COST Action 728:
Enhancing Mesoscale Meteorological Modelling Capabilities for Air Pollution and Dispersion Applications

Working Group 2:
Integrated systems of MetM and CTM: strategy, interfaces and module unification

OVERVIEW OF EXISTING INTEGRATED (OFF-LINE AND ON-LINE) MESOSCALE SYSTEMS IN EUROPE

Deliverable 2.1 Report

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Contents

1 Introduction

Historically air pollution forecasting and numerical weather predictions (NWP) were developed separately. This was plausible in the previous decades when the resolution of NWP models was too poor for meso-scale air pollution forecasting. Due to modern NWP models approaching meso- and city-scale resolution and using land-use databases and remote sensing data with finer resolution, this situation is changing. As a result the conventional concepts of meso- and urban-scale air pollution forecasting need revision along the lines of integration of mesoscale meteorological model (MetM) and chemical transport model (CTM).

The eventual integration strategy will not be focused around any particular model – instead it would possibly be to consider an open integrated system with fixed architecture (module interface structure) and with a possibility of incorporating different MetMs/NWP models and CTMs. Such a strategy may only be realised through jointly agreed specifications of module structure for easy-to-use interfacing and integration.

Both, off-line and on-line coupling of MetMs and CTMs will be considered in WG2. Thus, a timely and innovative field of activity will be to assess the interfaces between MetMs and CTMs and the MetM-for-CTM models, and to establish the basis for their harmonization and benchmarking. It will consider methods for the aggregation of episodic results, model down-scaling as well as nesting. The activity will also address the formulation of requirements of mesoscale meteorological models suitable as input to air pollution models.

The overall aim of WG2 is to identify the requirements for the unification of MetM and CTM modules and to propose recommendations for a European strategy for integrated mesoscale modelling capability.

The objective of this WG2 report is to compile a state-of-the-art report on existing methodologies, approaches, models and practice in different countries for building integrated (off-line and on-line) MetM and CTM mesoscale systems.

The report includes an overview and summary of existing integrated models and their characteristics as they are presently used in Europe mainly. The model contributions and descriptions were generally compiled from COST members' contributions concerning their own model systems or systems used in their countries. The editors performed some formal editing and inclusion of results into the summary tables but they did not aim at a system intercomparison or even rating of the various systems which would require careful checkings and intercomparisons beyond their scope or intention. The model coverage thus also necessarily remains patchy, especially for large countries like Germany with dozens of federal states and institutes developing and using own model systems or components. The model systems in countries not active in COST728, e.g. France, also remain unmentioned. Therefore, this information remains somehow subjective and qualitative and reflects the knowledge and opinions of single authors and not the whole COST or even European modelling community.

2 Methodology for model integration

As strategy of a new generation integrated Meteorology (MetM) and Atmospheric Chemical Transport (CTM) modeling systems for predicting atmospheric composition, meteorology and climate change it is suggested to consider air quality modelling as a combination and integration (at least) of the following factors: air pollution, urban climate/meteorological conditions and population exposure. This combination is reasonable due to the facts that:

(i) meteorology is the main source of uncertainty in air pollution and emergency preparedness models,

(ii) meteorological and pollution components have complex and combined effects on human health (e.g., hot spots in Paris, July 2003),

(iii) pollutants, especially aerosols, influence climate forcing and meteorological events (precipitation, thunderstorms, etc.).

In this context, several levels of the integration strategy are considered in the WG2 report:

1) off-line models:
   - separate CTMs driven by meteorological input data from meteo-preprocessors, measurements or diagnostic models,
   - separate CTMs driven by analysed or forecasted meteodata from NWP archives or datasets,
   - separate CTMs reading output-files from operational NWP models or specific MetMs at limited time intervals (e.g. 1, 3, 6 hours).

2) on-line models:
   - on-line access models, when meteodata are available at each time-step (possibly via a model interface as well),
   - on-line integration of CTM into MetM, where feedbacks may be considered. We will use this definition for on-line coupled modelling.

The on-line integration of meso-scale meteorological models and atmospheric aerosol and chemical transport models enables the utilisation of all meteorological 3D fields in CTMs at each time step and the consideration of the feedbacks of air pollution (e.g. urban aerosols) on meteorological processes and climate forcing. This very promising way for future systems of atmospheric environment forecasting is considered in the COST Action 728 (http://www.cost728.org) and realised in several partner teams, e.g. at DMI in the ENVIRO-HIRLAM system (Chenevez et al., 2004; Baklanov et al., 2004) or in the COSMO consortium for the Lokalmodell (Vogel et al., 2006, Wolke et al., 2003).

These model developments will lead to a new generation of integrated models for: (i) climate change modelling, (ii) weather forecast (e.g., in urban areas, severe weather events, etc.), (iii) air quality and chemical composition longer-term assessment and iv) chemical weather forecasting, an activity that is of increasing importance and is due to be supported by a COST action started in 2007.

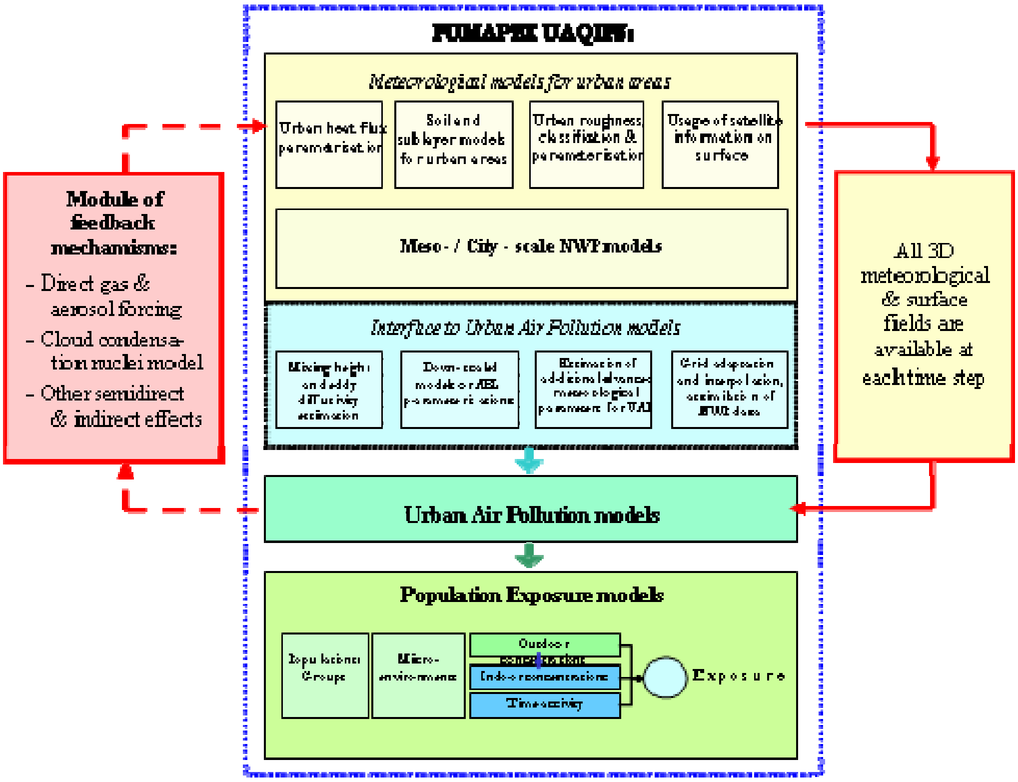

Figure 2.1: *Extended FUMAPEX scheme of Urban Air Quality Information & Forecasting System (UAQIFS) including feedbacks. Improvements of meteorological forecasts (NWP) in urban areas, interfaces and integration with UAP and population exposure models following the off-line or on-line integration (Baklanov, 2005; after EMS-FUMAPEX, 2005).*

Thus, the experience from various other communities will need to be integrated, as well as non-European Union countries experience, e.g. from America: the US EPA and other US and Canadian institutions (see WRF-Chem: Grell et al., 2005; Jacobson, 2005, 2006; Byun and Schere, 2006; Kaminski et al., 2005; etc.); from Russia, e.g. one of the first experience in on-line coupling of atmospheric pollution and meteorological models in the Novosibirsk scientific school (Marchuk, 1982; Penenko and Aloyan, 1985; Baklanov, 1988), for example for modelling of active artificial/anthropogenic impacts on atmospheric processes; from Japan: integrated chemical weather forecasting systems, based on the Earth Simulator (Uno et al., 2003, 2004).

As it was mentioned above, activities and investigation requirements are multiple but dispersed in Europe. Thus, a COST Action seems to be the best approach to integrate, streamline and harmonize these national efforts towards a leap forward for new breakthroughs beneficial for a wide community of scientists and users. The discussed European joint system strategy does not necessarily include just one model. It could be an open integrated system with fixed architecture (module interface structure) and with a possibility to incorporate different MetMs/NWP models and CTMs.

Such model integration should be realized following a joint elaborated specification of module structure for potential easy interfacing and integration. It might develop into a system, e.g. similar to the USA ESMF (Earth System Modelling Framework, see e.g.: Dickenson et al. 2002) or European PRISM (PRogram for Integrating Earth System Modelling) specification for integrated Earth System Models: http://prism.enes.org/ (Valcke at el., 2006).

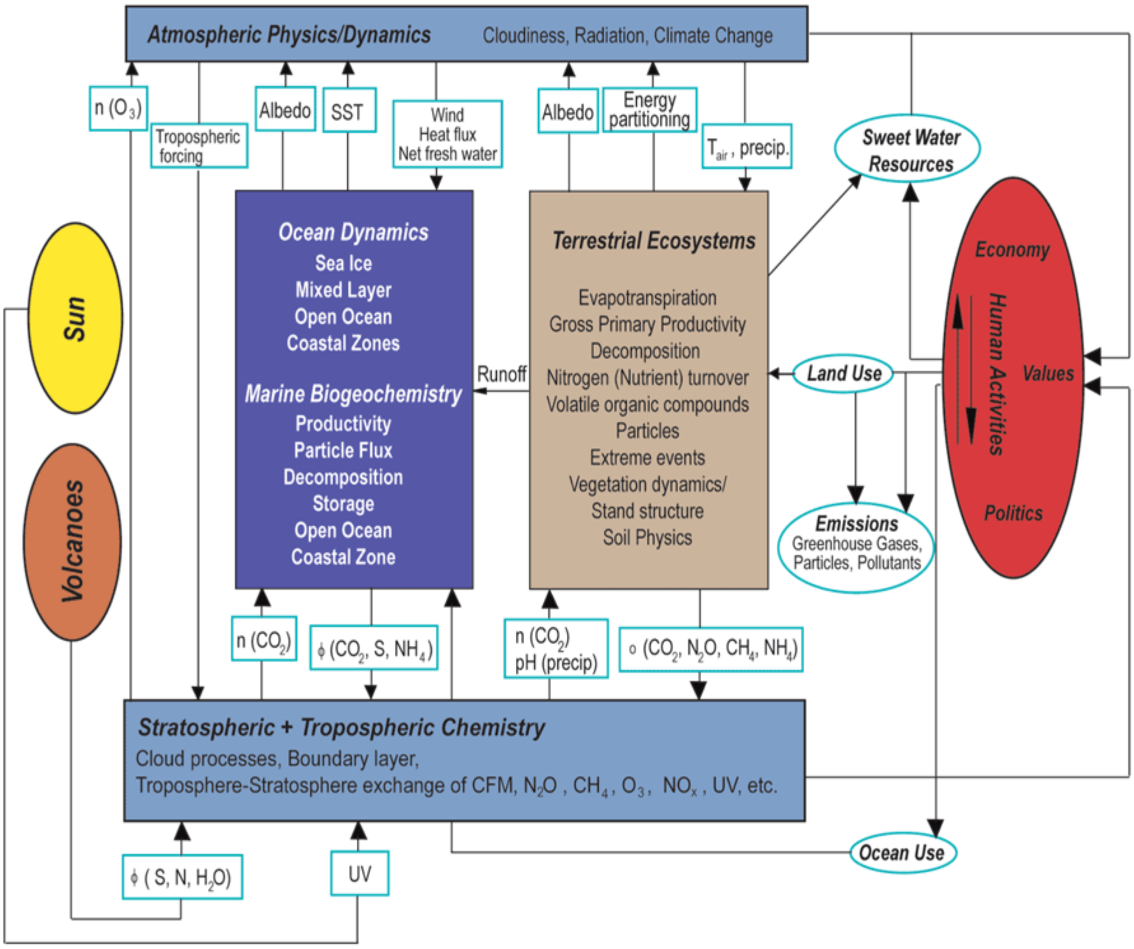

Figure 2.2. *COSMOS: **Community Earth System Models** Integrating Strategy (http://cosmos.enes.org)*

Community Earth System Models (COSMOS) is a major international project involving different institutes in Europe, in the US and in Japan, for the development of complex Earth System Models (ESM). Such models are needed to understand large climate variations of the past and to predict future climate changes (Claußen and Jacob, 2007).

Main differences of the COST 728 integrated strategy for meso-scale (MetM&CTM) models from the COSMOS integrating strategy (Figure 2.2) regard space and time scales of the considered phenomena. COSMOS is focused on the following processes and scales:

- Climate time-scale processes,
- General (global and regional) atmospheric circulation models,
- Atmosphere, ocean, cryosphere and biosphere integration.

A mesoscale integrated strategy will focus on forecast time scales of 1-4 days and omit the cryoshpere and the larger time and space scales in atmosphere, ocean and biosphere.

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3 Mesoscale off-line and on-line integrated Met&ACT models

(based on COST728 model database)

In COST728, a survey of the very many and diverse modelling communities in European countries was performed based on COST partner contributions.
The COST728 model inventory with detailed information on model qualities is available on the net (http://www.mi.uni-hamburg.de/costmodinv). The inventory is open to models of all scales and includes entries given in **Table 1**. Tables in Annex 2 summarize relevant information on models for COST 728 (see the details in WG4 reports and web-site). Contribution from COST 728 and 732 partners were solicited and compiled in this chapter.

Table 1: Model inventory containing all models from database of COST728, WG4, status 22 Dec 2006, see www.cost728.org plus WG2 partner contributions (no model cross-relation between table columns)

	Meteorology	**Chemistry & transport**	**Met & chem. & transport**
Microscale - COST 732	MITRAS	AERMOD MICTM	AERMOD AERMOD_Urban MICTM Chensi M-SYS MERCURE Meso-NH MIMO RCG VADIS
Mesoscale - COST 728	ALADIN ALADIN/A ALADIN/PL Lokalmodell aLMo ARPS CALGRID CLM FVM GEM/LAM GESIMA GME GRAMM Hirlam HRM Lokalmodell LAMI LAPS Lokalmodell LME LME_MH LMK MC2 MEMO (UoA-PT) MEMO (UoA-PT)	ADMS-Urban AERMOD ALADIN-CAMx ARGOS AURORA CAC CALGRID CAMx CHIMERE CHIMERE(ARPAIT) CMAQ CMAQ(GKSS) DERMA EMEP ENVIRO-HIRLAM EPISODE FARM FLEXPART FLEXPART/A FVM GEM/LAM-AQ GEOS-CHEM	BOLCHEM CALMET/CALPUFF CALMET/CAMx ENVIRO-HIRLAM GEM/LAM-AQ M-SYS MC2-AQ LM-ART LM-MUSCAT MCCM MEMO (UoT-GR) MERCURE Meso-NH RCG TAPM

	Meteorology	**Chemistry & transport**	**Met & chem. & transport**
	MERCURE MESO_NH METRAS MINERVE MM5 (UoA-GR) MM5 (UoA-PT) MM5 (UoH-UK) MM5(GKSS) NHHIRLAM RAMS SAIMM TAMOS TRAMPER UM WRF_ARW	GRAMM HYSPLIT LOTOS-EUROS LPDM MARS (UoT-GR) MARS (UoA-PT) MATCH MECTM MOCAGE MUSE NAME III OFIS RCG SILAM SPRAY 3 TAMOS TCAM TREX UAM-V	
Macroscale	GEM GME Hirlam TAMOS UM	CAC CAM-CHEM CHIMERE CHIMERE(ARPAIT) DERMA EMEP FLEXPART FLEXPART/A GEOS-Chem IMPACT LPDM MATCH MOCAGE NAME III SILAM STOCHEM TAMOS TCAM	ENVIRO-HIRLAM GEM_AQ

In the very many and diverse modelling communities in Europe, nevertheless, the model coverage necessarily remains patchy and model systems in countries not active in COST728, e.g. France, go unmentioned. Still, the contributions represent a wide spectrum of modelling complexity and effort in 16 European countries and about 40 institutions including ECMWF applying mopre than 25 integrated systems..

The majority of the presented systems are based on mesoscale meteorological models available at the national weather services or in weather forecasting consortia (i.e. HIRLAM, COSMO

(Lokalmodell), ALADIN, UM) and on international free community models developed by universities (i.e. MM5, WRF, MC2, RAMS).

Table 2: Main MetMs (top) and CTMs (bottom) from the COST728 community survey, applied by more than 2 groups.

MetM	MM5	COSMO LM	HIR-LAM	ECMWF	ALA-DIN	GME DWD	UM	RAMS	CAL-MET
No of groups using	11	9	6	6	3	3	3	3	3

CTM	CAMx	Chimere	CAL-GRID	CMAQ
No of groups using	5	4	3	3

This approach allows the air quality modelling community to take advantage and benefit from the development, testing, and model validations done for the purpose of weather prediction. At the same time it provides users without large own development capacities or with the need for a standard system to apply model systems supported by a wider community.

The modelling components that deal with transport and transformation of atmospheric pollutants are more diverse than the MetMs, ranging from a simple passive tracer along a trajectory (i.e. CALPUFF) to a complex treatment of reactive gases in an Earth system (i.e. MESSy).

This survey points out a wide range of model applications with the COST partners:
- diagnostic / climatologic: transport, AQ assessment and impact scenarios,, episode analysis, source apportionement,
- forecasting: transport and chemistry, AQ (urban AQ, coastal and industrial AQ), management policy advice covering gases incl. ozone, PM, pollen grains
- radioactivity (and environment) emergency forecasting.

A full list of applictions is provided in the Annex in Table A2.4.
This large variety of modelling systems can be considered a scientific richness but creates problems of model result inter-comparison and underlines difficulties in model development collaboration in Europe.

The overview also shows quite a surprising number of at least 10 more or less complex on-line coupled MetM and CTM model systems already being used in Europe (America and Australia):
- ENVIRO-HIRLAM (DMI, Denmark),
- COSMO LM-ART (Inst. for Meteorology and Climatology, FZ Karlsruhe, Germany),
- COSMO LM-MUSCAT (IfT Leipzig, Germany),
- MCCM (Inst. of Atmospheric Environmental Research at FZ Karlsruhe, Germany),

- MESSy: ECHAM5 (MPI for Chemistry, Mainz, Germany),
- MC2-AQ (York Univ, Toronto, University of British Columbia, Canada, and Warsaw University of Technology, Poland),
- GEM/LAM-AQ (York Univ, Toronto, University of British Columbia, Canada, and Warsaw University of Technology, Poland),
- WRF-Chem: Weather Research and Forecast and Chemistry Community modelling system (NCAR and many other organisations),
- OPANA = MEMO + CBM IV + SMVGear (Univ. of Madrid, Spain)
- BOLCHEM (CNR ISAC, Italy).
- ECMWF (passive pronostic stratos. ozone tracer in IFS, GEMS modelling)
- MESSy: ECHAM5-Lokalmodell LM planned at MPI-C Mainz, Univ. of Bonn, Germany.
- GME (global NWP model of DWD, Germany, passive progn. stratos. ozone tracer)

Table 3 shows some characteristics of the above mentioned on-line coupled MetM and CTM systems. However, it is necessary to mention, that many of the above mentioned on-line models were not build for mesometeorological scale, and they (e.g. GME, ECMWF GEMS, MESSy) are globale-scale modelling systems and are originated from the climate modelling community. Becides, at the current stage most of the on-line coupled models do not consider feedback mechanisms or include only simple direct effects of aerosols on meteorological processes (like COSMO LM-ART and MCCM). So, only two meso-scale on-line integrated modelling systems (WRF-Chem and ENVIRO-HIRLAM) consider feedbacks with indirect effects of aerosols.

Table 3: On-line coupled MetM - CTMs

Model name	**On-line coupled chemistry**	**Time step for coupling**	**Feedback**
BOLCHEM	Ozone as prognostic chemically active tracer		None
ENVIRO-HIRLAM	Gas phase, aerosol and heterogeneous chemistry	Each HIRLAM time step	Yes
WRF-Chem	RADM+Carbon Bond, Madronich+Fast-J photolysis, modal+sectional aerosol	Each model time step	Yes
COSMO LM-ART	Gas phase chem (58 variables), aerosol physics (102 variables), pollen grains	each LM time step	Yes (*
COSMO LM-MUSCAT (**	Several gas phase mechanisms, aerosol physics	Each time step or time step multiple	None
MCCM	RADM and RACM, photolysis (Madronich), modal aerosol	Each model time step	(Yes) (***
MESSy: ECHAM5	Gases and aerosols		Yes
MESSy: ECHAM5-COSMO LM (planned)	Gases and aerosols		Yes

MC2-AQ	Gas phase: 47 species, 98 chemical reactions and 16 photolysis reactions	each model time step	None
GEM/LAM-AQ	Gas phase, aerosol and heterogeneous chemistry	Set up by user – in most cases every time step	None
Operational ECMWF model (IFS)	Prog. stratos passive O3 tracer	Each model time ste	
ECMWF GEMS modelling	GEMS chemistry	Each model time step	Yes
GME	Progn. stratos passive O3 tracer	Each model time step	
OPANA=MEMO+CBMIV		Each model time step	

*) Direct effects only; **) On-line access model; ***) Only via photolysis

Further model synopsis tables are provided in Annex 2.

Main advantages of On-line & Off-line modelling approaches from first preliminary look are the following:

On-line coupling

- Only one grid; No interpolation in space;
- No time interpolation;
- Physical parameterizations are the same; No inconsistencies;
- All 3D meteorological variables are available at the right time (each time step); No restriction in variability of meteorological fields;
- Possibility to consider feedback mechanisms;
- Does not need meteo- pre/post-processors.

Off-line coupling

- Possibility of independent parameterizations;
- Low computational cost (if NWP data are already available and no need to run meteorological model);
- More suitable for ensembles and operational activities;
- Easier to use for the inverse modelling and adjoint problem;
- Independence of atmospheric pollution model runs on meteorological model computations;
- More flexible grid construction and generation for ACT models,
- Suitable for emission scenarios analysis and air quality management.

Coupling issues and problems involve:

- input data (measurements or prognostic model data including input data formats and coupling time step),
- downscaling / nesting with high resolution requirements for special topographies and circulation conditions, achieved through (self-)nesting of MetMs and/or CTMs including 2-way interactive nesting for MetMs: MM5, RAMS and an experimental COSMO-LM,

- modularity (requirements for high modularity and high compatibility, e.g. no COMMON blocks but direct parameter passing),
- flexible IO strategies,
- interfaces (described in the following).

The communication between off-line coupled meteorological and AQ models is a problem of often underestimated importance. The multitude of modelling systems previously introduced give rise to different approaches and methods implemented within interface modules. Tasks covered by interfaces are minimised in coupled systems relying on surface fluxes, turbulence and dispersion parameters (i.e. eddy viscosity) provided by the meteorological driver. Other systems use interface modules implementing surface and boundary layer parameterisations to estimate dispersion parameters. Sometimes these last choices are due to the need to rely on “standard” meteorological products and to guarantee the AQ modelling robustness for practical applications. In other cases interfaces are used to enhance local physiographic data resolution and possibly introduce advanced parameterisations (e.g. urbanisation). Atmospheric physics parameterisations, and even default or limit values assumed for some key parameters, can have relevant effects on pollutant concentration fields in critical conditions (e.g. low wind and stable conditions). Moreover, interface modules involve the evaluation of emissions of some relevant species that can be strongly influenced by meteorology, like biogenic VOC, windblown dust and sea salt spray (see e.g. Figure 3.1).

In the diverse landscape of European modelling, model harmonisation remains an important issue despite earlier efforts, e.g. COST710 (1994-1998) which are continued in the regular Harmonisation conferences.. A sample of current projects involved with issues of integrated met and chemistry modelling is given below showing the large effort and complexity but also stressing the need for cooperation:

- PRISM (FP5): Earth system modelling, software infrastructure,
- PRISM support: COSMOS, OASIS coupler,
- ENSEMBLES (FP6): climate change ensemble prediction system for Earth system models,
- ENES European system for Earth system modelling,
- ESMF Earth system modeling framework (US),
- FLUME flexible Unified Model Eenvironment (UK MetOffice),
- CURATOR info on earth system/climate models,
- intercomparison projects and IPCC assessments (US),
- GEMS (6FP) global and regional Earth system monitoring using satellites and in-situ data, ECMWF, data assimilation and forecasting
- GENIE Grid ENabled integrated Earth system model (UK),
- GO-ESSP global organisation of Earth system science portal (UK,NOAA,NASA, etc.).

Modular modelling, flexible IO strategies and adaptable interfaces following agreed guidelines for off-line and on-line integrated modelling, which are applied by all including the large consortia and community models, would greatly facilitate model improvement and applicability for European users, and a large COST action like 728 appears as a very suitable means for advancing this aim.

The results of this model overview will be used to identify frequent or common weaknesses and problems and will serve to highlight areas of improvement and to formulate recommendations. Other important questions only marginally covered in this overview are the topics of interfaces coupling MetMs and CTMs (their necessity, degree of complexity and kind of additional information provided), and the questions of feedback of CTMs on MetMs which will be treated in subsequent reports of WG2.

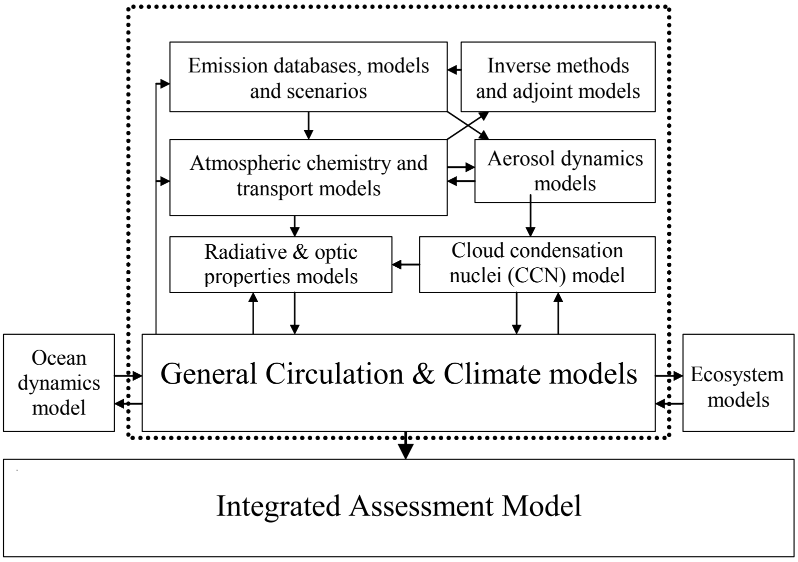

Figure 3.1. *The integrated system structure for studies of the meso-scale meteorology and air pollution, and their interaction.*

4 Overview of integrated models of COST728 partners

(information mainly provided by WG2 partners)

4.1 Integrated modelling at Central Institute for Meteorology and Geodynamics (ZAMG), Austria

(contribution by Ulrike Pechinger et al., ZAMG)

MetM: ALADIN
CTMs:

- FLEXPART, i.e. the mesoscale version of the ZAMG emergency response modelling system for nuclear accidents
- CAMx run to support ozone forecasting

only off-line coupling
interfaces: meteorological fields from MetM ALADIN, some only re-formatted, others interfaced using methods from literature, the MM5 CAMx pre-processor or the CTM CHIMERE

1. FLEXPART

At ZAMG the mesoscale model ALADIN is run twice a day and produces forecasts up to 48 hours with a horizontal resolution of 9.6km (289x259 grid cells) and 45 levels. The model runs on a SGI-origin3400 computer with 28 processors and produces a special binary output, which is not portable to other computers without the required ALADIN software. Therefore on the ALADIN computer the output had to be converted to the machine independent data format netCDF and then transferred to the central file server of ZAMG. The applications run on different computers (SUN workstations or linux server) and can access the data from the file server over NFS or from local copies of the netCDF files.

