

Description of Work for month 37-54

Version 1 April 2008

2.3 *Activity 3: Large-scale Chemistry Effects (Isaksen, Van Velthoven)*

Active work package descriptions

WP 3.1.1 Evaluation of multi-model performance against observations (Schnadt, ETH Zürich)

WP number	3.1.1	Period month 37-54	Start date :	1	End date	48
Participant id	DLR-IPA	ETH Zürich	CEA	KNMI	MPICHEM	UIO
Person-months	0	8.4	0	0	0	1
Participant id	UCAM-DCHEM					
Person-months	0					

Objective

O.3.1.1.1 To evaluate the latest versions of the models against observations focusing on key processes for correct simulation of the effects of transport emissions (M3.1.1.3).

Description of work

Model simulations for 2003 have been defined and carried out including diagnostics of key processes relevant for the effects of the different modes of transportation. The model output is compared with observations from the established *ETHmeg* observational database in order to evaluate the current performance of the ACMs. The *ETHmeg* model evaluation webpage (http://www.megdb.ethz.ch/index.php?site=model_validation) presents the most recent results from model evaluation with observations and model-model intercomparisons. Focus of the model evaluation has been stratosphere-troposphere exchange of ozone and NO_x, boundary layer venting, and convective transport of pollutants from the surface. Point-to-point comparison of observational and model data has already been carried out using the SPURT and MOZAIC observational data by ETH. A first report on the model performance is already available (D3.1.1.9).

In year 3 ETH has requested a shift of the final report on model evaluation to month 48 to enable them to spend all planned budget, since their postdoc has had unexpected periods of leave (related to pregnancy). The coordinator of QUANTIFY has already agreed to this shift. Therefore this WP is prolonged to month 48. This also allows us to include further model output in the evaluation.

For month 37-48 a further comparison of the model output with additional observations (CONTRACE, surface data) is planned. It is also planned to evaluate some new model outputs with respect to the recent near-surface observations from the QUANTIFY ship campaigns 2007. This will be done in autumn/winter 2008 when new model simulations will have been repeated using the final QUANTIFY emissions data sets, as planned in WP3.1.2.

Deliverables

D3.1.1.10 Second report on the performance of the models (month 48, ETH Zürich)

Milestones

None

WP 3.1.2 Current chemical composition changes from different modes of transport (Lelieveld, MPICHEM)

WP number	3.1.2	Period month 37-54		Start date :	3	End date	48
Participant id	DLR-IPA	CNRS-LSCE	KNMI	MPICHEM		UIO	UCI
Person-months	0	3	0	3		1	0
Participant id	UCAM-DCHEM						
Person-months	0						

Objectives

- O.3.1.2.1 To provide input data on chemical change for impact studies
O.3.1.2.2 To estimate the current change in chemical composition from different modes of transport

Description of work

An ensemble of model runs evaluating the current impact of the transport sectors has already been finished and reported (D3.1.2.9). Supplementary simulations with 20 and 100% (instead of 5%) perturbations of the transport sector emissions have been performed by UCAM and UIO to quantify the degree of non-linearity and non-additiveness of the impacts on radiative forcing.

The above simulations have been done with preliminary emissions available about 1 year after the start of the project. In the meantime these emission data sets have been improved by Act. 1 and also scenarios have been constructed for use in WP3.3.1-2. The scenarios have become available in gridded form by the end of last year and are currently being evaluated and preprocessed. Final model simulations of the current impact have to be performed using these updated emissions in order to estimate the difference between future and current impact in a consistent manner.

Due to remaining problems with the coupling between chemistry and dynamics in the MPICHEM model, the original deliverable D3.1.2.10 concerning calculated perturbation fields was found not be scientifically reasonable and has been cancelled. Instead a detailed simulation in high resolution mode of the ship campaign measurements (performed in 2007 by Activity 5) will be performed in year 4 by MPICHEM. Here, the focus will be on a ship corridor effects rather than on single plumes. It must be noted that MPICHEM, as leader of WP3.1.2, has spent quite a lot of effort on the analysis of the output from the whole set of models, and the reporting of this WP, including the preparation of a joint paper. We also note that output from additional model (MOCAGE from CNRM/Meteo-France) has been used in the analysis. Hence the total number of models contributing to model output is as has been as planned.

