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# Operational, regional-scale, chemical weather forecasting models in Europe

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Received: 17 January 2011 – Accepted: 22 January 2011 – Published: 21 February 2011

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## Abstract

Numerical models that combine weather forecasting and atmospheric chemistry are here referred to as chemical weather forecasting models. Eighteen operational chemical weather forecasting models on regional and continental scales in Europe are described and compared in this article. Topics discussed in this article include how weather forecasting and atmospheric chemistry models are integrated into chemical weather forecasting systems, how physical processes are incorporated into the models through parameterization schemes, how the model architecture affect the predicted variables, and how air chemistry and aerosol processes are formulated. In addition, we discuss sensitivity analysis and evaluation of the models, user operational requirements, such as model availability and documentation, and output availability and dissemination. In this manner, this article allows for the evaluation of the relative strengths and weaknesses of the various modelling systems and modelling approaches. Finally, this article highlights the most prominent gaps of knowledge for chemical weather forecasting models and suggests potential priorities for future research directions, for the following selected focus areas: emission inventories, the integration of numerical weather prediction and atmospheric chemical transport models, boundary conditions and nesting of models, data assimilation of the various chemical species, improved understanding and parameterization of physical processes, better evaluation of models against data and the construction of model ensembles.

## 1 Introduction

Chemical weather is defined here as the short-term (less than two weeks) variability of the atmospheric chemical composition. This definition is complementary to the traditional meteorological definition of weather, which is commonly characterized only by physical variables (e.g., temperature, wind, mass, radiation, humidity). Methods that include a combination of weather forecasting and atmospheric chemistry simulations are

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here referred to as chemical weather forecasting (CWF). CWF can therefore be seen as a specific category of air-quality forecasting, where air-quality forecasting models using numerical weather prediction (NWP) models are CWF models, but air-quality forecasting models using statistical methods are not (Kukkonen et al., 2009c). Similarly, for accuracy and consistency in replacing the traditional term *air-quality forecasting and information system*, we introduce a new term *chemical weather forecasting and information system* (CWFIS) to represent the integrated system responsible for the prediction and dissemination of chemical weather forecasts.

Sometimes the term biological weather forecasting is used to refer to forecasting of biological constituents in the air, such as various pollen species and airborne allergens. This paper does not specifically address biological weather forecasting, although some of the considered models include treatments for airborne pollen species.

Lawrence et al. (2005) have previously reviewed the then-current state of CWF and emerging research challenges. Baklanov et al. (2008a, 2010) and Schluenzen and Sokhi (2008) summarized existing mesoscale modeling systems and capabilities as an initial step to formulate recommendations for a unified integrated framework for modeling systems, although they did not compare the mathematical architecture of the various modeling systems. Baklanov (2010) also presented some gaps in our current understanding and recommended directions of future research for integrated CWF systems, although a valuable addition would be a more comprehensive set of recommendations summarizing the most urgent gaps of knowledge and research needs.

There are currently tens, possibly more than a hundred, of CWFIS's on a local, regional and continental scale in Europe and worldwide. Although abundant literature exists on the properties of individual models, scientific articles presenting compilations or synthesis of this information are scarce. Furthermore, the evaluation of models against data – defined here as the detailed analysis and evaluation of the mathematical structure of such models or modelling systems in terms of the underlying physics and chemistry – are more limited. No scientific evaluations have been presented of a larger number of CWF models. Despite a plethora of modelling options, it is far from obvious,

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which are the optimal ones in most cases. Thus, a systematic review of these options could substantially assist in evaluating the strengths and weaknesses of the various methods, and thus contribute to the development of better and more robust modelling methods in the future. Consequently, this present article aims to bring the field up to date with the most comprehensive summary and assessment of the state of CWF.

## 1.1 European-wide projects on chemical weather modeling

This study is part of the European Cooperation in Science and Technology (COST) ES0602 action, which provides a forum for benchmarking approaches and practices in data exchange and multi-model capabilities for CWF and near real-time (NRT) information services in Europe (<http://www.chemicalweather.eu>). The action was initiated by the Network of European Meteorological services (EUMETNET, <http://www.eumetnet.eu>) and the European Environment Agency (EEA). The content of this COST action, its main objectives and organisation have been reviewed by Kukkonen et al. (2009a,b), and the main results by Kukkonen et al. (2009c). The COST action includes participants from 20 countries, and its duration is from 2007 to 2011.

The COST ES0602 action has constructed a European open-access CWF portal (ECWFP) that includes access to a substantial number (more than 20) of available chemical weather forecasting systems and their numerical forecasts; these cover in total 31 areas in Europe (Balk et al., 2010; <http://www.chemicalweather.eu/Domains>). This portal can be used to find out, which CWF services are available for a specific domain, for specific source categories or for specific pollutants. Such a single point of reference for European CWF information has not previously been operational. The Action has also investigated and reviewed existing chemical weather information systems and services (e.g., Karatzas and Kukkonen, 2009). This study has also been part of the EU-funded projects MEGAPOLI, Megacities: Emissions, urban, regional and Global Atmospheric POLLution and climate effects, and Integrated tools for assessment and mitigation (<http://www.megapoli.info>) and TRANSPHORM, Transport related Air Pollution and Health impacts – Integrated Methodologies for Assessing Particulate

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Matter (<http://www.transphorm.eu/>).

There are several prominent ongoing European projects that address CWF. Some of the most important operational CWF programs lie within the EU-ESA (European Space Agency) programme GMES (Global Monitoring for Environment and Security, <http://www.gmes.info>), viz. the GEMS (Global and regional Earth-system (Atmosphere) Monitoring using Satellite and in-situ data, <http://gems.ecmwf.int>) and PROMOTE (PROtocol MONiTORing for the GMES Service Element, <http://www.gse-promote.org>; Poupkou et al., 2006) projects. The GMES Atmospheric Services focus on operational monitoring and forecasting of atmospheric composition, dynamics and thermodynamics through advanced exploitation of satellite and in-situ data, on a European, national and local level.

There are also other related EU-funded projects, such as CITYZEN (megaCITY – Zoom for the Environment, <https://wiki.met.no/cityzen>), EUCAARI (The European Integrated project on Aerosol Cloud Climate and Air Quality Interactions, <http://www.atm.helsinki.fi/eucaari>) and EUSAAR (European Supersites for Atmospheric Aerosol Research, <http://www.eusaar.net>). Within the GEMS project, analyses and 72 h forecasts have been presented using 12 state-of-the-art regional air-quality models on a quasi-operational daily basis (<http://gems.ecmwf.int>). The models rely on the operational meteorological forecasts of the European Centre for Medium-Range Weather Forecasts (ECMWF), as well as on GEMS global chemical weather data. They all consider the same high-resolution (5 km horizontal grid spacing) anthropogenic and biogenic emissions inventories.

An example of a small-scale network of a few operational air-quality services has been constructed within the first and second stages of the PROMOTE project. Although GEMS and PROMOTE CWF services have constituted major advances in this field – and are evidently valuable for a range of stakeholders – a limitation is that these projects have had a closed membership and have been fairly oriented around development. There is a need to involve additional stakeholders in a more comprehensive way, such as the national environmental agencies. This is also the task of the continuation

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projects of GEMS and PROMOTE, the MACC and PASODOBLE projects.

Another relevant program is Global Earth Observation and Monitoring (GEOmon, [www.geomon.eu](http://www.geomon.eu)), the goal of which is to build an integrated European ground-based observational network of atmospheric composition to complement satellite observations. It lays the foundation for a European contribution to GEOSS (Global Earth Observation System of Systems, <http://www.epa.gov/geoss>) and optimizes the European strategy of monitoring atmospheric composition measurements (Tørseth and Vik, 2009).

## 1.2 Aims and scope of this study

Given the huge variety of existing modelling systems and options, we must limit the scope of this article. Specifically, we select 18 operational CWF models on regional and continental scales (distance scales of approximately 10–6000 km) in Europe for more detailed analysis. These models are among the most widely used in Western European countries, as well as in Eastern and Central-Eastern European countries. However, this collection of models is by no means exhaustive. Moreover, some of these models have been mainly developed elsewhere, especially in the United States.

This paper has three main aims. (i) The first aim is to gather information on the selected operational CWF models in a systematic and harmonized format. (ii) The second aim is to evaluate preliminarily and to provide information that makes it possible for the readers to evaluate the relative strengths and limitations of the various models, and the components of the modeling systems. However, it is not the goal of this study to rank the models, or advocate one model over another. (iii) The third aim is to highlight the most prominent gaps of knowledge in CWF and to suggest priorities for future research directions.

We do not address purely diagnostic models, which do not include forecasting capabilities. The emergency preparedness models (such as those developed in case of nuclear and chemical accidents) are also outside the scope of this study. Because this article focuses on regional-scale models, we do not address modelling on global or

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urban scales. This study also addresses only operational CWF models. In comparison with genuine research models, and versions of operational models that are used only for research purposes, such operational models can include simplifications, such as a reduced resolution, smaller domains, and less sophisticated physics and chemistry modules. This article does not contain any new numerical intercomparisons of model predictions, or any novel evaluation of model predictions with data.

### 1.3 Organization of this article

This article is organized in the following manner. Section 2 introduces the 18 different CWF models and overviews some of the relevant physical processes. Section 3 discusses the numerical weather prediction components of the models. Section 4 discusses the processes in the atmospheric dispersion and chemistry modelling components. Section 5 discusses the evaluation of the models. Section 6 discusses user operations of the model, including availability, computer requirements, documentation, user interfaces, sensitivity analyses, and dissemination. Section 7 looks forward to discuss emerging issues in the CWF community, including the identification of major gaps of knowledge and future research needs. Finally, Sect. 8 concludes this article.

The main characteristics of the selected 18 CWF models considered in this study have been summarised and inter-compared in several tables. Overviews of the main properties of the CWF and NWP models are first presented in Tables 1 and 2. The atmospheric dispersion, chemistry and aerosol modelling, and deposition components are reviewed in Tables 3–7. The natural emissions, and the grid spacings and coordinate systems are presented in Tables 8 and 9. The evaluation of each CWF model, and the availability, user communities, documentation, and presentation of forecasts in the internet are presented in Tables 10–12. Finally, in relation to future research needs, adjoint (inverse) dispersion modelling is reviewed in Table 13.

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## 2 Introduction to operational chemical weather models

This section addresses some key concepts and introduces the main physical and chemical processes that are relevant for CWF. We have selected 18 operational, regional and continental scale CWF modeling systems for a more detailed examination.

For readability, this section contains an introduction on the selected main properties of those models, before we present a more detailed analysis and inter-comparison of model treatments for specific processes.