The ALADIN netCDF files are used for emergency response modelling with the trajectory model FLEXTRA (Stohl, 1998) and the dispersion model FLEXPART (Stohl, 1997) and for the ozone forecast with the CAMx model. In addition the data are used for pre-processing the meteorological input for the near-range dispersion model in RODOS.

The interface between the meteorological model and the dispersion part was developed in the view of an operational use. A couple of important changes considering input format and grid specifications had to be done to FLEXPART and FLEXTRA.

2. CAMx

The operational regional weather forecast model ALADIN-Austria, which is run at the Central Institute for Meteorology and Geodynamics (ZAMG) is used to implement a forecast system for tropospheric ozone for Austria (Baumann-Stanzer, 2005). The new air quality model system consists of three parts that are linked together (meteorology, emissions, dispersion model). The combination of the two major parts, the meteorological input provided by ALADIN and the chemical model CAMx, was implemented for the first time in this study.

CAMx (Comprehensive Air qualtity Model with extensions, http://www.camx.com) simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested 3D grids. A two grid nesting is used with a coarse grid over Europe and a finer grid for the core area covering Austria with the best possible spatial resolution of 9.6 km (according to the present grid of ALADIN-Austria).

The model needs meteorological fields as input which are supplied by the limited area model ALADIN (http://www.cnrm.meteo.fr/aladin/). It is run twice a day at the ZAMG and renders forecasts for 48 hours. The meteorological fields have a temporal resolution of one hour. The data is provided on 45 model-levels (only the lower 33 are used in CAMx) and has a horizontal resolution of 9.6 km. The majority of the necessary fields are extracted right away out of the ALADIN dataset and has only to be converted into CAMx readable input files. Those fields are horizontal wind (3D), temperature (3D), pressure (3D), convective and large scale precipitation (2D), snow cover(2D), solar radiation (2D) and specific humidity (3D).

Additionally CAMx needs, cloud optical depth (3D), height and pressure of the model levels (3D), cloud water content (3D) and precipitation water content (3D). These parameters are determined from the available ALADIN fields. One of the main challenges was to find appropriate methods to derive those fields. For that purpose already approved methods where investigated from literature as well as the MM5-CAMx – pre-processor (available on the CAMx homepage) or the chemical transport model CHIMERE (http://euler.lmd.polytechnique.fr/chimere/).

For each of the selected parameters computer programs were developed and implemented in the module. Some of the already existing code from the MM5CAMx or the CHIMERE pre-processor software could have been adopted with minor changes concerning programming language (Fortran 90 instead of Fortran 77) and structure. The corresponding citations are given in the following section which provides an overview on the parameterisations and assumptions for the different parameters.

2.) Parameterisations

2.1.) Measures for humidity

Mixing ratio (m), saturation vapour, water vapour content, dew point, relative humidity and virtual temperature (T_v) are obtained from the according ALADIN fields (Deutscher Wetterdienst, Aspirations – Psychrometer - Tafeln,1976). The respective relationships were included in the code.

2.2.) Pressure and height of model levels

The pressure at different model levels and the corresponding heights are needed to set up the CAMx modelling grid using a terrain-following vertical coordinate system.

Model level heights are derived with the barometric height formula (Pichler, 1997) based on the vertical pressure distribution and the virtual temperature (T_v) for every air column:

2.3.) Vertical diffusivity coefficient Kv

The vertical diffusivity coefficient Kv is determined following the method from Louis (1979). Most of the existing MM5CAMx pre-processor code was adopted for this parameter. This approach uses the Richardson number. Kv depends on the height above ground, vertical wind shear and equivalent potential temperature.
The equivalent potential temperature is calculated with temperature T, pressure p and specific humidity q which are available from ALADIN fields.

2.4.) Optical depth

To obtain the vertical profile of the optical depth, an algorithm is applied which is used by the chemical transport model CHIMERE (http://euler.lmd.polytechnique.fr/chimere/). Parts of this code have been integrated into the new routines. This approach uses layer thickness and relative humidity. The contributions are summarized beginning by convention from the top of the modelling domain (k_{top}). It is differentiated between low, medium and high cloud cover depending on the vertical level k

2.5.) Cloud and rain water content

Cloud and rain water content can not be extracted out of the ALADIN Austria data. The cloud water content is obtained first by an parameterisation from the convective precipitation rate which is provided by ALADIN. The correlation between cloud water and optical depth is used to approximate the cloud water content for cases when no convective precipitation occurs. From the cloud water content together with the 2D precipitation fields the rain water content can be derived.

Parts of the code are already implemented in the MM5CAMx pre-processor. Changes had to been done concerning programming structure to integrate the existing code into the developed routines.

For cases with convective precipitation the cloud water content (cw) is obtained by the method from Scott (1978).
Two assumptions have to be made at this point. The contributions of rain water (r_e > 1000 µm), snow and graupel have to be omitted because they are not available. Additionally grid cells with temperatures bellow 0 C° are neglected because they would contribute to the ice water content.

Typical cloud drops have a radius of about 10 µm and for the water density 1000 kg/m³ is used. Together with the already obtained optical depth the cloud water content is parameterised.

Also already integrated in the MM5CAMx pre-processor is the derivation of the rain water content which is determined by the surface fields of large scale and convective precipitation (r_{gr}, r_{kon}). Only contributions with rain rates higher than 0.2 mm/h are considered. The rain water content rw for the surface layer is calculated by the relationship in (Scott, 1978).

Based on the surface values the rain water content values are calculated at higher levels. The levels are initialised first by the value of the level below and the fraction of the precipitation of the current level is assigned to the cloud water content and is therefore subtracted from the rain water content in the actual height. The rain water content above the 0 C° level are set to 0.

3.) Future work and further developments

During the winter 2005/2006 several improvements have been conducted based on the experiences of the forecasts during the summer 2005 (Krüger, 2006). These changes are: improved emission data, dynamic boundary conditions and the use of operational available ozone column data from the ECMWF to enable a better adjustment to the actual weather conditions.

A future goal is to improve the parameterisation schemes and maybe include additional parameters which will be available from ALADIN datasets. One of the parameters that will be considered in more detail is the vertical diffusivity coefficient. Several other parameterisations are known for the calculation of this coefficient. These are based on different physical approaches and will be tested in view of tropospheric ozone forecast modelling.

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4.2 Integrated modelling in Belgium

4.2.1 Integrated modelling at the Flemish Institute for Technological Research (VITO)

(contribution by Koen De Ridder, VITO)

VITO has developed an integrated off-line modelling system based on the 3-D prognostic models ARPS (MetM – Univ. Of Oklahoma, USA) and AURORA (CTM – developed at VITO). This system is employed for simulating urban- to regional-scale air quality, in forecasting mode as well as for purposes of urban air quality assessment and management.

MetM

The **Advanced Regional Prediction System (ARPS)** is a non-hydrostatic mesoscale meteorological model developed at the University of Oklahoma (Xue et al., 2000, 2001). The finite-difference equations of the model are discretised on the Arakawa C-grid, employing a terrain-following co-ordinate in the vertical direction. Advection is solved with a 4th order central differencing scheme and leapfrog time stepping. Turbulence is represented by the 1.5 order TKE model, and the Sun and Chang (1986) parameterisation for the convective boundary layer. ARPS contains detailed parameterisations for cloud microphysics, cumulus convection, and radiation transfer. The model has nesting capabilities, allowing large-scale atmospheric features to enter the domain through the lateral boundaries. A detailed land surface scheme (De Ridder and Schayes, 1997) was incorporated in ARPS, to calculate the energy and water fluxes between the land surface and the atmosphere, including the effects of vegetation and soils on the partitioning of incident radiant energy between the turbulent fluxes of sensible and latent heat, and the storage heat flux. In order to better represent urban surfaces, the land surface model was modified by including the Brutsaert (1975) temperature roughness parameterisation for “bluff-rough” surfaces.

CTM

AURORA ('Air quality modelling in urban regions using an optimal resolution approach') is an atmospheric transport-chemistry model developed at VITO (Mensink et al., 2001). Advection is treated using the Walcek (2000) scheme, which is monotonic, exhibits a relatively limited numerical diffusion, and comes at a reasonable computational cost. Vertical diffusion is calculated with the Crank-Nicholson method (De Ridder and Mensink, 2002). The chemical gas phase chemistry in AURORA is based on the CB-IV mechanism, upgraded to account for biogenic emissions of isoprenes and terpenes. For the calculation of particulate matter, a state-of-the-art aerosol module is currently (Fall 2006) being implemented, consisting of the Caltech Atmospheric Chemistry Mechanism (CACM, Griffin et al., 2002) and the Model of Aerosol Dynamics, Reaction, Ionisation and Dissolution 2 (MADRID 2, Zhang et al., 2004). CACM describes the formation of secondary organic aerosol precursors in the atmosphere in a mechanistic way. MADRID 2 treats the formation of secondary aerosols by means of equilibrium calculations between the gas phase and the aerosol phase. Also dynamic processes (e.g., nucleation of particles) are included in MADRID 2. The module for particulate matter is capable of calculating the mass concentration of PM10 and PM2.5, as well as its chemical composition (ammonium, nitrate, sulphate, primary inorganic components, elementary carbon, primary organic components, and secondary organic components).

Coupling and interfaces

The coupling between ARPS and AURORA is currently off-line (though it is not excluded that in the future both models will be integrated more tightly in on-line mode). The time step for the coupling is variable, but generally it is hourly. No separate interface module is required to couple AURORA to ARPS as both models employ exactly the same grid, hence no spatial interpolation is required. The AURORA model reads 3-D ARPS output fields, and directly employs the relevant variables provided by the latter (wind vectors, eddy diffusion coefficients, temperature, humidity, ...) to calculate transport and chemistry.

Downscaling/nesting

Both ARPS and AURORA have nesting capabilities. ARPS is generally nested within model output of a global meteorological model, either the ECMWF model (using model-level data or else pressure-level data, at 0.5° spatial resolution) or the Final Analysis (FNL) data from NCEP (pressure-level data, at 1° resolution). The time step used is generally 6-hourly. More recently, ARPS was nested within output fields of the MM5 model operated by the Rheinisches Institut für Umweltforschung (RIU – Universität zu Köln). Further downscaling is achieved by nesting higher-resolution domains of ARPS within coarse-resolution ARPS simulation output. AURORA is nested within output fields of continental-scale models, such as CHIMERE or the EURAD model. Downscaling is achieved as is the case for ARPS, i.e., by nesting AURORA within itself at increasingly high resolution.

Data assimilation/initialization

For the moment no data assimilation is being used in ARPS/AURORA. However, in the near future satellite cloud data will be used together with data assimilation techniques to improve simulated cloud, which is particularly important for a good estimate of photolysis coefficients. AURORA will be extended with the possibility to assimilate observed pollutant concentrations from ground-based networks such as AirBase. Initialization of atmospheric fields in both ARPS and AURORA is achieved by interpolation from the coarse-scale models used for the nesting (see above). Apart from that, particular attention is given to the initialization of surface properties. For applications in Europe land cover is interpolated from the CORINE or PELCOM land cover maps. For applications outside Europe use is made of the GLC2000 (global) data base. Terrain height is interpolated from the Global 30 Arc-Second Elevation Data Set (GTOPO30) distributed by the U.S Geological Survey. Sea surface temperature is derived from AVHRR or MODIS imagery. Vegetation abundance is specified as a function of the Normalised Difference Vegetation Index (NDVI) contained in imagery from the VEGETATION instrument onboard the SPOT satellite platform.

Applications

- ARPS contributed to the intercomparison study MESOCOM (Thunis et al., 2003), and was recently used to demonstrate the effect of the Brutsaert thermal roughness parameterization by comparing simulated surface temperature with values observed by satellite (De Ridder, 2006).
- Within the BUGS project ("Benefits of Urban Green Space", EU-FP5), ARPS and AURORA were applied to evaluate the effects of vegetation and urban morphology on air quality (De Ridder et al., 2004). In this context, simulations were performed for benzene, ozone, and particulate matter, on Antwerp (Belgium), the Ruhr area (Germany), and Budapest (Hungary).
- In the PROMOTE project (ESA-GMES), AURORA is being used to perform (1) air quality forecasts for Belgium, with a zoom on the 5 largest cities, and (2) a calculation of urban air quality indicators for European cities, combining modelling and observations.
- AURORA was recently used to produce spatial patterns of pollutants, in the context of a study that aimed at relating pollutant concentration patterns to adverse health effects.

In the near future ARPS/AURORA will be employed to evaluate air quality in booming Chinese

- cities (Shenyang, Yanghzou).

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4.2.2 Integrated modelling at Royal Meteorological Institute of Belgium

(contribution of Andy Delcloo, Royal Meteorological Institute, Brussels, andy.delcloo@oma.be)

Summary:
MetMs: ECMWF
CTMs: Chimere parallel version
Assimilation of ozone soundings into the CTM Chimere

Model descriptions (with text descriptions): ***www.ecmwf.int ;***

Met Ms: operational forecast ECMWF, grid resolution: 50 km, time resolution: 3-hourly

CTM's: V200603par-rc1.1 version

Off-line models / On-line models: off-line coupling

Interface modules: parallel version

***Downscaling/nesting*:** one-way nesting
Data assimilation/initialisation:
Project description: Assimilation of vertical ozone profile data in the chemical transport model Chimere coupled to weather prediction models

Current applications of the integrated modelling systems:

Model unification/harmonization/ further developments

It is the goal to run Chimere with a one-way nesting approach with Aladin, 7 km resolution

References: -

4.3 Integrated modelling systems in Denmark (selection)

(contribution by Alexander Baklanov, Ulrik Smith Korsholm and Allan Gross, DMI)

4.3.1 DMI-ENVIRO-HIRLAM on-line coupled system

Summary:

MetMs: DMI-HIRLAM

CTMs: on-line fully integrated ACTM, could also be used as off-line coupled (CAC or some other)

Interfaces: On-line coupling.

Model descriptions:

Currently the Danish Meteorological Institute (DMI) is developing a new version of the meteorological model HIRLAM (High Resolution Limited Area Model) which includes on-line coupled tracers (DMI-ENVIRO-HIRLAM) (based on Chenevez et al., 2004) and has implemented a versatile aerosol-cloud module and heterogeneous chemistry in their Atmospheric Chemical Transport Model (ACTM-CAC) (Gross and Baklanov, 2004). Implementation of the ACTM-CAC in the DMI-ENVIRO-HIRLAM makes the inclusion of regional to urban scale feedbacks between the ACTM-CAC and DMI-HIRLAM possible (see the red box and dashed arrows in Figure 2.1) (Baklanov et al., 2004; Baklanov et al., 2006; Korsholm et al., 2007). Simplified feedback mechanisms, including indirect aerosol forcing, are included in the current version of the ENVIRO-HIRLAM integrated model.

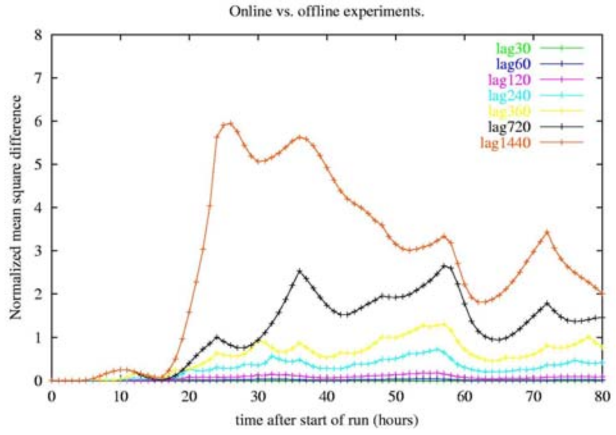

Figure 4.1. One example of On-line versus Off-line DMI-ENVIRO-HIRLAM runs for the ETEX experiment: normalized mean square difference (Korsholm et al., 2006). Simple test: only Advection part is differently coupled; On-line: each time step, Off-line: 0.5, 1, 2, 4, 6, 12, 24 hours; typical meteorological conditions (ETEX-1 case).

ENVIRO-HIRLAM is developing as an on-line integrated system with a possibility of the off-line coupling as well. The system realisation includes the following steps:
(i) nesting of models for high resolutions,
(ii) improved resolving boundary and surface layers characteristics and structures,
(ii) ‘urbanisation’ of the model,
(iii) improvement of advection schemes,
(iv) implementation of chemical mechanisms,
(v) implementation of aerosol dynamics,
(vi) realisation of feedback mechanisms,
(vii) assimilation of monitoring data.

The model is to be used for operational as well as research purposes and will comprise aerosol and gas transport, dispersion and deposition, aerosol physics and chemistry as well as gas-phase chemistry.

Several sensitivity tests of the off-line versus on-line coupling of MetM and CTM in ENVIRO-HIRLAM as well as their verification versus the ETEX experiment were considered and results discussed (Korsholm et al., 2006, 2007). Our preliminary tests of the off-line vs. on-line integrations of ENVIRO-HIRLAM (see e.g., Figure 4.1) show that the on-line integration of meso-scale meteorological models and atmospheric aerosol & chemical transport models with consideration of the feedbacks of air pollution (e.g. urban aerosols) on meteorological processes and urban climate is a very promising way for future systems of atmospheric environment forecasting.

4.3.2 The tropospheric Chemistry Aerosol Cloud (CAC) model

Summary:

MetMs: DMI-HIRLAM, ECMWF
CTMs: Chemistry Aerosol Cloud (CAC) model
Interfaces: Off-line coupling with own interface module.

Model descriptions:

Chemistry Aerosol Cloud (CAC) transport modelling system is a system which has been developed at DMI (Gross and Baklanov, 2004). The CAC modelling system is a highly flexible module based system. This makes it easy to perform changes of the chemistry, and apply the model to another emission inventory and/or meteorological data.

In the present version of CAC an updated version of CB-IV from 1999 with improved isoprene chemistry is used together with the Tropospheric Ultraviolet and Visible radiation model (TUV) to calculate photolysis rate coefficients, and emissions from EMEP. (A new aerosol module is in under development).

Currently the CAC modelling system is an off-line model. Therefore depending on the study item, different meteorological reanalysed archive data sets, numerical weather prediction (such as DMI-HIRLAM (Sass et al., 2002) or ECMWF) or climate models can be used as meteorological driver for the CAC modelling system. At present the transport in the model system can be solved either in the 3D Lagrangian or 3D Eulerian framework.

The horizontal and vertical resolution of the model depends on the resolution of the meteorological date and emission information. At present the model is run over a 0.2°×0.2° longitude-latitude grid.

The 3D version of the model has a vertical resolution of 25 heights. These heights are selected so they cover the lowest 3 km of the atmosphere. The amount of chemical compounds which is transported from the free troposphere into the atmospheric boundary layer is determined by the meteorological information and the concentration of the chemical compounds in the free tropospheric. These concentrations are longitude, latitude, land/sea and monthly dependent (Gross et al., 2005).

The model system is used for real-time regional scale forecasts of ground-level gas-phase air pollutants and regional scale modelling of historical ground-level gas-phase and aerosol air pollutant data.

4.3.3 The Danish Emergency Response Model of the Atmosphere (DERMA)

Summary:

MetMs: DMI-HIRLAM, ECMWF

CTMs: DERMA model

Interfaces: Off-line coupling with own interface module.

Model descriptions:

The Danish Emergency Response Model of the Atmosphere (DERMA) is a three-dimensional Lagrangian long-range dispersion model using a puff diffusion parameterisation, particle-size dependent deposition parameterisations and radioactive decay (Sørensen, 1998; Sørensen et al., 1998; Baklanov and Sørensen, 2001; Sørensen et al., 2007). Earlier comparisons of simulations with the DERMA model versus the ETEX experiment involving passive tracer measurements gave very good results (Graziani *et al*., 1998). The DERMA model can be used with different sources of NWP data, including the DMI-HIRLAM limited-area and the ECMWF global NWP models with various resolutions. The main objective of DERMA is the prediction of the atmospheric transport, diffusion, deposition and decay of a radioactive plume within a range from about 20 kilometres from the source up to the global scale. DERMA is run on operational computers at DMI. The integration of DERMA in ARGOS is effectuated through automated on-line digital communication and exchange of data. The calculations are carried out in parallel for each NWP model to which DMI has access, thereby providing a mini-ensemble of dispersion forecasts for the emergency management.

4.3.4 The Accident Reporting and Guidance Operational System (ARGOS)

Summary:

MetMs: LINCOM, DMI-HIRLAM, ECMWF

CTMs: The Local Scale Model Chain (LSMC) including RIMPUFF model; DERMA model

Interfaces: Off-line coupling, with LSMC meteorological pre-processor.

Models description:

The Danish nuclear emergency preparedness involves the Accident Reporting and Guidance Operational System (ARGOS), developed by the Danish Emergency Management Agency (DEMA) and collaborators (Hoe et al., 1999, 2002). The ARGOS system utilises meteorological forecast data for the prediction of contamination, doses and other consequences on local and

European scales. In Denmark such data are provided by DMI four times a day. The 3D data, which are transferred online to DEMA, are operationally extracted with 5 km (or experimentally 1.4 km) horizontal resolution forecasting up to 54 hours ahead. For Denmark the recent operational NWP system (Sass *et al., 2002*) consists of 2 nested models named DMI-HIRLAM-S05 and -T15, with horizontal resolutions of about 5 and 15 km, respectively. Within the FUMAPEX project for the urban version of ARGOS, DMI also runs experimental urbanised version of DMI-HIRLAM over Denmark with a horizontal resolution of 1.4 km and improvements of parameterisations of the urban sublayer processes and urban physiographic data classification (Baklanov *et al. (2005a,b)*).

In order to meet the input requirements of the ARGOS system, a meteorological pre-processing interface is translating and interpolating the NWP model output. The Local Scale Model Chain (LSMC) (Mikkelsen *et al.*, 1997) comprises a meteorological pre-processor, which calculates deposition and stability parameters and wind fields based on the data provided by the DMI-HIRLAM model. These data are pre-processed and interpolated to yield data input fields for the RIMPUFF local-scale dispersion model of ARGOS. The wind fields are interpolated either with the linearized flow model LINCOM (Mikkelsen et al., 1997; Astrup et al., 1996) or by $1/r^2$ weighting. The mixing height is included in the NWP output data or can be calculated by the LSMC using different methods.

The local-scale atmospheric dispersion model system LSMC, is used in ARGOS for the calculation of actual and forecasted ground-level air concentrations, wet and dry deposition, and ground-level gamma dose rates on short and medium range scales (up to about 100 km from the source). It includes the atmospheric local-scale dispersion model RIsø Mesoscale PUFF model (RIMPUFF) developed at the Risø National Laboratory (Mikkelsen *et al.*, 1984, 1997). At distances greater than about 20 kilometres from the source, the DMI DERMA model (see 4.3.3) can be used.

4.3.5 Other off-line integrated air pollution models in Denmark

There are several more (not presented in the report) ACT models off-line integrated with the DMI-HIRLAM model or other meteorological models or utilising NWP output data as meteo-drivers. They include, e.g. the following models:

- the DACFOS modelling system for operational ozone forecasting in DMI (Kiilsholm, 2000),
- the Kalman filter model for ozone forecasting (Chenevez and Jensen, 2001),
- the MOON air chemistry model, based on the RACM2 mechanism (Gross et al., 2005),
- the pollen statistical forecast model (Rasmussen, 2002) and Pollen-ENVIRO-HIRLAM system (Mahura et al., 2006; Rasmussen et al., 2006),
- CFD 3D local-scale obstacle-resolved air flow and pollution on-line coupled model (Baklanov 2000),
- the TOHR Air Pollution Forecast System, developed in the National Environmental Research Institute, Denmark (Brandt et al., 2000).

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4.4 Integrated modelling in Estonia

(contribution by Aarne Männik, Estonian Meteorological Hydrological Institute; Marko Kaasik, University of Tartu)

4.4.1 Integrated modelling at Estonian Meteorological Hydrological Institute (EMHI),

Summary: EMHI as national weather service is the main provider of meteorological information in Estonia. EMHI provides observations, meteofields from ECMWF and HIRLAM and meteofields from experimental setup of NHHIRLAM. EMHI has no responsibility for air pollution modeling, forecasting or emergency response duties in Estonia. However, it is planned to have „on the shelf“ system for emergency response based on ARGOS which will be in off-line mode driven by ECMWF or HIRLAM meteorological fields.

MetMs: HIRLAM, NHHIRLAM, ECMWF
CTMs: ARGOS
Interfaces: HIRLAM GRIB files containing forecast or analyses have to be converted into ARGOS specific format. The format is human readable and contains header and sections of single- and multi-level fields together with data tables. Only off-line coupling is used.

Model descriptions:
MetMs: HIRLAM model is described in section 4.3 and ECMWF model is well-known.
Description of NHHIRLAM follows under the section of University of Tartu.

CTMs: ARGOS is a Decision Support System (DSS) for emergency management (see Section 4.3.4). Its dispersion models supports short range: DERMA (Danish), MLDP (mesoscale modeling based on LSCM/RIMPUFF and long range dispersion which is based on several models Canada), SNAP (Norway) and MATCH (Sweden). ARGOS supports trajectory calculation and also urban dispersion modelling. Finer details on ARGOS model can be found on the web-page http://www.pdc.dk/argos/ .

4.4.2 Integrated modelling at University of Tartu,

Summary: University of Tartu is the main developer of NH HIRLAM. CTM SILAM from FMI was installed at University of Tartu in spring 2006 and it is being used for scientific research (Kaasik et al 2006). It is planned to use the output of NH HIRLAM for SILAM in „off-line“ mode in autumn 2007. Most of the research work related to mesoscale processes in air quality applications is expected to happen in University of Tartu as other air quality related institutions in Estonia are mainly focusing on operational usage.

MetMs: HIRLAM, NHHIRLAM, ECMWF

CTMs: SILAM
Interfaces: general GRIB interface
Only off-line coupling.

Model descriptions:
MetMs: HIRLAM model is described in section 4.3 and ECMWF model in section 4.16. NH HIRLAM is an extension module for limited area NWP model HIRLAM developed in University of Tartu. The main goal of NHHIRLAM is to extend initially hydrostatic model to nonhydrostatic domain while maintaining most of the parent model features. Explicit and semi-implicit Eulerian (Männik and Rõõm 2001; Rõõm and Männik 2002; Männik et al 2003) and semi-implicit Lagrangian integration (Rõõm et al 2006) schemes are supported. It is currently an adiabatic kernel using all HIRLAM physics parameterization schemes although the work is going to implement explicit representation of deep convection in HIRLAM.