Output fields of radiatively active species from the new model simulations of current impact will be made available to Activity 6 so that they can update their radiative forcing estimates.

Deliverables

- D3.1.2.10 Final current chemical perturbation fields from the DLR-IPA model (month 42, DLR-IPA)
D3.1.2.11 Final current chemical perturbation fields from the CNRS-LSCE model (month 42, CNRS-LSCE)
D3.1.2.12 Final current chemical perturbation fields from the KNMI model (month 42, KNMI)
D3.1.2.13 Final current chemical perturbation fields from the UIO model (month 42, UIO)
D3.1.2.14 Final current chemical perturbation fields from the UCAM-DCHEM model (month 42, UCAM-DCHEM)
D3.1.2.15 Report with final estimate of the current impact on atmospheric composition (month 48, MPICHEM)

Milestones

None

WP 3.1.3 Implementation of effective emissions (Hauglustaine, CNRS-LSCE)

WP number	3.1.3	Period month 37-54	Start date :	19	End date	48
Participant id	CNRS-LSCE	KNMI	MPICHEM	UIO	UCI	UCAM-DCHEM
Person-months	5	1	0	2	0	0

Objectives

- O3.1.3.1 To define or select suitable effective emissions for aviation, shipping and road transport
- O3.1.3.2 To implement apply these emissions in the ACMs
- O3.1.3.3 To estimate the effect of sub-grid scale chemistry and dispersion on chemical perturbations from aviation, shipping and road transport

Description of work

Currently emissions by transport activities are usually directly emitted into the coarse grid cells of global ACMs. These grid cells have sizes of typically 100-500 km. The uncertainty due to plume processing will be estimated by calculating the difference in pollutant concentrations between ACM simulations with and without effective emissions. For aviation the large uncertainty range in published calculations of effective emissions needs to be reduced. Preliminary estimates of aircraft plume processing have been made by UIO and KNMI. New effective emissions for are based on a parameterisation developed by CERFACS in Activity 2 that makes use of additional large scale fuel tracers. Coefficients for a parameterisation of aircraft plumes were supplied by CERFACS in month 23. During this third year of the project, the CNRS-LSCE has implemented the new CERFACS parameterisation (as described in D3.1.3.1) in their LMDz-INCA model (D3.1.3.2). The first results obtained in month 30 showed a very small impact of plume processing on aircraft produced ozone. Hence the parameterisation had to be reformulated by CERFACS (Act. 2) and evaluated once more in the LMDZ-INCA model. CNRS-LSCE has provided a first report on the latter estimates of aircraft plume processing (D3.1.3.8) in month 37. The results show that the introduction of the non-linearity of the atmospheric chemistry during the aircraft plume dispersion leads to NO_x and associated O₃ decreases along the major aircraft routes: Up to 5% (July) and 15% (January) of attenuation of the O₃ production from aircraft emissions is obtained in the high troposphere of Northern Hemisphere. These results compare well with alternative, already published approaches by UiO and KNMI. In our view it is quite satisfactory that conceptually quite different approaches yield similar results.

Because of the delays in the development of the parameterization and taking into account the delay of the future impact calculations (WP 3.3.1) that impacts Act. 6 downstream, we will not give priority to implementation of the new CERFACS plume parameterisation scheme in further models. We feel that in the end it is more interesting to have a comparison of fundamentally different approaches, than a comparison of results of implementation of the same parameterization in different models. The former gives a more comprehensive estimate of uncertainty. We plan, however, still to implement the new parameterization in the UIO model since this allows direct comparison of the new CERFACS approach to the older (Kraabøl) approach. This is scheduled for month 43-48, since WP3.3.1 gets priority. Hence original deliverables D3.1.3.3, D3.1.3.4, D3.1.3.5, D3.1.3.7 are cancelled, D3.1.3.6 is shifted to month 48, and this WP is prolonged from month 36 to month 48. An update of D3.1.3.8 will then be provided by CNRS-LSCE (before month 54).