### 2.1 Criteria for the selection of the models and the use of information sources

A fairly large number of models were first suggested by the participants of the COST ES0602 action for a more detailed examination; participants from more than 20 European countries (listed in Kukkonen et al., 2009c) were encouraged to volunteer for this activity. Finally, 18 models were selected for inclusion in this article.

The main criteria for the selection of the 18 models were (i) the prominence and wide usage of the models, and (ii) the sufficient availability of scientific literature and Web-based documentation on the relevant model properties. Most of the models addressed in this study are also contained in the Model Documentation System (MDS) of the European Environment Agency (EEA), accessible at <http://air-climate.eionet.europa.eu/databases/MDS/index.html>, and in the joint COST 728 and COST 732 Model Inventory (C728/732MI), accessible at <http://www.cost728.org> (Schluenzen and Sokhi, 2008). We also aimed to present a balanced geographical representation across Europe.

To obtain the most credible and up-to-date information, model properties were derived primarily from published literature and from the developers or users of each model. We also used secondary information sources from the Web, such as the MDS, C728/732MI and the various web pages of individual modelling systems. In some cases, we received conflicting information from these sources. When that has happened, we extracted the information from the published literature whenever available,

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and then contacted the model developers for confirmation.

## 2.2 The integration and coupling of NWP and CWF models

How NWP models couple with CWF models can be realized in one of two principal ways. Grell et al. (2005) and Baklanov et al. (2008a) suggested the following definitions.

*Off-line modelling systems* (also called one-way interactive models) contain a separate chemical transport model (CTM) driven by meteorological input data from meteorological pre-processors, measurements or diagnostic models, is driven by analysed or forecasted meteorological data from NWP archives or datasets, or reads output files from operational NWP models or specific meteorological models at limited time intervals (e.g., 1, 3, 6 h).

*On-line modelling systems* (also called integrated or two-way interactive models) can be on-line access models, when meteorological data are available at each time-step (possibly via a model interface), or on-line integration of a CTM into a NWP model, where two-way feedbacks may be considered. We will use this latter definition for on-line coupled modelling.

The on-line integration of NWP or other meteorological models, with atmospheric aerosol and chemical transport models (CTM) allows all meteorological three-dimensional (3-D) fields in CTM's at each time step to be used. It also facilitates the consideration of air-pollution feedbacks (e.g., those due to aerosols or greenhouse gases) on meteorological processes and climate forcing, and further on the chemical composition. Within the 18 CWF models considered here, only two models (EnviroHIRLAM and WRF-Chem) are realised as on-line integrated models with two-way interactions. Previously, Zhang (2008) has reviewed the history and current status of the development and application of online-coupled meteorology and chemistry models, with a focus on five representative models developed in the US including GATOR-GCMOM, WRF/Chem, CAM3, MIRAGE, and Caltech unified GCM. An overview and description of existing online coupled chemistry-meteorology models in Europe was

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done by Baklanov et al. (2010).

There are potential problems communicating between off-line coupled meteorological and CWF models. The wide variety of existing modelling systems has lead to a number of approaches and methods implemented in interface modules. Tasks performed by interfaces are minimised in some coupled systems (as on-line models do not need interfaces per se); these rely on surface fluxes, and turbulence and dispersion parameters (such as eddy viscosity) that are provided by the meteorological drivers.

Other modelling systems use interface modules that implement surface and boundary layer parameterisations to estimate dispersion parameters. In some cases interfaces are used to enhance the resolution of local physiographic data, and possibly introduce advanced parameterisations (e.g., those for urbanisation). Moreover, interface modules can include the evaluation of emissions of species that can be strongly influenced by meteorology, such as biogenic Volatile Organic Compound (VOC), wind-blown dust, sea salt, and pollen.

## 2.3 Overview of the models

The 18 models discussed in this article are now briefly introduced, presented in alphabetical order by their acronyms. A summary of selected main characteristics of these models appear in Table 1. The European countries of the model users are listed in the titles. In some cases, these countries may differ from the countries where these models were originally developed.

### 2.3.1 ALADIN-CAMx (Austria)

The air-quality model for Austria (AQA) consists of the meteorological model ALADIN-Austria (Sect. 3.2.5) and the chemical dispersion model CAMx (Comprehensive Air Quality Model with extensions; <http://www.camx.com>). The two models are coupled offline. The modelling system ALADIN-CAMx was implemented for the first time in Baumann-Stanzer et al. (2005). The forecasts, which are done in cooperation with

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the University of Natural Resources and Applied Life Sciences in Vienna (BOKU), are supported by the regional governments in Austria.

The SAPRC99 gas-phase photochemistry module (Carter, 2000) used in the operational AQA forecasts considers 76 different species and 217 reactions. The model system generally uses European Monitoring and Evaluation Programme (EMEP; <http://www.emep.int>) emissions for Europe. For the countries Austria, Czech Republic, Slovakia and Hungary, the original 50 km × 50 km data are downscaled to 5 km × 5 km based on an inventory from 1995. The EMEP data for 2005 (Vestreng et al., 2006) was used during summer 2007. In addition, a new highly resolved emission inventory for the City of Vienna (Orthofer et al., 2005) is used. Before 2008, terpene and isoprene emissions were calculated according to Guenther et al. (1993), and biogenic NO and NO<sub>2</sub> emissions were calculated according to Williams et al. (1987) and Stohl et al. (1996). For the operational air-quality forecasts in 2009, these methods were replaced by the BEIS3 (Biogenic Emission Inventory System) mechanism, which is implemented in the emission model SMOKE.

Monthly average (1991–2001) concentrations of the different species are used as boundary conditions for the coarse grid. The concentrations were obtained from model calculations (Krüger et al., 2008), which were conducted for the EU-project CECILIA (Central and Eastern Europe Climate Change Impact and Vulnerability Assessment, <http://www.cecilia-eu.org>). Forecasts of total column ozone are provided by the ECMWF IFS (Integrated Forecast System) model (Sect. 3.2.1).

### 2.3.2 CAMx-AMWFG (Greece)

The AM&WFG (Atmospheric Modeling and Weather Forecasting Group, National and Kapodistrian University of Athens, Greece) developed the air-quality forecasting system CAMx-AMWFG, which is based on the CAMx photochemical model. The system utilizes the SKIRON/Dust modeling system (Sect. 2.3.16) meteorological fields in order to prepare long-range transport of gases and particulate matter for Europe and the Mediterranean Region. The CAMx model was developed for regional-scale

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modeling of ozone and other pollutants (ENVIRON 1997, 2006). Products from this model are 48 h operational forecasts of O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, and particulate sulfate (PSO<sub>4</sub>) fields for the Mediterranean region and Europe every hour produced once per day (<http://forecast.uoa.gr/camxindx.php>). Additionally CAMx-AMWFG can provide the concentration and deposition for sodium and chloride (from sea-salt production), sulfate produced on dust (DSO<sub>4</sub>), and nitrate produced on dust (DNO<sub>3</sub>).

### 2.3.3 EURAD-RIU (Germany)

The EURAD model (European Air Pollution and Dispersion model) is an air-quality forecast model system for research and assessment. The model system was developed at the Rhenish Institute for Environmental Research (RIU) at the University of Cologne, Germany. The EURAD Air Quality Forecast System consists of three major components: MM5 (Sect. 3.2.8) to predict the needed meteorological variables, the EURAD Emission Module (EEM) to calculate the temporal and spatial distribution of the emission rates of the major pollutants, and the EURAD Chemistry Transport Model (EURAD-CTM) to predict the concentrations and deposition of the main atmospheric pollutants.

For the initial and boundary conditions, the NCEP GFS (National Centers for Environmental Prediction Global Forecast System) is interpolated onto the grids of the nested MM5 domains. The nesting enables consistent modelling from local to continental scales. Geographical information (e.g., orography, land-use type) is taken from the United States Geological Survey (USGS) database.

EURAD uses the RADM2 (Second generation Regional Acid Deposition Model) and its successor RACM (Regional Atmospheric Chemistry Mechanism) for computing the chemical processes and MADE (Modal Aerosol-Dynamics model for EURAD) for computing aerosol processes. RADM2 contains 63 reactive species treated in 158 chemical reactions. There is an option to run the code with the more sophisticated RACM chemistry as well. Detailed aqueous-phase chemistry is incorporated, as well. The horizontal and vertical transport is done by the fourth-order Bott advection scheme.

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Vertical mixing of the species is treated by an implicit vertical diffusion scheme. The sink at the lower boundary of the model is treated by wet and dry deposition parameterization. The major driver for wet deposition is the predicted precipitation. The dry deposition is calculated via the deposition velocity for each species, which depends upon the particle itself, the meteorological conditions and the land-use type.

The daily output of meteorological and atmospheric constituents covers Europe, Central Europe and the German States of North Rhine-Westfalia, Lower Saxony and Bavaria. These products are published on the EURAD website (<http://www.riu.uni-koeln.de>).

### 2.3.4 Enviro-HIRLAM (Denmark and others)

Enviro-HIRLAM (Environment – High Resolution Limited Area Model) is an online coupled NWP and CTM model for research and forecasting of both meteorological and chemical weather. The modelling system was developed by DMI (Danmarks Meteorologiske Institut) with other collaborators (Chenevez et al., 2004; Baklanov et al., 2008b; Korsholm et al., 2008) and included by the European HIRLAM consortium as the baseline system in the HIRLAM Chemical Branch ([http://hirlam.org/index.php?option=com\\_content&view=category&id=108:hirlam-chemistry-branch&layout=blog&Itemid=104&layout=default](http://hirlam.org/index.php?option=com_content&view=category&id=108:hirlam-chemistry-branch&layout=blog&Itemid=104&layout=default)).

To make the model suitable for CWF in urban areas, the meteorological part is improved by implementation of urban sublayer modules and parameterisations. The aerosol module in Enviro-HIRLAM has two parts: (i) a thermodynamic equilibrium model (NWP-Chem-Liquid) and (ii) the aerosol dynamics model CAC (tropospheric Chemistry Aerosol Cloud transport model). Parameterisations of aerosol feedback mechanisms in the Enviro-HIRLAM model are described in Korsholm et al. (2008) and Korsholm (2009).

Users have the option to choose one of several chemical models: RADM2, RACM or the newly developed economical NWP-Chem. Online Enviro-HIRLAM is used at DMI for operational pollen forecasting. The DMI operational system also includes the

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off-line version (the so-called CAC system), which is used operationally for CWF (e.g. in GEMS) and the Lagrangian model DERMA (Danish Emergency Response Model of the Atmosphere; Sørensen et al., 2007) for emergency preparedness modelling.

