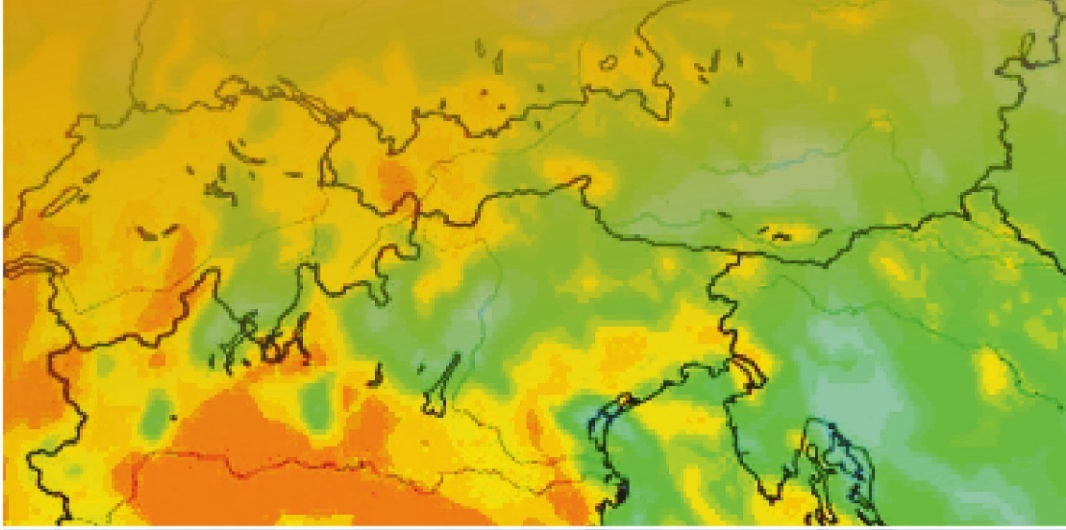

Alexander Baklanov · Alexander Mahura
Ranjeet S. Sokhi *Editors*

Integrated Systems of Meso-Meteorological and Chemical Transport Models

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Preface

Weather natural hazards, the environment and climate change are of concern to all of us. Especially, it is essential to understand how human activities might impact the nature. Hence, monitoring, research, and forecasting is of the outmost importance. Furthermore, climate change and pollution of the environment do not obey national borders; so, international collaboration on these issues is indeed extremely important.

In the future, the increasing computer power and understanding of physical processes pave the way for developing integrated models of the Earth system and gives a possibility to include interactions between atmosphere, environment, climate, ocean, cryosphere and ecosystems.

Therefore, development of integrated Numerical Weather Prediction (NWP) and Atmospheric Chemical Transport (ACT) models is an important step in this strategic direction and it is a promising way for future atmospheric simulation systems leading to a new generation of models. The EC COST Action 728 "Enhancing Mesoscale Meteorological Modelling Capabilities for Air Pollution and Dispersion Applications" (2004–2009) is aimed at identifying the requirements and propose recommendations for the European strategy for integrated mesoscale NWP-ACT modelling capability.

DMI strongly supports this development. Almost 10 years ago DMI initiated developing an on-line integrated NWP-ACT modelling system, now called Enviro-HIRLAM (Environment – HIgh Resolution Limited Area Model), which includes two-way interactions between meteorology and air pollution for NWP applications and chemical weather forecasting. Recently we also initiated organisation of the Chemical branch in the HIRLAM international consortium (http://hirlam.org), where this model is considered as the baseline model. The Enviro-HIRLAM became an international community model starting January 2009 with several external European organisations joining the research and development team (e.g., from the University of Copenhagen, Denmark; University of Tartu, Estonia; University of Vilnius, Lithuania; Russian State Hydro-Meteorological University; Tomsk State University, Russia; Odessa State Environmental University, Ukraine) with new coming participants.

During 2002–2005, DMI led EC FP5 project FUMAPEX (http://fumapex.dmi.dk), which developed a new generation Integrated Urban Air Quality Information and Forecasting System and implemented such a system in six European cities.

The new EC FP7 project MEGAPOLI (2008–2011) (http://megapoli.info), coordinated by DMI, is also focusing on further developments of integrated systems and studies of interactions between atmospheric pollution from mega cities and meteorological and climatic processes.