Act. 2 (CERFACS) will provide documentation (possibly including code) on how to implement the plume parameterization to UIO before month 43.

Deliverables

- D3.1.3.3 Output fields from ACM simulations with/without effective emissions (month 34, KNMI, cancelled).
- D3.1.3.4 Output fields from ACM simulations with/without effective emissions (month 34, MPICHEM, cancelled).

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| D3.1.3.5 | Output fields from ACM simulations with/without effective emissions (month 34, UCAM-DCHEM, cancelled). |
| D3.1.3.6 | Output fields from ACM simulations with/without effective emissions (month 34, UIO, will be shifted to month 48). |
| D3.1.3.7 | Output fields from ACM simulations with/without effective emissions (month 34, UCI, cancelled). |
| D3.1.3.8 | Report on the uncertainty in estimates of chemical perturbations from aviation and shipping due to sub-grid scale chemical conversions (month 36, CNRS-LSCE, delivered month 37) |

Milestones
M3.1.3.3 Provide documented parameterization for effective emissions to UIO (month 43, CNRS-LSCE/CERFACS)

WP 3.2.2 Aircraft induced sulphur impact on UTLS ozone (Rogers, UCAM-DCHEM)

WP number	3.2.2	Period month 37-54	Start date :	33	End date	48
Participant id	CEA-LSCE	MPICHEM	UIO	UCAM-DCHEM		
Person-months	2	0	1	3		

Objective

O3.2.2.1 To estimate the effect of aircraft sulphur emissions on UTLS ozone

Description of work

The impact on ozone of the increase in stratospheric aerosol density (SAD) due to aircraft sulphur emissions will be calculated. Recently published calculations of results from one model indicate (Pitari et al., 2002) that the downward transport of air depleted in ozone by the increased SAD is of the same order of magnitude as the ozone production from aircraft NO_x emissions. This effect needs to be investigated with other models, because it is highly sensitive to vertical transport in the UTLS and to the microphysics implementation. A sensitivity study will be performed with several ACMs with perturbed and unperturbed stratospheric background aerosol climatologies.

The set-up of the model simulations has been fixed and is described in a report (D3.2.2.1). UCAM has coupled the global stratospheric chemistry model SLIMCAT with an aerosol microphysical module (SAMM; Tripathi, 2004) and performed a 3 year run with NO_x, SO₂ and water vapour emissions based on AERO2K. The simulation period includes the Pina Tubo volcanic eruption causing a strong increase in background stratospheric aerosol density. The difference in the aircraft impact due to the increase in the sulphuric aerosol density has been calculated. Hence this WP is somewhat ahead of schedule.

In the coming period UCAM will extend its simulation to more years, and the other groups will perform their simulations.

Deliverables

- D3.2.2.2 Output from CEA model simulation with perturbed/unperturbed stratospheric aerosol (month 44, CEA)
- D3.2.2.3 Cancelled
- D3.2.2.4 Output from UCAM-DCHEM model simulation with perturbed/unperturbed stratospheric aerosol (month 44, UCAM-DCHEM)
- D3.2.2.5 Output from UIO model simulation with perturbed/unperturbed stratospheric aerosol (month 44, UIO)
- D3.2.2.6 Report on the effect of aircraft sulphur emissions (month 48, UCAM-DCHEM)

Milestones

- M3.2.2.1 Description available of model simulations to be performed (month 38, UCAM-DCHEM)
- M3.2.2.2 Model simulations carried out (month 44, UCAM-DCHEM)

WP 3.2.3 Impact of cirrus clouds (Van Velthoven, KNMI)

WP number	3.2.3	Period month 37-54	Start date :	19	End date	54
Participant id	KNMI					
Person-months	4					