### 2.3.5 FARM (Italy)

FARM (Flexible Air quality Regional Model) was originally derived from STEM-II (Sul-  
fur Transport and dEposition Model; Carmichael et al., 1998) and was later developed  
as an independent project by ARIANET s.r.l. (<http://www.aria-net.it>). The model de-  
velopment is presently supported by ENEA (Ente per le Nuove tecnologie, l'Energia  
e l'Ambiente; [www.enea.it](http://www.enea.it)) within the national project MINNI (Modello Integrato  
Nazionale a supporto della Negoziazione Internazionale sui temi dell'inquinamento at-  
mosferico; [www.minni.org](http://www.minni.org)) funded by the Italian Ministry of Environment. A short model  
presentation is available at <http://www.aria-net.it/front/ENG/codes/files/10.pdf>, a more  
detailed online description (in Italian) can be found at [http://www.minni.org/sistema/  
sistema-modellistico-atmosferico/modulo-chimico](http://www.minni.org/sistema/sistema-modellistico-atmosferico/modulo-chimico), and a comprehensive user's guide  
is provided on request. Recent applications are documented in Gariazzo et al. (2007),  
Silibello et al. (2008) and Calori et al. (2008).

The SAPRC-99 (Carter, 2000) and an updated version of the chemical mechanism  
implemented in the EMEP Lagrangian Acid Deposition Model (Hov et al., 1988), includ-  
ing the treatment of Persistent Organic Pollutants (POP's) and mercury, and gas-phase  
chemical mechanisms have been implemented into the model using KPP chemical  
pre-processor (KPP, Kinetic Pre-Processor: Damian et al., 2002; Sandu et al., 2003;  
Daescu et al., 2003). The integration of the chemical reactions is performed by means  
of the the following methods included in KPP: Rosenbrock (Sandu et al., 2003) and  
LSODE (Radhakrishnan and Hindmarsh, 1993). Photolysis reaction rates appearing  
in the mechanism can be estimated either using simple look-up tables or an on-line ver-  
sion of the Tropospheric Ultraviolet-Visible Model (TUV, Madronich, 1987). SAPRC99  
is coupled with the CMAQ aero3 module to include aerosol processes. In presence  
of a cloud layer a simplified aqueous phase mechanism is considered, to include the

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sulfate production in clouds.

FARM runs operationally at ARIANET coupled with the meteorological model RAMS (Regional Atmospheric Model System; Cotton et al., 2003) to produce national-scale air-quality forecasts (<http://www.aria-net.eu/QualeAria>). The model is run by some Italian Regional Environmental Protection Agencies (ARPA) to produce air-quality analyses and forecasts. In particular, ARPA Lazio runs the model driven by RAMS to produce urban air-quality forecasts for Rome (Finardi et al., 2009) available at <http://www.arpalazio.net/main/aria/sci/previsioni/roma/pm10.php>; ARPA Piemonte together with Novara and Torino Provinces use the model driven by COSMO I7 (Italian implementation of the LM model, formerly known as LAMI, Limited Area Model Italy, [http://www.arpa.emr.it/sim/?mappa\\_numeriche](http://www.arpa.emr.it/sim/?mappa_numeriche)) to forecast air quality over Torino City (Finardi et al., 2008) and Novara Province (Pittini et al., 2007), with results browsable at <http://www.provincia.novara.it/arianova/WEB/index.html>; and ARPA Lombardia uses FARM and a meteorological analysis using the ECMWF as a background field to compute near-real-time air-quality analyses ([http://ita.arpalombardia.it/ITA/qaria/doc\\_DistribSpazialeCalcolata.asp](http://ita.arpalombardia.it/ITA/qaria/doc_DistribSpazialeCalcolata.asp)).

### 2.3.6 LOTOS-EUROS (The Netherlands)

Several models have been developed in The Netherlands. Netherlands Organisation for Applied Scientific Research (TNO) developed LOTOS (Bultjes, 1992; Schaap et al., 2004) and the National Institute for Public Health and the Environment (RIVM) developed EUROS (de Leeuw and van Rheineck Leyssius, 1990; Matthijsen et al., 2002). During 2004, the two models were unified, resulting in the LOTOS-EUROS model version 1.0 (LONG Term Ozone Simulation – EUROpean Operational Smog model, Schaap et al., 2008; <http://www.lotos-euros.nl>). The model can be used to model the fate of pollutants such as photo-oxidants, aerosols, heavy metals and persistent organic pollutants (POPs) over Europe.

The model is used operationally to forecast air pollution over Europe and the Netherlands driven by the meteorology from ECMWF IFS. The model is used to perform 72 h

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European forecast (twice daily) at 30 and 15 km horizontal grid spacing and a smaller domain over the Netherlands at a 15 km horizontal grid spacing, including data assimilation of ozone measurements (van Loon et al., 2004). PM<sub>10</sub> (Particulate Matter <10 μm) forecasts are produced including a bias correction (Manders et al., 2009).

### 2.3.7 MATCH (Sweden)

The Multi-scale Atmospheric Transport and Chemistry (MATCH) model is a three-dimensional, Eulerian model developed at SMHI (Swedish Meteorological and Hydrological Institute). It is used in a range of applications from urban-scale studies with grid spacings on the order of a km or smaller (e.g., Gidhagen et al., 2005) to regional and continental-scale studies on eutrophic deposition and photochemistry (e.g., Langner et al., 2005; Engardt et al., 2005; Andersson et al., 2007). MATCH is used for air-quality assessment in Sweden and the Baltic Sea region and for forecasts of radioactivity in case of nuclear emergencies in Europe (Langner et al., 1998).

MATCH includes modules describing emissions, advection, turbulent mixing and dry and wet deposition. Depending on the application, specific modules describing chemistry or aerosol dynamics can be added to the basic transport model. The MATCH design has flexible horizontal and vertical resolution and allows for an arbitrary number of chemical compounds. The advection scheme (Bott, 1989) is fourth-order in the horizontal and second-order in the vertical. A complete description of the transport model can be found in Robertson et al. (1999) and in the on-line documentation (<http://www.smhi.se/sgn0106/if/meteorologi/match.htm>). Details on the photochemistry version of MATCH can be found in Andersson et al. (2007) and van Loon et al. (2007). Emissions used for the runs are based on EMEP2003.

The current MATCH operational system for CWF consists of two components, driven by HIRLAM and ECMWF meteorology, respectively. The MATCH-HIRLAM component uses meteorological data provided by the HIRLAM NWP model that is operational at SMHI. MATCH-HIRLAM is primarily targeted to ozone and is run once a day. A run consists of a hindcast of the previous day and forecasts for the present day and

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the next day. The model grid comprises nearly all of Europe with a horizontal grid spacing of 44 km (<http://www.airviro.smhi.se/MAQS>). MATCH-ECMWF is a part of the GEMS/MACC regional cluster and uses ECMWF Integrated Forecast System (IFS) meteorology. It is currently operated with a horizontal grid spacing of 0.5° (0.2° in preparation) and provides 72 h forecasts of such quantities as O<sub>3</sub>, NO, NO<sub>2</sub>, CO, SO<sub>2</sub>, PM<sub>2.5</sub>, PM<sub>10</sub>, visibility and AOD (<http://gems.ecmwf.int/>; <http://www.airviro.smhi.se/MAQS>).

### 2.3.8 MM5-CAMx (Greece)

MM5-CAMx is the combination of the limited-area, non-hydrostatic, terrain following and sigma-coordinate meteorological model MM5 (Sect. 3.2.8) coupled off-line with the three-dimensional Eulerian photochemical dispersion model Comprehensive Air quality Model with extensions (CAMx). The forecast system performs a 72 h forecast of daily mean and daily maximum O<sub>3</sub>, NO, NO<sub>2</sub>, CO, SO<sub>2</sub>, and PM<sub>10</sub> concentrations on three domains: two on the regional scale (Europe, Balkan Peninsula) and one on an urban scale (Athens) (<http://lap.phys.auth.gr/gems.asp>).

### 2.3.9 MM5-CHIMERE (France and Portugal)

MM5-CHIMERE consists of two models: The PSU/NCAR Mesoscale Model MM5 which is used to compute the meteorological variables that are needed to drive the chemistry-transport model, and the MM5-CHIMERE model (<http://www.lmd.polytechnique.fr/chimere/>), developed by IPSL (Laboratoire de Météorologie Dynamique), which is used to predict the concentrations and deposition of several tropospheric species. MM5-CHIMERE has been primarily designed to produce daily forecasts of ozone, aerosols and other pollutants and to make long-term simulations for emission control scenarios. MM5-CHIMERE is executed over a range of spatial scales from a global and regional scale (domains of several thousands of kilometers) to an urban scale (100–200 km) with horizontal grid spacings of 1–100 km. Products are daily 72 h forecasts for O<sub>3</sub>, NO<sub>2</sub>, PM<sub>2.5</sub>, PM<sub>10</sub> and desert dust (<http://prevair.org>).

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### 2.3.10 MM5/WRF-CMAQ (Spain, UK)

The CMAQ (United States Environmental Protection Agency, Community Multiscale Air Quality) model includes a suite of chemical as well as transport and dynamic schemes (Byun and Schere, 2006). It includes dynamical and chemical interactions between atmospheric pollutants on multiple scales in a modular framework. CMAQ has been designed for assessing the impact of multiple pollutants including tropospheric O<sub>3</sub> and other oxidants, speciated PM, and acid-deposition species on time scales from an hour to years.

CMAQ is a widely used chemistry transport model which has been linked to a number of meteorological models including MM5, Eta and WRF. Although WRF has superseded MM5, the MM5-CMAQ is used for example to provide 72 h forecasts for hourly, daily maxima and daily average information related to O<sub>3</sub>, NO<sub>2</sub>, CO, SO<sub>2</sub>, PM<sub>10</sub>, PM<sub>2.5</sub> and NH<sub>3</sub> ([http://verde.lma.fi.upm.es/cmaq\\_eu/](http://verde.lma.fi.upm.es/cmaq_eu/)).

Examples of CWF model forecasts can be found in Eder et al. (2006, 2009); they examine the performance of the model for forecasting 8 h ozone concentrations over the USA. CMAQ is also used operationally in the UK to predict footprints of industrial power plants for pollutants such as SO<sub>2</sub> and PM<sub>10</sub> (e.g., Yu et al., 2008). CMAQ is supported and distributed by the Community Modeling and the Analysis System center (CMAS, <http://www.cmascenter.org/>).

### 2.3.11 MOCAGE (France, Spain, Romania)

The MOCAGE (Modèle de Chimie Atmosphérique à Grande Echelle, Model of Atmospheric Composition at Large Scales) three-dimensional multi-scale CTM has been designed at Météo-France for both research and operational applications. MOCAGE is applicable to CWF, tracking and back-tracking of accidental point-source releases, trans-boundary pollution assessment, assimilation of remote-sensing measurements of atmospheric composition, and studies on the impact of anthropogenic emissions of pollutants on climate change, with more than 40 references in the international peer-

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reviewed literature (e.g., Dufour et al., 2004; Bousserez et al., 2007).

