 CPUh for each simulated year using a T42L19 grid. A climatologically significant simulation must cover at least 10 years. Furthermore, several different simulations are required to study separately the influence of each process or parameterisation on the model results. A set of 5 sensitivity experiments will consume about 30000 CPUh.
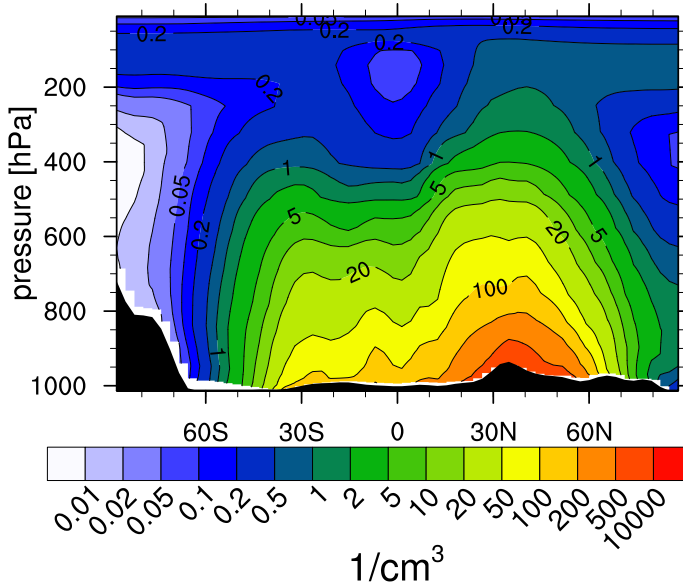

Fig. 1.1 Zonal annual mean number concentration of potential ice nuclei.

1.4.2 Impact of ship emissions on atmospheric composition and climate

Emissions from international shipping contribute significantly to the total budget of anthropogenic emissions and have been recognised as a growing problem by both scientists and policymakers. Already in 2000, shipping contributed with around 2.7% to all anthropogenic CO_2 emissions, with around 15% to nitrogen oxide (NO_x) emissions and with around 8% to sulfur dioxide (SO_2) emissions [3]. If no control measures were taken beyond International Maritime Organisation (IMO) regulations that existed in 2005, NO_x emissions were predicted to further increase to values of today's emissions from road transport, and SO_2 emissions were predicted to double until 2050 [4]. We aim at quantifying the impact of gaseous and particulate ship emissions on the chemical composition of the atmosphere and on climate for present day conditions and for several scenarios of future development.

A variety of important results have been achieved. One of the major findings was that the potential of particle emissions or their precursors from shipping to modify the microphysical and optical properties of clouds (the so-called *indirect aerosol effect*) is significant [9]. The additional aerosol particles brighten the clouds above the oceans, which then are able to reflect more sunlight back into space (see Fig. 1.2). The model results indicate that the cooling due to altered clouds far outweighs the warming effects from greenhouse gases such as CO_2 or ozone from shipping, overall causing a negative radiative forcing today. The indirect aerosol effect of ships on climate is found to be far larger than previously estimated, contributing up to 39% to the total indirect effect of anthropogenic aerosols. This contribution is high because ship emissions are released in regions with frequent low marine clouds in an otherwise clean environment and the potential impact of particulate matter on the radiation budget is larger over the dark ocean surface than over polluted regions over land. The main reason for the high impact on clouds is the high average sulfur content in maritime fuels.

We are planning to study how climate impacts of particulate and gaseous emissions from large diesel engines change when fuels from renewable sources are used. As a first step we have repeated the [9] simulations on LRZ/ALTIX and are now running simulations where heavy fuel oil is replaced with bio fuels in the international shipping fleet. Each experiment encompasses a period of 6 years (1999–2004), preceded by a spin-up time of one year, and uses the relaxation technique. The cost of each modelled year is around 400 CPUh, with a total output for each simulation of about 450 GB. Preliminary simulations suggest that replacing heavy fuel oil with bio fuels (e.g. palm oil) significantly reduces the near-surface sulfate (SO_4) concentration as well as the effect of shipping emissions in enhancing cloud reflectivity.