Objective

O3.2.3.1 To estimate the effect of cirrus clouds on the impact of transport emissions

Description of work

Cirrus clouds are not only important for climate, but also for the UTLS ozone budget. Recent modelling studies suggest that chemical ozone loss on these ice particle surfaces is comparable in magnitude, but of opposite sign to aviation induced ozone production. Model studies have also demonstrated the significance of cirrus cloud particles for irreversible HNO₃ removal in the upper troposphere, significantly reducing NO_x-catalysed chemical ozone production. However, only a few modelling studies on these issues have been performed so far. Recent laboratory research and observations, both in-situ and space-borne, have supplied new findings of key parameters that allow very useful following-up modelling efforts that have currently not been performed.

Currently, new recommendations for reaction rates have been implemented by KNMI in the TM4 model, leading to significant changes in some of them (J_{MGLY} , k_{OH-CO} , J_{HCHO} , etc.). Experiments with a modified ice cloud scheme are set up, including an evaluation of the parameterization of Kärchner&Lohmann (2002). The goal is to estimate the influence of cirrus on the impact of transport on ozone.

As noted in the third periodic progress report reported, KNMI suffers from delays due to the premature departure of their postdoc. In the meantime a new postdoc has been hired. However, most of the work in WP3.2.3 still has to be done. This is rescheduled to the second half of the 4th year, since priority needs to be given to the simulations for WP3.3.1 on future composition changes because Act. 7 depends on this output. A prolongation until e.g. month 54 of QUANTIFY might be useful to perform the work in full depth.

Deliverables

- D3.2.3.1 Description of a new parameterisation for ice cloud interaction based on recently determined parameters (month 30, shifted to month 38)
- D3.2.3.2 Report on the effect of cirrus clouds on the chemical perturbations by transport (month 36, shifted to month 48)

Milestones

- M3.2.3.1 A new parameterisation for ice cloud interaction based on recently determined parameters available (month 30, shifted to month 38)
- M3.2.3.2 Model simulations carried out (month 34, shifted to month 46)

WP 3.3.1 Future chemical composition changes from different modes of transport (Isaksen, UIO)

WP number	3.3.1	Period month 37-54	Start date :	8	End date	48
Participant id	DLR-IPA	CNRS-LSCE	KNMI	MPICHEM	UCI	UIO
Person-months	3	6	4	2	3	7
Participant id	UCAM-DCHEM					
Person-months	2					

Objectives

- O3.3.1.1 To provide input data of future chemical changes for impact studies (M3.3.1.4)
- O3.3.1.2 To estimate the changes in future chemical composition from different modes of transport (M3.3.1.5)

Description of work

The global scale CTMs will be used to perform first-order studies of future chemical impacts. Changes in distributions will be calculated for O₃, CH₄ (through changes in its lifetime) and for particle distributions (sulphate, organic carbon aerosols). Time slice calculations for the target year 2050 will be performed with meteorology from 2003. These simulations will use gridded transport emission inventories for 2050 that have been provided by Activity 1, but still require some reprocessing, rescaling and evaluation.

For all transport sectors, emissions were provided for the 4 marker scenarios A1, A2, B1, and B2. In Act.3 we have decided to start with the high emission scenario A1 and the low emission scenario B1. In the case of aviation the “A1i” (moderate to good fuel efficiency, moderate NO_x improvements) and the “B1” (good fuel efficiency improvement, good NO_x improvements) versions will be used.

As was done for the current impact simulations in WP3.1.2, we will reduce one transport sector at a time in the future runs (i.e. three runs with 5% reduction in aviation, road, shipping, respectively), in addition to a reference future run with all emissions included.

For initialisation of well-mixed GHG it has been decided to use the SRES recommendations. So far, UiO have provided tables for the A1b scenario. Source data for sea surface temperatures has still to be decided. Chlorine and bromine levels from WMO2006 will be used in those models that have stratospheric chemistry. Tables were provided by UiO.