MOCAGE has the flexibility to be run in different configurations with different parameterizations depending upon its application. The model considers the troposphere and stratosphere on the planetary scale and over limited-area sub-domains at higher horizontal resolution. The model provides (by default) its own time-dependent chemical boundary conditions.

MOCAGE has been run daily since 2001. In 2004, Météo-France joined the partnership consortium and operational platform “Prév’Air” (<http://www.prevoir.org>; Rouil et al., 2009) in charge of the pollution monitoring and forecasting for the French Ministry of Environment. Within this platform, 72 h forecasts are delivered daily to Prév’Air users, including ozone, precursors and aerosol over the globe (horizontal grid spacing of 2°, Europe (0.5°) and France (0.1°)).

MOCAGE is also run daily in the context of GMES atmosphere projects (GEMS and now MACC, <http://www.gmes-atmosphere.eu/services/raq>), participating in the pre-operational ensemble forecasting system. The configuration used in this context has two domains and covers the globe at 2° horizontal grid spacing and Europe (15° W–35° E and 35° N–70° N) at 0.2° grid spacing. MOCAGE is also run by the Spanish and Romanian national meteorological services for their research and operations. MOCAGE is coupled to the computational fluid dynamics software PALM (<http://www.cerfacs.fr/~palm>) and can assimilate using variational methods (3d-var, 3d-fgat or 4d-var) profiles, columns or surface measurements of key atmospheric pollutants (see for instance: El Amraoui et al., 2010).

### 2.3.12 NAME (the UK)

NAME (Numerical Atmospheric dispersion Modelling Environment) is an off-line Lagrangian dispersion model developed by the Met Office (Jones et al., 2007). It provides a flexible modelling environment able to predict dispersion over distances ranging from kilometres to the whole globe and for time periods from minutes upwards. This flexibility allows the model to be used in a variety of applications, including emergency

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response (e.g., Webster et al., 2007) and routine air quality forecasting.

NAME uses meteorology from the Met Office Unified Model (MetUM), in either global or limited area configuration. Chemical modelling within NAME employs the scheme originally derived for the STOCHEM model (Collins et al., 1997). This scheme models gaseous and aqueous phase chemistry and has 40 advected and 18 non-advected tracers, 140 reactions and 23 photolytic reactions; 16 species are emitted. The dry deposition scheme used is based on a resistance network analogy for deposition velocity modelling. Particles can also be removed from the model atmosphere by the following processes; ((i) fall out due to gravity, ((ii) impaction with the surface, ((iii) washout by falling precipitation, and iv) rainout, where the pollutant is absorbed directly into cloud droplets as they form.

Emissions are pre-processed using three datasets: (i) the UK National Atmospheric Emission Inventory at 1 km resolution; (ii) a 5 km resolution inventory for shipping emissions around the UK; (iii) the EMEP 50 km inventory outside the UK. The UK routine air quality forecast configuration of NAME employs a nested configuration, with an outer domain covering Western Europe and an inner domain covering the UK. The effective model grid for the inner domain corresponds to a resolution of around 8 km. The model provides forecasts out to 5 days and routine output parameters include atmospheric concentrations of ozone, CO, NO<sub>2</sub>, SO<sub>2</sub>, PM<sub>10</sub> and secondary aerosol species.

### 2.3.13 OPANA (Spain and others)

OPANA is an Operational version of ANA model (Atmospheric mesoscale Numerical pollution model for urban and regional Areas). OPANA is designed to operate under routine basis to forecast 5–7 days of air concentrations. OPANA produces daily air-quality forecasts in Leicester City Council (UK), Madrid Municipality (Spain) and Las Palmas de Gran Canaria (Spain). It is also used as an impact assessment system for industrial installations. Numerical products include daily 72 h forecasts for O<sub>3</sub>, NO<sub>2</sub>, CO, SO<sub>2</sub>, and PM<sub>10</sub> (<http://artico.lma.fi.upm.es/>).

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### 2.3.14 RCG (Germany)

The urban-scale photochemical model CALGRID (California Grid Model; Yamartino et al., 1992) and the regional-scale model REM3 (Regional Eulerian Model; Stern, 1994) were used as the starting point for the urban/regional scale model, REM-CALGRID (RCG, Stern, 2003). The RCG model has been designed to fulfill the requirements of the ambient air-quality framework directive 96/62/EC of the European Commission (Stern et al., 2008). RCG is run in off-line mode. For long-term diagnostic applications, the meteorological driver is prepared by the analysis system TRAMPER (Tropospheric Realtime Applied Meteorological Procedures for Environmental Research).

For operational forecasting, the meteorology derives from the GME model (Sect. 3.2.2). The model is part of a model system development including statistical and fuzzy models (Reimer and Dlabka, 2000) and Eulerian model RCG (Flemming and Reimer, 2000) to forecast especially surface ozone concentrations. The full system is documented in Reimer et al. (2000). After transformation of GME data to RCG coordinates, the boundary layer parameters are determined anew by the TRAMPER boundary layer module.

The forecast system was developed with respect to local abatement strategies for German authorities in application of the so-called German ozone law in the 1990s. With the introduction of EU directives, the diagnostic tests on emission scenarios became much more important than real-time forecasts. The RCG model has been operational for more than 10 y, running every day at 12:00 UTC and producing a 72 h forecast over Central Europe (<http://www.trumf.de/>).

### 2.3.15 SILAM (Finland, Estonia, Russia, Lithuania and Spain)

The SILAM modelling system (Air Quality and Emergency Modelling System) includes both Eulerian and Lagrangian dynamic kernels (e.g., Sofiev et al., 2006a,b; Saarikoski et al., 2007; Siljamo et al., 2008; Sofiev et al., 2009; Saarnio et al., 2010; <http://silam>).

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fmi.fi). The model applications range from global to meso-beta scale (grid spacing down to 1 km). The SILAM model is an open access system, and the source code is publicly available on the web. The model is the official air-quality forecasting tool on regional and larger scales in Finland and Lithuania. The model is also used for research purposes in Estonia, Russia, Lithuania and Spain.

The model has been used operationally in the EU-funded GEMS and MACC (<http://www.gmes-atmosphere.eu>) and EU-funded PROMOTE (<http://www.gse-promote.org>) and PASODOBLE projects. The predicted species include the concentrations of O<sub>3</sub>, NO<sub>x</sub>, SO<sub>x</sub>, NH<sub>x</sub>, VOCs, sea salt, anthropogenic PM<sub>2.5</sub> and PM<sub>10</sub>, as well as pollution from wildland fires (e.g., Saarikoski et al., 2007; Sofiev et al., 2009; Saarnio et al., 2010) and for selected biogenic aerosols, such as allergenic pollen (e.g., Sofiev et al., 2006b, 2011; Siljamo et al., 2008; Veriankaitė et al., 2010). The model is capable of four-dimensional variational data assimilation (Sofiev and Atlaskin, 2004). The model has recently been applied to evaluate the dispersion of primary PM<sub>2.5</sub> emissions in the whole of Europe and in more detail in Finland, and the resulting adverse health impacts (Tainio et al., 2009, 2010; Karvosenoja et al., 2010).

The meteorological information is extracted most commonly from the FMI variant of the weather forecasting model HIRLAM, which is used as a downscaling tool for ECMWF Integrated Forecast System forecasts (which are also used without modifications), and from the regional AROME model simulations for Southern Finland and the Baltic States. The products are 54 and 72 h forecasts for Finland, the Baltic States, and Europe (<http://silam.fmi.fi>).

### 2.3.16 SKIRON/Dust (Greece)

SKIRON/Dust is a modelling system that couples the National Oceanic and Atmospheric Administration (NOAA) Eta NWP model (Sect. 3.2.6) off-line with a dust transport model. As of this writing, SKIRON's NWP component runs at 5 km horizontal grid spacing, using the nonhydrostatic version with the Betts–Miller–Janjic convective parameterization scheme. Other modifications to the Eta model in SKIRON include

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a different radiative transfer scheme, differences in the soil properties in the surface parameterization, more soil and vegetation categories, and the incorporation of sloped surfaces in the surface energy balance.

The dust module of the system is based on the work of Nickovic et al. (2001). The dust transport submodel includes eight size bins of dust particles (Marticorena and Bergametti, 1995; Zender et al., 2003; Pérez et al., 2006), the calculation of AOD and the correction of radiative transfer through look-up tables (Kaufman et al., 2002). Dry and wet deposition schemes have been improved, and the in-cloud scavenging has been included (Kumar et al., 1995; Seinfeld and Pandis, 1998; <http://forecast.uoa.gr/dustindx.php>).

### 2.3.17 THOR (Denmark)

THOR is an integrated air-pollution forecast and scenario management system (Frohn and Brandt, 2006; <http://thor.dmu.dk>), consisting of an off-line coupled three-dimensional NWP model Eta (Sect. 3.2.6) and several air pollution models (e.g., Danish Eulerian Hemispheric Model DEHM, Urban Background Model UBM, point source model OML, Operational Street Pollution Model OSPM, accidental release model Danish Rimpuff and Eulerian Accidental release Model DREAM). The model covers most of the Northern Hemisphere with one two-way coupled nest over Europe. The system is capable of 72 h forecasts of weather and air pollution from regional scale over urban background scale and down to individual street canyons in cities. DREAM can be used for any accidental release from power plants, industrial sites, natural and human made fires, etc. ([http://www2.dmu.dk/1\\_Viden/2\\_miljoetilstand/3\\_luft/4\\_spredningsmodeller/5\\_Thor/default\\_en.asp](http://www2.dmu.dk/1_Viden/2_miljoetilstand/3_luft/4_spredningsmodeller/5_Thor/default_en.asp)).

The system can be used for information and warning of the public in cases of high air-pollution levels and for policy management (e.g., by emission reduction or traffic scenarios) of many different chemical compounds. The THOR system is executed up to four times every day. The products are 72 h forecast and daily maximum of O<sub>3</sub>, NO, NO<sub>2</sub>, SO<sub>2</sub>, and SO<sub>4</sub> for Denmark and Europe

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([http://www2.dmu.dk/1\\_Viden/2\\_Miljoe-tilstand/3\\_luft/4\\_udsigt/Default.asp](http://www2.dmu.dk/1_Viden/2_Miljoe-tilstand/3_luft/4_udsigt/Default.asp)).