These remarks show the importance to organise a workshop to share and analyse international experience in integrated modelling worldwide. The first workshop on "Integration of meteorological and chemical transport models" (http://netfam.fmi.fi/Integ07) was arranged at DMI (Copenhagen, Denmark) on 21–23 May 2007. The workshop was organised in the framework of the COST Action 728 and in cooperation with the Nordic Network on Fine-scale Atmospheric Modelling. Almost 50 participants, including invited experts in integrated modelling and young scientists, from 20 countries attended this event to discuss the experience and further perspectives of coupling air quality and meteorology in fine-scale models. The workshop was aimed at joining both NWP and air quality modellers to discuss and make recommendations on the best practice and strategy for further developments and applications of integrated and coupled modelling systems "NWP and Meso-Meteorology – Atmospheric Chemical Transport". Main emphasis was on fine-resolution models applied for local chemical weather forecasting and considering feedback mechanisms between meteorological and atmospheric pollution (e.g. aerosols) processes. The following topics were in the focus of presentations and discussions:

- Online and offline coupling of meteorological and air quality models
- Implementation of feedback mechanisms, direct and indirect effects of aerosols
- Advanced interfaces between NWP and ACT models
- Model validation studies, including air quality-related episode cases

As a follow-up a young scientist summer school and workshop on "Integrated Modelling of Meteorological and Chemical Transport Processes / Impact of Chemical Weather on Numerical Weather Prediction and Climate Modelling" was organised by DMI and Russian State Hydrometeorological University during 7–15 July 2008 in Russia.

This book, written mostly by invited lectors/speakers of the Copenhagen workshop, is focused on above mentioned workshop topics, summarizes presentations, discussions, conclusions, and provides recommendations. The book is one of the first attempts to give an overall look on such integrated modelling approach. It reviews the current situation with the on-line and off-line coupling of mesoscale meteorological and air quality models around the world (in European countries, USA, Canada, Japan, Australia, etc.) as well as discusses advantages and disadvantages, best practice, and gives recommendations for on-line and off-line coupling of NWP and ACT models, implementation strategy for different feedback mechanisms, direct and indirect effects of aerosols and advanced interfaces between both types of models.

It is my hope that this book will be useful for first of all to those interested in the modelling of meteorology and air pollution, but also for the entire meteorology and atmospheric environment communities, including students, researchers and practical users.

Copenhagen, Denmark DMI Director General, Peter Aakjær

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Chapter 1
Introduction – Integrated Systems: On-line and Off-line Coupling of Meteorological and Air Quality Models, Advantages and Disadvantages

Alexander Baklanov

1.1 Introduction

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 (due to advances in computing power) and the use of 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 meso-scale meteorological models (MetMs) and atmospheric chemical transport models (ACTMs). For example, a new Environment Canada conception suggests to switch from weather forecasting to environment forecasting. Some European projects (e.g. FUMAPEX, see: fumapex.dmi.dk) already work in this direction and have set off on a promising path. In case of FUMAPEX it is the Urban Air Quality Information and Forecasting Systems (UAQIFS) integrating NWP models, urban air pollution (UAP) and population exposure models (Baklanov et al. 2007b), see Fig. 1.1.

In perspective, integrated NWP-ACTM modelling may be a promising way for future atmospheric simulation systems leading to a new generation of models for improved meteorological, environmental and "chemical weather" forecasting.

Both, off-line and on-line coupling of MetMs and ACTMs are useful in different applications. Thus, a timely and innovative field of activity will be to assess their interfaces, and to establish a 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 requirements of meso-scale meteorological models suitable as input to air pollution models.

The COST728 Action (http://www.cost728.org) addressed key issues concerning the development of meso-scale modelling capabilities for air pollution