All modelling groups participating in the current impact simulations described in 3.1.2 will participate in these simulations of future impact. However, DLR-IPA will only calculate perturbations for the sum of all transport sectors and combine the results with simulations with the changed climate of 2050, as described in WP3.3.2.

Deliverables D3.3.1.2, D3.3.1.3, D3.3.1.5, D3.3.1.6, and D3.3.1.7 (future chemical perturbation fields from the CNRS-LSCE, KNMI, UCI, UCAM-DCHEM, and UIO models, respectively) were all due by month 36, but are delayed and will be delivered by month 42 (for one scenario at least). The reason for the delay is primarily the late delivery of gridded emission scenarios, most of which were delivered in month 33, and in month 35 in the case of aviation, instead of month 30.

The output fields for 2050 of radiatively active constituents will be provided to Activities 6 and 7 (month 42) for calculation of radiative forcing and for simulations with (simplified) climate models.

Act. 1 will rescale the current and scenario numbers for aviation to total fuel used. They will also provide emission totals, so that re-gridding of the emission fields for use in the models can be easily checked.

Deliverables

- D3.3.1.2 Future chemical perturbation fields from the CNRS-LSCE model (month 36, CNRS-LSCE, now planned month 42)
- D3.3.1.3 Future chemical perturbation fields from the KNMI model (month 36, KNMI, now planned month 42)
- D3.3.1.4 Future chemical perturbation fields from the MPICHEM model (month 42, MPICHEM). May be joint with DLR-IPA (D3.3.1.8).
- D3.3.1.5 Future chemical perturbation fields from the UCI model (month 36, UCI, now planned month 42)
- D3.3.1.6 Future chemical perturbation fields from the UCAM-DCHEM model (month 36, UCAM-DCHEM, now planned month 42)
- D3.3.1.7 Future chemical perturbation fields from the UIO model (month 36, UIO, now planned month 42)
- D3.3.1.8 Future chemical perturbation fields from the DLR model (month 42, DLR)
- D3.3.1.9 Report with estimate of the future chemical impact (month 46, UIO)

Milestones

- M3.3.1.2 Results from simulations of future impact from CTMs available (month 36, UIO, now planned month 42)
- M3.3.1.3 All results from simulations of future impact available, including those from CCMs (month 42, UIO)

WP 3.3.2 Impact of future climate change (Grewe, DLR-IPA)

WP number	3.3.2	Period month 37-54	Start date :	25	End date	48
Participant id	DLR-IPA	CNRS-LSCE	MPICHEM	UiO		
Person-months	4.7	9	6	4		

Objectives

O3.3.2.1 To estimate the effect of atmospheric chemistry-climate feedbacks on the future impact of emissions from transport (M3.3.2.3)

Description of work

Significant changes in climate parameters such as H₂O, temperature, and dynamics (transport of stratospheric ozone) are expected to occur in the future global atmosphere. These changes will affect the oxidation process and thereby the atmospheric concentrations of climate gases such as ozone and methane. In a first step existing global CCM simulations will be analysed with regard to the impact of climate variability and of chemistry-climate feed-backs on traffic induced ozone changes.

In a second step each participating group will perform 4 simulations (the first two of which are in common with WP3.3.1, i.e. A and BR):

A: A simulation with meteorology/climate for 2000 and all emissions for 2050.

BR: A simulation with meteorology/climate for 2000 and all emissions for 2050 except for a reduction of the emissions from transport by -5%.

C: Same as A but with meteorology/climate for 2050.

DR: Same as BR but with meteorology/climate for 2050

The set-up for these model simulations is described in the already available report D3.3.2.1.

The WP3.3.2 runs will use consistent SST boundary conditions provided by DLR (V. Grewe, M3.3.2.2). The consistency of chemistry-climate runs performed here and the climate runs performed in Activity 6 by CNRM has been discussed. CNRM will generate its own SSTs but use historical composition fields from a climate-chemistry run with E39C to CNRM for their transient runs.