### 2.3.18 WRF-Chem (Spain and others)

The Weather Research and Forecast (WRF; <http://www.wrf-model.org/>) model coupled with Chemistry (WRF-Chem; Grell et al., 2005) provides the capability to simulate chemistry and aerosols from cloud scales to regional scales. WRF-Chem was developed by the NOAA with contributions from National Center for Atmospheric Research (NCAR), Pacific Northwest National Laboratory (PNNL), EPA, and university scientists (<http://www.acd.ucar.edu/wrf-chem/>).

WRF-Chem is an on-line model; it solves the chemistry every 10 min and the meteorological time step is 5 min. The Emission Model (EMIMO) (Compures Science School – Technical University of Madrid, UPM) provides emission data for every grid cell, per hour and per primary pollutant, based on TNO European emissions. Products are daily 72 h O<sub>3</sub>, NO<sub>2</sub>, SO<sub>2</sub>, CO, PM<sub>10</sub>, PM<sub>2.5</sub> and NH<sub>3</sub> forecasts for Europe ([http://verde.lma.fi.upm.es/wrfchem\\_eu/](http://verde.lma.fi.upm.es/wrfchem_eu/)).

## 3 Numerical weather prediction models

Nearly all operational air-quality models have two components, a numerical weather prediction (NWP) component and an air-pollution chemistry and physics component. The purpose of this section is twofold. First, we discuss the characteristics of NWP models that affect the ability of the coupled model to produce accurate forecasts of air quality. Second, we provide a brief overview of the different NWP models in operational air-quality models in Europe. Tribbia and Anthes (1987) provide a review of the scientific basis for numerical weather prediction, and Stensrud (2007) reviews physical parameterization schemes.

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### 3.1 Characteristics of NWP models

In this section, the model architectures and physical processes in the NWP models are discussed.

#### 3.1.1 Formulation of NWP models

5 NWP models can be broken into hydrostatic and nonhydrostatic models. Hydrostatic models assume that the accelerations of vertical velocity are small relative to that of gravity. Nonhydrostatic models, on the other hand, are capable of modeling vertical accelerations exceeding that of gravity, such as are found in deep, moist convection. Most models with horizontal grid spacings less than 10 km are run using nonhydrostatic models.

10 Another aspect is the vertical coordinate used in the formulation of the governing equations. Some models use pressure as their vertical coordinate, whereas others use a terrain-following sigma coordinate, where  $\sigma = (p - p_s) \div (p - p_t)$ ,  $p$  is pressure,  $p_s$  is surface pressure, and  $p_t$  is pressure at the top of the model (usually fixed at 100, 50, or 15 10 hPa). Others are hybrid systems that blend sigma coordinates near the surface and pressure coordinates aloft, obtaining the benefits of both coordinate systems (simpler formulation of governing equations in pressure coordinates and better representation of near-surface flows along sigma surfaces).

#### 3.1.2 Cloud microphysical parameterizations

20 Accurate forecasting of the size and number concentrations of cloud and precipitation water particles is important for deposition, photochemistry and aerosol-cloud-radiation interaction in CWF models. On the grid scale, cloud and precipitation processes are handled by cloud microphysical parameterizations. When grid-cell-sized regions of the model atmosphere become saturated, model clouds begin to form. Because these processes act on scales smaller than the grid-scale, cloud 25

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microphysical parameterizations handle the distributions and the conversions of condensed water substance between cloud water, rain water, cloud ice, snow, graupel, and hail. Schemes range in sophistication from (i) those that neglect ice processes to (ii) one-moment schemes (predicting only mixing ratios of each hydrometeor species) and to (iii) two-moment schemes (predicting number concentrations and mixing ratios). Because of the relative lack of knowledge about microphysical processes, higher-moment schemes and more sophisticated parameterizations do not necessarily lead to better predictions of clouds and precipitation. Straka (2009) presents a recent review of cloud microphysical parameterizations and principles.

### 3.1.3 Convective parameterization schemes

The choice of convective parameterization scheme in the numerical weather prediction model is important for two reasons. As Baldwin et al. (2002) lament, “All convective parameterizations contain arbitrary parameter settings and have characteristic behaviors that are sometimes inconsistent with reality.” First, the morphology and evolution of the convective systems that form in the model may depend on the convective scheme. For example, Bukovsky et al. (2006) showed that curved convective lines often formed in an operational model with a modified Betts–Miller scheme, but did not initiate in the right place and time, whereas convective systems formed with the Kain–Fritsch scheme did not form bowing segments as frequently, but did initiate in the right place and time.

Second, how the convective parameterization changes the model atmosphere may not resemble what happens in reality. For example, Baldwin et al. (2002) showed that a modified version of the Betts–Miller scheme does not produce observed cold pools in the wake of convective systems and may eliminate convective inhibition more quickly than in reality.

Models with horizontal grid spacings less than 5 km are often considered to be convection-permitting models, meaning that convective parameterizations can be omitted (at least partly for large-scale convection storms), allowing convective instabilities to be handled on the grid scale. In these models, the cloud microphysical

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parameterizations must do all the work of relieving instability. Another limitation of convective parameterization schemes is that only heat and moisture are redistributed. Momentum is generally not, partially because methods to handle such redistribution have not been developed.

5 A common assumption is that convective parameterization schemes exist to parameterize convective precipitation. In fact, convective parameterization schemes exist to relieve the model of gravitational or buoyant instability in the vertical. Any precipitation created by the adjustment of the atmosphere back to stability because of the convective parameterization scheme (called convective precipitation or subgrid-scale precipi-  
10 tation) is merely a byproduct of the readjustment. Models usually have two schemes for releasing moist gravitational instability, one for deep convection such as thunderstorms, and one for shallow convection such as the stratocumulus clouds that cap the planetary boundary layer in the subtropics.

Many convective parameterization schemes are developed from research on tropi-  
15 cal convection. Most of these schemes release the conditional instability almost as quickly as it is formed, maintaining convective neutrality. These are called statistical-equilibrium schemes, following the terminology in Emanuel (1994, Sects. 11.2 and 12.3) and Mapes (1997). Such schemes include the Kuo (1965, 1974), Arakawa-Schubert (1974), Betts-Miller (1986), and Tiedke (1989) schemes.

20 Convection in the mid and high latitudes, however, often does not behave in this manner. Instability may build up over hours or days, kept from being released by a lower-tropospheric stable layer or inversion called a cap or lid, measured by an energy barrier called the convective inhibition. Convection is released by some mechanism to lift unstable parcels past the layer of convective inhibition to release the instability. Such  
25 schemes are called activated or triggered schemes (Sects. 11.2 and 12.3 in Emanuel, 1994; Mapes, 1997). Such schemes include the Kain-Fritsch (Kain and Fritsch, 1990, 1993; Kain 2004) scheme and its derivatives (e.g., Bechtold et al., 2001).

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### 3.1.4 Boundary layer parameterization schemes for NWP models

Similar to convective parameterizations that redistribute heat and moisture when the atmosphere becomes unstable to moist processes, boundary-layer parameterizations serve a similar purpose for the near-surface layer of air. Some way is needed for models to distribute the heat, moisture, and momentum as the free atmosphere joins with the surface through the unresolved scales of turbulence present in the planetary boundary layer. The stability of the planetary boundary layer affects how this redistribution occurs, so some schemes work better for stability stratified situations (i.e., surface inversions), others work better for unstably stratified situations (i.e., convective boundary layers), and yet others work better for neutrally stratified situations (i.e., well-mixed boundary layers).

Despite their sophistication, the schemes used in NWP models have limitations, and these limitations can be critical for CWF applications. For example, CWF models may need greater vertical resolution within the boundary layer or improved surface sub-layer parameterizations, especially for urban-scale air-pollution modeling where low-level emissions within the surface layer are occurring (from traffic, for example). Mixing height is a quantity needed for boundary layer parameterizations, and it may be quite variable, especially over different land categories in urban areas or due to internal boundary layers, blending heights, etc. Furthermore, in some situations, the mixing height may even be poorly defined. Therefore the boundary layer parameterisations in NWP models used for CWF should be further improved, as discussed in the overview in Baklanov and Grisogono (2007) and Sokhi et al. (2010).

### 3.1.5 Initial and lateral boundary conditions

Initial conditions come from the observations collected worldwide and transmitted through the Global Telecommunications System. In addition, local sources of data such as Doppler radars, satellites, mesoscale observations, and buoys may also be included. The process by which observations are ingested into the model, interpo-

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lated onto the model grid, and balanced to produce a dynamically consistent set of initial conditions is called *data assimilation*. Some data assimilation systems are three-dimensional variational assimilation approaches (3DVAR), whereas others also include assimilating data in time (4DVAR). Some of the newest data-assimilation approaches involve ensemble Kalman filtering, an approach that recognizes that the initial conditions are not (and can never be) perfectly known.

NWP models can cover a global domain or be limited-area models, with a regional domain. Limited area models have to accommodate lateral boundary conditions from some larger-scale (usually global) model. Because output from global models is infrequent (usually only stored every 3 or 6 h) and the limited-area models need input at their domain boundaries every model time step (usually tens of seconds), the data along the lateral boundaries is usually interpolated linearly in time. For situations where the flow may be changing or new features are moving into the limited-area domain through the boundaries, large errors may be introduced (Nutter et al., 2004).

## 3.2 NWP models

In this section, we discuss the different NWP models that commonly are used to provide meteorological data to the operational air-quality models. The characteristics of each model are summarized in Table 2.

### 3.2.1 ECMWF IFS

Widely regarded as the most accurate NWP model in the world, the European Centre for Medium-Range Weather Forecasts (ECMWF) was developed from a European COST action to provide global medium-range weather forecasts (Woods, 2006). At the time of this writing (August 2010), the nonhydrostatic ECMWF model known as the Integrated Forecast System (IFS) is T1279, an equivalent grid spacing of about 16 km, with 91 vertical hybrid-coordinate levels. The model is run twice a day at 00:00 UTC and 12:00 UTC. The nonhydrostatic dynamical core comes from the ALADIN model

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(Sect. 3.2.5). The convective scheme is a modified Tiedke (1989) scheme (Nordeng 1994), testing for shallow, deep, and midlevel convection (e.g., above a frontal zone or inversion). The surface scheme is Tiled ECMWF Scheme for Surface Exchanges over Land (TESSEL) and has been revised to include surface hydrology and the choice of a global soil texture (Balsamo et al., 2009). Access to the model and its output is proprietary for 18 European member states and 10 states with co-operation agreements.

### 3.2.2 GME

GME (global model) from German Weather Service (DWD) is a hydrostatic model and is designed for the routine forecast of complex weather development on synoptic scales (Majewski et al., 2002). The vertical domain is extended up to the stratosphere. For regional weather forecasts, the nonhydrostatic limited area models COSMO-EU and COSMO-De (Consortium for Small Scale Modeling) are used with boundary conditions from GME (www.dwd.de). The global model GME is defined on an icosahedral grid with about 60 km resolution. Within the postprocessing all fields are transformed to the latitude-longitude geographical grid.