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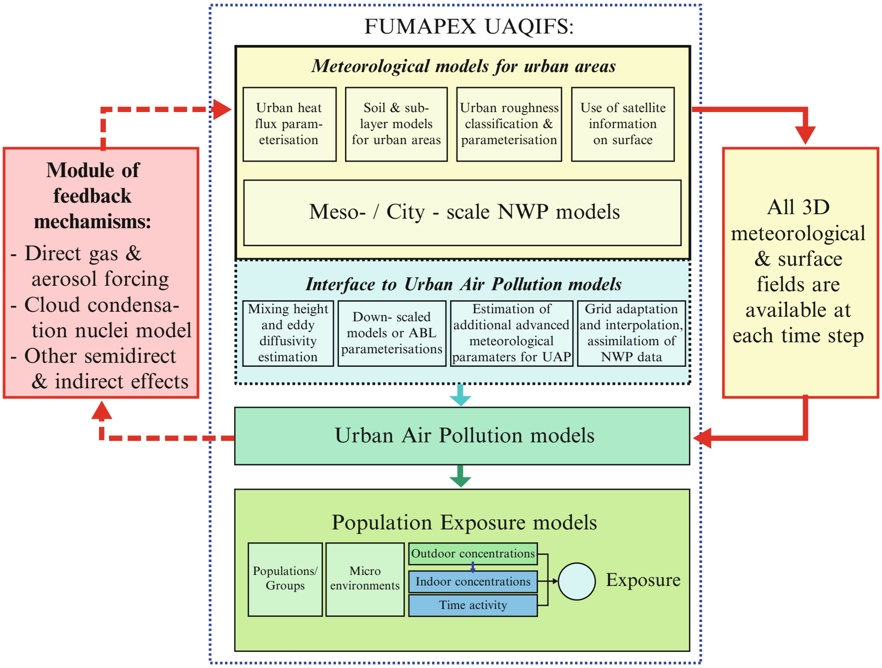

Fig. 1.1 Extended FUMAPEX scheme of Urban Air Quality Information & Forecasting System (UAQIFS) including feedbacks. Improvements of meteorological forecasts (NWP) in urban areas, interfaces and integration with UAP and population exposure models following the off-line or on-line integration (Baklanov 2005; after EMS-FUMAPEX 2005)

and dispersion applications and, in particular, it encouraged the advancement of science in terms of integration methodologies and strategies in Europe. The final integration strategy will not be focused around any particular model; instead it will be possible to consider an open integrated system with fixed architecture (module interface structure) and with a possibility of incorporating different MetMs/NWP models and ACTMs. Such a strategy may only be realised through jointly agreed specifications of module structure for easy-to-use interfacing and integration.

The overall aim of working group 2 (WG2) of the COST 728 Action, “Integrated systems of MetM and ACTM: strategy, interfaces and module unification”, is to identify the requirements for the unification of MetM and ACTM modules and to propose recommendations for a European strategy for integrated meso-scale modelling capabilities. The first report of WG2 (Baklanov et al. 2007a) compiles existing state-of-the-art methodologies, approaches, models and practices for building integrated (off-line and on-line) meso-scale systems in different, mainly European, countries. The report also includes an overview and a summary of existing integrated models and their characteristics as they are presently used. The model contributions were compiled using COST member contributions, each focusing on national model systems.

1.2 Methodology for Model Integration

The modern strategy for integrating MetMs and ACTMs is suggested to incorporate air quality modelling as a combination of (at least) the following factors: air pollution, regional/urban climate/meteorological conditions and population exposure. This combination is reasonable due to the following facts: meteorology is the main source of uncertainty in air pollution and emergency preparedness models, meteorological and pollution components have complex and combined effects on human health (e.g., hot spots in Paris, July 2003), pollutants, especially aerosols, influence climate forcing and meteorological events (such as, precipitation and thunderstorms).

In this context, several levels of MetM and ACTM coupling/integration can be considered:

Off-Line

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

On-Line

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

The main advantages of the On-line coupled modelling approach comprise:

- Only one grid is employed and no interpolation in space is required
- There is no time interpolation
- Physical parametrizations and numerical schemes (e.g. for advection) are the same; No inconsistencies
- All 3D meteorological variables are available at the right time (each time step)
- There is no restriction in variability of meteorological fields
- Possibility exists to consider feedback mechanisms, e.g. aerosol forcing
- There is no need for meteo- pre/post-processors.

However, the on-line approach is not always the best way of the model integration. For some specific tasks (e.g., for emergency preparedness, when NWP data are available) the off-line coupling is more efficient way.

The main advantages of Off-line models comprise:

- There is the possibility of independent parametrizations
- They are more suitable for ensembles activities
- They are easier to use for the inverse modelling and adjoint problem
- There is the independence of atmospheric pollution model runs on meteorological model computations
- There is more flexible grid construction and generation for ACTMs
- This approach is suitable for emission scenarios analysis and air quality management.

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 ACTMs at each time step and the consideration of two-way feedbacks between air pollution (e.g. urban aerosols), meteorological processes and climate forcing. These integration methodologies have been demonstrated by several of the COST action partners such as the Danish Meteorological Institute, with the DMI-ENVIRO-HIRLAM model (Chenevez et al. 2004; Baklanov et al. 2004, 2008; Korsholm et al. 2007) and the COSMO consortium with the Lokal Modell (Vogel et al. 2006; Wolke et al. 2003).