CTMs: For SILAM and interface description please refer to FMI-s contribution

4.4.3 Integrated modelling at Estonian Environmental Research Centre,

Summary: Estonian Environmental Research Centre has rather unique nationwide air-quality system. The system consists of cascade of models (receptor model, gaussian model, gridpoint model, street canyon model, heavy gas model, MATCH model) based on AIRVIRO software from SMHI. The „off-line“ installation of MATCH model is driven currently by HIRLAM meteorological fields from Swedish Meteorological Institute, but it is planned to get meteorological fields from EMHI in future.

MetMs: HIRLAM (fields from SMHI)
CTMs: MATCH
Interfaces: Specific interfaces to the MetMs built into MATCH itself.
Only off-line coupling.

Model descriptions:
MetMs: HIRLAM model is described in section 4.3

CTMs: For MATCH model description please refer to contribution 4.12.1 by SMHI

4.4.4 Integrated modelling at Radiation Protection Centre ,

Summary: The Radiation Protection Centre has the responsibility of emergency response modelling in case of radiation danger. The Radiation Protection Centre has installation of ARGOS system in „off-line“ mode which is driven with meteorological fields supplied by Danish Meteorological Institute HIRLAM.

MetMs: HIRLAM (fields from DMI)
CTMs: ARGOS
Interfaces: Only off-line coupling.

Model descriptions:
MetMs:HIRLAM model is described in section 4.3

CTMs: ARGOS system was described in section 4.12.1 for SMHI

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4.5 Integrated modelling in Finland

4.5.1 Regional-to-meso-scale system SILAM

(Contribution by M.Sofiev, FMI)

MetM: HIRLAM
CTM: SILAM (Sofiev *et al,* 2006c)
Emissions: EMEP database, Finnish national inventories, sea salt and pollen modules of SILAM (Sofiev *et al.*, 2006a)
Only off-line coupling; both meteorological drivers are in hot-swap and can be selected by operators.
Interfaces:
The meteorological pre-processor and input decoders are made universally applicable to virtually any modern NWP models providing that this model is capable of writing WMO GRIB standard format. Under these conditions, adaptation of the system to the new dataset should not require recompilation of the model but rather extending the GRIB-code tables to the new model. An experiment is being conducted in Estonia when SILAM will be coupled with non-hydrostatic HIRLAM version. Feedback mechanisms are at the planning stage.

Current applications of the integrated modelling systems:
Model development and verification was based on (i) numerous emergency-type tests and inert-comparisons including ETEX, Chernobyl, EU-ENSEMBLE, NKS MetNet, etc. In all cases the SILAM system was coupled with the appropriate NWP driver – either one operational at the time of the specific experiment or the modern NWP system re-run for the corresponding period of time.

Long-term simulations and evaluation has been performed for 2000-2002 for various aerosol-type species and sulphur oxides and sulphates (Sofiev *et al*, 2006a).

Presently, the system is used for the operational forecasts available at http://silam.fmi.fi, which include primary anthropogenic aerosol, sulphur oxides and sulphates, pollen (Sofiev *et al.*, 2006b), and fine primary particles originating from biomass burning.

Future developments:

The on-going development is concentrated on several directions: (i) completion and evaluation of new Eulerian SILAM v.4.0; (ii) completion of the full-chemistry mechanism with simplified ozone chemistry in the SILAM v.4.0, (iii) further development of the fire assimilation system, (iv) refining the pollen forecasts and further development of pollen emission module, (v) operational implementation of two-scale forecasts with zooming over Finland; link to city-scale model (see next sub-section).

Research includes (i) further development of off-line coupling interface with downscaling possibilities and feedback mechanism, (ii) development and implementation of aerosol dynamics, (iii) variational data assimilation experiments and inverse problem solution.

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4.6 Integrated modelling in Germany (selection)

4.6.1 Integrated modelling at the German Weather Service (DWD)

(contribution by Barbara Fay, DWD, Germany)

MetMs: COSMO-Lokalmodell (LM) with COSMO-LMK (very short term LM), COSMO climate LM (CLM), HRM, LM-MH (mixing heights)

CTMs: Trajectories, LPDM, photochemistry CTM, trajectory box-model

No interfaces needed as identical grids used in METMs and CTMs.

Only off-line coupling.

MetMs:

COSMO-Lokalmodel (LM) – nonhydrostatic mesoscale NWP model (refer to COST728 WG4 model database), developed by COSMO (consortium for small-scall modelling of 7 national/regional weather services incl. Germany, Switzerland, Poland, Greece, Italy and ARPA-SIM Bologna), version LME for Europe and N. Africa, operational 7km, 45 layers.
Climate extension of COSMO-LM as CLM (COSMO Climate LM), mainly developed by Potsdam Institute for Climate Impact Research (PIK) and Research Center Geesthacht (GKSS) and operational in LM version 3.18 (Mar 2006). Currently used for consortial simulations in the IPCC (International Panel on Climate Change).

COSMO-LMK (LM Kürzestfrist (German for: very short-range)), now pre-operational, 2.8km, 50 layers, 18h forecast 8 times/day, for nowcasting in Germany and Alps. Explicitly resolved deep convection, shallow convection still parameterised, 6-class could microphgysics (incl. graupel). Under preparation: COSMO-LMK ensemble with 20 members.

Global Model (GME) of DWD (refer to WG4 database), global, operational 40km, 41 layers. GME-data transferred to several countries as initial/boundary data for world-wide mesoscale models (see LM and HRM, plus Bulgaria, Jugoslavia, Kenia).

High-resolution Mesoscale Model (HRM) of DWD (not in COST728 database), mesoscale, based on LM predecessor Deutschlandmodell, operational 6 – 28km resolution, 20-35 layers, operational in 9 national/regional weather services in Brazil (DHN and INMET), Ghanghzou (China), Israel, Italy, Oman, Romania, Spain, Vietnam. Initial and boundary data provided by GME to all users twice daily via internet.

LME-MH (LM mixing heights) of DWD (refer to WG4 database): Gradient Richardson scheme based on turbulence parameterisation of LM, operational for emergency preparedness and research.

CTMs:

Trajectory model, operational, based on LME, GME, HRM with corresponding resolutions (not in COST728 database). High-accuracy (2nd order) numerical scheme, timesteps 1-5min only. Also used by MeteoSwiss. Operational for all applications (radioactivity preparedness, backtracking for measurements incl. climatologies, campaign planning etc.).

LPDM (Lagrangian Particle Dispersion Model, refer to WG4 database), operational, based on LM and GME, mainly for radioactivity emergency preparedness incl. CTBTO backtracking.

Photochemistry CTM (Eulerian model, RADM chemistry, not in database), mesoscale, was pre-operational for ozone forecasting.

Trajectory box model (based on above trajectory model, MH model and photochemistry CTM, not in database), mesoscale, research version.

Off-line models, interfaces

All models off-line, only GME carries ozone on-line as a passive tracer and prognostic variable. Usually hourly input data. Generally **no interfaces needed** because all MetMs and CTMs fully adapted to their 'predecessor' models.
No on-line coupling of models planned for near future at the DWD.

Downscaling/nesting:

Operational: COSMO-LME once nested non-interactively into GME
Research: non-interactive COSMO-LM self-nesting down to 1km, pre-operational 2.8km COSMO-LMK-version (short-term forecasting). Also 2way interactive self-nesting for COSMO-LM, experimental.

Data assimilation/initialisation:

Operational: GME: 3hourly Optimal Interpolation, Digital Filter Initialisation (Lynch, 1997), sea surface temperature (SST), sea ice boundaries, ozone mixing ratio from ECMWF.
COSMO-LME: continuous nudging analysis plus SST plus snow height plus sea ice (refer to WG4 model database).
Chemical substances: no assimilation of measurements.

Model unification/harmonization

Harmonised model development and application in COSMO for LM. Also trajectories (and mixing heights). HRM used in 9 national/regional weather services as operational NWP model.

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4.6.2 Institute for Tropospheric Research (IfT), Leipzig, Germany:

Online coupling:

COSMO LM-MUSCAT (Multiscale Chemistry Aerosol Transport). Both COSMO-LM and MUSCAT operate in one executable file but there is no real online coupling as the MUSCAT simulation follows the LM one for each time step. Several gas phase mechanisms, aerosol physics. The model system can be used for

- air quality studies with special emphasis on the compliance with EU guidelines for air quality and impact of pollutants (Renner, 2002),
- scenario calculations to evaluate different reduction strategies to lower particulate matter occurrence in European areas by adequate emission reductions of particle sources and/or of gaseous pollutants which may have the potential to form particles in the troposphere,
- multiscale air pollution simulations from the regional to urban scale.

The performance of the model system is demonstrated in the ongoing CITY-DELTA project, an European intercomparison of long term model responses to urban scale emission reduction scenarios with special focus on ambient level of ozone and particulate matter (Wolke et al., 2003). The further development of the model is focussed on a more detailed treatment of the formation of secondary particles.

Actual projects: Modeling of the formation and dispersion of secondary particles from coal- fired large-scale power plants in Saxonia, Germany. Radiative Effects of Saharian Desert Aerosol.

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4.6.3 Institute for Meteorological and Climate Research in the Troposphere (IMK-TRO) of the Forschungszentrum Karlsruhe (Karlsruhe Research Centre, FZK)

(contribution by Heike Vogel, IMK-TRO)

On-line coupling:

COSMO LM-ART (**Aerosols and Reactive Trace Gases within LM**): enhanced model system to simulate the spatial and temporal distribution of reactive gaseous and particulate matter. In addition to the transport of a non reactive tracer the dispersion of chemical reactive species and aerosols can be calculated using on-line coupling of gas phase chemistry (58 additional variables) and aerosol physics (102 additional variables) and pollen grains in LM with the transport mechanisms of the operational LM. Secondary aerosols which are formed from the gas phase, directly emitted components like soot, mineral dust, sea salt and biological material are represented by log normal distributions. Processes as coagulation, condensation and sedimentation are taken into account. The emissions of biogenic VOCs, dust particles, sea salt and pollen are also calculated online, taking into account the dependencies on the meteorological variables. For efficient calculation of the photolysis frequencies a new method was developed using the GRAALS radiation scheme (Geleyn and Ritter, 1992) that is already implemented in LM. For studying the interaction of the aerosol and radiation, the so-called direct aerosol effect the climatological aerosol optical properties, which are used in the standard LM version, are replaced by parameterized ones that take into account current modal aerosol mass densities. By comparing different simulation results obtained with parameterized and climatological aerosol optical properties, the impact of the aerosol not only on the radiation, but also on other meteorological variables as the temperature can be quantified.

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4.6.4 Institute for Meteorology and Climate Research, Atmospheric Environmental Research (IMK-IFU), Forschungszentrum Karlsruhe GmbH (FZK)

(contribution by Peter Suppan, IMK-IFU)

Summary: Fully on-line coupling, focus on coupling of atmospheric with hydrological and biosphere models

CTMs: MCCM (MM5/chem); fully on-line coupled meteorology-chemistry model.

MetMs: MM5, WRF-ARW: focus on offline coupling with microscale, lagrangian, and hydrological models

Interfaces: On-line coupling for meteorology and atmospheric chemistry in MCCM, on-line coupling between MCCM and biosphere model.

Off-line coupling between MM5 or meteorological output of MCCM and GRAMM/GRAL and hydrological models (PREVAH and WaSiM).

Use of MCCM output to supply initial profiles for the canopy-chemistry model CACHE (Forkel et al., 2006).

Model descriptions:

Mesoscale Climate Chemistry Model MCCM (MM5/chem)

The online coupled regional meteorology-chemistry model MCCM (Grell et al. 2000) has been developed at the IMK-IFU. MCCM is based on the non hydrostatic NCAR/Penn State University mesoscale model MM5 (http://www.mmm.ucar.edu/mm5, Grell et al., 1995). Similar to MM5 MCCM runs can be applied over a range of spatial scale from the continental scale to the urban scale. Possible horizontal resolutions are between 100 km and 1 km. The advantage of the on-line approach against an off-line approach was demonstrated by Grell et al. (2004).

MCCM includes three online coupled tropospheric gas phase chemistry modules (RADM, RACM, RACM-MIM [Stockwell et al., 1990, 1997, Geiger et al., 2003]). As MCCM is designed for the implementation of chemistry modules that are prepared using the KPP preprocessor (Damian et al., 2002), further chemistry mechanism can be easily implemented. Photolysis frequencies for the chemistry mechanisms are computed online at each grid point with the Madronich photolyis module considering the values of temperature, cloud water and ice content, and tropospheric ozone which were currently predicted by the model. Aerosol processes are described with the modal MADE/SORGAM aerosol module (Schell et al., 2001) which considers as single compounds sulphate, nitrate, ammonium, water, and 4 organic compounds. For the Aitken and the accumulation mode the gas phase/particle phase partitioning of the secondary sulphate/nitrate/ammonium/water aerosol compounds is based on equilibrium thermodynamics. The organic chemistry assumes that secondary organic aerosol compounds (SOA) interact with the gas phase and form a quasi-ideal solution.

BVOC emissions and the emission of NO from soils are computed online depending on the local land use and on the actual simulated values of temperature and incoming solar radiation. Anthropogenic emissions of primary pollutants, like NOx, SO2, and hydrocarbons, as well as emissions of primary particulate matter have to be supplied as gridded data sets either at hourly intervals or as yearly data.

Besides the full version including gas phase chemistry aerosol physics MCCM can also be run with meteorology and gas phase chemistry without aerosol as well as the meteorology part without any chemistry. The meteorological output of MCCM can also be used as driver for offline models such as GRAL (Graz Lagrangian Model, Öttl et al., 2001).

Validation studies with MCCM have shown its ability to reproduce observed meteorological quantities and pollutant concentrations for different conditions and regions of the earth (Grell et al., 2000; Jazcilevich et al., 2003; Forkel et al., 2004; Suppan and Schädler, 2004, Forkel and Knoche, 2006; Haas et al, 2007).

Applications of MCCM at the IMK-IFU include short term studies such as simulations of high pollutant episodes for Mexico City (Forkel et al., 2004), receptor analysis (Suppan and Schädler, 2004) as well as long term studies such as climate-chemistry simulations (Forkel and Knoche, 2006), simulations of yearly pollution conditions in the Alpine region, and daily real time forecasts of ozone and particulate matter for Germany. Current activities include online coupling of MCCM with a biosphere model.

Mesoscale Model MM5

The NCAR/Penn State University model MM5 (http://www.mmm.ucar.edu/mm5, Grell et al., 1995) is a well tested community model. The modelling system includes pre processing tools for the preparation of input for MM5 from the output of various global meteorology models. The main features of MM5 are non hydrostatic dynamics, terrain following non equidistant vertical coordinates, several different options for the description of cloud and precipitation process, 4d data assimilation, and nesting capabilities.

At IMK-IFU the outputs of MM5 hindcast/forecast runs are used to provide input for various kinds of models, e.g. 3d-fields for the mesoscale model GRAMM (Almbauer et al., 2000) and the lagrangian particle model GRAL (Graz Lagrangian Model, Öttl et al., 2001) and 2d-fields for hydrological models WaSiM-ETH and PREVAH (Gurtz et al., 2003). The results of the respective models are used for adopting both, their own physical parameters and the MM5 configurable setups, to the location and scale of the respective areas and scenarios.

Weather and Research Forecast Model WRF-ARW

The Weather Research and Forecasting Model (WRF, http://www.wrf-model.org/index.php) is a mesoscale numerical weather prediction system designed to serve operational forecasting and atmospheric research needs. It can be denoted as successor of the mesoscale model MM5 with newly designed, flexible model components.

The equations of the ARW (Advanced Research WRF) solver are fully compressible, Euler non-hydrostatic and conservative for scalar variables. A description about the model WRF can be found at Skamarock, et al. (2005).

At IMK-IFU, WRF-ARW v2.2 is currently used in stand-alone mode for numerical weather prediction. For flood forecasting purposes, the hydrological water balance model WaSiM was coupled off-line to WRF (Marx, 2007).

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4.6.5 Max-Planck-Institute (MPI) of Chemistry in Mainz, Germany:

On-line coupling:

MESSy system (Modular Earth Submodel System): definition of infrastructure for the coupling of various programs (some similarity to the PRISM system) where all used programs are to be unified in one executable file.

In 2006, several chemistry components may be coupled to a GCM (**ECHAM5**, MPI for Meteorology, Hamburg) where a choice of different CTMs may be made for the same task.

In cooperation with the Universities of Mainz (Professor Wernli) and Bonn (Prof. Bott) in 'operational atmospheric chemistry in multiscale models'.

Plans for on-line coupling:

There are plans to integrate the LM into MESSy leading to a coupling of ECHAM5-LM, both simulating chemistry. Bonn university plans the introduction of a tracer into LM investigating advection algorithms, turbulent and convective tracer transport, interactions atmosphere/soil and trace gases/aerosols.

4.6.6 Institute of Atmospheric Physics, Department of Atmospheric Dynamics of DLR (German Aerosopace Centre), Oberpfaffenhofen near Munich.

Off-line and on-line coupled models.

Mesoscale meteorological models: MM5, MESOSCOP, REWIH3D driven with ECMWF analyses, satellite products

Global models, esp. coupled dynamics-chemistry model ECHAM/CHEM

Numerical models for sound propagation in the inhomogenous atmosphere (AKUMET, AKU3D).

4.6.7 Rhenian Institute for Environmental Research (RIU) of the University of Cologne, Cologne, Germany

Off-line coupled model system in **EURAD project and model system** (European Dispersion and Deposition Model). www.eurad.uni-koeln.de

CTM system EURAD simulates the dynamic, physical and chemical processes which are important for emission, chemical production, transport and deposition of atmospheric trace constituents.Various applications in AQ assessment and field experiment evaluation, forecasting and strategy development mainly on scales of 1km to 1000km also using data assimilation techniques, refer to www.eurad.uni-koeln.de.

MM5 driven by ECMWF and NCEP meteorological data.
EEM (EURAD emissions model), also emission data from TNO (Netherlands), EMEP, German EPA, federal EPAs and IER (Univ. of Stuttgart)
EURAD CTM: using RADM (and RACM) mechanisms
also aerosol models MADE (Modal aerosol dynamics model for Europe) and secondary organic aeorosl model SORGAM (Secondary Organic Aerosol model, Schell et al., 2001)

4.6.8 Integrated modelling at the Free University of Berlin, Intitute for Meteorology

(contribution by Eberhard Reimer, FU Berlin)

Only off-line one-way coupling.

MetM:
meteorological drivers for CTM are determined in different ways:

1. numerical analysis scheme TRAMPER with isentropic vertical coordinate. Data used for interpolation are radiosondes, surface and satellite data from weather services and archives from FU Berlin. The scheme uses statistical interpolation and the boundary parameters (mixing height, u*, Monin-Obukov ….) are prepared by boundary layer modelling including the adjustment to topography, sloping terrain and mass consistency. The area of interest is Europe with about 25km^2 grid down to smaller arrays within Europe with grid sizes down to 1km^2. The data are transformed to pressure and sigma coordinates.
2. The first guess for analysis is given by simple large scale analysis, by forcast data from German Weather Service GME and ECMWF.
3. for comparison the meteorological forecast from mesoscale models MM5, LM and Aladin are used.

CTM:
The chemical transport model REM-CALGRID is an urban/regional scale model development designed to fulfil the requirements of the ambient air quality framework directive 96/62/EC of the European Commission. The urban-scale photochemical model CALGRID and the regional scale model REM3 were combined into the new urban/regional scale model, REM-CALGRID (RCG). The premise was to design an Eulerian grid model of medium complexity that can be used on the regional, as well as the urban, scale for short-term and long-term simulations of oxidant and aerosol formation.

The model includes the following features:

- A generalized horizontal coordinate systems, including latitude-longitude coordinates;

- A vertical transport and diffusion scheme that correctly accounts for atmospheric density variations in space and time, and accounts for all vertical flux components when employing either dynamic or fixed layers;
- A new methodology to eliminate errors totally from operator-split transport and ensure correct transport fluxes, mass conservation, and that a constant mixing ratio field remains constant;
- Inclusion of the recently improved and highly-accurate, monotonic advection scheme developed by Walcek (2000). This fast and accurate scheme has been further modified to exhibit even lower numerical diffusion for short wavelength distributions;
- Updated releases of the SAPRC-93 and CBM-IV photochemical reaction schemes;
- Two equilibrium aerosol modules, that treat the thermodynamics of inorganic aerosols; An equilibrium aerosol module, that treat the thermodynamics of organic aerosols;
- Simple modules to treat the emissions of sea salt aerosols and wind blown dust particles;
- A simple wet scavenging module based on precipitation rates;
- An emissions data interface for long term applications that enables on-the-fly calculations of hourly anthropogenic and biogenic emissions

The trajectory model is used for source/receptor statistics in backward and forward mode, for interpretation of the CTM REM/CALGRID. The quantitative cross boundary transports of chemical species (PM10, SO2 …) for special areas are determined by long term statistics of 3D-trajectories and observations.
The scheme uses a mix of dynamic and kinematic equations with second order schemes considering energy balance on isentropic surfaces in the troposphere and stratosphere and sigma coordinate in the planetary boundary layer.

Model information:

The CTM is used for long term modeling in relation to EU directives for PM10, PM2,5, ozone and NO2. Emission scenarios are modeled to support regional and urban assessment and abatement strategies prepared by environmental agencies and administrations.
For short term purposes a 3 day forecast of PM10 and ozone is prepared for real time presentation.
The meteorological driver is prepared for 3 and 1 hourly cycles for CTM and trajectories depending on the horizontal grid size.

The RCG model requires annual emissions of VOC, NOx, CO, SO2, CH4, NH3, PM10, and PM2.5, split into point and gridded area sources. Mass-based, source group dependent NMVOC profiles are used to break down the total VOC into the different species classes of the chemical mechanisms. Hourly emissions are derived during the model run using sector-dependent, month, day-of-week and hourly emissions factors.
European-wide annual anthropogenic emission averages for 2000 for CO, NOX, NMVOC, SOX, NH3 and PM10 on a 50 km * 50 km grid are taken from the EMEP data base [Vestreng, 2003] and were transformed into the geographical RCG-grid.. For the nested region Berlin/Brandenburg, highly resolved emissions data were obtained from regional administrations. To ensure consistency

between the urban-scale and the continental-scale emissions, the Berlin/Brandenburg data were scaled sector-by-sector to the level of the EMEP data.

Special emphasis is taken on the further improvement of the meteorological driver TRAMPER by a more complex boundary layer module and by satellite data with respect to 3D clouds and precipitation for new deposition scheme.

The RCG model will be used for further scenario runs for PM2,5 and in general for other non European regions. All models are used in measurement campaigns, for real time information and for modeling within several project from EU, BMBF, the German Environmental Agency and local administrations.

4.6.9 Integrated modelling at the Meteorological Institute, University of Hamburg

(contribution by Heinke Schlünzen, Meteorological Institute, University of Hamburg, Germany)

Summary:

MetMs: MITRAS, METRAS, METRAS PC, M-SYS

CTMs: MICTM, MECTM, M-SYS

Interfaces: no interfaces needed within microscale (MITRAS/MICTM) and mesoscale (METRAS/MECTM) MetMs and CTMs; in M-SYS several grids are used and interface modules are available

All models are currently off-line coupled / on-line coupling version in development; the 1999 online version was not further used (not developed for parallel computers).

Model descriptions

All models developed in different consortia.

MetMs:

Non-hydrostatic models with 3D non-uniform grids, solves wind, temperature, humidity, cloud- and rainwater as well as concentration equations (flux form) and derives pressure from the (diagnostic) anelastic equation.

MITRAS (microscale transport and flow model)

Main developers Meteorological Institute, University of Hamburg; Alfred-Wegener-Institute for Polar and Marine Research, Bremerhaven; Institute for Tropospheric Research, Leipzig; Fraunhofer-Institut for Atmospheric Environmental Research, Garmisch-Partenkirchen; Forschungszentrum Jülich. MITRAS resolves buildings using the blocking approach and vegetation by using the viscosity approach. Orography and temperature effects are considered, open lateral boundaries are used (alternative: prescribed inflow). MITRAS model output can be used as meteorological input for MICTM. MITRAS is part of the model system M-SYS.

METRAS (mesoscale transport and flow model)

Main developers Meteorological Institute, University of Hamburg; Alfred-Wegener-Institute for Polar and Marine Research, Bremerhaven; Forschungszentrum Jülich; Rechenzentrum Universität Karlsruhe; Institute f. Geometry and Applied Math RWTH Aachen; Federal Research Center for Forestry and Forest Products, Grosshansdorf; Ocean University of Qingdao, PR China; University of Birmingham, UK. METRAS can be used for resolutions from ~500m to ~10km. Per grid-cell several sub-grid-scale land use characteristics are considered by using flux aggregation with blending height concept. METRAS is nested in results of coarser resolving models (e.g. weather forecast, analysis or regional climate model). At the model top absorbing layers are used, or the nesting technique is applied. METRAS includes passive tracer transport. A multi-scale version and are in development. METRAS is part of M-SYS. METRAS is suitable as training model for (undergraduate) students.

METRAS PC (public domain PC version of METRAS):

Main developers Meteorological Institute, University of Hamburg and METCON Pinneberg. Public domain operational version of METRAS used by more than 50 consultants for environmental impact assessment studies or for investigating wind energy potential. Similar to METRAS, but more simple to apply.

M-SYS:

M-SYS is a multi-scale mesoscale-microscale meteorology and chemistry model system, a combination of METRAS / MECTM in several resolutions and MITRAS / MICTM. Applicable to investigate meteorology as ell as concentration fields of several pollutants (e.g. NO_x, O_3, SO_2 , NH_3, Pb, nitrate, sulphate) including chemical transformations and deposition at the ground can be calculated dependent on the sources (industry, power stations, household, car and ship traffic). Emission scenario studies can be performed.

CTMs:

The chemistry models use the meteorology results of the corresponding models and the same grids. Prognostic equations are solved for several pollutants (e.g. NO_x, O_3, SO_2 , NH_3, nitrate, sulphate). Chemical transformations are included using the RADM2 gas phase chemistry from Stockwell et al.,. The lateral and upper model boundaries are open or results of a coarser model are used. Biogenic emissions and directly simulated. The dry deposition is calculated from a resistance model, it depends on pollution and surface characteristics.

MICTM (microscale chemistry transport model):

Main developers are Meteorological Institute, University of Hamburg, Forschungszentrum Jülich, University of Birmingham, UK. MICTM uses MITRAS meteorology and is part of M-SYS.

MECTM (mesoscale chemistry transport model):

Main developers are Meteorological Institute, University of Hamburg; Ocean University of Qingdao, University of Birmingham. MECTM is using METRAS output for the meteorology and is part of M-SYS. Simple aerosol dynamics as well as the sectional aerosol model SEMA of von Salzen and Schlünzen (1999) can be selected to calculate aerosol influences.

Off-line models / On-line models:

The above mentioned models are currently all off-line coupled when chemical transformations are included. For passive tracer transport of specific applications (e.g. pollen transport) on-line coupling is used.

Interface modules:

For meteorology/chemistry interfaces are not needed since the same grid structure is used.

Downscaling/nesting:

One-way nesting is available for all models; an off-line approach is used. In test is a two-way nesting method.

Data assimilation/initialisation:

For data assimilation a nudging method is used for meteorology and chemistry.

Current applications of the integrated modelling systems

Maps on air pollution and quality in different scale, urban and coastal pollution studies.

Model unification/harmonization/ further developments

It is intended to further harmonise the mesoscale and microscale models to eventually receive a consistent multi-scale atmospheric model for micro and mesoscale which includes chemical reactions. For this purpose new numerical schemes will be developed, an error control technique be developed and introduced and scale dependent parameterisations be developed and used.