### 3.2.3 Unified model

The Unified Model (UM; Cullen, 1993) was developed by the UK Met Office and introduced in 1990. The Unified Model can serve as a global model or a nonhydrostatic limited-area model (Davies et al., 2005). The model vertical coordinate is height, and the convective parameterization is based on Gregory and Rowntree (1990), and the boundary-layer scheme is described by Brown et al. (2008). The Unified Model is a proprietary model and has limited access to those outside the UK Met Office.

### 3.2.4 HIRLAM

The High Resolution Limited Area Model (HIRLAM; Undén et al., 2002; http://hirlam.org) derives from a consortium of European meteorological institutes (Denmark,

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Estonia, Finland, Iceland, Ireland, Norway, The Netherlands, Spain, and Sweden, with France as a research partner). HIRLAM is run at a variety of grid spacings from 50 km to 1.5 km, depending on country, with the reference version being run at Finnish Meteorological Institute (FMI). HIRLAM is a hydrostatic model, although a nonhydrostatic version also exists. Three convective parameterization schemes are available: STRACO (Soft TRAnSition COvection), which is a modified Kuo scheme that aims to produce a smooth transition between convective clouds and large-scale condensation, Rasch and Kristjánsson (1998), and Kain and Fritsch (1990, 1993). HIRLAM is available to member states, but the access can be granted for other users by a special agreement.

### 3.2.5 ALADIN, ARPEGE, and AROME

ALADIN (Aire Limitée Adaptation Dynamique INitialisation) is a limited-area version of the French global model ARPEGE (Action de Recherche Petite Echelle Grande Echelle, which was the basis for the ECMWF IFS), growing out of a French-led consortium. ALADIN uses a modified version of the Bougeault (1985) convective scheme and a terrain-following–pressure hybrid vertical coordinate. ALADIN and HIRLAM consortia joined together starting in 2004 to form the HARMONIE consortium (Hirlam Aladin Research on Meso-scale Operational NWP in Euromed) in which a new model has been developed (AROME, Applications of Research to Operations at MESoscale; Seity et al., 2010).

### 3.2.6 Eta

The Eta model was the operational limited-area hydrostatic model from June 1993 to June 2006 in the United States. The model uses a unique step-coordinate vertical coordinate called the eta (hence the name of the model), a modified version of the sigma coordinate (Mesinger et al., 1988; Janjic, 1990, 1994). The Eta model uses a version of the Betts-Miller convective scheme (Betts and Miller, 1986; Janic, 1994; Baldwin et al., 2002). Research versions of the Eta included a sigma-coordinate

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version, a nonhydrostatic version, and a version with the Kain–Fritsch convective parameterization scheme (Baldwin et al., 2002; Kain et al., 2003). One problem with the Eta model is that it fails to reproduce strong surface winds associated with downslope windstorms, partially as a result of the way that the mountain waves are handled in the eta coordinate system (Gallus, 2000; Gallus and Klemp, 2000).

### 3.2.7 MEMO

MEMO (MEscale MOdel) is a nonhydrostatic mesoscale model for simulating wind flow. MEMO was developed by the Aristotle University of Thessaloniki and the University of Karlsruhe. MEMO has been used to study the wind fields around urban areas (e.g., Kunz and Moussiopoulos, 1995). The model uses a terrain-following coordinate and has two physical parameterizations of importance – radiative transfer (Moussiopoulos, 1987) and *K*-theory for the planetary boundary layer – but neglects moist processes by assuming the atmosphere is unsaturated. MEMO is coupled with the photochemical dispersion model MARS (Model for the Atmospheric Dispersion of Reactive Species) to produce the European Zooming Model (EZM; Moussiopoulos, 1995). Because MEMO does not contain moist atmospheric processes, its applicability when clouds and precipitation are present is limited.

### 3.2.8 MM5

The fifth-generation Pennsylvania State University/National Center for Atmospheric Research Mesoscale Model (MM5) is a nonhydrostatic limited-area model that has been one of the most popular open-source mesoscale models in the world (Dudhia, 1993; Grell et al., 1994; <http://www.mmm.ucar.edu/mm5>). MM5 is a terrain-following sigma-coordinate model with a large degree of flexibility in choosing and nesting domains, grid spacings, and model physics. For example, as of the writing of this article, users of the MM5 can choose from six convective parameterizations, seven resolvable-scale cloud microphysics parameterizations, six planetary boundary layer parameterizations,

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seven surface parameterizations, and four atmospheric radiation schemes, although many of these schemes are outdated, overly simple, or inappropriate for some weather situations. As such, care is needed when configuring the model to ensure optimal performance.

### 3.2.9 WRF

The successor to the MM5 is the open-source Weather Research and Forecasting model (WRF, pronounced *worf*, like the *Star Trek* character; Skamarock and Klemp, 2008; Wang et al., 2009). The goal of WRF is to produce a common architecture for both research and operations to build upon (<http://wrf-model.org>). WRF has two nonhydrostatic dynamic cores, the ARW (Advanced Research WRF), developed primarily by the National Center for Atmospheric Research, and the NMM (Nonhydrostatic Mesoscale Model; Janjic et al., 2001; Janjic, 2003), developed primarily by the NOAA/National Centers for Environmental Prediction. The WRF-ARW uses a sigma vertical coordinate in either a limited-area or global domain, whereas the WRF-NMM uses a hybrid sigma–pressure vertical coordinate. One of the recent additions to WRF is the positive-definite advection scheme, which improves the conservation of advected quantities and prevents negative quantities such as mixing ratio and chemical concentrations (Skamarock, 2006; Skamarock and Weisman, 2009).

## 4 Air chemistry models: architectures and physical processes

CWF models are also commonly called chemical transport models (CTM), as they simulate processes controlling the distribution of chemical species in space and time. To calculate atmospheric concentrations of pollutant species, the modelling framework needs to incorporate several key processes: (i) horizontal and vertical transport (i.e., advection, diffusion, convection), (ii) chemical transformation, (iii) temporal allocation and distribution of emissions, and iv) deposition of the pollutants. Although there are

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a large number of three-dimensional CWF models available, most of these are based on similar frameworks for linking these four types of interactions, and they all solve the continuity equations for mass conservation of the pollutants in the atmosphere.

Transport of pollutant species involves both advection and diffusion. Advection refers to the movement of pollutant species by the mean wind fields, whereas diffusion involves sub-grid-scale turbulent mixing of pollutants. By definition, advection transports the pollutants without a significant change in the concentration in the considered volume, whereas diffusion involves mixing and hence leads to lowering of pollutant concentrations. In an Eulerian frame of reference, the computational domain of a CWF model consists of a matrix of contiguous grid cells forming a finite three-dimensional volume (also called a box). As this box is a subset of the entire atmospheric globe, lateral boundary conditions define the advection into the modelling grid. It is typical to assume that horizontal advection is dominant and that there is no exchange at the top boundary of the domain. The following sections describe the main processes that are included in CWF models.

One of the key problems in atmospheric composition modelling is knowing the accuracy and reliability of the numerical schemes applied. A less appreciated, but also an important issue, is to ensure the compatibility between the schemes applied in different modules of the modelling system. Usually, the model construction follows the process-wise split (e.g., Seinfeld and Pandis, 2006), thus distinguishing the advection scheme, diffusion algorithm, chemical transformation module, dry, and wet deposition, data assimilation control module, and a set of supplementary modules including meteorological pre-processor. Of these, advection and diffusion are usually closely linked.

The main physical and chemical components of the selected 18 models have been summarized in Table 3.

## 4.1 Advection and convection

Existing advection schemes can be categorized by one of four approaches: finite-difference, flux, semi-Lagrangian, and spectral. The basic principles of these schemes

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were formulated several decades ago and, with certain modifications, are still applied.

The finite-difference schemes involve direct discretization of the dispersion equation and involve various types of interpolation functions to evaluate derivatives of the concentration fields, as reviewed by Riehtmyer (1962), Leith (1965), and Roach (1980).

5 Examples of specific developments are van Leer (1974, 1977) and Russel and Lerner (1981). These once-popular schemes usually suffer from substantial numerical viscosity and limited stability, which sets very stringent limitations to the Courant number (the ratio of the maximum distance passed during the model time step to the model grid cell size). Consequently, interest has largely shifted towards flux and semi-Lagrangian schemes for practical applications.

10 Flux-type schemes are based on an evaluation of the admixture fluxes at the borders of the grid cells using some interpolation procedure for determining the concentrations and wind speed (e.g., Odman, 1998). Probably the most widely used flux-type scheme is Bott (1989, 1992, 1993), and its derivatives (e.g., Syrakov, 1996; Syrakov and Galperin, 1997, 2000) involving different approximation functions (i.e., Bessel functions instead of Lagrangian polynomials). Although these schemes suffer from both stability and viscosity problems, they are superior to finite-difference approaches. Flux-type schemes also require special efforts to maintain mass conservation.

20 Semi-Lagrangian schemes (e.g., Crowley, 1967, 1968; Egan and Mahoney, 1972; Pedersen and Prahm, 1974; Smolarkevich, 1982; Prather, 1986; Williamson and Rach, 1989; Staniforth and Cote, 1991, and references therein; Galperin, 1999, 2000; Sofiev, 2000b) represent the concentrations as a set of masses distributed according to certain rules inside the grid cell and advect like Lagrangian particles but some properties are conserved. A sub-class of these schemes include purely Lagrangian schemes (Eliassen, 1978; Eerola, 1990; Stohl et al., 2005) where the masses are essentially independent and transported individually with the follow-up reprojection to the computational grid. These schemes have better numerical viscosity, which can be made exactly zero (Galperin, 2000), and stability (i.e., their working range of Courant number is probably the widest out of all types of the advection schemes). However, many

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semi-Lagrangian schemes exhibit large non-monotonicity and other distortions of the transported field, which require substantial efforts and computational resources to be kept under control.

By comparison, Lagrangian schemes are rarely used for chemistry composition computations, mainly due to the unbearable overhead of meeting the requirements posed by nonlinear chemical transformation mechanisms. Nevertheless, such schemes are theoretically possible. Such schemes naturally resolve the numerical diffusion problem, which plagues the performance of almost all Eulerian schemes. Although the diffusion problem is seemingly inevitable in Eulerian schemes, Lagrangian advection schemes do not suffer this problem because they lack explicit discretization of horizontal movement, which is performed in continuous space rather than in predefined grid meshes. As a result, numerical viscosity of purely Lagrangian schemes is always zero. Such a result comes at a price of 100% non-monotonicity of the concentration fields, which originates from limited spatial representativeness of a single Lagrangian particle.