The WP3.3.2 runs have not started yet, for the same reason as in WP3.3.1: the gridded future emission data were delivered rather late by Act. 1 and still require further evaluation and preprocessing, which are currently underway. It is still planned to finish the simulations by month 42.

Deliverables

D3.3.2.2 Future chemical perturbation fields including climate feedbacks from the DLR-IPA model (month 42, DLR-IPA)

D3.3.2.3 Future chemical perturbation fields including climate feedbacks from the CNRS-LSCE model (month 42, CNRS-LSCE)

D3.3.2.4 Future chemical perturbation fields including climate feedbacks from the MPICHEM model (month 42, MPICHEM). May be joint with DLR-IPA (D3.3.2.2).

D3.3.2.5 Future chemical perturbation fields including climate feedbacks from the UIO model (month 42, UIO)

D3.3.2.6 Report on the effect of climate feedbacks on future impact (month 48, DLR-IPA)

Milestones

M3.3.2.2 2050 SSTs distributed among Act.3 partners (month 38, DLR-IPA)

M3.3.2.3 Historical composition fields distributed to CNRM-Act. 6 (month 38, DLR-IPA)

M3.3.2.4 Model simulations ready (month 42, DLR-IPA)

WP 3.3.3 Possible mitigation strategies (Isaksen, UIO)

WP number	3.3.3	Period month 37-54	Start date :	19	End date	40
Participant id	CNRS-LSCE	KNMI	MPICHEM	UIO	UCAM-DCHEM	
Person-months	5	2	1	1	1	

Objective

O3.3.3.1 To investigate options for reducing the impact of individual transport modes

Description of work

Model runs with the global scale CTMs will be performed to estimate different options for reduced climate impact. The model runs will look at contributions from individual modes of transport and from different regions. Analysis and recommendations for combination of options that efficiently reduce the impact of emissions will be made.

D3.3.3.1 (description of model setup for calculating effects of mitigation options) was submitted in month 30. As the provision of mitigation scenarios of emissions is not included in the work plan for Activity 1, alternative solutions had to be found. The plan is now to run the “B1 ACARE” scenario, provided by Activity 1, for aviation as a mitigation scenario. B1 ACARE has the lowest emissions due to the implementation of the ACARE targets for fuel and NOx: this can be described as a mitigation scenario as the fuel efficiency improvements are most likely to be implemented due to concern over climate change. B1 ACARE can be seen as a very optimistic but feasible scenario.

For road it was originally envisaged to create a hydrogen scenario that assumes increased use of hydrogen on top of scenario B1. However, at the third annual project meeting in Budapest, it was found that the future scenario for road traffic produced by Activity 1 already looks more or less like a mitigation scenario (having taken into account significant planned reductions), while for the future shipping and aviation scenarios this is not the case. Therefore, it was decided to create a ‘policy failure’ scenario for road emissions. It is now planned that this scenario will replace the hydrogen scenario that was previously planned. Act. 1 (DLR-V) will provide this summer 2008.

Since Act. 1 can not provide all input for the mitigation runs before month 42 the execution of the runs has been postponed from month 36 to month 43-45.

Deliverables

D3.3.3.2 Datasets from the CNRS-LSCE model with chemical perturbations for different mitigation options (shifted from month 36 to 45, CNRS-LSCE)

D3.3.3.3 Datasets from the KNMI model with chemical perturbations for different mitigation options (shifted from month 36 to 45, KNMI)

D3.3.3.4 Cancelled.

D3.3.3.5 Datasets from the UCAM-DCHEM model with chemical perturbations for different mitigation options (shifted from month 36 to 45)

D3.3.3.6 Datasets from the UIO model with chemical perturbations for different mitigation options (shifted from month 36 to 45, UIO)

D3.3.3.7 Report on mitigation strategies (month 40, UIO, shifted to month 48)

Milestones

M3.3.3.2 Gridded mitigation scenarios available from Act. 1 (month 42, UIO)

M3.3.3.3 Model simulations ready; provision of output data to Activity 7 accomplished (month 46 UIO)