In 2010, we plan to study the effect of parameterising the gas phase chemical processes in subgrid scale engine exhaust plumes of aviation and shipping. This study should allow a better representation of the impact of these emissions in particular on the tropospheric ozone burden.
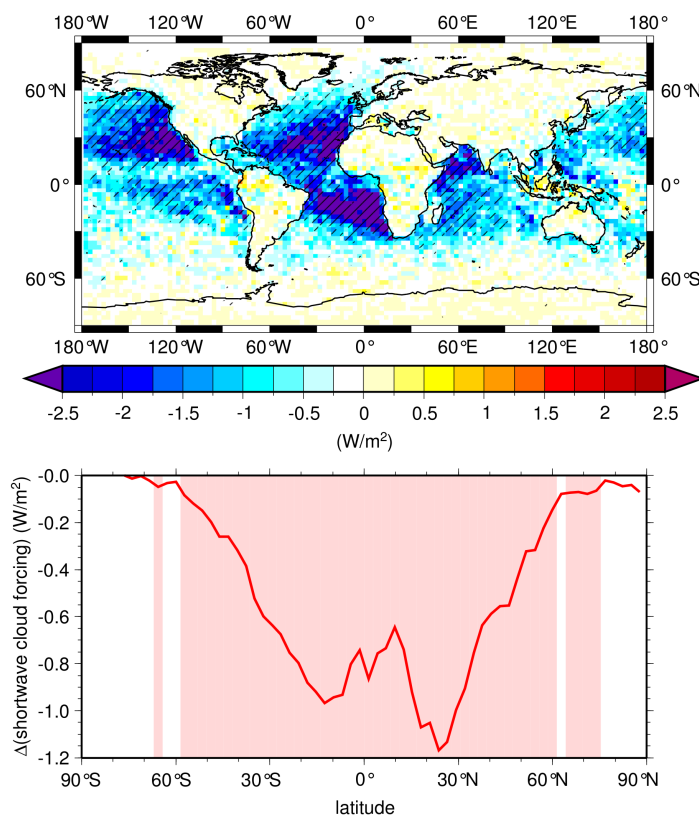
Fig. 1.2 Multi-year average of simulated changes in short-wave cloud forcing due to shipping at the top of the atmosphere in W/m^2. Upper panel shows the geographical distribution, lower panel zonal averages. Hatched areas (upper panel) and light-red shaded areas (lower panel) show differences which are significant at the 99% confidence level compared to the inter-annual variability (from [9]).

1.5 Final remarks

The high-performance computing facility LRZ/ALTIX represents an excellent platform for the numerical-simulation activities by the Institute of Atmospheric Physics of the German Aerospace Center. We use the model system EMAC to conduct simulations for a variety of scientific tasks that are related to questions concerning Earth's climate, atmospheric chemical composition, and aerosol characteristics. EMAC's major benefit is its ample flexibility to incorporate new code due to a modular architecture and the possibility of doing coupled chemistry-climate simulations.

In its current setups, the performance of EMAC on LRZ/ALTIX allows for multidecadal simulations which is necessary to obtain climatologically significant results. EMAC is a model system that comprises various different numerical concepts, from spectral transformation and time integration to linear algebra and Lagrangian meth-

ods, with different types of distributed-memory parallelisation. Hence, the good performance demonstrates that LRZ/ALTIX represents a flexible computing platform.

Many of our modelling activities on LRZ/ALTIX are aiming at creating EMAC setups required for present and future scientific tasks. These setups comprise a new upper-boundary representation, a decoupling of chemistry and climate to allow for chemistry-transport simulations, the inclusion of a mixed-layer ocean, and full-Lagrangian transport and dynamics.

The future is going to bring even higher demands on computing performance. One reason is the need for higher model resolution in order to resolve more and more of the small-scale parameterised physics. Another reason is the need for climate simulations that do not only account for radiation-coupled atmospheric dynamics and chemistry but also for ocean feedback. Future versions of EMAC will have improved parallel scalability so that simulations on a greater number of cores will be feasible.

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