Spectral models (e.g., Kreiss and Olinger, 1972; Prahm and Christensen, 1977; Zlatev and Berkowicz, 1988) use Fourier transformation to convert the differential equations into algebraic ones, which are then solved analytically. Such schemes are more commonly used in NWP models than chemical transport models.

One new line of development, often based on semi-Lagrangian schemes, is adaptive-grid advection algorithms (e.g., Staniforth and Cote, 1991 and references therein; Lagzi et al., 2004; Jablonowski, 2004 and references therein; Jablonowski et al., 2006). These schemes are geared at solving the problems with sharp gradients in the computed variables and with a wide range of spatial and temporal scales of input forcing. The advantage of more accurate computations in the sub-domains that require high resolution outweighs the extra errors introduced by repeated reprojection of the main fields, as well as the extra computational time needed for the grid transformation.

The diversity of advection routines developed during the last 50 years and still under construction is explained by a long list of requirements to such schemes. The most important ones are: positive definiteness to the scheme, minimal numerical viscosity,

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limited non-monotonicity, sufficiently high stability, absence of phase error, local and global mass conservation, and sufficiently high numerical efficiency. Unfortunately, meeting all requirements simultaneously is not possible. For example, more numerical viscosity smoothes the result, thus improving monotonicity.

5 The most important criteria when selecting a scheme seems to be the positive definiteness of the algorithm (i.e., a guarantee that mass will remain positive after the advection step) and monotonicity (i.e., minimizing high-frequency fluctuations of the field). These two criteria can be optimised to some extent at a cost of substantial numerical viscosity, which is a common problem for most of the Eulerian advection schemes.  
10 Only the scheme of Galperin (1999, 2000) has exactly zero numerical viscosity, but at a somewhat increased non-monotonicity of instant concentration fields and additional memory requirements.

Other criteria, sometimes mentioned but rarely taken with the highest priority, are: minimization of phase error (i.e., correct representation of the transport velocity), the scheme transportivity (i.e., shift of the centre of mass of a puff from the analytical solution), and additivity (i.e., correct treatment of superimposed puffs). Two features of the schemes have somewhat outstanding importance: the conservation of mass and costs of the computations. The mass-conservation problem is usually considered as the highest priority in the chemistry-transport models, so that schemes that significantly  
20 violate this requirement are excluded from consideration. Finally, the efficiencies of the advection schemes (both in terms of the computational time and memory) are potentially important, but rarely considered more important than positive definiteness or mass conservation.

25 Interestingly, these two features are not the most important aspects to be considered for NWP models. Although the conservation of mass is desirable in NWP models, this criterion is usually compromised, if an algorithm that is not exactly conservative has a better performance or monotonicity.

Within the 18 models considered in this review, only a few use the same type of solutions. There is, however, a general lack of detail regarding the descriptions of

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the advection mechanisms in the publications for each of the models, which suggests that the schemes are implemented with minor, if any, deviations from the original source. Examples of the schemes used by the selected models are: Bott (1989) (CAMx, Enviro-HIRLAM, MATCH), Piecewise Parabolic Method (PPM) of Colela and Woodward (1984) (CAMx and CHIMERE), Walcek (2000) (RCG, LOTOS-EUROS), Yamartino (1993) and Wicker and Skamarock (2002) (CMAQ, WRF-Chem and FARM), Williamson and Rash (1989) (semi-Lagrangian scheme of MOCAGE), Eerola (1990) (Lagrangian SILAM kernel), Galperin (1999, 2000) (Eulerian SILAM kernel), Janjic (1997) (SKIRON/Dust), Zlatev (1995) (THOR), and Cullen (1993) (NAME).

Some models have more than one advection algorithm. In particular, CAMx has an alternative between Bott and PPM, as well as an optional Plume-in-Grid formulation for representing the large point sources in the lower-resolution grid. The Plume-in-Grid option is also available in CMAQ. Enviro-HIRLAM has as options also semi-Lagrangian schemes, in particular the CISL (Kaas, 2008). SILAM has two dynamic kernels: Lagrangian and Eulerian, either can be selected for a particular run via a switch in the model control file.

## 4.2 Horizontal and vertical turbulent diffusion

Meteorological models drive the chemistry transport models for solving atmospheric diffusion equations for trace species. Diffusion is treated fully in meteorological models, whereas only horizontal and vertical turbulent diffusion is treated in chemistry transport models.

The horizontal diffusion is based on the Smagorinsky approach (1963) within the models ALADIN-CAMx, SKIRON/Dust, FARM, CAMx-AMWFG and MM5-CAMx. The models MM5-CHIMERE, MM5-CAMx and MM5-CMAQ use the Medium Range Forecast Planetary Boundary Layer (MRF PBL) scheme. The MM5 model uses several PBL schemes: Bulk PBL, high resolution Blackadar PBL, Burk Thompson PBL, Eta PBL, Gayno-Seaman PBL and Pleim-Chang PBL. The SILAM system involves two approaches, depending on the kernel: the solution with the Lagrangian kernel uses

prescribed horizontal diffusion via random particle relocation at each model time step (Eerola, 1990); the Eulerian one includes an embedded algorithm that reflects the main features of the  $K$ -closure model; the horizontal eddy diffusivity is dependent on the wind speed.

5 For the description of the vertical diffusion, the  $K$ -diffusion scheme is widely used, but otherwise, there are not many similarities between different models. In ALADIN-CAMx and MOCAGE, the vertical diffusion is calculated according to the Louis (1979) approach, which uses the Richardson number and the mixing length. Two convective boundary layer schemes are implemented in OPANA: Blackadar and the Asymmetric  
10 Convective Model (ACM, Pleim and Chang, 1992). OPANA also includes local diffusion, vertically continuous integration, smooth transition from stable to convective and faster matrix solver, and updated eddy diffusion scheme.

RCG's vertical turbulent mixing formulation uses  $K$ -diffusion in combination to mixing height, which is treated as one layer above a 50-m surface layer. Its stable and convective boundary layer diffusion coefficients are based on PBL scaling regimes. Therefore,  
15 vertical mixing is dominated by the time-dependent evolution of the mixed layer.

FARM also uses  $K$ -diffusion, eddy viscosities can be produced by the meteorological driver or by the preprocessor SURFPRO (SURface atmosphere interFace PROcessor), which can choose among different parameterisations, based on atmospheric  
20 boundary layer (ABL) scaling. In MM5-CHIMERE, the vertical turbulent mixing takes place only in the boundary-layer. The formulation uses  $K$ -diffusion, without the counter-gradient term. The vertical diffusion is mainly modelled with the ACM2 in MM5-CMAQ; WRF/CHEM uses the PBL parameterization by the Yonsei University (YSU).

The Eulerian kernel in SILAM is modelled according to the  $K$ -closure, with the approach of Genikhovich et al. (2004) used for the evaluation of  $K_z$ . The Lagrangian kernel within SILAM assumes a well-mixed ABL and fixed random-walk parameters in the  
25 free troposphere. Exchange between the ABL and the troposphere in the Lagrangian version takes place due to variation of the ABL height. In MATCH the turbulence is parameterized using three primary parameters: the surface friction velocity, the surface

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sensible heat flux and the boundary layer height.

The main limitation of the Lagrangian system of SILAM is the assumption of a well-mixed ABL. For the Eulerian SILAM variant, the  $K$ -closure is used for diffusion in the vertical direction and also for horizontal diffusion. The eddy diffusivity of the vertical profile is evaluated at every time step by Sofiev et al. (2010). The limitations on a large scale originate partly from the simplified free-troposphere diffusion. The Lagrangian kernel assumes fixed mixing coefficient, while the Eulerian one assumes 10% of the ABL maximum  $K_z$  value. In LOTOS-EUROS, the mixing layer is treated as one layer and the ground level output is generated by assuming a vertical profile near the ground based on the deposition velocities.

### 4.3 Chemistry

Presently the main air-pollution issues in Europe are the human health impacts of exposure to particulate matter and ozone, and to a lesser extent nitrogen dioxide, sulphur dioxide, carbon monoxide, lead and benzene (EEA, 2007). Ozone is formed in the atmosphere in photochemical reaction cycles, which brings the ozone precursors (i.e.  $\text{NO}_x$ , VOCs) and their gas-phase atmospheric chemistry, to the focus of CWF. All state-of-the-art chemical modules in most of the modelling systems in this review include these reaction cycles.

The choice of a chemical scheme for a CWF model is always a compromise between its complexity, the requirements and restrictions of the modeling system, how it is applied, and the available computational resources. Basic gas phase inorganic chemistry is usually included in all models, and the schemes are often quite similar because inorganic atmospheric chemistry is well established.

A photochemical oxidation mechanism of VOCs is a must in any CWF model aiming to predict the ozone concentrations – here the models may differ considerably, with different levels of detail and different parameterisations. In addition to the anthropogenic VOCs, the oxidation of biogenic VOCs should be included, especially if the model domain covers regions with dense forests. Aqueous oxidation of the sulphur compounds

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and transfer of species from the gas phase into aqueous and solid phases can also be included, depending on the focus of the modeling system. Several approaches have been developed, which typically involve the simplification of more comprehensive chemical schemes to include only the key chemical constituents and processes. In the following, concise descriptions of some viable approaches are given.

The most commonly used chemical sub-model types among the chemical weather prediction models to be discussed in this review are (in alphabetical order): CBM-IV, ISORROPIA, MELCHIOR, NWP-Chem, RADM2, SAPRC-99, and UNI-OZONE. Some characteristics of these chemical submodels are compared in Table 4.

The implementation of the chemical mechanisms in the chemical weather prediction systems often involves adaptations, updates or other modifications of the original scheme. These changes are not always well documented or transparent. Therefore only the general features of the original chemical schemes are discussed below. In the following, the models using the different chemical modules are listed in brackets in the titles. More information about the details of the implementation of any chemical submodule in a particular CWF system can be found at the web sites of the prediction systems. A list of references on the comparisons of various chemical submodules is presented in Table 5.

Carter's one-product isoprene oxidation scheme (Carter, 1996) is adopted for biogenic compounds in several models, and the ISORROPIA thermodynamic equilibrium scheme (<http://nenes.eas.gatech.edu/ISORROPIA/>, Nenes et al., 1998a,b) is used to determine the physical state and composition of inorganic aerosols in many modeling systems. ISORROPIA does not consider aerosol size distributions or aerosol micro-physical processes, which is why it is included in this section with other purely chemical schemes, instead of in Sect. 4.4.

#### 4.3.1 CBM-IV (CAMx, CMAQ, LOTOS-EUROS, OPANA, RCG, SILAM)

The Carbon bond mechanism IV (CBM-IV, also called CB-IV; Gery et al. 1989; <http://airsite.unc.edu/soft/cb4/cb4main.html>) is a lumped-structured condensed mechanism.