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4.7 Integrated modelling at the National and Kapodistrian University of Athens (NKUOA)

Contribution by Maria Tombrou/Elissavet Bossioli

Summary:
MetMs: MM5, MM5_urban (Dandou et al., 2004)
CTMs: UAM-V, CAMx

Model descriptions:

MetMs: MM5_urban model, whereby urban features have been introduced both in the thermal and dynamical parts. In particular, the released anthropogenic heat is given as a temporal and spatial function of the diurnal variation of the anthropogenic emissions. The objective hysterisis model (OHM) (Grimmond et al. 1991) has also been incorporated for the calculation of the heat storage term. The surface fluxes were also modified according to Akylas et al. (2003) and Akylas and Tombrou (2005), following recent advances in ABL structure over rough surfaces under unstable conditions. Finally, the eddy diffusivities for the stable cases were modified according to King et al. (2001).

CTMs: UAM-V and CAMx are 3D multi-scale photochemical grid models. UAM-V treats only gaseous pollutants while CAMx treats both gaseous and particulate pollutants.

Off-line models / On-line models:

Interface modules:

Interfaces: Meteorological and chemical models are off-line coupled on an hourly basis. Most interfaces (land use, grid, meteorological data, emissions) have been developed upon the specific models' needs.

- The meteorological interface provides 3D fields of horizontal wind speed, temperature, precipitation, pressure, humidity, and vertical diffusion coefficients.
- CAMx also uses 'mm5camx' pre-processor (available at the url location http://www.camx.com/down/support.php), which translates MM5 output meteorological fields to CAMx inputs.
- The development of a new meteorological interface is planned for the future in order to provide the chemical models with 2D fields of Monin Obukhov length, UV albedo, surface roughness and friction velocity.
- The development of an interface coupling a global CTM with the mesoscale photochemical models is planned for the future in order the boundary conditions to be more accurately described.

Issues identified during the coupling procedure

1. UAM-V and CAMx models, diagnose the vertical velocity from the divergence, instead of using MM5 model's vertical velocities directly. It was shown (Bossioli et al., 2006) that this

issue as well as several other compatibility problems between the two models (e.g. temporal consistency, UAM's dependence on hydrostatic balance) can cause inappropriate changes to vertical velocities, especially over complex topographies.

2. The current assumption of the photochemical models (as in the case of UAM-V) of not treating the surface inversion as a solid lid during the night but allowing ozone and its precursors to be mixed and diluted through the vertical layers weakens the ozone accumulation aloft. On the contrary, when predetermined mixing heights are considered (as in UAM-IV model), higher ozone values are calculated.
3. Applying the MM5 model with and without nesting can change the ozone spatial distribution significantly, under local circulation conditions (e.g. sea-breeze).
4. Modifications depicting the urban structure influence the concentrations, especially in the suburban areas.

Downscaling/nesting:

All models are applied with two-way nesting down to 0.67km.

The data extracted from the process of satellite images - spatial resolution 30m (land use and AOT) are further used for several applications such as:

- Downscaling of relatively course mesh model output
- Urban density
- Updating the anthropogenic emission inventory based on urban density.
- Distribution of the biogenic emissions inside the urban sector based on a vegetation index

Data assimilation/initialisation:

No data assimilation.

The initial and lateral boundary conditions for the MM5 model are provided by the European Center for Medium range Weather Forecast (ECMWF) numerical prediction model.

Chemical models initialisation with measured data

Current applications of the integrated modelling systems

MM5-UAM-V and MM5-CAMx systems are mostly applied over Greece nested over the Greater Athens Area.

Meteorological simulations.

The detailed information, derived from the satellite image, is used in order to construct new fields for various parameters, such as the roughness length, the semi-empirical coefficients for the heat storage and the albedo. For example, if the albedo field for the base case albedo scenario (buildings albedo 0.18) is replaced by the albedo field for the high albedo scenario (buildings albedo 0.85), due to environmentally friendly paintings, the air temperature (at 2 m agl) will be decreased.

The MM5-UAM-V modelling system have been applied during national and international projects:

ICAROSNET

Mapping air pollution in Greece

Impact assessment (e.g. power plants, national road)

The MM5-UAM-V and MM5-CAMx modelling systems has been applied for scientific purposes:

Investigation and quantification of the effect of critical factors that conduce to the ozone formation and accumulation during ozone episodes. The research revealed that the factors that lead to a more realistic description of the urban mixture and thus of the ozone production.
Development and application of comprehensive parameterization for SSA emissions over Attica peninsula.The size range modeled (0.03μm – 40μm) is divided into 10bins, with the chemical speciation of sea-water (Na^+, Cl^-, $ssSO4^{2-}$ and the rest).The parameterization includes open-sea and surf-zone SSA production.
The application of the dynamic mechanism for mass transfer between gas and aerosol phases. The significance of different mass transfer mechanisms is studied. Aerosol modeling includes both equilibrium and dynamic mechanisms for the mass transfer between gas and aerosol phases. The equilibrium method assumes instantaneous equilibrium between phases, which is true for small particles, though wrong for larger particles and treats aerosol mass as "bulk". As a result, Na^+ becomes associated with fine $SO4^{2-}$ (a quick reaction that equilibrium "captures") and no NaCl is available for its reaction with HNO3 (a slow reaction that equilibrium cannot "capture"). On the other hand, the dynamic method assumes variable mass transfer rates e.g. NO3 are transferred continuously between gas and aerosol phases and interact with most of the aerosol components (e.g. NaCl reaction). Additionally, it does explicit integration of mass transfer equations for each bin separately. As a result, NaCl is available for its reaction with HNO3 (a slow reaction that "is captured" for the coarse bins), towards coarse aerosol nitrate and particle Cl^- is displaced by $NO3^-$ and evaporates to gaseous HCl. Our applications use a combination of both mechanisms – the hybrid approach, which involves the equilibrium method between gases and fine aerosols (for PM2.5 mass – 6 bins) and the dynamic method for the coarse mass (for PM2.5-40 mass – 4 bins).

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4.8 Integrated modelling in Italy (selection)

4.8.1 Integrated modelling at Arianet, Milano, Italy

(contribution by Sandro Finardi, Arianet, Milano)

Arianet has developed integrated modelling systems **off-line** coupling diagnostic and prognostic meteorological models with CTMs and Lagrangian particle models. The modelling systems are used for regional/urban air quality assessment and management, urban air quality forecast and real-time industrial emission control.

MetMs:

- **RAMS (Regional Atmospheric Modelling System)** – non-hydrostatic mesoscale NWP model (in database), developed by Colorado State University (http://rams.atmos.colostate.edu) and ATMET (http://www.atmet.com). The model implements a full set of non-hydrostatic, compressible Reynolds-averaged primitive equations, plus conservation equations for scalar quantities, supplemented with parameterisations for turbulent diffusion, solar and terrestrial radiation, moist processes, kinematic effects of terrain, cumulus convection, and sensible and latent heat exchange between the atmosphere and the surface, described by multiple soil layers, vegetation, snow cover, canopy air, and surface water.
- **MINERVE** - mass-consistent diagnostic meteorological model developed by Aria Technologies (www.aria.fr). (Aria Technologies, 2001; Finardi et al., 1993; Desiato et al., 1998). is a. It reconstructs 3D wind fields starting from vertical profiles and near-ground wind measurements, through a two-step procedure: a) interpolation of wind observations over the computational mesh, b) adjustment of the wind field to satisfy mass conservation. MINERVE also produces an interpolated temperature field, keeping into account the variation of temperature with terrain height.
- **LAPS (Local Analysis and Prediction System)** – high resolution meteorological analysis model, developed by NOAA (http://laps.noaa.gov/). It allows to build meteorological analyses integrating data from local networks of surface observing systems, Doppler radars, satellites, wind and temperature profilers, as well as aircraft. LAPS can be used to initialise RAMS, MM5, WRF, and ETA models.

CTMs:

- **SPRAY3** - Lagrangian Particle Dispersion Model (to be included in database, described in EIONET - Model Documentation System), developed by Arianet and CNR/ISAC (Tinarelli et al., 1994). The behavior of the airborne pollutant is simulated through “virtual particles” whose mean movement is defined by the local wind and the dispersion is determined by velocities obtained as solution of Lagrangian stochastic differential equations (Thomson, 1987), reproducing the statistical characteristics of the turbulent flow.
- **FARM (Flexible Air quality Regional Model)** - Eulerian chemical transport model (to be included in database, described in EIONET - Model Documentation System), developed by Arianet (Silibello and Calori, 2003). FARM can be configured with different gas-phase chemical mechanisms (e.g. SAPRC-90 or SAPRC99), it allows to choose between two modules for the description of aerosols: the CMAQ aero3 modal approach and a simplified bulk aerosol module (aero0), based on the approach adopted by the EMEP Eulerian Unified model (EMEP). The models implements one- or two-way nesting capability with an arbitrary number of computational grids.

Off-line models:

All models are coupled off-line, usually on a hourly frequency basis.

The air quality models can be coupled with any meteorological data source providing 3D and 2 meteorological fields thanks to the interface module that is not tailored on a specific MetM. FARM is interfaced to LAMI (Italian version of Lokal Modell) in ARPA Piemonte (Environmental Protection Agency of Piemonte Region) to produce urban air quality forecast for the cities of Torino and Novara.

No **on-line** coupling of models is planned at the moment.

Interface modules:

Meteorological and air quality models are connected by the interface module **GAP/SURFPRO** (Calori et al., 2006; Finardi et al., 2005).

GAP (Grid AdaPtor) is a grid interpolation tool interfacing FARM chemical-transport model with any NWP and meso-meteorological models. GAP interpolates a sequence of 2D and 3D atmospheric fields from a source grid identified by mesh points, geographic coordinates and altitudes, to a target grid defined using UTM projections and terrain-following vertical coordinates. The set of 2D/3D variables to be interpolated is freely configurable, and different interpolation techniques for sparse data can be selected.

Starting from topography and land-use data managed by the modelling system and gridded fields of meteorological variables (e.g. wind, temperature and humidity) **SURFPRO (SURface-atmosphere interFace PROcessor)** (ARIANET, 2002) can compute 2D gridded fields of turbulence scaling parameters (i.e. roughness length, sensible heat flux, friction velocity, Monin Obukhov length, mixing height and convective velocity scale) as well as 3D fields of horizontal and vertical diffusivities and 2D fields of deposition velocities for a given set of chemical species. The computational schemes implemented in SURFPRO are based on the Monin-Obukhov similarity theory, when computing radiation and energy budgets, the processor can take into account water bodies, terrain slopes and related solar shading effects. An updated version of SURFPRO (Finardi et al., 2005) has been developed within the FUMAPEX project, including the objective hysteresis model of Grimmond and Oke (1999), to enhance the description of the urban surface energy budget, and mixing height computational schemes accounting for inhomogeneities and advection effects (Gryning and Batchvarova, 1996; Zilitinkevich and Baklanov, 2002).

Downscaling/nesting:

- **RAMS** has two-way nesting capability and it is used to downscale larger scale NWP models outputs for both operational and case studies activities.
- **FARM** offers one- or two-way nesting possibilities. Emissions and meteorological fields must be provided for every grid at the proper space resolution.

Data assimilation/initialisation:

RAMS implements nudging type of four-dimensional data assimilation with observational data. Nudging is based on 3D fields produced by RAMS Isentropic Analysis (ISAN) pre-processor.

No data assimilation is available for air quality models.

Current applications of the integrated modelling systems

The RAMS-FARM modelling system has been adopted by the ENEA and Ministry of the Environment for the national project called MINNI (National integrated model to support atmospheric pollution international negotiation). A web site is under development and presently available in draft version (only in Italian) at http://www.minni.org.

The MINERVE-FARM modelling system (based on diagnostic meteorological fields reconstruction) is presently used at ARPA Piemonte, Valle d'Aosta and Lombardia (Environmental Protection Agencies of Piemonte, Valle d'Aosta and Lombardia Regions) for air quality assessment and management activities. In particular Regione Piemonte decided to implement the modelling system as a permanent air quality assessment tool to support its air quality institutional activities. ARPA Piemonte is in charge to perform modelling applications on a yearly basis (Bande et al, 2006) to provide concentration fields for the main atmospheric pollutants on a hourly basis and to compute all the indicators required by EU legislation.

FARM is interfaced to LAMI (Italian version of Lokal Modell) to produce urban air quality forecast for the cities of Torino and Novara. The forecasting system is installed at ARPA Piemonte, while a client application is installed at Provincia di Novara to allow access to the modelling system results for statistical and graphical elaboration.

The MINERVE-SPRAY3 and RAMS-SPRAY3 modelling systems are used for real-time industrial emission control and air pollution forecast in the industrial area of Priolo, near Siracusa. The forecasting system (Finardi et al ., 2006) is projected to provide CIPA (Industrial Consortium for Environmental Protection) with information useful to support the prevention and management of air pollution episodes, and to inform local authorities and population before or during the possible episodes.

The MINERVE-SPRAY3 and RAMS-FARM modelling systems are used for industrial and urban air quality assessment analysis at ISPESL (Institute for occupational safety, health and prevention of the National Health Service, Ministry of Health).

Model unification/harmonization

Interfaces and air quality models development follows the needs highlighted by major users' application and takes advantage of the cooperation with major partners, in particular ENEA, ARPA Piemonte, ISPESL and CNR/ISAC.

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4.8.2 Integrated modelling at CNR/ISAC (National Research Council/Institute of Atmospheric Sciences and Climate), Bologna

(contribution by Alberto Maurizi, CNR-ISAC)

Summary: on-line coupling

Meteo: BOLCHEM (hydrostatic, Limited Area Model)
Chemistry: SAPRC90 and CBIV chemical mechanisms
Aerosol: M7

The on-line modelling system BOLCHEM consists of a meteorological limited area hydrostatic model (BOLAM) coupled with different gas chemistry modules (SAPRC90 and CB-IV chemical mechanisms), an aerosol module (M7, work in progress) and a Lagrangian dispersion module for both forward and backward computation of trajectories.

Model description

The BOLCHEM model (BOLam + CHEMistry) is the result of an on-line coupling between the mesoscale meteorological model BOLAM (BOlogna Limited Area Model, http://www.isac.cnr.it/~dinamica/bolam/index.html) (Buzzi et al., 1994, Buzzi et al., 2003) and modules for transport and transformation of chemical species.

BOLAM dynamics is based on hydrostatic primitive equations, with wind components, potential temperature, specific humidity, surface pressure, as dependent variables. The vertical coordinate system is hybrid-terrain-following, with variables distributed on a non-uniformly spaced staggered Lorenz grid. The horizontal discretisation uses geographical coordinates on an Arakawa C-grid. The time scheme is split-explicit, forward-backward for gravity modes. A 3-d WAF (Weighted Average Flux) advection scheme coupled with semi-Lagrangian advection of hydrometeors is implemented. A fourth order horizontal diffusion of the prognostic variables (except for ps), a second order divergence diffusion and damping of the external gravity mode are included. The lateral boundary conditions are imposed using a relaxation scheme that minimises wave energy reflection. The initial and lateral boundary conditions are supplied from the ECMWF (European Centre for Medium-range Weather Forecasts) analyses available at 0.5° x 0.5□‹ resolution. Hybrid model level data are directly interpolated on the BOLAM grid.

Transport (advection and diffusion) of tracers (both passive and reactive) is performed on-line at each meteorological time-step using WAF scheme for advection and a "true" (second order) diffusion, with diffusion coefficient carefully estimated from experiments. Vertical diffusion is performed using one-dimensional diffusion equation with a diffusion coefficient estimated by means of an E-l turbulence closure scheme. Dry deposition is computed through resistance-analogy scheme and is provided as boundary condition to the vertical diffusion equation. Furthermore, vertical redistribution of tracers due to moist convection is parameterised consistently with the Kain-Frisch scheme used in the meteorological part for moist convection.

Physical/chemical processes are treated separately for gas phase, aerosol classes and generic tracers (e.g. radioactive species, Saharan dust, ...). Gas phase is treated using the SAPRC90 or CB4 chemical mechanisms. Aerosol is modelled using M7 module from ECHAM5 (coupling still in progress) and generic species are case by case user defined by providing chemical/physical properties and equations.

More technical details can be found in the COST 728/732 model inventory:
http://www.mi.uni-hamburg.de/
List_classification_and_detail_view_of_model_entr.567.0.html?&user_cost728_pi2[showUid]=80

Downscaling/nesting:

Within the hydrostatic approximation limit, BOLCHEM can be nested in itself.

Data assimilation/initialisation:

Optimal interpolation of surface/profile composition data.

Current applications of the integrated modelling systems

BOLCHEM is being used within the GEMS EU project.

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4.8.3 Integrated modelling at CNR/ISAC (National Research Council/Inst. Of Atmospheric Sciences and Climate), Torino

(contribution by Silvia Trini Castelli, ISAC-CNR, Torino, Italy)

ISAC-Torino developed **off-line** integrated modelling system RMS, coupling the prognostic meteorological model RAMS with the Lagrangian particle model SPRAY, through the boundary layer and turbulence interface module MIRS. The modelling systems is used for regional down to local and urban environmental impact studies and air quality assessment and management.

MetMs:

- **RAMS (Regional Atmospheric Modelling System)** – non-hydrostatic mesoscale NWP model (in database), developed by Colorado State University (http://rams.atmos.colostate.edu) and ATMET (http://www.atmet.com). RAMS is fundamentally a limited-area model, but may be configured to cover an area as large as a planetary hemisphere for simulating mesoscale and large-scale atmospheric systems and, on the other hand, because of its no lower limits in the domain size or to the mesh cell size of the model's grid, microscale phenomena can be simulated. The model includes also a large number of configuration options for the description of atmospheric processes. The main options comprehend hydrostatic and non-hydrostatic versions, two-way interactive grid nesting, terrain-following coordinates, stretched vertical coordinates, nudging system, different options of numerical schemes, several top and lateral boundary conditions and a conjunct of physical parameterisations.

- **RAMS6.01_mod:** a modified version of latest RAMS6.0 model. In RAMS6.01_mod our group implemented new alternative turbulence closures, standard k-l and k-ε turbulence models (Trini Castelli et al., 2001; Ferrero et al., 2003, Trini Castelli et al., 2005) and a so-called anisotropic version of k-l model (Trini Castelli et al., 2006). Adopting this kind of closures enables RAMS to simulate more properly the mesoscale flow at relatively high-resolution, of the order of few hundreds metres. Lately, also the renormalization group version of k-ε (RNG- k-ε) was introduced (Reisin et al., 2006): k-ε type closure, jointly with the Cartesian grid and the so called ADaptive Aperture method available in RAMS6.0, allows to downscale towards the urban scale, using very high resolution, in the order of metres. RAMS6.01_mod is under test in different case studies.

CTMs:

. **SPRAY3** - Lagrangian Particle Dispersion Model, developed by Arianet and ISAC-CNR (Tinarelli et al., 1994). The code operates the transport and diffusion of chemically neutral airborne species in complex real conditions (orography presence, landuse heterogeneity, low wind regime) characterized by non-homogeneity in space and time of meteo-diffusive variables (wind vertical shears, breezes caused by non-uniform terrain). SPRAY reconstructs the concentration fields determined by point, line, area and volume sources. Different portions of the emitted plumes can experience different atmospheric conditions, allowing more realistic reproductions of complex phenomena (low wind-speed conditions, strong temperature inversions, flow over topography, presence of terrain discontinuities such us land-sea or urban rural). The latest version of SPRAY includes recent developments regarding the formulation of the Langevin stochastic equations, new modules for the specific treatment of low wind conditions and new more efficient methods for the particle time-stepping. The latter allows the model to perform more efficient complex simulations, taking into account a large number of emissions of several origins.

Off-line models:

The meteorological and dispersion models are coupled off-line through a parameterisation interface module, usually on an hourly frequency basis even if, in principle, any other time frequency can be chosen.

The dispersion model can be coupled also with different meteorological data sets, since the interface module can ingest and process generic 3D and 2D meteorological fields and it is not tailored on a specific MetM.

No **on-line** coupling of models is planned at the moment.

Interface module:

The meteorological and air quality models are connected by the interface module **MIRS** (Trini Castelli and Anfossi, 1997; Trini Castelli, 2000). MIRS ingests the meteorological fields produced by RAMS or, alternatively, other kind of data fields, deriving by observations or diagnostic models. Topography, wind speed, potential temperature is the minimum information requested, then turbulent kinetic energy, diffusion coefficients and surface fluxes are treated when available. MIRS calculates the surface layer and boundary layer parameters, the friction velocity, the temperature scale and Monin-Obukhov length, the PBL height, the convective velocity , the variances of the velocity fluctuation , the local velocity decorrelation time scale and the third and fourth moments of the vertical velocity fluctuations. Several alternative options are available for the parameterisations of the atmospheric boundary layer and turbulence processes. The fields of data are then processed to prepare a meteorological file in the appropriate format and with the temporal sequence of interest to be used by SPRAY as input information. The output format can be easily adapted for other Lagrangian models. An updated version of the module, **MIRS4.0,** coupling the RAMS6.01_mod version with SPRAY, is under development.

Downscaling/nesting:

- **RAMS** has two-way nesting capability and it is used to downscale larger scale NWP models outputs for both operational and case studies activities.

Data assimilation/initialisation:

RAMS implements nudging type of four-dimensional data assimilation with observational data. Nudging is based on 3D fields produced by RAMS Isentropic Analysis (ISAN) pre-processor.

No data assimilation is available for air quality models.

Current applications of the integrated modelling systems

The RMS modelling system is presently used in the Project ALPNAP - Alpine Space, INTERREG III B "*Monitoring and Minimisation of Traffic-Induced Noise and Air Pollution Along Major Alpine Transport Routes*" (http://www.alpnap.org).

Some latest examples of applications in environmental impact studies are listed in the following.

PROJECT BRENNER BASIS TUNNEL: Brenner Project – Italian Side: dispersion modelling of vehicle traffic along the Brenner highway and main South-Tyrol roads, in collaboration with Arianet srl. (2005-2006)

AEM (Municipal Electricity Company) assignment: Impact assessment of the pollutant dispersion in atmosphere from power plants in the urban site of Torino and from traditional heating systems – evaluation of alternative solutions. (2005)

E-ON-Italia assignment: Modelling study of the pollutant dispersion in atmosphere – the thermoelectric power plant in Livorno Ferraris. (2005)

TRM S.p.A. (Consortium for the Incinerator in Turin) assignment: Modelling study of the atmospheric dispersion of the emissions from an Incinerator in different emissive and meteorological scenarios in the Province of Torino. (2004)

Model unification/harmonization

RMS modelling system is under continuous improvement, in collaboration with major partners Arianet Srl (Italy), DISTA-Univ. Piemonte Orientale (Italy), ATMET Ltd (USA) and taking advantage of the contributions in developments and applications from CESI Ricerca (Italy), SOREQ Nuclear Research Centre (Israel), Mitsubishi Heavy Industries (Japan), Universities of São Paulo and Santa Maria (Brazil).

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4.8.4 Integrated modelling at ARPA/ER, Bologna

MetM: LAMI (Italian version of the Lokalmodell, COSMO consortium) and hourly analyses from LAMA data set. CALMET_SIM,,.
CTM: regional version of CHIMERE, statistical pollution model OPPIO (Ozone and PM10 Polynomial Inference based on Observations)
only offline-coupling
suitable interface from LAMI to CHIMERE was constructed.

4.8.5 Integrated modelling at Brescia University

(contribution by Giovanna Finzi, Claudio Carnevale, Enrico Pisoni, Marialuisa Volta)

MetM: RAMS, CALMET,MM5
CTM: TCAM
Interfaces: met. Interface PROMETEO for format conversion
Only off-line coupling, no **on-line** coupling of models is planned at the moment.

The Environmental System Modelling and Control Group of the Department of Electronics for Automation (at University of Brescia) has developed integrated modelling systems **off-line** coupling diagnostic and prognostic meteorological models with eulerian CTMs. The modelling systems are used for regional air quality assessment and management.

MetMs:

- **RAMS (Regional Atmospheric Modelling System)** – is a non-hydrostatic mesoscale NWP model, developed by Colorado State University and ATMET company. The model is based on non-hydrostatic, compressible Reynolds-averaged primitive equations, plus conservation equations for scalar quantities. It also uses parametrisations for turbulent diffusion, solar and terrestrial radiation, moist processes, kinematic effects of terrain, cumulus convection, and sensible and latent heat exchange between the atmosphere and the surface, described by multiple soil layers, vegetation, snow cover, canopy air, and surface water.

- **CALMET** – is a diagnostic meteorological model that includes a diagnostic wind field module, and micrometeorological modules. The diagnostic wind field module uses a two step approach to compute the wind fields. At first calculating an initial-guess wind field. Then implementing an objective analysis to introduce observational data into the wind field determined in the former step. The micrometeorological module uses two boundary layer parametrisations applied to land and water grid cells, respectively. The principal parameters needed to describe the boundary layer structure are the surface heat flux, surface momentum flux and the boundary layer height. Several parameters, i.e. friction velocity, convective velocity scale, mixing height and Monin-Obukhov length are derived from these.

CTMs:

- **TCAM** - The Transport Chemical Aerosol Model (TCAM) is an eulerian photochemical three-dimensional multi-phase model. The TCAM model solves the mass balance equations by means of a splitting operator. The horizontal advection scheme is derived by the CALGRID model code; it implements a finite difference scheme based on Chapeau functions and on the non linear Forester filter. The diffusivity parameters are calculated evaluating Pasquill-Gifford stability classes. The vertical transport is solved using either an explicit or an implicit scheme based on the value of horizontal diffusivity, calculated by taking into account meteorological parameters such as Monin-Obukhov length, mixing height, friction velocity and convective velocity. The dry deposition is described using a resistance-based algorithm which takes into account pollutant (gas and particulate matter) properties, local meteorology and terrain features. The wet deposition module for gas and particles describes dissolution in droplets and precipitation scavenging. The model implements different chemical mechanisms based both on lumped molecule (SAPRC90, SAPRC97, COCOH97) and on lumped structure (CB-IV) approaches. The gas phase chemistry is solved by the IEH algorithm which treats the slow reacting species and the fast reacting ones separately. The TCAM model also includes and harmonizes a module describing aerosol dynamics by means of a fixed-moving approach. A generic particle is represented with an internal core containing the non volatile material, like elemental carbon, crustal and dust. The dimension of the core of each size class is established at the beginning of the simulation on the basis of a logarithmic distribution and is held constant during the simulation. The volatile material is supposed to reside in an outer shell of the particle whose dimension is evaluated by the module at each time step on the basis of the total mass and total number of suspended particles. Both shell and core are suppose to be internally mixed. The aerosol module is coupled to COCOH97 chemical mechanism, an extended version of SAPRC97. It describes the dynamics of 21 chemical compounds. The inorganic species are twelve (H2O, SO4=, NH4+, Cl-, NO3-, Na+, H+, SO2(aq), H2O2(aq), O3(aq), elemental carbon and other). The organic species are 9, namely a generic primary and 8 classes of secondary organic species, each of them corresponding to one of the Condensable Organic Compounds included in the gas phase chemical mechanism. Such chemical compounds are split in 10 size bins, so that the prognostic variables solved by the module are 210. TCAM describes the most relevant aerosol processes: the condensation, the evaporation, the nucleation of H2SO4 and the aqueous oxidation of SO2. The estimation of equilibrium pressures of the condensing inorganic species is computed by means of the SCAPE2 thermodynamic module.