These model developments will lead to a new generation of integrated models for: climate change modelling, weather forecasting (e.g., in urban areas, severe weather events, etc.), air quality, long-term assessments of chemical composition and chemical weather forecasting (an activity of increasing importance which is supported by a new COST action ES0602 started in 2007).

1.3 Overview of European On-Line Integrated Models

The experience from other European, as well as non-European union communities, will need to be integrated. On our knowledge on-line coupling was first employed at the Novosibirsk scientific school (Marchuk 1982; Penenko and Aloyan 1985; Baklanov 1988), for modelling active artificial/anthropogenic impacts on atmospheric processes. Currently American, Canadian and Japanese institutions develop and use on-line coupled models operationally for air quality forecasting and for research (GATOR-MMTD: Jacobson, 2005, 2006; WRF-Chem: Grell et al. 2005; GEM-AQ: Kaminski et al. 2005).

Such activities in Europe are widely dispersed and 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.

Such a 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 et al. 2006).

Community Earth System Models (COSMOS) is a major international project (http://cosmos.enes.org) 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.

The main differences between the COST-728 integrating strategy for meso-scale models and the COSMOS integration strategy regards the spatial and temporal scales. COSMOS is focusing on climate time-scale processes, general (global and regional) atmospheric circulation models and atmosphere, ocean, cryosphere and biosphere integration, while the meso-scale integration strategy will focus on forecast time-scales of 1 to 4 days and omit the cryosphere and the larger temporal and spatial scales in atmosphere, ocean and biosphere.

The COST728 model overview (Baklanov et al. 2007a) shows a surprisingly large (at least ten) number of on-line coupled MetM and ACTM systems already being used in Europe (see also more information in Table 1.1):

- BOLCHEM (CNR ISAC, Italy)
- ENVIRO-HIRLAM (DMI, Denmark)
- LM-ART (Inst. for Meteorology and Climate Research (IMK-TRO), KIT, Germany)
- LM-MUSCAT (IfT Leipzig, Germany)
- MCCM (Inst. for Meteorology and Climate Research (IMK-IFU), KIT, 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)
- WRF-CHem: Weather Research and Forecast and Chemistry Community modelling system (NCAR and many other organisations)
- MESSy: ECHAM5-Lokalmodell LM planned at MPI-C Mainz, Univ. of Bonn, Germany

However, it is necessary to mention, that many of the above on-line models were not build for the meso-meteorological scale, and several of them (GME, MESSy) are global-scale modelling systems, originating from the climate modelling community. Besides, 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 (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.

Table 1.1 On-line coupled MetM – ACTMs (Baklanov et al. 2007a)

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[a]
COSMO LM-MUSCAT[b]	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)[a]
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 step	Yes
ECMWF GEMS modelling	GEMS chemistry		
GME	Progn. stratos passive O3 tracer	Each model time step	
OPANA=MEMO +CBMIV		Each model time step	

[a]Direct effects only
[b]On-line access model

1.4 Feedback Mechanisms, Aerosol Forcing in Meso-meteorological Models

In a general sense air quality and ACTM modelling is a natural part of the climate change and MetM/NWP modelling process. The role of greenhouse gases (such as water vapour, CO_2, O_3 and CH_4) and aerosols in climate change has been highlighted as a key area of future research (Watson et al. 1997; IPCC 2007, 2001; AIRES 2001). Uncertainties in emission projections of gaseous pollutants and aerosols (especially secondary organic components) need to be addressed urgently to advance our understanding of climate forcing (Semazzi 2003). In relation to aerosols, their diverse sources, complex physicochemical characteristics and large spatial gradients make their role in climate forcing particularly challenging to quantify. In addition to primary emissions, secondary particles, such as, nitrates, sulphates and organic compounds, also result from chemical reactions involving precursor gases such as SO_x, DMS, NO_x, volatile organic compounds and oxidising agents including ozone. One consequence of the diverse nature of aerosols is that they exhibit negative (e.g. sulphates) as well as positive (e.g. black carbon) radiative forcing characteristics (IPCC 2007, 2001; Jacobson 2002). Although much effort has been directed towards gaseous species, considerable uncertainties remain in size dependent aerosol compositional data, physical properties as well as processes controlling their transport and transformation, all of which affect the composition of the atmosphere (Penner et al. 1998; Shine 2000; IPCC 2007, 2001). Probably one of the most important sources of uncertainty relates to the indirect effect of aerosols as they also contribute to multiphase and microphysical cloud processes, which are of considerable importance to the global radiative balance (Semazzi 2003).