- **CALGRID** - The photochemical model CALGRID is an Eulerian three-dimensional model for gas phase simulations. It implements an advection-diffusion scheme in terrain-following coordinates with vertical variable levels. The CALGRID chemical module implements the SAPRC90 and the CBIV mechanisms. The QSSA (Quasi Steady State Approximations) algorithm solves the kinetic equations. The SAPRC90 chemical mechanism includes 54 species (10 fast reacting species, 30 slow reacting species, 5 constant and 9 steady-state), and 128 reactions (16 photolytic ones). The mechanisms have been evaluated using the results of a variety of environmental chamber experiments. The results show that the scheme is able to simulate maximum ozone concentrations and rates of NO oxidation and ozone formation to within 30% of the experimental measurements for 63% of the simulation tests, although there was a slight bias towards over-predicting maximum ozone concentrations in experiments designed to represent ambient mixtures.

Off-line models:

All models are coupled off-line, usually on a hourly frequency basis.
The air quality models have been used considering different meteorological fields, i.e. using RAMS or MM5 fields. This is possible due to the PROMETEO meteorological interface, that transforms original meteorological fields in the requested projection/resolution/format.

No **on-line** coupling of models is planned at the moment.

Interface modules:

Meteorological and air quality models are connected by the interface module **PROMETEO.**
This interface performs following steps:

1. A grid projection and interpolation, interfacing the chemical-transport model with the meso-meteorological models. This can be useful to transform 3D atmospheric fields from a source grid identified by mesh points, geographic coordinates and altitudes, to a target grid defined using UTM projections and terrain-following vertical coordinates.
2. Starting from topography and land-use data and gridded fields of meteorological variables (e.g. wind, temperature,..) , **PROMETEO** computes 2D gridded fields of turbulence scaling parameters (friction velocity, Monin Obukhov length, mixing height, convective velocity scale, Pasquill-Gifford stability class), as well as 3D fields of vertical wind and vertical diffusivities. The computational schemes implemented in **PROMETEO** for turbulence scaling parameters are based on Holtslag and van Ulden scheme (1983). For vertical diffusivities calculation different techniques can be used (i.e. the integration methodology developed by Byun et al. (1999) for CMAQ).

Downscaling/nesting:

- **RAMS** has a two-way nesting capability and it is used to downscale larger scale NWP models outputs.
- **TCAM** has a one-way nesting capability.
- **CALGRID** has a one-way nesting capability.

Data assimilation/initialisation:

RAMS implements nudging type of four-dimensional data assimilation with observational data. Nudging is based on 3D fields produced by RAMS Isentropic Analysis (ISAN) pre-processor.

No data assimilation is available for air quality models.

Current applications of the integrated modelling systems

CALMET-CALGRID has been used to perform both episode and long-term gas simulation and to evaluate the effectiveness of suitable emission control strategies over the Lombardia region. The modelling system has been applied during the CityDelta-CAFE intercomparison modelling excercise (phase I) to a northern Italy domain to evaluate the impact of selected emission control strategies on ozone and nitrogen oxides. The modelling system has also been used to perform episode simulation during PIPAPO campaign (1-6 June 1998).

CALMET-TCAM has been applied to a northern Italy domain in the frame of CityDelta-CAFE project (phase I and phase II) in order to simulate the entire 1999 year and to evaluate the impact of current legislation and most feasible emisison reduction on ozone and PM10 at 2010. The modelling has also been used to perform episode simulation during PIPAPO campaign (1-6 June 1998).

MM5-PROMETEO-TCAM has been applied to a northern Italy domain in the frame of CityDelta-CAFE project (phase III), in order to simulate the entire 2004 year and to evaluate the impact of current legislation and most feasible emission reduction on ozone and PM10 at 2020. The input/output data of TCAM model in this configuration (and in the previous one) has been used to identified source-receptor modelling to be implemented in multi-objective problem for the selection of effcient emission control strategies.

RAMS has been used to drive TCAM model studing a pollution episode of the PIPAPO campaign, to perform a comparison between prognostic and diagnostic drivers of CTMs.
Furthermore, still in an experimental way, it is planned to use RAMS with improved Sea Surface Temperature (SST) fields based on daily AVHRR satellite image, instead of the RAMS standard Monthly SST dataset. In the framework of a PM2.5 Measurement Campaign performed in the Brescia area, in cooperation with London Imperial College and ENI, it is also planned to use RAMS, to reconstruct meteorological fields of the Campaign period.

Model unification/harmonization

Interfaces and air quality models development follows the air quality community recommendations.

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4.9 Integrated modelling in Poland

4.9.1 Integrated modelling at Warsaw University of Technology, Warsaw, Poland

(contribution by Joanna Struzewska)

MetM-CTM: MC2-AQ, GEM/LAMAQ
On-line coupling

MC2-AQ (Mesoscale Compressible Community – Air Quality)

MC2-AQ is a three-dimensional air quality model developed for studying oxidant chemistry on regional to urban scales. The modelling system is based on the Canadian Mesoscale Compressible Community (MC2) Model (Tanguay et al. 1990; Laprise et al. 1997), a non-hydrostatic meteorological model, to which modules permitting on-line calculations of chemical transformations, anthropogenic and biogenic emissions, and deposition were added. The transport of chemical species is done on the same grid and with the same advection, convection, and diffusion schemes as are used for the meteorological fields. The model system is flexible and was adapted to different scales by allowing for self-nesting (Plummer,1999; Kaminski et al. 2002).

Spatial discretization

MC2-AQ can be run on a Polar Stereographic projection (true at 60^{o}N), a rotated Mercator projection and a true lat-lon coordinate system. The discretization of the space derivatives is done by finite differences on an Arakawa C-type staggered grid for the horizontal and a Tokioka B-grid (Tokioka 1978) in the vertical. The orography is introduced using the Gal-Chen height coordinates (Gal-Chen and Somerville, 1975).

The model top and the number of vertical levels are set up by the user. For most of simulations carried out for Europe 35 - 45 vertical levels with model top at 16 - 20 km were used.

Initial and boundary conditions

Time-varying boundary conditions are provided to MC2-AQ using a one-way nesting scheme based on the work of Davies (1976). The model variables are gradually blended with those of the driving model over a 'sponge', or transition, zone of specified width.

Following options were used to provide initial and boundary conditions for MC2-AQ simulations over Europe:

- Operational objective analysis for meteorology + 3D chemical fields from a global chemistry transport model
- MC2-AQ model results form lower horizontal resolution run (in '*self – nested*' mode)
- output from a global on-line model GEM-AQ

A number of fields and parameters are needed to specify surface characteristics and are obtained from analysed, climatological and geophysical datasets. These include surface roughness, land–sea mask, albedo, deep soil temperature, ice cover, and topography. The surface roughness length is influenced by topography and vegetation type.

Model dynamics

The model is an extension of the fully compressible limited area model developed by Tanguay, Robert and Laprise (Tanguay et al. 1990; Laprise et al. 1997). The numerics of the model are based on a semi-Lagrangian, semi-implicit time stepping procedure, which allows for comparatively large time steps despite the presence of rapidly propagating sound waves (Tanguay et al. 1990; Benoit et al. 1997a). The horizontal diffusion coefficient is automatically adjusted to the grid resolution ($2^{nd}/4^{th}$ order implicit/explicit horizontal diffusion are used).

Vertical transfers due to turbulent air motion are parameterized in the form of vertical diffusion (Benoit et al. 1989). The effect is strongly dependent on the vertical diffusion coefficient, which is locally evaluated every time step. Also, vertical diffusion is modified to control excessive divergence near the top of the models.

Transport of the chemically active tracers is calculated using the three time-level semi-Lagrangian advection scheme native to the MC2 mdoel. Unconstrained cubic Lagrange interpolation is used to calculate values of the advected field at the upwind endpoint of the trajectory.

The vertical transfer of trace species due to subgrid-scale turbulence is parameterized using eddy diffusion for heat transfer calculated by the host meteorological model. The effect of shallow convection on the vertical distribution of tracers is calculated as a special case of turbulent diffusion.

Model physics

The physics package consists of a comprehensive set of physical parameterization schemes (Benoit et al. 1989; Mailhot et al. 1989a; Mailhot 1994):

- Over land, the surface (skin) temperature is predicted from a heat budget using the “force–restore” method (Deardorff 1978; Benoit et al. 1989) combined with a stratified surface layer. Over oceans, the sea surface temperature is kept fixed during the integration. Over land, a soil moisture availability factor (percentage of field capacity) is used for calculating evaporation (Budyko bucket method or semipotential approach). Recently the ISBA scheme (Interactions Soil-Biosphere-Atmosphere) has been added to the package.
- The planetary boundary layer is based on a prognostic equation for turbulent kinetic energy (Benoit et al. 1989). A shallow convection scheme for nonprecipitating clouds is included to give a more realistic description of cloud-topped boundary layers. Shallow convection accounts for the formation of small cumuli that generally produce little precipitation but transport a large quantity of moisture vertically and play an important role in the atmospheric water cycle. Shallow convection is simulated with a method described by Mailhot (1994) and is treated as a special case of the turbulent planetary boundary layer to include the saturated case in the absence of precipitation.
- Condensation processes at resolvable scales account for the formation of stratiform precipitation and, if mesh is sufficiently fine that individual convective cloud cells can be resolved, explicit convective precipitation. The explicit condensation process is represented by the isobaric condensation, which removes moisture when relative humidity exceeds a saturation point. Advanced microphysical equations are also incorporated in the model: versions of so-called Kuo-symmetric, relaxed Arakawa-Schubert (Moorthi and Suarez 1992), explicit cloudwater schemes with mixed phases (Tremblay et al. 1996a) and detailed microphysics (Kong and Yau 1997).
- Deep convective processes are handled with a Kuo-type convective parameterization (Kuo 1974; Mailhot et al. 1989a). A description of microphysical processes similar to that of the stratiform precipitation is also included. However, due to the complexity of evaporation

from convective clouds, which strongly depends on the cloud internal dynamics (such as moist downdrafts, not included in the Kuo scheme), evaporation of convective precipitation is not considered. Recently the more sophisticated convection schemes such as the Fritsch–Chapell (Fritsch and Chappell 1980) and the Kain–Fritsch (Kain and Fritsch 1990) schemes have been developed.

- The radiation subpackage contains detailed radiation schemes that are fully interactive with clouds. The infrared radiation scheme (Garand 1983; Garand and Mailhot 1990, Yu et al. 1997) includes the effects of water vapor, carbon dioxide, ozone, and clouds. The solar radiation scheme is essentially the one described by Fouquart and Bonnel (1980). It takes into account the effects of water vapor, carbon dioxide, ozone, clouds, Rayleigh diffusion, and multiple scattering. Cloud–radiation interactions represented in these schemes are an important effect.
- Gravity wave drag parameterization is based on a simplified linear theory for vertically propagating gravity waves generated in statically stable flow over mesoscale orographic variations (McFarlane 1987; McLandress and McFarlane 1993). It makes use of a representation of the subgrid-scale orography (also called launching height) for exciting the gravity waves.

Chemistry

Gas phase:

Chemical scheme used in MC2-AQ is similar to ADOM IIB (Lurmann et all, 1986; Venkatram et al., 1988). The mechanism is comprised of 47 species, 98 chemical reactions and 16 photolysis reactions. The species are solved depending on their lifetime and reaction rates. Very short lived species such as atomic oxygen are assumed to be in photochemical steady state. A semi-implicit method is used for long lived species and the implicit Newton's method is used for species that interact rapidly with others.

Spatially and temporally varying clear-sky photolysis rates are derived from a pre-calculated look-up table. Photolysis rates are stored for 10 height levels up to 20 km, 13 solar zenith angles and 5 different values of the surface albedo, with linear interpolation used to derive photolysis rates at intermediate values of these variables. Correction of the clear-sky photolysis rates for the presence of clouds is performed with the method proposed by Chang et al. (1987).

Aerosol and wet chemistry are not incorporated

Removal processes:

The effects of dry deposition are calculated as a loss term in the chemistry solver. Dry deposition velocities are calculated from a multiple resistance model, based on Wesley’s approach. Wet deposition scheme is based on SMHI Report No 82, Sep. 1998

Emissions

The effects of emissions of trace species are calculated as production part of the chemistry. Area emissions, defined as all anthropogenic and biogenic emissions, are assumed to be emitted at the surface and injected to the lowest model level. Emissions from major point sources may occur directly into model layers above the surface. Biogenic emissions are calculated ‘on-line’, at each chemical time step, using standardized emission rates from the Biogenic Emissions Inventory System (BEIS II) (Geron et al., 1994).

Results processing for model evaluation:
For comparison with observations, modelled values in the grid square corresponding to the station location are used (no spatial interpolation applied). For comparison with lidars / vertical soundings linear interpolation to measurement levels is used.

MC2-AQ applications over Europe

- Impact of large scale meteorological conditions on the formation of high ozone concentration in the lower troposphere
- Model study of the transport and transformation of ozone and its precursors in the frontal zone
- Impact of the emission reduction on summer smog episodes in urban areas. The model study . (State Committee for Scientific Research project)
- Influence of the local circulation on air quality over Gdansk-Sopot-Gdynia agglomeration.
- CityDelta European Modelling Exercise
- ESCOMPTE modelling exercise - model evaluation and intercomparison (METEO-France)

GEM/LAM-AQ applications over Europe (the GEM/LAM-AQ modelling system is described by the group from Canada)

- Integrated modelling study for Krakow agglomeration (JRC) "From toxic emission to heath effects"
- Impact of moorland and forest fires in Eastern Europe on PMs concentration over Poland
- Photooxidants' formation and transport over Europe during the heat wave period in July 2006

4.9.2 Integrated modelling at the Institute Meteorology and Water Management (IMGW) Section Krakow, Poland

(contribution by Wieslaw Kaszowski, Jolanta Godlowska, Wojciech Rozwoda)

MetM: ALADIN, CALMET
CTM: CALPUFF
Interfaces: Interface between ALADIN and CALMET for format conversion
Only off-line coupling now,
on-line coupling of models ALADIN/ MM5/CALMET/CALPUFF is planned at the moment.

The modelling system is used for regional (Malopolska Region) air quality assessment and management.

MetMs:

- **ALADIN** – is a hydrostatic mesoscale NWP model, developed by METEO France and collaborated 15 countries. The model use the spectral technique for the horizontal representation of fields. Model **ALADIN-Poland** is run twice a day in Krakow and produces forecasts up to 48 hours with a horizontal resolution of 13.5km and 31 levels. Domain size is 2270 km. For system ALADIN/CALMET/CALPUFF we use the ALADIN data (surface and upper air data) from 11 grid points near Krakow. We treat forecast the ALADIN data as a diagnostic data.
- **CALMET** – is a diagnostic 3-dimensional meteorological model that includes a diagnostic wind field module, and boundary layer modules. The diagnostic wind field module uses a two

step approach to compute the wind fields. At first calculating an initial-guess wind field. Then implementing an objective analysis to introduce observational data into the wind field determined in the former step. There are two boundary layer parametrisations in CALMET, applied to land (Energy Balance Method) and water (Profile Method) grid cells, respectively. CALMET iterpolate meteorological data (surface and radiosoundins) also using kinematic effects, slope flow, blocking effects. It includes divergency minimization procedure and micrometeorological model for overland and overwater boundary layers. In Krakow we replace radiosoundings and synoptic data by data from ALADIN/PL.

CTMs:

- **CALPUFF** – is non-steady-state Lagrangian Gaussian Puff Model containing modules for complex terrain effects, overwater transport, coastal interaction effect, wet (empirically-based scavenging coefficient method (e.g. Maul 1980)) and dry (based on the dry deposition resistance model (Slinn et al. 1978)) removal and simple chemical transformation. There is pseudo-first-order chemical reaction mechanism for the conversion SO2 to $SO4^{--}$ and NOx to $NO3^{-}$ based on scheme used in the MESOPUFF II model (Scire et al. 1984) or The RIVAD/ARM3 scheme (Morris et al. 1988) for clear non-urban areas. CALPUFF contains algorithms for near source effects such as building downwash, transitional plume rise, partial plume penetration, subgrid scale terrain interaction. The CALPUFF need emission inventory for point, line, volume and area sources. We use inventory prepared by Krakow Government.

Off-line models:

Models are coupled off-line, usually on a 6 hour frequency basis.

Coupling of models ALADIN/ MM5/CALMET/CALPUFF is planned at the moment.

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Interface modules:

Meteorological interface transforms meteorological data from ALADIN in the requested CALMET format. CALMET and CALPUFF are compatible and don’t need interfaces.

Downscaling/nesting:

- **ALADIN** is a double nested model
- **CALMET** has a one-way nesting capability.
- **CALPUFF** has a one-way nesting capability.

Data assimilation/initialisation:

ALADIN – 3D-Var assimilation scheme

CALMET- an objective analysis procedure introduce observational data from synoptic and radiosounding stations

No data assimilation is available for air quality model.

Current applications of the integrated modelling systems

ALADIN/CALMET/CALPUFF has been used to evaluate the effectiveness of suitable emission control strategies over the Malopolska region.

Model unification/harmonization

Interfaces and air quality models development follows the air quality community recommendations.

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4.10 Integrated modelling in Portugal

(contribution by Ana Isabel Miranda, University of Aveiro)

Integrated modelling at GEMAC – University of Aveiro

(contribution by Ana Miranda, Helena Martins)

Summary:
MetMs: MM5, MEMO
CTMs: CHIMERE, CAMx, MARS
Only off-line coupling (MM5-CHIMERE, MM5-CAMx, MM5-MARS, MEMO-MARS).

Model descriptions :
MetMs:
MM5: The nonhydrostatic Pennsylvania State University/National Center for Atmospheric Research Mesoscale Meteorology Model MM5 (Dudhia, 1993; Grell et al., 1994) is a powerful meteorological model that contains comprehensive descriptions of atmospheric motions; pressure, moisture, and temperature fields; momentum, moisture, and heat fluxes; turbulence, cloud formation, precipitation, and atmospheric radiative characteristics. It's a nested-grid primitive-equation model that uses a terrain-following sigma (nondimensionalised pressure) vertical coordinate.

MEMO: The mesoscale meteorological model MEMO (Flassak and Moussiopoulos, 1987) is a three-dimensional Eulerian non-hydrostatic prognostic model, which describes the atmospheric boundary layer for unsaturated air. The atmospheric physical phenomena are simulated by numerically approximating a set of equations in terrain-following co-ordinates, including mass continuity and momentum and transport equations for scalar quantities.

CTMs:
CAMx: The Comprehensive Air quality Model with extensions (CAMx) is an Eulerian photochemical dispersion model that allows for an integrated "one-atmosphere" assessment of gaseous and particulate air pollution (ozone, PM2.5, PM10, air toxics, mercury) over many scales ranging from sub-urban to continental. CAMx simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids. It contains five chemical mechanisms, four of them based on the Carbon Bond Mechanism version 4 (CB-IV) and the other one on the SPARC99 (ENVIRON, 2002). Other important features are: the two-way nested grid structure, several chemical kinetics solver options, horizontal advection solver options: and an advanced photolysis model:

CHIMERE: CHIMERE is a three-dimensional chemistry-transport model, that simulates gas-phase chemistry (Schmidt et al., 2001), and aerosol formation, transport and deposition (Bessagnet et al.,

2004) from European to urban scales. Horizontal transport is taken into account by calculating pollutant fluxconvergence from the boundaries of each model cell. The numerical scheme used to interpolate fluxes at cell boundaries is the Parabolic Piecewise Method (Collela and Woodward, 1984), for slow species (ozone and precursors), and a first-order scheme is used for the other species. Vertical transport is assumed to balance horizontal mass divergence/convergence. The chemical mechanism uses 44 species and 116 reactions and was derived from the original complete scheme MELCHIOR. In order to reduce the computing time it follows the formalism of ‘‘chemical operators’’ (Aumont et al., 1997). The hydrocarbon degradation is fairly similar to the EMEP gas phase mechanism. Adaptations are made in particular for low NOx conditions and NO3 nitrate chemistry. The impact of cloud on hotolytic reaction rates is included in a highly parameterized fashion: in the presence of clouds a radiation attenuation coefficient is taken into account throughout the model layers.

MARS: The MARS model, a 3D Eulerian model, numerically simulates photo-oxidants formation considering the chemical transformation process of pollutants together with its transport in the atmospheric boundary layer (Moussiopoulos et al., 1995). The EMEP mechanism describes the tropospheric gas-phase chemistry with 66 species and 139 photochemical reactions, including 34 photolysis reactions; VOC speciation: methane, ethane, n-butane, ethane, propene, o-xylene, formaldehyde, acetaldehyde, methylethylketone, methanol, ethanol and isoprene. The KOREM mechanism, which is simpler, includes 39 chemical reactions and 20 reactive pollutants. KOREM results from the combination of inorganic reactions of the CERT mechanism (Atkinson et al., 1982) and organic reactions of the compact mechanism of Bottenheim and Strausz (1982); VOCs are lumped in five classes: methane, alkanes, alkenes, aromatics and aldehyds.

Off-line models, Interfaces:

All models off-line. No interfaces needed since MetMs and CTMs are compatible, except for the case of MM5/MARS application. An interface between MM5 and the photo-chemical model MARS was developed. With this interface all the needed meteorological parameters to calculate photo-chemical air pollutants advection, production, and removal are fed into the photo-chemical model with the necessary time-step resolution. The meteorological variables are interpolated from theMM5 Arakawa B horizontal grid to the MARS C grid (further details on Arakawa grids in Alder et al. (1977)). 2D fields of Monin–Obukhov length and non dimensional roughness, ln(Z/Z0), are also included.

Downscaling/nesting:

Both MM5, CHIMERE and CAMx incorporate two-way grid nesting.

Initialisation:

MM5: MM5 simulations are initialised with the global reanalysis data from the National Center for Environmental Prediction and from the National Center for Atmospheric Research (NCEP/NCAR).

CHIMERE: Monthly climatologies of O3, NO2, CO, PAN, CH4, C2H6, HCHO and HNO3 taken from the MOZART second generation model (Horowitz et al., 2003) force the coarser grids simulations the lateral and top boundaries. Therefore, the large-scale runs concentrations of 22 slow species including ozone and precursors (VOC and reactive nitrogen species) are passed as lateral boundary values to the small-scale runs.

CAMX, MARS: Boundary conditions are calculated based on top concentrations of 21 particulate and gaseous species in the case of CAMx, and 8 gaseous species in MARS.

Current applications of the integrated modelling systems

The system MM5/CHIMERE is being applied for the long-term assessment of particulate matter, over Portugal, with a 10km grid size resolution. The simulations are performed in time slices of 5 consecutive days, each new period being initialized by concentrations obtained at the end of the previous one. Boundary conditions are provided by a prior large-scale simulation, covering Western Europe with a 0.5º resolution. Boundary conditions for the regional simulation are taken from monthly averages of the GOCART model. More details about this application can be found in Borrego et al. (2006a).

The performance of the CHIMERE photochemical model in simulating ozone and nitrogen dioxide in Portugal over a long-term summer period has also been examined. The analysis focused on comparisons against the available measurements during the 2001 summer season. The model was applied to the Continental region of Portugal, with a horizontal domain of 290x580km and a 10 km horizontal resolution. The meteorological forcing of the model was given by the European Centre for Medium-Range Weather Forecasts (ECMWF) 3-hourly short-term forecasts. The Portugal model run was nested within a continental-scale run, using the same physics and a simple oneway technique: the coarse grid long-term simulation was performed with CHIMERE over a regional area from10.5 W to 22.5 E and from 35 N to 57.5 N. More details about this application can be found in Monteiro et al. (2005a).

The system MM5/CHIMERE is currently running operationally for air quality forecast in Portugal, including particulate matter. The Portugal model run (10km resolution) is nested within a continental scale run (50 km resolution). More details about this forecast can be found in Monteiro et al. (2005b).

Nowadays, the system MM5/CAMx is being used to assess the human exposure to urban air pollutants over Oporto urban area. The MM5 runs consist in four nested domains (the larger one covering Western Europe with 30 km horizontal resolution, the smaller one covering the Oporto urban area with 1 km horizontal resolution) with two-way nesting simulations. The CAMx is applied to all domains, except the larger one, also with two-way nesting.

The MEMO/MARS system has been applied to assess the potential impacts of urban planning strategies, namely different land use patterns, on urban air quality. More details about this application can be found in Borrego et al. (2006b).

Model unification/harmonization/ further developments

For the assessment of the human exposure to urban air pollutants an exposure module is being developed for CAMx. The exposure calculation methodology has already been developed for the local scale (Borrego et al., 2006c).

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4.11 Integrated modelling at the University of Madrid, Spain

Contribution by R. San José, Environmental Software and Modelling Group (ESMG) – Technical University of Madrid (UPM)

Summary:
MetMs: MEMO, MM5, WRF
CTMs: CHIMERE, CAMx, CMAQ
Interfaces:
MEMO is coupled on-line with SMVGEAR chemical solver for CBM-IV (Name of the model: OPANA on-line)
MM5 is coupled off-line with CAMx and CMAQ

MetMs:
MEMO is a numerical mesoscale meteorological model representative of the second generation of limited area mesoscale non-hydrostatic meteorological models.

CTMs:
CMAQ is a numerical transport and chemical model which is developed by EPA (US) and is implemented in a full modular approach. It means that the user can select different chemical schemes (CBM-IV, V, SAPRAC-99, RADM, etc.) and different numerical schemes (SMVGEAR, MEBI, QSSA, etc.). It has different capabilities such as: Process analysis, IRR analysis, etc.)

CAMx is a similar model to CMAQ. It has different parameterizations and capabilities (OSAT, etc.)

CHIMERE is a numerical transport model which has a more modern development and uses a similar approach to CMAQ or CAMx.

Off-line models / On-line models:
OPANA model is a system which integrates the meteorological and the chemical model in on-line and off-line modes for different meteorological and chemical transport models. OPANA is included in the European Air Quality Database for models (http://pandora.meng.auth.gr/mds/qstart.php?MTG_Session=405880ab6137a896434f02e9351985b8)

Interface modules:
The interface modules are built adhoc for each model.

Downscaling/nesting:
The mentioned models include downscaling and nesting capabilities

Data assimilation/initialisation:
The MM5 includes 3DVAR and 4DVAR data assimilation. We have extended the mathematical approach to passive pollutants into CMAQ.

Current applications of the integrated modelling systems

Currently the integrated models are being used internally in the laboratory since they are in the process to be optimized and validated. The operational applications are currently carried out with off-line models except for Madrid city, which we use a 2000 version of the OPANA model which includes a full on-line version of the OPANA (MEMO+CBM-IV (SMVGEAR)).

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4.12 Integrated modelling in Sweden

4.12.1 Integrated modelling in Sweden at the Swedish Meteorological and Hydrological Institute (SMHI)

(contribution by Christer Persson and Valentin Foltescu, SMHI)

MetMs:

- **HIRLAM** – operational hydrostatic NWP model. The model runs at SMHI for 22, 11 and 5 km resolutions, 4 times/day, 48h forecast for 22 and 11 km versions, 24h forecast for 5 km version
- **ECMWF** – global model
- **ALADIN/AROME** – hydrostatic and non-hydrostatic model versions run for research purpose, 5 km resolution for hydrostatic version, 2.5 km resolution for non-hydrostatic version, 1 time/day
- **MESAN** – real-time system for mesoscale univariate analyses of selected meteorological parameters, run 4 times/day.

CTM:

- **Trajectory model** based on HIRLAM
- **MATCH** off-line model, no plans to implement on-line coupling in the near future. Specific interfaces to the MetMs given above built into the MATCH code.

Integrated modelling:

Since 1990 the Swedish Meteorological and Hydrological Institute, SMHI, has developed an off-line model system for regional dispersion of atmospheric pollutants, **MATCH** (Multi-scale Atmospheric Transport and Chemistry model) (Robertson et al., 1999). The MATCH-model can today be applied on a range of different scales and atmospheric dispersion problems. MATCH is built on a modular concept and there are a number of options available, which may suit different applications, depending on the available input and requested output.

MATCH is the only Eulerian grid-point dispersion model used for policy support in Sweden. Recently, MATCH has been used in the NEPAP-project of the EU (Network for the support of European Policies on Air Pollution) in close collaboration with both DG Research and CAFE mainly for studies of the inter-annual variability as a result of variations in meteorological conditions.

Different versions of the MATCH model are presented, assessed and verified in a number of articles and reports. The applications on national scale (MATCH-Sweden) are presented in Langner et al. (1995 and 1996). Examples of regional studies for Europe, the Swedish West Coast, for Stockholm, and for two regions south and west of Stockholm are presented in Foltescu et al. (2005), Persson et al. (1994), Persson and Ullerstig (1997), Engardt et al. (2002), Gidhagen et al (2005). MATCH is also used on the European scale in an operational application for emergency response in case of nuclear accidents (Langner et al., 1998) as well as for studies of tropospheric chemistry and ground level ozone (Langner et al, 2005). The MATCH model has previously been used to study sulfur deposition over Asia (e.g Engardt et al., 2005) and over Southern Africa (Zunckel et al., 2000). The model has also been applied to Central Chile to simulate dispersion of particulate arsenic emitted from copper smelters (Gidhagen et al., 2002) and sulfur compounds (Olivares et al., 2002; Gallardo et al., 2002). MATCH has recently been implemented within the Internet AIRVIRO-system for supporting policy on air quality in Estonia.

Model down-scaling/nesting, incl. data assimilation

The MATCH model requires three-dimensional, time-resolved information for a number of meteorological variables including horizontal winds, temperature, humidity, cloudiness and precipitation. This information is derived from some kind of meteorological model. MATCH accepts inputs from different meteorological models but normally data is used from HIRLAM (High Resolution Limited Area Model) or from the European Centre for Medium range Weather Forecasts (ECMWF) global model. Also 2-D meso-scale meteorological analyses, based on observations, for surface parameters such as precipitation, snow cover, visibility, 2m temperature and 10m wind can be utilized in MATCH. Such meso-scale analyses, performed by the MESAN system (Häggmark, 2000), are at present available at SMHI for the time period 1990-present covering Europe at 11 km horizontal resolution.

MATCH currently (2006) runs with (hydrostatic) HIRLAM fields at 11 km horizontal resolution producing hindcasts and forecasts (up to 48 hours ahead four times per day). In the near future MATCH will also be run with fields from the non-hydrostatic HIRLAM-ALADIN at a resolution of 2.5 km. A procedure for local adaptations by Kalman-filter is available.

Annual air pollution assessment studies for Sweden have been performed since the mid 1990-ies as a support to the Swedish environmental protection authorities, based on a specific version of the MATCH model, where air and precipitation chemistry measurements at background locations over NW Europe are utilized in combination with model calculations. Model calculated contributions from emissions on local/meso scale are subtracted from observed concentrations in air and precipitation in order to obtain pollution concentration fields which only vary smoothly and thus are suitable for interpolation using the same technique as in conventional meteorological data assimilation. So far the Optimum Interpolation (OI) technique has been used. This includes a method for deriving long-range transport contributions to concentrations in air and precipitation. The long-range contributions of concentrations are then run through the dry- and wet deposition modules of the MATCH model in order to map the total deposition to different land-use classes.

The method first applied for Sweden is described in Persson et al. (1994, 1996) and Langner et al. (1995, 1996). For the deposition of base cations and other sea-salts empirical coast-class correction factors have been introduced (Lövblad et al., 2004) based on measurements of sea-salt at varying distances from the coast combined with basic information concerning oceanographic and meteorological conditions. The coast-class correction factors make it possible to perform the OI analyses on smoothly varying fields with much weaker gradients compared to the direct observations. The analysis is currently being refined by implementing 2D-variational analysis instead of OI and applied for sulphur and nitrogen compounds, ozone and base cations.

MATCH has also been applied for more detailed deposition assessments with higher horizontal resolution (5 km) in regions of Sweden. In these cases a coupling has been made with the operational air pollution assessment work on the national scale. The coupled system can then provide information on contributions from long-range transport, national (Swedish) emissions and regional emissions to the total observed deposition within a region. For studies of urban air pollution (particle number concentration) horizontal resolutions below 1 km have been tested successfully in the Stockholm area (Gidhagen et al., 2005).

The meteorological data is read into the MATCH model, usually on a three hourly basis. Data for each grid point and vertical level is then interpolated to hourly values. The overall time step in the transport part of the model is 5-10 minutes depending on horizontal resolution. For certain parts of the calculations, e.g. in the chemistry code, a shorter time step is applied. Interfaces between MetMs and the MATCH-CTM are built into MATCH and controlled by switches which are set depending on the type of input (e.g. HIRLAM, ECMWF, MM5,…).

Initial state and time dependent boundary conditions are read from data in GRIB format. The update frequency of boundaries may be set individually for each component. The one-way nesting is straight forward as output from MATCH is produced in GRIB format. Initial state can be taken from other model runs (at any model resolution) or based on the boundary concentrations specified by the user (interpolated to fill the model volume). A full data assimilation scheme is not yet implemented. The adjoint transport scheme is though available.

The model accounts for up to 6 different projections on input and output. The grid could either be defined by the input weather data, or be specifically set up. For the latter interpolation of weather data (if needed) is made on the fly. The model is mainly adapted to weather data on so called hybrid vertical coordinates, and the vertical coordinates of weather data generally define the model vertical coordinates.

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4.12.2 Integrated modelling at Stockholm University, Department of Meteorology

On-line coupled systems

- **MIUU photochemistry model** – meso-scale hydrostatic model which for research purpose has been developed to include on-line coupled photochemistry. (Researcher Gunilla Svensson).
- **MITCRM, Cloud Resolving Model including chemistry** – meso-scale non-hydrostatic model, model area 200x200 km, which has been applied in research projects. (Researcher Annika Ekman).

4.13 Integrated modelling in Switzerland

(contribution by Alain Clappier, EPFL)

The main objective of the COST-728 Action is to develop advanced conceptual and computational frameworks to enhance significantly European capabilities in mesoscale meteorological modelling for air pollution and dispersion applications. Currently, the weather forecasting and air quality communities are overlapping but somewhat disparate. In the framework of the COST 728 Action, different Swiss partners will contribute to bring together these communities developing better interfaces between NWP models and air quality models all run in off-line mode.

The Swiss partners are:

- Laboratoire de Pollution de l'Air et des Sols (LPAS)
Swiss Federal Institute of Technology in Lausanne (EPFL)
- Laboratory of Atmospheric Chemistry (LAC),
Paul Scherrer Institute (PSI) in Villigen.
- MeteoSwiss in Zürich
- Material Sciences & Technology (EMPA) in Dubendorf
- Société d'Etude en Environnement (SEDE) in Vevey
- Applied Scientific Computing (ASCOMP) in Zürich.

These partners are working on four different projects.

4.13.1 Linking meteorological and photo-chemical dispersion models: development and tests of an interface with improved turbulence schemes: PSI (LAC) and EPFL (LPAS).

MetM. MM5, Lokalmodell (Swiss version aLMo)
CTM: CAMx
Only off-line coupling, improvement of interfaces

Numerous air quality simulations at PSI with the 3-dimensional meteorological model MM5 and the Comprehensive Air Quality Model (CAMx) showed that the parameters of the interface that links the two models might significantly affect the concentration of pollutants. One of the key processes is the vertical turbulent diffusion implemented in the interface. The current schemes are not capable of simulating vertical transport correctly.

In this project an improved parameterization for turbulent diffusion shall be developed and applied to a test case. The investigation will be done in the frame of a PhD thesis jointly carried out by PSI / LAC and EPFL / LPAS. There are common interests of both institutions regarding air quality modelling, and of MeteoSwiss. Today, the Swiss weather service runs the forecast model aLMo developed by the Consortium for Small Scale Modelling (COSMO) operationally and provides the output to both PSI and EPFL for air pollution studies. MeteoSwiss itself derives wind trajectories and uses a Lagrangian particle dispersion model for emergency response purposes. EMPA uses the same dispersion model in time-inverted mode in the frame of source apportionment studies. All four institutions will benefit from an improved version of the current turbulence schemes.

After having become familiar with the main features of the meteorological and photochemical dispersion models used at PSI, the PhD student will spend a few weeks at EPFL to become acquainted with turbulent transport and its parameterization. He will implement the most promising schemes into an interface that links MM5 and CAMx. In the first phase the various approaches shall be tested for a given domain including complex topography, urban and rural areas. Their impact on meteorology and finally on the concentrations will be investigated and the optimum parameterization will be determined. In a second phase the model package shall be applied to more extended domains covering Switzerland and northern Italy.

For a potential use of aLMo as direct pre-processor for CAMx (i.e. without MM5) the interface has to be extended for the aLMo output. Currently, this makes sense only if the CAMx grid cells are larger than the aLMo resolution (about 7 km). In the next future, however, a high-resolution version aLMo2 with a grid cell size of about 2 km will be available. As soon as aLMo2 is in its pre-operational phase (planned for 2007), the PhD student will run the model at the Swiss National Supercomputing Centre (CSCS) at Manno in close cooperation with MeteoSwiss.

4.13.2 Linking high-resolution NWP and Lagrangian dispersion modeling (LILA): MeteoSwiss and EMPA

MetM: Lokalmodell (Swiss version aLMo), downscaled
CTM: LPDM
Only off-line coupling, improvement of interfaces

MeteoSwiss and Empa use a Lagrangian particle dispersion model to simulate the transport of radioactive nuclides and non-decaying airborne substances. This dispersion model uses the same parameterisations as the numerical weather prediction (NWP) model. These parameterisations are based on assumptions appropriate for the synoptic scale, but are of limited accuracy on the small scales as needed for dispersion modelling. While the inaccuracies are not a significant problem for weather forecasting, they are of major concern for dispersion modelling especially in the complex orography of the Alpine region.

Through the advancement of high-resolution NWP modelling to mesh sizes of 1 – 3 kilometres, the weather processes on that scale become much better represented. Nevertheless, the problem of inaccurate parameterisations for sub-grid scale effects remains even with higher resolution. The goal of this project is the development, implementation, and testing of an elaborate interface between the NWP model of the Consortium for Small Scale Modelling (COSMO) and a Lagrangian particle dispersion model. The interface will, in particular, include improved parameterisations for dispersion applications. The project thus perfectly fits with one of the objectives of the COST Action 728, improving areas of parameterisation that are poorly treated with regard to requirements for air pollution and dispersion applications.

A simple version of the proposed interface between the meteorological model and the dispersion model will be developed at an early stage of the project in synergy with the companion project proposed by PSI and EPFL. After that, the PhD student of the partner proposal by PSI and EPFL will focus on the implementation of an advanced turbulence scheme for a downscaling of the NWP-derived parameters. The primary task for the PhD thesis suggested in this proposal will be to test the influence of the future high-resolution parameters on the dispersion. The higher resolution will primarily have an effect on the dispersion close to the source. With increasing distance from the source, the spread of the plume increases and the smaller scales become less important, allowing the modelling of the dispersion with a lower resolution of the NWP-derived parameters. The proposed interface will have to handle the transition between the fine resolution close to the source and the coarser resolution further away.

The newly developed modelling system will be verified with observations. The Empa will combine emission data with pollution transport simulations to derive synthetic concentration time series that can be compared to actual concentration measurements. The successful application will allow the apportioning of strength and location of source regions for the air pollutants reaching the measurement site.

With the envisaged interface, the existing COSMO model can be used as driving meteorological model for air quality and pollutant transport modelling. This also opens the valuable opportunity to use the existing archives covering several years of hourly COSMO model analyses for air pollution modelling, for the benefit of all institutions operating dispersion models on a regional range.

4.13.3 Enhanced dispersion modelling through meteorological model integration in complex terrain: SEDE and EPFL (LPAS)

MetM: Lokalmodell (Swiss version aLMo)
CTM: POLYTOX (multi-box model)
Only off-line coupling, improvement of interfaces

SEDE SA has developed an Eulerian non-stationary multi-box model of pollution dispersion, POLYTOX, whose original approach has already been validated with multiple impact studies. As an efficient 3D code, It is simple enough for fast computations, but includes however vertical and horizontal diffusion parameterization. It represents an approach directed towards maximizing the use of measurements available, usually performed at ground level by weather stations. It is thus possible to calculate the dispersion of pollutants with a resolution of 100 meters on a surface of

5000 km2, on a one year period in a few hours. Such a high resolution is necessary for an adequate modelling of primary pollutants, especially when determining their peak values close to the most important emission sources.

This approach looses however its accuracy when transported concentrations are proportionally important, as it is often the case for ozone and particle matter in the troposphere. There is also another issue, namely that the wind field measured at a few seldom weather stations is also insufficient for describing with the required accuracy the overall wind flow.

The emerging high resolution NWP models should make it possible to provide initial and boundary conditions with sufficient accuracy, so that the simplified method embedded into POLYTOX can provide results with good accuracy within a small computing time.

The project will thus first carry out the integration of an NWP, like aLMo, and POLYTOX. Wind interpolation, mixing height and diffusion coefficients parameterization will be undertaken.

The integrated model will then be used to improve the modelling of dispersion under very low wind speed conditions, and for also improving the urban primary pollutant modelling, using the urban diffusion parameterization developed at EPFL - LPAS. Comparisons with former air quality impact studies will be undertaken to assess the enhancements achieved.

4.13.4 Multi-scale flow analysis in the urban sublayer using large-eddy simulation: ASCOMP and EPFL (LPAS)

MetM: LES model
(CTM: CAMx, AUSTAL,MISKAM)

Air quality becomes a serious health concern in modern societies, and this has connections with the growth of urban areas. Millions of people are today exposed to high levels of pollutant concentrations. Emission control strategies have to be envisaged and rigorously practiced, with the help of pollution forecast models. Numerical prediction should again play a crucial role in this context, but various roadblocks need first to be alleviated before gaining in credibility. Air quality models require an integrated approach to simulate the local urban scale (< 1-5 km) and surrounding mesoscale (1-200 km). This is synonymous to couple large-scale weather forecasting models (NWP) with sub-scale air quality models (AQ). Only under these conditions can the “boundary conditions” between the two environments be transcended and accounted for rigorously. The increasing predictive -or resolving- capabilities of NWP’s is allowing these to penetrate (in terms of resolution) deeper within the sub-scale or city-scale domains. Air quality models (such as CAMx, AUSTAL, MISKAM) require, on the other hand, a sort of “super-scale boundary conditions” that can be provided only by NWP’s, e.g. MM5. The link between the two is therefore obvious, and that is the pillar of our project. Existing sub-scale models have proven disappointing in describing the flow and turbulence fields accurately enough to be used for pollution transport studies. Difficulties also arise from the treatment of heterogeneous surface characteristics such surface roughness, and phase-change processes (evaporation). Particle dispersion in low momentum conditions is an additional challenge that requires more attention. The same is true for production of secondary pollutants, such as ozone during mesoscale transport. Flow and turbulence models constitute therefore the cornerstone of the assessment process and can influence substantially the results of subsequent modules (e.g. physico-chemistry). With this proposal we intend to help develop a better subscale parameterization model by use of a sophisticated modelling approach, transcending RANS. We intend to use the Large-eddy Simualtion (LES) approach for the flow around a matrix of cubical obstacles, representing a typical sub-urban area. Expected outcome of this work include: improving the urban parameterization in the mesocale models, and promote the knowledge on the interactions between urban sub-scale and large-scale phenomena. This will increase the credibility of existing pollutant concentration simulation codes, which form the main instrument for defining appropriate actions.

4.14 Integrated modelling in the UK (selection)

4.14.1 Integrated modelling at the UK MetOffice

(contribution by Maria Athanassiadou, info by Matthew Craig Hort and Andrew Jones, Atmospheric Dispersion Group, Met Office

A. CTMs used in the MetOffice, UK

Only off-line one-way coupling with MetMs

I. NAME III

The Met Office atmospheric dispersion modelling capabilities are based on the NAME III dispersion model driven by 3-d meteorological fields from the Met Office's numerical weather prediction model, the Unified Model. The interaction is a one-way coupling (i.e. NAME III is run off-line using output fields of certain meteorological parameters). A regional scale model, covering the UK and Western Europe, is used for air quality/chemistry applications.

1) MetM: Numerical weather prediction model: Met Office Unified Model ('UM')

- grid-point NWP model
- hybrid vertical coordinate system ('height-based eta' - terrain following at surface blending to constant height surfaces)
- operational versions at global, regional and mesoscale resolutions;
- experimental high-resolution mesoscale versions (down to 250 m resolution).
- Global version:
    - horizontal resolution (~ 40 km),
    - 50 vertical levels
- Regional version (North Atlantic and European area):
    - horizontal resolution (~ 12 km),
    - 38 vertical levels
- Mesoscale version (United Kingdom area):
    - horizontal resolution (~ 4 km),
    - 38 vertical levels
- operational models run 4 times daily at 00 UTC, 06 UTC, 12 UTC and 18 UTC.
- reference: "Cullen, M. J. P. (1993) The unified forecast/climate model. Meteorological Magazine 1449, 81-94."

2) Atmospheric dispersion model: NAME III

- Lagrangian particle dispersion model
- originally developed as a nuclear accident model following the Chernobyl accident, today NAME is used in a wide range of applications (e.g. environmental emergency response, volcanic ash modelling, air quality forecasting, source detection and attribution)
- includes:
  - plume rise (buoyant/momentum-driven releases)
  - radioactive decay (radionuclides)
  - virus decay (biological species)
  - chemical transformations
  - dry and wet deposition
- uses UM fields files (can also use single-site observations for short-range applications)
- global/regional met at 3-hourly intervals
- mesoscale met at hourly interval
- uses lowest 31 UM model levels only (troposphere/lower stratosphere)
- met parameters as full 3-d fields:
  - mean wind (u, v, w components),
  - temperature,
  - specific
  - humidity,
  - pressure,
  - dynamic cloud liquid water,
  - dynamic cloud ice
- met parameters as surface/single-level fields:
  - surface stress,
  - surface sensible heat flux,
  - surface pressure,
  - mean sea level pressure,
  - convective cloud amount/base/top,
  - high/medium/low dynamic cloud amount,
  - roughness length,
  - dynamic/convective rain rate,
  - dynamic/convective snow rate,
  - boundary layer depth

- chemistry scheme:
  - represents gas and aqueous-phase chemistry (sulphate/nitrate/ozone)
  - chemical reactions derived from the Met Office's global atmospheric chemistry model, STOCHEM
  - chemistry calculated on a static 3-dimensional grid after each main advection time-step

- Reference "Jones, A. R., Thomson, D. J., Hort, M. and Devenish, B. (2004) 'The U.K. Met Office's next-generation atmospheric dispersion model, NAME III', in 'Air Pollution Modeling and its Application XVII', Borrego, Carlos; Norman, Ann-Lise (Eds.), Springer, 2006, ISBN-10: 0-387-28255-6."

II. Other CTMs used in the MetOffice

CHEMET

- This is an emergency response service provided by the UK MetOffice on a 24/7 basis to UK emergency services and UK government.
- It uses ADMS as the dispersion model.
- The service provides the dispersion prediction on a GIS map background along with a synopsis of current and expected meteorological conditions.
- A request is instigated by phone, email and/or fax.
- Output is in a standard format and is disseminated by fax and email directly to responding services and agencies.
- Guidance can be updated as frequently as 1 hourly.

HYSPLIT (HYbrid Single-Particle Lagrangian Integrated Trajectory) model

- The model does dispersion and trajectories.
- The dispersion of a pollutant is calculated by assuming either puff or particle dispersion.
- The model can be run interactively on the Web through the READY system on the Met Office site or the code executable and meteorological data can be downloaded to a Windows PC.
- Also used by:
  - Some academics in UK.
  - Americans and Australians in various systems e.g. Volcanic ash prediction.
- Web site: http://www.arl.noaa.gov/ready/hysp_info.html#DATA
- Met data: Gridded 3D NWP.

B. Further CTMs used in the UK

I. SCIPUFF (Second-order Closure Integrated Puff) model

- It is the dispersion model in HPAC (Hazard Prediction and Assessment Capability model suit) which is a military based model system (contains lots of source and effects models in addition to the dispersion bit) used and developed by dstl, AWE, and others for military applications.
- American Offline model.
- Free to download off web
  - http://www.titan.com/products-services/abstract.html?docID=336
- Met data: Fixed winds, surface or profile observations or gridded meteorological input accepted
- The SCIPUFF is a Lagrangian puff dispersion model that uses a collection of Gaussian puffs to represent an arbitrary, three-dimensional time-dependent concentration. The turbulent diffusion parameterisation is based on turbulence closure theory.
- SCIPUFF has been validated against a number of laboratory and field experiments. It has been recommended as an alternative model by the EPA which can be used on a case-by-case basis for regulatory applications.

II. ADMS (plus ADMS Urban and all the other varieties) -

Used by:

- Many companies
- Local councils for air quality assessment
- Environment Agency (EA) for environmental impact assessment and emergency response
- Food Standard Agency for emergency response.
- Some emergency services.
- Met Office within CHEMET service

Integrated modelling within the Centre of Atmospheric & Instrumentation Research (CAIR), University of Hertfordshire, UK

(contribution by C. Chemel, Y. Yu, R.-M. Hu, and R. S. Sokhi, CAIR, UH, UK)

Summary: A variety of MeMs and CTMs are used by the Atmospheric Dynamics & Air Quality group (ADAQ) at the Centre of Atmospheric & Instrumentation Research (CAIR), University of Hertfordshire, UK. The on-going modelling activities in our group focus on the development and application of MeMs and CTMs to investigate the transport, mixing, transformation and impacts of pollutants across scales ranging from global to micro-scales. MeMs and CTMs are eventually considered within an integrated framework depending on the applications. The models support studies that are mainly conducted for research purposes. In the following section, an overview of the models and applications are given.

MetMs: MM5, WRF, ARPS, PUM
CTMs: CMAQ, WRF/Chem, GEOS-Chem, GEM-AQ
Interfaces: off-line coupling for CMAQ, online coupling for WRF-Chem, GEOS-Chem, GEM-AQ

A. Model descriptions:

a. MeMs:

MM5 (PSU/NCAR Mesoscale Model, 5th generation) – Limited-area model developed jointly by Penn State University and NCAR (http://www.mmm.ucar.edu/mm5/) (Grell *et al.*, 1995). This is a community based model with external contributions worldwide that has been used extensively worldwide for many years to investigate a variety of atmospheric processes taking place from meso- to local scales, including the urban scale. The model uses ‘by default’ land-cover data from USGS, for which urban areas are classified only by one urban land-cover class. In our group, more detailed land cover data from CEH have been used to refine the representation of urban areas in the UK, by distinguishing continuous urban and suburban areas (see for instance Kitwiroon, 2006). Indeed, about one half of the London metropolitan area may be classified actually as suburban area. Furthermore, the modelling system has been systematically used until 2006 to provide CMAQ with meteorological fields.

WRF (Weather Research and Forecasting) – Limited-area model developed as a community model (http://www.wrf-model.org) (Skamarock et al., 2005). This next-generation community based model is mainly developed at NCAR, NOAA, AFWA, NRL, OU and FAA. The modelling system is designed for both operational forecasting and atmospheric research needs for a broad spectrum of applications across scales ranging from a few meters to thousands of kilometres. The model includes two dynamical cores (namely ARW and NMM), and is very flexible, offering advanced physics and numerics options. In our group, it has been applied to investigate a variety of atmospheric flows, e.g. flows over complex terrain such as mountainous and urban areas, strong convective systems over Northern Australia. Note that WRF has naturally replaced MM5 for most of the on-going studies. Furthermore, it has been straightforward to replaced MM5 by WRF to be coupled with CMAQ thanks to the MCIP interface in the Models-3 framework (see the section on CMAQ below and § B).

ARPS (Advanced Regional Prediction System) – Limited-area model developed by University of Oklahoma (http://www.caps.ou.edu/ARPS/). This non-hydrostatic, compressible LES model is devoted to meso- and small-scale (down to a resolution of a few meters) atmospheric flows. Xue *et al.* (2000; 2001) gave an extensive description of the model formulation and applications (see also the contribution to this report by K. de Ridder, VITO, Belgium). This code has been used extensively in our group for studying atmospheric flows over complex terrain, such as mountainous (e.g. Brulfert et al. 2005) and urban areas. It has also been used to investigate turbulence and mixing in the boundary layer (e.g. Chemel and Staquet, 2007). A MCIP-type interface (as used in the Models-3 framework; see § B) has been developed to couple ARPS with CMAQ as well as with the Transport and Air POllution Model (TAPOM) developed by A. Clappier, EPFL, Switzerland.

PUM (Ported Unified Model) – Multi-scale model based on the Unified Model (UM) developed by the UK Met. Office (http://www.metoffice.gov.uk/research/nwp/numerical/unified_model) (see also the contribution to this report by M. Athanassiadou and co-workers, as well as Cullen, 1993). The model has been released to the user community for research purposes in 2006. The modelling system is made up of a number of sub-models that enable for instance oceanic and atmospheric applications to be coupled. The model can be applied to global and regional domains over a wide range of temporal and spatial scales. Currently, it is being used within CAIR to investigate the representation and the impact of the urban canopy of the London metropolitan area for modelling urban- and regional-scale air quality. To enable air quality research investigations, the model has been coupled with CMAQ through a MCIP-type interface (see § B)(see § B).

b. CTMs

CMAQ (Community Multiscale Air Quality) – Multi-scale, multi-pollutant model developed by US EPA (http://www.cmaq-model.org) (see also the contribution to this report by K. Schere, US EPA, USA, as well as Byun and Schere, 2006). Different chemical mechanisms (CB-IV, CB05, SAPRAC-99 and RADM2) and solvers (EBI, SMVGEAR) are available. The model is embedded within the Models-3 framework, which includes interfaces to prepare for instance emissions (SMOKE), initial (ICON) and lateral boundary conditions (BCON). Note that the emission processor SMOKE has been adapted to include European (from EMEP and EPER) and UK (from NAEI) scale anthropogenic emissions as well biogenic emissions (as calculated from the method proposed by Guenther et al., 1995). This work was performed as part of a project funded by the UK Environment Agency and the FP6 project AIR4EU. The modelling system (coupled with either MM5, WRF, ARPS or the UM) can be used to investigate regional- to local-scale (including urban-scale) air quality. In our group, it has been applied for instance for studying the air quality in the London metropolitan area (e.g. Sokhi, et al. 2006) and for evaluating contribution of industrial point emissions to regional air quality (Yu et al., 2007).

WRF/Chem (WRF coupled with Chemistry) – Multi-scale, multi-pollutant model developed collaboratively by several groups (NOAA/NCEP, NOAA/ESRL, NCAR) (see the contribution by G. Grell, NCAR, USA, as well as http://ruc.fsl.noaa.gov/wrf/WG11/ and Grell *et al.*, 2005). Many choices of chemical mechanisms (e.g. RADM2, CBM-Z) are available. The model is embedded within the WRF framework and is fully coupled with the dynamical core (for instance ARW or NMM). At the moment, a program is available to prepare emission input from the US EPA emission inventory. Consequently, the modelling system has been used and tested essentially for

US applications. It is used in the US for semi-operational simultaneous forecasting of weather and air quality and has been evaluated with retrospective simulations. Within CAIR, it has been applied to the UK regional scale by switching off the chemistry whilst a detailed inventory for anthropogenic emissions is being finalized. The model will complement models such as CMAQ and UKCA (which is currently developed jointly by NCAS and the UK Met. Office).