In addition to better parameterisations of key processes, improvements are required in regional and global scale atmospheric modelling (IPCC 2005; Semazzi 2003). Resolution of regional climate information from atmosphere-ocean general circulation models remains a limiting factor. Vertical profiles of temperature, for example, in climate and air quality models need to be better described. Such limitations hinder the prospect of reliably distinguishing between natural variability (e.g. due to natural forcing agents, solar irradiance and volcanic effects) and human induced changes caused by emissions of greenhouse gases and aerosols over multidecadal timescales (Semazzi 2003). Consequently, the current predictions of the impact of air pollutants on climate, air quality and ecosystems or of extreme events are unreliable (e.g. Watson et al. 1997). Therefore it is very important in the future research to address all the key areas of uncertainties so as provide an improved modelling capability over regional and global scales and an improved integrated assessment methodology for formulating mitigation and adaptation strategies.

In this concern one of the important tasks is to develop a modelling instrument of coupled “Atmospheric chemistry/Aerosol” and “Atmospheric Dynamics/Climate” models for integrated studies, which is able to consider the feedback mechanisms, e.g. aerosol forcing (direct and indirect) on the meteorological processes and climate change (see Fig. 1.2).

Chemical species influencing weather and atmospheric processes include greenhouse gases which warm near-surface air and aerosols such as sea salt, dust, primary and secondary particles of anthropogenic and natural origin. Some aerosol particle components (black carbon, iron, aluminium, polycyclic and nitrated aromatic compounds) warm the air by absorbing solar and thermal-IR radiation, while others (water, sulphate, nitrate, most of organic compounds) cool the air by backscattering incident short-wave radiation to space.

It is necessary to highlight those effects of aerosols and other chemical species on meteorological parameters have many different pathways (such as, direct, indirect and semi-direct effects) and they have to be prioritized and considered in

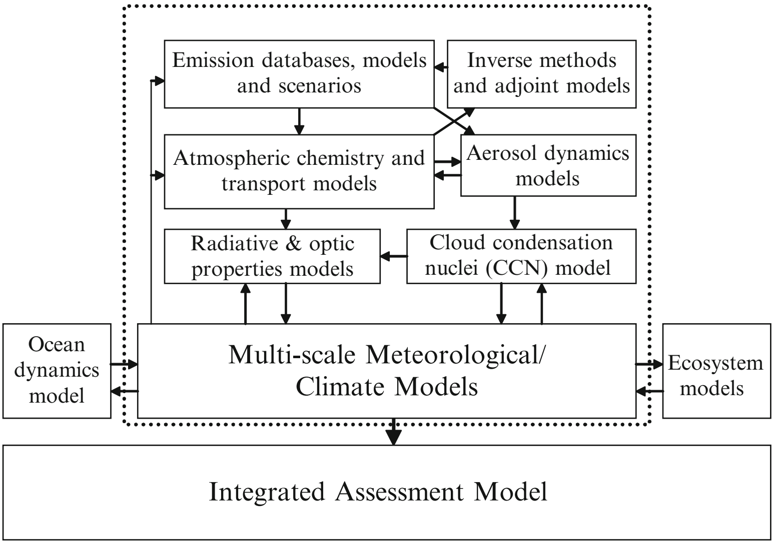

Fig. 1.2 The integrated system structure for studies of the meso-scale meteorology and air pollution, and their interaction

on-line coupled modelling systems. Following Jacobson (2002) the following effects of aerosol particles on meteorology and climate can be distinguished:

- Self-Feedback Effect
- Photochemistry Effect
- Smudge-Pot Effect
- Daytime Stability Effect
- Particle Effect through Surface Albedo
- Particle Effect through Large-Scale Meteorology
- Indirect Effect
- Semi-direct Effect
- BC-Low-Cloud-Positive Feedback Loop

Sensitivity studies are needed to understand the relative importance of different feedback mechanisms. Implementation of the feedbacks into integrated models could be realized in different ways with varying complexity. The following variants serve as examples:

One-Way Integration (Off-Line)

- The chemical composition fields from ACTMs may be used as a driver for Regional/Global Climate Models, including aerosol forcing on meteorological processes. This strategy could also be realized for NWP or MetMs.