GEOS-Chem (Goddard Earth Observing System coupled with Chemistry) – Global-scale model of atmospheric composition driven by assimilated meteorological observations from GEOS at the NASA Global Modeling and Assimilation Office (http://www-as.harvard.edu/chemistry/trop/geos/, see also Bey *et al.*, 2001). The modelling system can be used to investigate a wide range of atmospheric composition problems, including future climates and planetary atmospheres using general circulation model meteorology to drive the model (e.g. Park *et al.*, 2004). It has been applied to generate vertical profiles for satellite retrievals (Hu *et al.*, 2007) as well as initial and boundary conditions for regional air quality and climate models.

GEM-AQ (Global Environmental Multiscale coupled with Air Quality) – Multi-scale model based on GEM, which is developed by Environment Canada for operational weather prediction in Canada (e.g. Côté *et al.*, 1998; Gong *et al.*, 2003) (see the contribution to this report by J. W. Kaminski, York University, Canada). The modelling system can be used to investigate atmospheric processes and air quality over a broad range of scales, from the global scale down to the meso-gamma scale. It has been applied mainly for regional air quality and climate change studies (e.g. Hu *et al.*, 2005).

B. Interfaces for off-line models:

Among the CTMs that we use only CMAQ needs an interface to be coupled with a MeM. To proceed, we take advantage of the Models-3 framework. Indeed, within this framework, an interface is available for MM5 and WRF, namely the Meteorology-Chemistry Interface Processor (MCIP) (see the contribution to this report by K. Schere, US EPA, USA). A detailed description of this interface is given by Byun and Ching (1999). As for ARPS and UM models, interfaces based on the original MCIP have been developed. Note that the interface for the UM can handle data either from BADC (operational archived data at a 12-km horizontal resolution, http://badc.nerc.ac.uk), UM or PUM. This interface, known as UMMCIP, was developed in collaboration with Aeolus, UWERN and the UK Met. Office.

C. Downscaling / nesting:

All the abovementioned models can be run using one-way nesting when focusing on limited-area domains. A two-way interactive nesting technique is available in MM5, WRF, WRF/Chem and GEM-AQ. For typical global-scale applications, PUM, GEOS-Chem and GEM-AQ are run down to a 1° horizontal resolution. For typical regional-scale applications using any of the models (e.g. MM5, WRF, ARPS or UM with CMAQ), three to four domains are nested down to a horizontal resolution of 3 to 5 km. Five domains are usually necessary for a downscaling down to the urban scale (namely horizontal resolution as fine as 1 km or less). In practice, when focusing on a limited area, GEM-AQ is often run down to a horizontal resolution of 15 km.

D. Data assimilation / initialization:

Data assimilation (FDDA nudging and 3D-Var) is available in almost all the abovementioned MeMs. In practice, data assimilation is not fully available in PUM (not released by the UK Met. Office). As for the CTMs, no data assimilation is currently implemented for chemical variables. However, note that data assimilation is naturally implemented in GEOS-Chem since it is driven by assimilated data from GEOS. Many applications focus mainly on retrospective simulations with the use of initial and boundary conditions for the MeMs employed from gridded re-analyses from ECMWF or NCEP. Regarding the CTMs, no such re-analyses are available. Monthly mean data from the UK Met. Office global-scale CTM STOCHEM (Collins et al., 1997) are used to provide initial and boundary conditions for CMAQ and WRF/Chem. As for GEM-AQ, the model is initialized from climatological datasets.

E. Model unification / harmonization:

The models should actually be considered within an integrated framework, designed to be a plug-compatible platform, which enables scales and processes to interact. Also, each model contains specificities, which are often suitable for certain applications. Furthermore, atmospheric dynamics and chemistry can strongly interact through feedback processes (e.g. the radiative forcing of aerosols). Hence, current research focuses on ways to couple efficiently atmospheric dynamics and chemistry for both off- and on-line models as well as identifying for which problems these approaches are appropriate. In addition, basic research is undertaken to address specific issues (such as, stable atmospheric conditions, representation of the urban canopy, aerosol treatment in CTMs). A heavy technical work is also being conducted to adapt the non-UK modelling systems to the UK (for instance, preparation of emissions, speciation profiles for different chemical mechanisms, refined land-cover data, etc).

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Development of the UM meteorology-chemistry interface processor (UMMCIP)

4.15 Integrated modelling at ECMWF (European Centre for Medium-Range Weather Forecasts, Reading, UK)

As part of the GEMS sub-project on global reactive gases (GRG), ECMWF performs coupled modelling of meteorology and atmospheric chemistry on the global scale in collaboration with the following partners:

- Forschungszentrum Juelich & MPI-Hamburg (MOZART)
- meteo-france (MOCAGE)
- KNMI (TM5)

Further, the GEMS sub-project on aerosols (AER) is working on the integration (in-line coupling) of aerosol processes in ECMWFs integrated forecast system (IFS).

Summary:

MetMs:

- ECMWFs integrated forecasts system (IFS, www.ecmwf.int) including tracer transport and application of external tendencies describing source and sink processes (emissions, chemistry and deposition) provided by one of three CTMs

CTMs:

- TM5, MOCAGE, MOZART-3

Interfaces:

- Coupler OASIS4 http://www.prism.enes.org/PAEs/coupling_IO/software_OASIS4.php)

Model descriptions (with text descriptions):

MetMs:

The GEMS-GRG system is a 3D two-way coupled system: IFS provides 3D and 2D atmospheric fields at high temporal resolution to drive the CTMs, and IFS receives 3D tracer concentration fields and tracer tendencies due to source and sink processes from the CTM. A further coupling option is the feedback of concentration fields from the IFS to the CTM

The GRG coupled system can be run in three modes:

- CTM forecast mode (one-way coupling)
- IFS tracer forecast mode (two- way coupling, and optional concentration feedback from the IFS to the CTM)
- IFS tracer data assimilation mode (two way coupling, and feedback concentration feedback from the IFS)

For details of the IFS see http://www.ecmwf.int/research/

CTMs

- TM5:http://www.phys.uu.nl/~tm5/, for
- MOCAGE : http://www.lmd.jussieu.fr/~hourdin/AMMA/MODELS/AMMA_MOCAGE.pdf
- MOZART-3: http://gctm.acd.ucar.edu/mozart/

Downscaling/nesting:

- CTM run at a T63 resolution or similar and the IFS at T 159.
- Horizontal interpolation (bicubic or bilinear) is performed by the coupler OASIS4 software
- Vertical resolution (60 layer in a sigma-hybrid coordinate) is identical

Data assimilation/initialisation:

- Data assimilation of satellite observations of atmospheric composition using ECMWFs 4DVAR system.
- Initialisation of the IFS tracers by the CTM data.

Current applications of the integrated modelling systems

- Currently data assimilation of MOPITT CO and SCHIAMCHY NO2 and O3, more observations to be included

- Near-real time forecasts in research mode: http://www.ecmwf.int/products/forecasts/d/inspect/catalog/research/gems/grg/realtime/

Model unification/harmonization/ further developments

- Integrating aerosol, global reactive gases and greenhouse gases into one production system at ECMWF.

4.16 Non-European integrated modelling

4.16.1 Integrated modelling supported by CSIRO Marine and Atmospheric Research, Aspendale, Victoria 3195, Australia

(contribution of Peter Hurley, CMAR, Aspendale, Australia)

Summary:
MetMs: TAPM http://www.csiro.au/products/ps1gu.html
CTMs: TAPM
Interfaces:
Only on-line coupling.

Model descriptions:
MetMs:
The Air Pollution Model (TAPM)
TAPM is a PC-based, nestable, prognostic meteorological and air pollution model driven by a Graphical User Interface (GUI). It was designed to be easy to use and fast to run, but also to be based on comprehensive science. Datasets of the important inputs needed for meteorological simulations accompany the model, allowing model set up for any region, although user-defined databases can be connected to the model if desired. The only user-supplied data required for air pollution applications are emission information. The model outputs can be examined easily and quickly, with various types of output processing options provided.

The meteorological component of TAPM is an incompressible, optionally non-hydrostatic, primitive equation model with a terrain-following vertical coordinate for three-dimensional simulations at typically 25 levels. It includes parameterisations for cloud/rain micro-physical processes, turbulence closure, urban/vegetative canopy and soil, and radiative fluxes. The model equations neglect the curvature of the earth and assume a uniform distance grid spacing across the domain, so that the horizontal model-domain size should be restricted to be less than 1000 x 1000 km. The maximum altitude is 8 km, so there is no stratosphere. These restrictions mean that high-impact weather may not be simulated well — such conditions are generally not associated with important air pollution events.

TAPM uses the fundamental equations of atmospheric flow, thermodynamics, moisture conservation, turbulence and dispersion, wherever practical. The meteorological component of the model is nested within synoptic-scale analyses/forecasts that drive the model at the boundaries of the outer grid. The coupled approach taken in the model, whereby mean meteorological and turbulence fields are passed to the air pollution module every five minutes, allows pollution modelling to be done accurately during rapidly changing conditions such as those that occur in sea-breeze or frontal situations. The use of integrated plume rise, Lagrangian particle, building wake, and Eulerian grid modules, allows industrial plumes to be modelled accurately at fine resolution for long simulations.

CTMs:

The air pollution module of TAPM consists of various sub-modules, including the Eulerian Grid Module (EGM), the Lagrangian Particle Module (LPM), the Plume Rise Module (PRM) and the Building Wake Module (BWM). Wet and dry deposition processes are included. The use of a condensed chemistry scheme also allows nitrogen dioxide, ozone, and particulate mass to be modelled for long periods. A range of pollutant emission configurations can be used, including point sources, line sources, area/volume sources and gridded surface sources. The optional gridded surface emission files can include general gridded surface emissions, biogenic surface emissions, wood heater emissions, and vehicle exhaust and evaporative emissions for a range of fuel types (petrol, diesel, LPG). Some of these emission files need to be supplied at fixed temperature and/or radiation level, with the model making adjustments in emissions for variations in these meteorological variables as a simulation progresses.

Off-line models / On-line models:

On-line model.

Interface modules:

Interfaces are not needed.

Downscaling/nesting:

For computational efficiency, TAPM includes a one-way nested approach for meteorology and air pollution, with the pollution grids optionally able to be configured for a sub-region and/or at finer grid spacing than the meteorological grid, which allows a user to zoom-in to a local region of interest quite rapidly. Up to four nests can be set directly through the GUI.

Data assimilation/initialisation:

TAPM contains an option to nudge to meteorological observations. Default initialisation is via the Australian Bureau of Meteorology’s Global AnalysiS and Prediction (GASP) analyses set, which are available with TAPM. However any analysis set (e.g. ECMWF, NCEP) can easily be used for initialisation.

Current applications of the integrated modelling systems

TAPM is used to model winter and summer meteorology and photochemical smog and particulates in urban areas, fumigation from elevated point sources in coastal areas, and medium-range transport. Year-long simulations to determine extreme (high) pollution statistics in urban areas and industrial complexes are also carried out. References to these works and to verification studies can be found in Hurley et al. (2005).

European applications include regulatory policy development, process research, impact assessment studies, and air quality forecasting.

Model unification/harmonization/ further developments

A complex chemical transport model developed at CMAR (Cope et al. 2005) has recently been coupled with TAPM in an online mode for use in more complex chemistry situations. This system is referred to as **TAPM-CTM.**

TAPM is also applied in further European countries: Greece, Norway, Portugal, Spain

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4.16.2 Multiscale Air Quality Modelling in Canada

(Contribution by Jacek W. Kaminski York University, Toronto, Canada)

MetM-CTM: GEM-AQ (Global Environmental Multiscale Air Quality model)
On-line coupling

The Global Environmental Multiscale Air Quality model (GEM–AQ) is based on the model developed by the Environment Canada for operational weather prediction (Côté et al., 1998a), The host meteorological model can be configured to simulate atmospheric processes over a broad range of scales, from the global scale down to the meso-gamma scale. GEM–AQ can be run in a global uniform configuration, global variable resolution, where the grid has a uniform core and moving away from the core, the grid size increases by a constant factor. In addition, a limited area configuration (LAM) is also available. The model has a flexible vertical coordinate system and can be used either with sigma or pressure hybrid (Laprise and Girard, 1990) with the top at 10 hPa. For a properly account of stratospheric/tropospheric exchange in polar regions and, in particular, ozone inflow from the stratosphere a hybrid coordinate system is required.

Spatial discretization

To meet the needs of operational weather forecasting and research, Environment Canada proposed a unified strategy based on the use of a global variable-resolution model, run with different configurations:

- a uniform-resolution 'medium-range' configuration, for global-scale problems such as medium- and long-range weather forecasting
- a variable-resolution 'continental-scale' configuration for more detailed forecasts to 2 days; and
- variable-resolution 'meso-[beta]-scale' and 'meso-[gamma]-scale' configurations for yet-more-detailed forecasts and simulations at correspondingly-shorter time periods.

An arbitrarily-rotated latitude-longitude mesh focuses resolution on any part of the globe. Such approach provides an efficient and conceptually simple solution to the nesting problem for regional forecasting: the planetary waves are adequately resolved around a high-resolution subdomain (which resolves mesoscale disturbances), there are no artificial lateral boundaries with their attendant problems, and there is no abrupt change of resolution across an internal boundary since the resolution varies smoothly away from the area of interest.

In the vertical GEM uses the generalized sigma vertical coordinate system. It has terrain-following sigma surfaces near the ground and in the model atmosphere. The top level is 10 hPa. Medium and long-range forecasts by the global version of the model is done on the uniform lat-lon grid with 0.9 degree resolution and 28 vertical levels. The current version of GEM regional forecast uses the non-uniform horizontal grid with 15 km resolution over central window, rotated at ~90 degrees and 58 vertical levels. A sponge layer is present to prevent spurious heat increase at the top of the model, and to facilitate the assimilation of upper-atmospheric satellite observations. The sponge acts on the top four model levels. The model top and the number of vertical levels are set up by the user. For most of simulations carried out for Europe 28 and 58 vertical levels with model top at 10 hPa were used.

Initial conditions

A number of fields and parameters are needed to specify surface characteristics and are obtained from analysed, climatological and geophysical datasets. These include surface roughness, land–sea mask, albedo, deep soil temperature, ice cover, and topography. The surface roughness length is influenced by topography and vegetation type.

Model dynamics

The set of non-hydrostatic Euler equations (with a switch to revert to the hydrostatic primitive equations) maintain the model's validity right down to the meso-[gamma] scales. The time discretization of the model dynamics is fully implicit, 2 time-level (Côté et al. 1998a; Côté et al. 1998b). A semi-Lagrangian treatment of advection overcomes the stability limitations encountered in Eulerian schemes due to the convergence of the meridians and to strong jets.

The spatial discretization for the adjustment step employs a staggered Arakawa C grid that is spatially offset by half a mesh length in the meridional direction with respect to that employed in previous model formulations. It is accurate to second order, whereas the interpolations for the semi-Lagrangian advection are of fourth-order accuracy except for the trajectory estimation (Yeh et al., 2002).

The semi-Lagrangian scheme used in the GEM regional model is already diffusive, so that the horizontal diffusion coefficient does not need to be very strong. Furthermore, if the diffusion were applied to both the temperature and the specific humidity, the resulting fields could lose some of their intrinsic coherence. For these reasons, in the GEM regional model (~15km) a delta^6 horizontal diffusion with a small diffusion coefficient (0.04) is used only on the momentum variables.

Vertical diffusion scheme is fully implicit scheme based on turbulent kinetic energy (Benoît et al., 1989).

Model physics

The physics package consists of a comprehensive set of physical parameterization schemes (Benoit et al. 1989; Mailhot et al. 1989a; Mailhot 1994):

1 Over land, the surface (skin) temperature is predicted from a heat budget using the "force–restore" method (Deardorff 1978; Benoit et al. 1989) combined with a stratified surface layer. Over oceans, the sea surface temperature is kept fixed during the integration. Over land, a soil moisture availability factor (percentage of field capacity) is used for calculating evaporation (Budyko bucket method or semipotential approach). Recently the ISBA scheme (Interactions Soil-Biosphere-Atmosphere) has been added to the package.

2 The planetary boundary layer is based on a prognostic equation for turbulent kinetic energy (Benoit et al. 1989). A shallow convection scheme for non-precipitating clouds is included to give a more realistic description of cloud-topped boundary layers. Shallow convection accounts for the formation of small cumuli that generally produce little precipitation but transport a large quantity of moisture vertically and play an important role in the atmospheric water cycle. Shallow convection is simulated with a method described by Mailhot (1994) and is treated as a special case of the turbulent planetary boundary layer to include the saturated case in the absence of precipitation.

3 Condensation processes at resolvable scales account for the formation of stratiform precipitation and, if mesh is sufficiently fine that individual convective cloud cells can be resolved, explicit convective precipitation. The explicit condensation process is represented by the isobaric condensation, which removes moisture when relative humidity exceeds a saturation point. Advanced microphysical equations are also incorporated in the model: versions of so-called Kuo-symmetric, relaxed Arakawa-Schubert (Moorthi and Suarez 1992), explicit cloud water schemes with mixed phases (Tremblay et al. 1996a) and detailed microphysics (Kong and Yau 1997).

4 Deep convective processes are handled with a Kuo-type convective parameterization (Kuo 1974; Mailhot et al. 1989a). A description of microphysical processes similar to that of the stratiform precipitation is also included. However, due to the complexity of evaporation from convective clouds, which strongly depends on the cloud internal dynamics (such as moist downdrafts, not included in the Kuo scheme), evaporation of convective precipitation is not considered. Recently the more sophisticated convection schemes such as the Fritsch–Chapell (Fritsch and Chappell 1980) and the Kain–Fritsch (Kain and Fritsch 1990) schemes have been developed.

5 The radiation subpackage contains detailed radiation schemes that are fully interactive with clouds. The infrared radiation scheme (Garand 1983; Garand and Mailhot 1990, Yu et al.

1997) includes the effects of water vapor, carbon dioxide, ozone, and clouds. The solar radiation scheme is essentially the one described by Fouquart and Bonnel (1980). It takes into account the effects of water vapor, carbon dioxide, ozone, clouds, Rayleigh diffusion, and multiple scattering. Cloud–radiation interactions represented in these schemes are an important effect.

6 Gravity wave drag parameterization is based on a simplified linear theory for vertically propagating gravity waves generated in statically stable flow over mesoscale orographic variations (McFarlane 1987; McLandress and McFarlane 1993). It makes use of a representation of the subgrid-scale orography (also called launching height) for exciting the gravity waves.

Chemistry

Gas phase:

Air quality modules are implemented on-line in the host meteorological model. Currently, there are 37 advected and 14 non-advected gas phase species in the model. Transport of the chemically active tracers by the resolved circulation is calculated using the semi-Lagrangian advection scheme native to GEM. The vertical transfer of trace species due to subgrid-scale turbulence is parameterized using eddy diffusion calculated by the host meteorological model. The effects of shallow convection on the vertical distribution of tracers are calculated as a special case of turbulent diffusion. Large scale deep convection in the host model depends on the resolution: in this version we have the mass flux scheme of Zhang and McFarlane (1995) for tracer species.

The gas-phase chemistry mechanism currently used in the GEM-AQ model is based on a modification of version two of the Acid Deposition and Oxidants Model (ADOM) (Venkatram et al., 1988), derived from the condensed mechanism of Lurmann et al. (1986). The ADOM-II mechanism comprises 47 species, 98 chemical reactions and 16 photolysis reactions.All species are solved using implicit Newton's method. In order to account for background tropospheric chemistry, 4 species (CH_3OOH, CH_3OH, CH_3O_2 and CH_3O_3H) and 22 reactions were added to the chemical solver. Heterogeneous hydrolysis of N2O5 is calculated using the online distribution of aerosol.

Although the model meteorology is calculated to 10 mb the focus of the chemistry is in the troposphere and perhaps mid- and high-latitudes regions of the UTLS region. Thus all species are transported throughout the domain for ozone and NOy we replace the field with climatologies after each transport time step. For ozone we used the HALOE climatology above 100 hPa while for NOy we replace it using the NOy fields from the CMAM model (e.g. de Grandpre et al. 2001).

Photolysis rates (J values) are calculated on-line every time step using the method developed by Landgraf and. Crutzen (1998). In this method radiative transfer calculations are done using delta-two stream approximation for 8 spectral intervals in UV and visible applying pre-calculated effective absorption cross sections. Cloud cover and water content are provided by the host meteorological model. The J value package that is used was developed for the Modular Earth Submodel System (MESSy) (Jöckel,, et al., 2005) and has been adopted for GEM-AQ.

Aerosols

Th current version of GEM-AQ has 5 size-resolved aerosols types viz., sea salt, sulphate, black carbon, organic carbon, and dust. The microphysical processes which described formation and transformation of aerosols are calculated by the Canadian Aerosol Module (CAM) (Gong et al., 2003). The particle mass is distributed into 12 logarithmically spaced bins from 0.005 to 10.24 microns radius. The following aerosol processes are accounted for in the model: nucleation, condensation, coagulation, sedimentation and dry deposition, in-cloud oxidation of SO2 , in-cloud scavenging, and below-cloud scavenging by rain and snow.

Removal processes:
The effects of dry deposition are included as a flux boundary condition in the vertical diffusion equation. Dry deposition velocities are calculated from a 'big leaf' multiple resistance model (cf. Wesely 1989, Zhang, et al., 2002) with aerodynamic, quasi-laminar layer, and surface resistances acting in series.

Emissions
Despite the fact that a new inventory (EDGAR3.0 and 3.2) is available, the emission dataset used for global simulation was compiled using EDGAR2.0 (archived in 2000, valid for 1990) and GEIA global inventories (Olivier et al. 1999; Olivier et al. 2001). EDGAR2.0 data was chosen for its detailed information on NMVOC speciation. Emission data compiled for GEM-AQ includes global fields of anthropogenic emission fluxes with 1°x1° resolution and natural emissions with 5°x5° resolution. Yearly averaged anthropogenic emissions contain different industrial sectors and non-industrial activity such as burning of agricultural wastes and fuel wood, for 14 gaseous pollutants. Monthly averaged biogenic, ocean and soil emission fluxes, as well as biomass burning (forest and savannah) emissions, have been derived for 9 species (7 VOC species, CO and NO_2). The various species for which emissions are included, along with source type, viz., anthropogenic combustion, biomass burning.

In the upper troposphere/lower stratosphere region (UTLS) sources of NOx are small, from large scale convective updrafts, stratospheric sources and lightning. For lightning we have used the monthly mean totals of lightning NOx from the GEIA inventory (scaled from 12.2 Tg/yr to 5 Tg/yr) and distributed them in the horizontal according to the convective cloud distribution of the model. In the vertical, the lightning NOx is distributed according to the profiles given by Pickering, 1998.

Results processing for model evaluation:

The GEM-AQ model has been run for a number of scenarios ranging from a global uniform domain, global variable resolution for regional scenarios, to very high resolution limited area for local air quality studies. Before a model can be used as a tool for environmental assessments such as chemical weather forecasting and data assimilation an intensive model evaluation must be carried out to learn about model behaviour, weaknesses and strengths. GEM-AQ has been exercised with a 5 year run (2001-2005) on a global uniform 1.5°x1.5° resolution domain (240 x 120 grid points) and 28 hybrid levels extending to 10hPa. The objectives of this simulation were to derive a multi-year model climatology, to examine seasonal variation and regional distribution, evaluate global emissions, and provide chemical initial and boundary conditions for high resolution model simulations.

The model was evaluated using the following observations

- Logan ozonesonde climatology (Logan 1999, Logan 1994)
- GOME tropospheric column ozone (Liu et al. 2005)
- tropospheric CO from MOPIT and AURA-MLS
- aircraft in-situ observarvations (Emmons et al., 2000)

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4.16.3 Integrated Modelling in the US (selection)

4.16.3.1 The Weather Research and Forecast and Chemistry (WRF/CHem) Community modelling system (http://www.wrf-model.org/WG11)

(contribution of Georg Grell, NCAR, Boulder, CO.)

MetMs: ARW-WRF and NMM-WRF, WRF/CHEM

Summary:

This fully coupled modeling system is based on the Weather Research and Forecast (WRF) model. WRF is designed to be modular, and a single source code is maintained that can be configured for both research and operations. WRF has two different dynamic cores, the Advanced Research Version (ARW) model, and the Nonhydrostatic Mesoscale Model (NMM). It offers numerous physics options, thus tapping into the experience of the broad modeling community. Advanced data assimilation systems are being developed and tested in tandem with the model. Although the model is designed to improve forecast accuracy across scales ranging from cloud to synoptic, the priority emphasis on horizontal grid resolutions of 1-10 kilometers makes WRF particularly well suited for newly emerging Numerical Weather Prediction (NWP) applications in the non-hydrostatic regime. Meteorological details of this modeling system can be found in Skamarock et al. (2005); the details of the chemical aspects are covered in Grell et al. (2005), and Fast et al. (2006).

Model descriptions

Although WRF has several choices for dynamic cores, the mass coordinate version of the model, called Advanced Research WRF (ARW) was the first to have all chemistry options included. The prognostic equations integrated in the ARW model are cast in conservative (flux) form for conserved variables; non-conserved variables such as pressure and temperature are diagnosed from the prognostic conserved variables. In the conserved variable approach, the ARW model integrates a mass conservation equation and a scalar conservation equation. These equations are discretized in a finite volume formulation, and as a result the model exactly (to machine roundoff) conserves mass and scalar mass. The discrete model transport is also consistent and preserves tracer correlations (c.f. Lin and Rood (1996)). The ARW model uses a spatially 5th order evaluation of the horizontal flux divergence (advection) in the scalar conservation equation and a 3rd order evaluation of the vertical flux divergence coupled with the 3rd order Runge-Kutta time integration scheme. The time integration scheme and the advection scheme is described in Wicker and Skamarock (2002). Skamarock et al. (2005) also modified the advection to allow for positive definite transport.

WRF is a community effort, and will replace MM5, also the Rapid Update Cycle model (RUC), and the forecast model from the National Center for Environmental Prediction (NCEP) from the National Weather Service (NWS), the ETA model. It includes almost all physics options from these various modeling system. In addition new physics options were developed that allow for interaction of chemistry and meteorology, in particular, to account for the aerosol direct, indirect, and semi-indirect effect. WRF/Chem is also a community effort (http://www.wrf-model.org/WG11), with many different modelers being involved in the development of this modeling system.

The chemistry package consists of dry deposition ("flux-resistance" method), three options for biogenic emissions (online, offline, or online modification of offline reference fields), and many choices to treat the gas phase chemistry. These choices include the well known RADM2 mechanism, the CBM-Z Carbon Bond mechanism, but also a version of the Kinetic PreProcessor (KPP), implemented by Salzman and Lawrence (2006). Photolysis routines include a Madronich scheme (1987) and FAST-j (Wild et al. 2000). The photolysis schemes are coupled with hydrometeors and aerosols. To model aerosols, WRF/Chem includes a modal approach (MADE/SORGAM, Schell et al. 2001) as well as a sectional method. The sectional aerosol module was also coupled to an atmospheric radiation scheme as well as to a second moment microphysics parameterization. Aqueous phase chemistry effects have recently been included. WRF/Chem allows for both 1-way and 2-way nesting of meteorology and chemistry, or it may use global boundary conditions. Data assimilation methods are available for meteorology (3dvar, FDDA nudging, advanced 4dvar under development). Plans exist to expand the data assimilation systems to chemistry. Initial fields for model simulations can come from these analysis systems, other modeling systems (such as GFS or ECMWF), or forecasts.

In addition to simulating the weather or -- in its most complicated form -- the air quality, this numerical modeling system may also be used as a coupled weather prediction and chemical dispersion model in order to forecast the release and transport of atmospheric tracers (through grid and subgrid-scale transport, emissions, and deposition).

Current applications of the integrated modelling systems

WRF/Chem is used for semi-operational simultaneous forecasting of weather and air quality and has been evaluated with retrospective simulations with data from the 2002 and 2004 New England Air Quality Study (NEAQS). It currently is also under evaluation with data from the Texas 2006 field campaign. Evaluation focused on a combined look at chemistry and meteorology, for surface data as well as upper level data. Other applications include – but are not restricted to - its use for research related to emissions (Kim et al. 2006, Frost et al. 2006), processes that are important for global climate change (Fast et al. 2006), and use of ensemble methods in forecasting (Pagowski and Grell 2006).

Model unification/harmonization/ further developments

Current development efforts and plans thereof focus on more coupling approaches for aerosols, more choices for aerosol modules, and extension of the KPP capabilities, as well as the development of data assimilation systems.

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4.16.3.2 Integrated modelling at the Atmospheric Modeling Division, U.S. Environmental Protection Agency (EPA), Research Triangle Park, North Carolina, U.S.A.

(contribution by Kenneth Schere, EPA)

Summary:

MetMs: MM5, WRF/arw

CTMs: CMAQ model

Interfaces: The Meteorology-Chemistry Interface Processor (MCIP) is used to prepare meteorology data from the MM5 or WRF for use in the emissions modelling system and the chemical-transport model (CMAQ). All models are currently off-line coupled with one-way transfers of data. On-line coupling version in development.

Model descriptions

MetMs:

Mesoscale Model Version 5 (MM5)

The PSU/NCAR mesoscale model (known as MM5) is a limited-area, nonhydrostatic, terrain-following sigma-coordinate model designed to simulate or predict mesoscale atmospheric circulation. The model is supported by several pre- and post-processing programs, which are referred to collectively as the MM5 modeling system. The MM5 modeling system software is mostly written in Fortran, and has been developed at Penn State and NCAR as a community mesoscale model with contributions from users worldwide. The MM5 modeling system software is freely provided and supported by the Mesoscale Prediction Group in the Mesoscale and Microscale Meteorology Division, NCAR http://www.mmm.ucar.edu/mm5/

Weather Research and Forecast Model- Advanced Research WRF (WRF/arm)

The Weather Research and Forecasting (WRF) Model is a next-generation mesocale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. It features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility. WRF is suitable for a broad spectrum of applications across scales ranging from meters to thousands of kilometers. The effort to develop WRF has been a collaborative partnership, principally among the National Center for Atmospheric Research (NCAR), the National Oceanic and Atmospheric Administration (the National Centers for Environmental Prediction (NCEP) and the Forecast Systems Laboratory (FSL), the Air Force Weather Agency (AFWA), the Naval Research Laboratory, Oklahoma University, and the Federal Aviation Administration (FAA). WRF allows researchers the ability to conduct simulations reflecting either real data or idealized configurations. WRF provides operational forecasting a model that is flexible and efficient computationally, while offering the advances in physics, numerics, and data assimilation contributed by the research community. WRF has a rapidly growing community of users, and workshops and tutorials are held each year at NCAR. WRF is currently in operational use at NOAA/NCEP.

http://wrf-model.org/wrfadmin/docs/arw_v2.pdf

CTMs:

Community Multiscale Air Quality (CMAQ) Model:

The U.S. EPA developed the Models-3 Community Multiscale Air Quality (CMAQ) system to apply a “one atmosphere” multiscale and multi-pollutant modeling approach based mainly on the “first principles” description of the atmosphere. The multiscale capability is supported by the governing diffusion equation in a generalized coordinate system that handles many map projections and vertical coordinate systems, a scheme that maintains dynamic consistency with the upstream (i.e., off-line) meteorology model, a nesting approach, and a sub-grid plume-in-grid modeling technique. The multi-pollutant (i.e., tropospheric ozone, acid deposition, particulates, air toxics, mercury, nitrogen loading, and visibility) capability is provided by the generalized chemistry mechanism description, general numerical solver, and comprehensive description of gaseous and aqueous chemistry and modal aerosol dynamics. The CMAQ numerical grid model uses the MM5 or WRF meteorological models and the SMOKE emissions model as upstream driver models.

The CMAQ modeling system was designed to have a flexible community modeling structure based on modular components. The CMAQ chemical transport model includes the following process modules:

Horizontal advection
Vertical advection
Mass conservation adjustments for advection processes
Horizontal diffusion
Vertical diffusion
Gas-phase chemical reaction solver

Aqueous-phase reactions and cloud mixing
Aerosol dynamics and size distributions
Plume chemistry effects
Aerosol deposition velocity estimation
Photolytic rate computation
Process analysis

www.cmaq-model.org

Off-line models / On-line models:

The above mentioned models are currently all coupled off-line.

Interface modules:

The CMAQ consists of six interface processors:
Meteorology-chemistry interface processor (MCIP)
Photolysis rate processor (JPROC)
Initial conditions processor (ICON)
Boundary conditions processor (BCON)

Downscaling/nesting:

One-way nesting is available for the CMAQ model. One- or two-way nesting is implemented in the MM5 and WRF/arw models, although when used with CMAQ applications, only the one-way nested mode is used. .

Data assimilation/initialisation:

For data assimilation a Newtonian nudging method is used for meteorology. No data assimilation is currently implemented in the CMAQ model

Current applications of the integrated modelling systems

Multiple applications and evaluations of the CMAQ modelling system, from urban to regional to hemispheric scales have been conducted. See, for example, proceedings of the annual CMAQ model conferences: www.cmascenter.org/conference/archive/cfm

Model unification/harmonization/ further developments

A two-way on-line version of the WRF/arw-CMAQ system is under development, consistent with the existing off-line model.

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5 Summary

The objective of this report is to provide an overview of the existing mesoscale modelling systems and capabilities in Europe as presented by their developers or users. Contribution from COST 728 partners were solicited and compiled in this report. In the very many and diverse modelling communities in Europe, nevertheless, the model coverage necessarily remains patchy and model systems in countries not active in COST728, e.g. France, go unmentioned. Still, the contributions represent a wide spectrum of modelling complexity and effort in 16 European countries and 40 institutions including ECMWF. In addition, descriptions of modelling systems developed and used in Canada and USA were included in this report.

The majority of the presented systems are based on mesoscale meteorological models available at the national weather services or in weather forecasting consortia (i.e. HIRLAM, COSMO (Lokalmodell), ALADIN, GEM) and on models developed by university consortia (i.e. MM5, WRF, MC2, RAMS). This approach allows the air quality modelling community to take advantage and benefit from the development, testing, and model validations done for the purpose of weather prediction.

The modelling components that deal with transport and transformation of atmospheric pollutants are much more diverse ranging from a simple passive tracer along a trajectory (i.e. CALPUFF) to a complex treatment of reactive gases in an Earth system (i.e. MESSy).

This survey points out a wide range of model applications with the COST partners:

- diagnostic / climatologic: AQ assessment, episode analysis, source apportionement,
- forecasting: AQ, urban AQ,
- radioactivity (and environment) emergency forecasting.

The overview also shows quite a surprising number of on-line coupled MetM and CTM model systems already being used in Europe (and America):

- BOLCHEM (CNR/ISAC, Bologna, Italy),
- ENVIRO-HIRLAM (DMI, Denmark),
- LM-ART (Inst. for Meteorology and Climatology, FZ Karlsruhe, Germany),
- LM-MUSCAT (IfT Leipzig, Germany),
- MCCM (Inst. of Environmental Atmospheric Research at FZ Karlsruhe, Germany),
- MESSy: ECHAM5 (MPI-C Mainz, Germany),
- MC2-AQ (York Univ, Toronto, University of British Columbia, Canada, and Warsaw University of Technology, Poland),
- GEM/LAM-AQ (York Univ, Toronto, University of British Columbia, Canada, and Warsaw University of Technology, Poland),
- MESSy: ECHAM5-Lokalmodell LM planned at MPI-C Mainz, Univ. of Bonn, Germany,
- WRF-CHem: Weather Research and Forecast and Chemistry Community modelling system (NCAR and many other organisations),
- [Global models GME (German Weather Service) and IFS (ECMWF) with integrated passive ozone tracer.]

However, many of the above mentioned on-line coupled models were not build for the meso-meteorological scale, and they (e.g. GME, ECMWF GEMS, MESSy) are globale-scale modelling systems and first of all for climate change modelling. Becides, at the current stage most of the on-line coupled models do not consider feedback mechanisms or include only direct effects of aerosols on meteorological processes (like COSMO LM-ART and MCCM). Only two meso-scale on-line integrated modelling systems (WRF-Chem and ENVIRO-HIRLAM) consider feedbacks with indirect effects of aerosols.

The results of this report will be used to identify frequent or common weaknesses and problems and will serve to highlight areas of improvement and to formulate recommendations. Other important questions only marginally covered in this overview are the topics of interfaces coupling MetMs and CTMs (their necessity, degree of complexity and kind of additional information provided), and the questions of feedback of CTMs on MetMs which will be treated in subsequent reports of WG2.

It is anticipated that in the course of the COST 728 Action a unified approach to off-line and on-line integrated modelling will be developed. The presented overview of the available modelling systems provides the basis for the development of such an approach. Future activities of the WG2 will use and benefit from the practical expertise of the partners. The unified approach will be developed in the form of recommendations for a common modelling strategy rather than a single modelling system. This will allow for an implementation of the ‘best practice’ approach facilitating model intercomparison and exchange of information.

It is recognized that priorities and expectations of individual users and centres are very diverse as it is shown in the body of this report. However, a common modelling strategy is imperative for the development and implementation of attainable air quality standards in the context of sustainable economic development.

Ultimately, information and expertise compiled by the COST 728 Action will inspire and guide the individual user and institutes to improve their modelling systems and practices. At the same time it will provide an opportunity especially for users without large own development capacities or with the need for a standard system to migrate to a model system supported by the wider community. In addition, the common modelling strategy will facilitate and solidify the development and growth of observing platforms (i.e. satellite instruments and observing networks) that will provide initial chemical conditions for the purpose of air quality or ‘chemical weather’ modelling.

Annex 1: WG2: Integrated systems of MM and CTM: strategy, interfaces, module unification.

The ***overall aim*** of WG2 is identifying requirements and building an European strategy for integrated mesoscale modelling capabilities.

Specific objectives of this WG are:

- identifying requirements for an integrated mesoscale modelling capability/strategy for Europe;
- the development of a guidance and strategy for on-line coupling of MM and CTMs, including requirements for module unification;
- formulation of requirements of meso-scale MMs suitable as input to air pollution models and improved meteorological pre-processors and model interfaces capable to connect meso-scale MM results to CTMs;
- recommended methods for the model down-scaling and nesting, as well as assimilation techniques.

This strategy of integrated modelling and on-line coupling of meso-meteorological and air chemistry/pollution models has a good perspective in future, therefore this Action will help building such a strategy and base for the new generation of integrated 'environment - weather' forecast and assessment mesoscale models.

Historically, air pollution forecasting and numerical weather prediction (NWP) were developed separately. This was plausible in the previous decades when the resolution of NWP models was too poor for meso-scale air pollution forecasting. Due to modern NWP models approaching meso- and city-scale resolution and using land-use databases with a fine resolution, this situation is changing nowadays and requires a revision of the conventional conception of meso- and urban-scale air pollution forecasting and correspondingly an integration of MM and CTM. For example, a new Environment Canada conception suggests to switch from the weather forecast to the environment forecast. Some European projects (e.g. FUMAPEX) already work in this direction and have set off on a very promising path. In case of FUMAPEX it is the Urban Air Quality Information and Forecasting Systems (UAQIFS) integrating NWP models to UAP and population exposure models (Baklanov et al., 2002).

As it was mentioned above, activities and investigation requirements are multiple but dispersed in Europe. Thus, a COST Action seems to be the best approach to integrate, streamline and harmonize these national efforts towards a strong leap forward for new breakthroughs beneficial for a wide community of scientists and users. The discussed European joint system strategy does not include compulsory the only model. It could be an open integrated system with fixed architecture (module interface structure) and with a possibility to incorporate different MMs/NWP models and CTMs. Such a model integration should be realized following a joint elaborated specification of module structure for possible easy interface and integration. It can be, e.g., a system similar to the PRISM specification for integrated Earth System Models: http://prism.enes.org/.

All of these involve urban/rural transitions, including recirculations and feedbacks. These locally forced features interact with synoptic scale processes, such as fronts and convection. They are a challenge for both weather predictions and for simulating regional pollution transport. Even more, the interaction of meteorology (e.g. cloud formation) and pollution transport (cloud nuclei, precipitation) is very important in the regional scales, where clouds no longer can be treated as sub-grid-scale and falling rain drops are explicitly simulated. These aspects yield a close coupling between weather forecasting and air quality. Therefore both: off-line and on-line coupling of MMs and CTMs will be considered in WG2.

Additionally, NWP models are not primarily developed for air pollution modelling and their results need to be designed as input to meso-scale air quality models or they have to be integrated into joint modelling system for air quality forecasting and assessments. In fact, any high-resolution CTM run requires preparing its own meteorological fields by using the type of MetM-for-CTM model fed from some true NWP model. Thus, a timely and innovative field of activity would be to assess the interface between METMs and CTMs - the MetM-for-CTM models, and to set the basis for their harmonisation.

WG2 will also review practical aspects of running meso-scale models, e.g., gaining access to meteorological and geophysical data sets, running models, accessibility of model codes and data sets. It will consider methods for the aggregation of episodic results, model down-scaling as well as nesting and assimilation techniques. The activity would also address the formulation of requirements of meso-scale meteorological models suitable as input to air pollution models. This activity should be the main space for interactions and dialogue between the meteorological and air pollution community.

Especially assimilation techniques should receive a dedicated attention, as it has been shown that powerful assimilation techniques may be more critical for achieving accurate forecasts than complex models, at least on the short-range (1-2 days). In this respect, the Action could aim at inspecting requirements for assimilation techniques with a view to proposing development of monitoring networks. Meteorological networks are under a transition phase with many manual stations changed into less numerous automatic stations together with the use of remote sensing, but which are still under development. Chemical networks are still very coarse and their resolution cannot generally cope with high-frequency meteorological processes.

Both CTM and NWP meso-scale models require and are dependent on specific input data that may also influence the final outputs: land-use and topographical data, parameters coupled with land-use (e.g., albedo) and emission data. The Action should assess existing datasets and methods in order to propose recommendations for the basic characteristics required for these models as to these ancillary datasets with respect to spatial and temporal resolution, classes split, etc. Especially the use of remote sensing (e.g., through GMES activity) should be tested.

The following ***activities*** are planned in WG2 to achieve the WG2 objectives:

- Overview of existing integrated (off-line and on-line) systems in Europe and outside Europe.

- Discussion of the advantages and disadvantages of different ways of the integration of MM and CTM.
- Development of a guidance and strategy for on-line coupling of MM and CTMs
- Overview of existing module structures of MMs & CTMs, and recommendations and requirements for module unification.
- Formulation of requirements of meso-scale MMs suitable as input to air pollution models and improved meteorological pre-processors and model interfaces capable to connect meso-scale MM results to UAP models.
- Recommended methods for the model down-scaling and nesting, as well as assimilation techniques.
- Identifying requirements for an integrated mesoscale modelling capability/strategy for Europe.

Deliverables:

1. Overview of existing integrated (off-line and on-line) mesoscale systems (Year 1).
2. Overview of existing module structures of MMs & CTMs, recommendations and requirements for module unification (Years 2 and 4).
3. Requirements of meso-scale MMs suitable as input to CTMs, assessed meteorological pre-processors and model interfaces between MMs and CTMs (Year 3).
4. Recommended methods for the model down-scaling and nesting, as well as assimilation techniques (Year 4).
5. Requirements for an integrated mesoscale modelling capability/strategy for Europe (Year 5).

Wider Benefits:

The Action will provide an independent, authoritative forum for the discussion of a joint European strategy for an integrated mesoscale modelling capability. The Action will also help building such a strategy and base for the new generation of integrated 'environment - weather' forecast and assessment mesoscale models. Improvement of meteorological pre-processors and construction of model interfaces capable to connect NWP model results and measurement data to AP models input needs leading to an improved capability to forecast and assess air pollution episodes.

Inputs to the Activity:

Inputs to the activity will be the information on CTM, MM, NWP models, used and developed in different countries, their experience of model integration, as well as existing module interface structures. As to data requirements, it would include meteorological data and chemical data.

Range of activities:

For achieving the objectives of WG2 about two work group meeting will take place every year, including two open workshops during the years 3 and 5. Much of the compilation work will be done using open literature, internet, e-mail and questionnaires in close cooperation with EC and national projects.

Dissemination:

The results of the Action will be disseminated through the usual methods for scientific research. These will include a web site, COST reports (years 1, 3 and 5), conference and peer reviewed publications. For the dissemination work existing European networks and bodies (e.g., EUROMET, EEA, EURASAP, CLEAR cluster, ACSENT) will be used.

References

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Annex 2: Tables with detailed information on model qualities based on the COST728 model inventory

Table A2.1:
Self-nesting of MetMs and data supply (only selected models)

Model name	One way	Two way	Online	Offline	Data exchange by	Time step for data exchange
ARPS	●			●	file	1 hour
ENVIRO-HIRLAM	●		●		array	1 hour or every time step
FVM	●				array	
GME					array	
GRAMM	●				array	10 time steps of the larger model
Hirlam	●			●	file	6h
LME	●	●	●	●	file	1 hour
LME_MH	●			●	array	1 hour
MC2	●		●		array	Depends on resolution, in most of application every 1 hour
MEMO	●			●	array	
METRAS	●			●	file	According to the resolution, in typical applications once per hour
MM5 (UoA-GR)	●	●	●	●	file	runs three timesteps for each parent step before feeding back information to the parent domain
MM5 (UoA-PT)	●	●	●	●	file	runs three timesteps for each parent step before feeding back information to the parent domain
MM5 (UoH-UK)	●	●	●	●	array	every time step
NHHIRLAM	●				file	6h
RAMS		●	●		array	each model domain corresponding time step
SAIMM					array	
TAMOS					array	
UM	●			●	file	Fully flexible. Usually 5-15 min at 1km, 1-3h at 12 km.

Table A2.2:

Input Data for CTMs (selected CTMs)

Model name	Orography	Land use	Meteorology
ADMS-Urban	(x,y,z) terrain data	Surface roughness	Flexible; can use minimum standard met observations. Hourly values.
AERMOD	(x,y,z) terrain data	surface roughness	hourly values of surface meteorological observations and daily values (night) of vertical profiles
CALGRID	Orography height for each grid location	None -used by CALMET meteorological preprocessor	Hourly 3D wind gridded fields of wind components, air temperature and liquid water content. Hourly 2D fields of mixing height, Monin-Obukhov lenght (L), PGT class, friction velocity (u*), convective scale velocity (w*).
CMAQ		Optional used to diagnose missing PBL parameters and deposit velocity	2D and 3D time dependent variables and 2D and 3D time independent variables calculated from MM5
EPISODE	Yes	Yes	Temperature (stability) and wind measurements in at least one meteorological mast is the minimal amount of meteorological data which must be provided. Gridded wind fields are usually calculated separately, by using a wind field model which takes into effect the influences of the topography on the wind field depending on stability. Other meteorological parameters such as cloud cover, relative humidity and precipitation may also be given as input data, usually based on measurements. Hourly gridded values of turbulence (sigma-v and sigma-w) and mixing height are calculated using a separate boundary layer meteorological preprocessor. This preprocessor also calculates other parameters used by the model, such as the Monin-Obukhov length, the friction velocity, the Lagrangian time scales and the mixing height. Alternatively, some or all of these meteorological data may also be calculated externally by using other meteorological model systems, and input to the model via data files.
FLEXPART		ECMWF, ALADIN	ECMWF, ALADIN in Gridded Binary (GRIB) format
FVM	Yes	Yes	Geostrophic wind and vertical atmospheric stability, boundaries for wind, potential temperature, density, turbulent quantities, moisture
GRAMM	Gauß –Krueger Coordinates	CORINE	Interpolated field measurements
LOTOS-EUROS	from meteo	PELINDA and CORINE/SMIATEK	TRAMPER(Tropospheric Realtime applied meteorological procedures for Environmental Research)
LPDM	LME and GME parameters used	LME and GME parameters used	all meteorological input data are direct output fields of the operational NWP models LME or GME.
MECTM	GLOBEFILE (1 km resolution); higher resolution if available	Smiatek data (based on CORINE data set and satellite images)	results of METRAS
SILAM	from the meteo files	own compilation	ECMWF - operational and ERA-40 HIRLAM any other GRIB-formatted meteo input data
TAMOS	as in ECMWF and	as in ECMWF and	all meteorological input data are output fields of the

Table A2.3:
Nesting for chemistry & transport (selected models)

Model name	One Way	Two Way	Other	Variables nested	Nesting online	Nesting offline	Data exchange by	Time step for data exchange	Method
ENVIRO-HIRLAM		●			●		Array	Each	
FVM							Array		
GEM/LAM-AQ							Array		
GRAMM							Array		
MC2-AQ							Array		
MEMO (UoT-GR)							Array		
MERCURE							Array		
TAMOS							Array		
TCAM	●					●			

Table A2.4:
Coupling of MetMs to CTMs (selected models as in chapter 4)

MetM	CTM	user	Interface	Application
LM, GME	LPDM	DWD, Germany	None needed, direct use of NWP model out	Radioactivity emergency, CTBTO backtracking
LM-ART	LM-ART (on-line)	Inst. for Met. And Climate Research of Karlsruhe Research Centre (FK), Germany	-	contribution of transport and chemistry on air pollution on different scales, effective fluxes of primary and secondary pollutants incl. pollen grains into the free troposphere
LM-MUSCAT	LM-MUSCAT	Inst. For Tropospheric Research,(IfT)., Leipzig, Germany	-interface for program flow organisation	EC directives,AQ and reduction scenarios, CityDelta, Saharan dust transport
ECHAM5 In MESSy Modular Earth Submodel System	Modular Earth Submodel System (incl. LM with chemistry (planned).)	Max-Planck_Inst. (MPI) for Chemistry And Univ. Mainz, Mainz, Germany	-	
GME,ECMWF,TRAMPER, MM5, LM, Aladin	RCG (REM-CALGRID)	Free Univ. Of Berlin, Berlin, Germany	TRAMPER	EC directive modelling, PM10, PM2.5, ozone, NO2
ENVIRO-HIRLAM (on- and off-line) DMI-HIRLAM-Tracer	ACTM	DMI, Copenhagen, DK		
MM5	UAM-V	National and Kapodistrian Univ. Of Athens, Greece	Interfacing problems Recognised and discussed	Photochemistry
UM	NAME III	UK MetOffice		Radioact. And environment

				emergency response, AQ, source detection and attribution
UM	STOCHEM	UK MetOffice	None needed ?	Global atm. Chem.. model
UM ?	ADMS-Urban	Many companies	?	Environm. impact assessm., emergency response
METRAS	METCM	Univ. of Hamburg, Germany	not needed due to same grid. In M-SYS several grids are used and interface modules are available	Maps on air pollution and quality in different scale, urban and coastal pollution studies
MM5 (UoA-PT)	MEMO(UoA-PT)	Univ. of Aveiro, Portugal	Not needed except for MM5/MARS	Long-term AQ, AQ forecasts, urban AQ studies
MM5 (UoH-UK)	CMAQ	Univ. of Hertfordshire, UK		AQ scenarios
MM5, MEMO, WRF	CHIMERE,CAMx,CMAQ	Univ. of Madrid, Spain	Interfaces needed, built adhoc	Impact studies and AQ modelling for industrial emissions, ozone prediction
MM5 , aLMo (Swiss LM)	CAMx	PSI and EPFL, Switzerland	Improved interface development for turbulence	AQ, source apportionment
aLMo (Swiss LM) downscaled	LPDM (of DWD)	MeteoSwiss and EMPA, Switzerland	Improved interface development for downscaled dispersion parameterisations	Radioactive and passive tracers
aLMo (Swiss LM	POLYTOX (multibox model)	SEDE and EPFL, Switzerland	Improved interface for very high resolution (100m)	Primary and secondary pollutants
RAMS, MINERVE, LAPS	SPRAY3, FARM	Arianet	GAP and	Industrial and

		Milano, Italy	SURFPRO	urban AQ,industrial emission contral and AQ forecasting, AQ assessment in N. Italy.
RAMS, CALMET, MM5	TCAM, CALGRID	Univ. of Brescia, Italy	PROMETEO	Episode and long-term gas simulation, control strategies for Lombardia region and CityDelta for ozone and PM10, source-receptor modelling
LAMI (Italian LM)	FARM	Arianet, Milano, Italy	GAP and SURFPRO	AQ forecasts for Torino and Novara
LAMI (Italian LM)	CHIMERE	ARPA-SIM, Bologna, Italy	Dedicated interface	UA forecasting for Bologna And region
BOLCHEM	BOLCHEM (on-line)	CNR/ISAC Bologna, Italy	?	?
HIRLAM NH-HIRLAM, ECMWF	SILAM, IairViro, ARGOS	Univ. of Tartu, Estonian Met. Hydrol. Service, Eston. Environm. Research Centre, Estonia		Emergency response, AQ Modelling
HIRLAM , ECMWF, MESAN and others	MATCH	SMHI, Sweden	Interfaces contained in MATCH	Regional studies, emergency preparedness, tropos chem., ground ozone, ind. pollut., AQ (Estonia)
ALADIN,CALMET	CALPUFF	IMGW, Krakow, Poland	Interface ALADIN-CALMET for format conversion	Regional AQ assessment and management
ALADIN	FLEXPART CAMx	ZAMG, Vienna, Austria	Dedicated interface using	Radioactivity emergency

			methods from literature, the MM5 CAMx pre-processor or the CTM CHIMERE	Ozone forecasting
MC2-AQ	MC2-AQ (on-line)	Warsaw University of Technology, Poland	-	Photochemical episodes – from regional to urban scale
GEM/LAM-AQ	GEM-LAM-AQ (on-line)	York University, Toronto, Canada, Enivronment Canada Warsaw University of Technology, Poland	-	Multiscale tropospheric chemistry modelling
HIRLAM,ECMWF,MM5, MESAN	MATCH	Swedish Met. And Hydrol. Inst., Stockholm	Specific interfaces to MetMs built into MATCH	Policy support, e.g. air pollution also in Estonia, nuclear emergency response, tropos. Chemistry, ground ozone, uslfur depos. In Asia and SAfrica, Chile.
MM5, CFD MIMO	CMAQ, CAMx CHIMERE	Technical University of Madrid, Spain		Sens. And AQ assessment studies incl. dioxins and furans, operational system to provide boundary cond. For regional chem.. modelling in Spain, very-high resolution emission dat with CFD

				MIMO emission modelling incl. inverse simulations, industrial AQ forecasts for Madrid surroundings.
ARPS	AURORA	VITO, Belgium	none needed, direct use of ARPS output (same grid)	urban- to regional-scale AQ assessment and forecast