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The carbon bond approach is used to lump organic species. The code treats the reactions of four different types of species: inorganic species, explicit organic species, organic species represented by carbon surrogates and organic species that are represented by molecular surrogates. Inorganic chemistry is represented explicitly with no lumping. Organics represented explicitly are formaldehyde, ethene and isoprene. Carbon bond surrogates describe the chemistry of different types of carbon bonds commonly found as parts of larger molecules. CBM-IV is widely used in research and regulatory air quality models as Models-3/CMAQ (Byun and Ching, 1999).

#### 4.3.2 ISORROPIA (CAMx, CHIMERE, CMAQ, LOTOS-EUROS, RCG, FARM)

ISORROPIA (“equilibrium” in Greek) is a thermodynamic equilibrium aerosol module designed for the calculation of equilibrium concentrations of semi-volatile inorganic species (Nenes et al., 1998a,b; Fountoukis and Nenes, 2007). The aerosol system consists of sulphate, nitrate, ammonium, sodium, chloride and water, partitioned between gas, liquid and solid phases. Aerosol particles are assumed to be internally mixed (i.e. all particles of the same size have the same composition), and the model also determines the water content of the particles. In ISORROPIA, four distinct chemical species are possible in the gas phase, twelve in the liquid phase and nine in the solid phase. The number of species and equilibrium reactions solved in the calculation is determined by the relative abundance of each aerosol precursor ( $\text{NH}_3$ , Na,  $\text{HNO}_3$ , HCl,  $\text{H}_2\text{SO}_4$ ) and the ambient relative humidity and temperature.

ISORROPIA has been optimized for speed and robustness for application in urban, regional and global air-quality models. The performance of ISORROPIA has been evaluated against several in-situ datasets (e.g., Nowak et al., 2006) and compared to other thermodynamic equilibrium schemes (e.g., Nenes et al., 1998b; Ansari and Pandis, 1999a,b; Yu et al., 2005). A new version of the ISORROPIA module, called ISORROPIA II (not used at the moment in any of the discussed CWF models), which includes the treatment of the crustal species (Ca, K, Mg), is available online at <http://nenes.eas.gatech.edu/ISORROPIA/>.

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### 4.3.3 MELCHIOR (CHIMERE)

The MELCHIOR (Modele Lagrangien de Chimie de l'Ozone a l'échelle Régionale; <http://www.lmd.polytechnique.fr/chimere/>; Schmidt et al., 2001) chemical mechanism was originally developed from an earlier version of the EMEP model chemistry (Simpson, 1992; Vautard et al., 2001), with special attention to low NO<sub>x</sub> conditions and nighttime (NO<sub>3</sub>) chemistry. The original extended version of the mechanism includes more than 300 chemical reactions of 80 gaseous species, whereas the reduced version (MELCHIOR2) treats 44 species and about 130 reactions. MELCHIOR2 has explicit oxidation schemes for methane, ethane, *n*-butane, ethene, propene and *o*-xylene. Biogenic compounds are represented by isoprene,  $\alpha$ - and  $\beta$ -pinene, and lumped terpene, humulene and ocimene classes. Eight chemical operators (Carter, 1990; Aumont et al., 1996) are introduced in the reduced mechanism as surrogates for groups of reactive intermediates. In addition to the MELCHIOR2 gas-phase chemical mechanism, the CHIMERE modeling system also incorporates a sectional aerosol module with primary and secondary particles, multiphase sulphur and nitrogen chemistry, and the thermodynamic equilibrium scheme ISORROPIA (Nenes et al., 1998a,b).

The model has been applied e.g. to the simulation of air-pollution episodes at regional and urban scales and ozone-trend analyses (Beekmann and Vautard, 2009, and references therein). The CHIMERE/MELCHIOR modeling system has also been used in operational forecasting of pollutant levels over Western Europe for several years, and it has been extensively compared to observations (<http://www.prevoir.org>; Honoré et al., 2008).

### 4.3.4 NWP-Chem (Enviro-HIRLAM)

The NWP-Chem scheme is an economical scheme designed at DMI for operational forecasting (Korsholm et al., 2008). It consists of the NWP-Chem-Gas gas-phase chemistry scheme and thermodynamic equilibrium model NWP-Chem-Liquid. The scheme includes 27 main reactions and describes the basic chemistry of the photo-

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oxidation of VOC to peroxy radicals, the most important  $\text{NO}_x$  reactions, the most important ozone formation reactions, sulphur (DMS = dimethyl sulfide is included) and isoprene chemistry (biogenic emissions of isoprene  $\alpha$ -pinene and other terpenes affects gas-phase chemistry – such as ozone – as well as aerosol formation). In the present version of NWP-Chem-Gas, the ordinary differential equations are solved using the quasi-steady-state approximation (Hesstvedt et al., 1978).

#### 4.3.5 RADM2 (CAMx, CHEM, CMAQ, Enviro-HIRLAM, EURAD, OPANA, WRF/CHEM) and RACM (Enviro-HIRLAM, EURAD, MOCAGE)

The second-generation Regional Acid Deposition Model (RADM2) gas-phase chemical mechanism (Stockwell et al., 1990) was developed from the earlier RADM mechanism (Stockwell, 1986). The emissions were aggregated into model species based on similarities in chemical reactivity, organic functional groups and the reactivity of the organic compounds with OH. The aggregation factors, rate parameters and product yields for the organic reactions were derived from the organic emissions aggregated into each model species (Middleton et al., 1990).

An evolution of RADM2-RADM, RACM (Regional Atmospheric Chemistry Mechanism), was proposed in (Stockwell et al., 1997). The absorption cross sections and quantum yields that are required input for a program that calculates photolysis rate constants from calculated actinic flux (Madronich, 1987). The mechanism was evaluated against data obtained from the University of California, Riverside, environmental chamber database (Carter et al., 1995).

#### 4.3.6 SAPRC-99 (ALADIN-CAMx, CMAQ, FARM, OPANA)

The chemical mechanism developed at the Statewide Air Pollution Research Center in Riverside, California (SAPRC-99) is a detailed mechanism for the gas-phase atmospheric reactions of volatile organic compounds (VOCs) and oxides of nitrogen ( $\text{NO}_x$ ) in urban and regional atmospheres (<http://www.engr.ucr.edu/~carter/SAPRC99/>). The

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scheme can be used in airshed models to determine absolute and relative ozone reactivities of the many types of VOCs that can be emitted into the atmosphere, and for other control strategy and research applications. This mechanism represents a complete update of the Carter's (1990) SAPRC-90 mechanism and incorporates recent reactivity data from a wide variety of VOCs. The mechanism has assignments for about 400 types of VOCs and can be used to estimate reactivities for about 550 VOC categories.

A condensed version of SAPRC-99 was developed for use in regional models. A unique feature of this mechanism is a computational system to estimate and generate complete reaction schemes for most non-aromatic hydrocarbons and oxygenates in the presence of  $\text{NO}_x$ , from which condensed mechanisms for the model can be derived. The mechanism was evaluated against the results of approximately 1700 environmental chamber experiments carried out at the University of California, Riverside, including experiments to test ozone reactivity predictions for over 80 types of VOCs. The mechanism was used to update the various ozone reactivity scales developed by Carter (1994), including the widely used Maximum Incremental Reactivity (MIR) scale. However, the reactivity estimates for many VOC classes are uncertain, which must be taken into account when using these data for regulatory applications. For this reason, uncertainty classifications have been assigned to all VOCs, and upper limit MIRs for VOCs with uncertain mechanisms are presented.

A new version of the SAPRC chemical mechanism called SAPRC-07 (not used at the moment in any of the discussed CWF models) is available online at <http://www.engr.ucr.edu/~carter/SAPRC>, including references to detailed description about improvements and new compounds in the new version.

#### 4.3.7 SILAM acid basic (SILAM)

The scheme is a further development of the DMAT model algorithm (Pressman et al., 1991; Galperin and Sofiev, 1998; Sofiev, 2000) and is oriented for the treatments of the production processes of the secondary inorganic aerosols, such as sulphates, nitrates

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and ammonia. It includes 29 species, 12 photochemical, 27 inorganic and 12 methane and ethane reactions. Most of reactions take place in the gas phase and constitute the oxidation of SO<sub>x</sub>, NO<sub>x</sub>, and NH<sub>x</sub>.

The ozone cycle is considered via the photostationary equilibrium shifted in the presence of organic species. This approach does not lead to an accurate ozone estimation but is sufficient for partitioning of NO<sub>x</sub> to NO and NO<sub>2</sub>. Aqueous-phase and heterogeneous reactions are responsible for within-droplet SO<sub>2</sub> oxidation, N<sub>2</sub>O<sub>5</sub> hydrolysis and three-component equilibrium between ammonium, ammonium nitrate, and nitric acid, the description of which generally follows Finlayson-Pitts and Pitts (1998).

The previous version of the scheme has been evaluated within the scope of EMEP programme (Sofiev et al., 1994) and a multi-annual evaluation was made by Sofiev (2000). The current scheme version is used in the MACC project with daily operational evaluation (<http://www.gmes-atmosphere.eu>). A comparison with NO<sub>2</sub> total column observed by OMI instrument onboard of Aura NASA spacecraft has been performed by Huijnen et al. (2010).

#### 4.3.8 UNI-OZONE (EMEP model, MATCH (EMEP-MS-C-W))

The chemical scheme of the Unified EMEP Model (UNI-OZONE, <http://www.emep.int/OpenSource/index.html>; Simpson et al., 2003) contains full oxidant chemistry, gas and aqueous oxidation of SO<sub>2</sub> to sulphate, ammonium chemistry, nighttime production of HNO<sub>3</sub> and nitrate, coarse nitrate particle formation, as well as the advection of primary particles. Therefore, the scheme provides comprehensive chemistry for both photo-oxidant and acidification studies. The VOC scheme is lumped, with explicit oxidation mechanisms for methane, ethane, ethanol, *n*-butane, ethene, propene, *o*-xylene and isoprene.

The EMEP model is under constant revision by the Executive Body for the Convention on Long-range Transboundary Air Pollution (LRTAP). In the 1990s, the EMEP models also became the reference atmospheric dispersion model for use in the Integrated Assessment Models supporting the development of air-quality policies under

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the EU Commission. The chemical schemes of the EMEP model have been extensively intercompared with other atmospheric chemistry models (e.g., Kuhn et al., 1998; Andersson-Sköld and Simpson, 1999; Gross and Stockwell, 2003; Jimenez et al., 2003; Cuvelier et al., 2007; Vautard et al., 2007).

### 4.3.9 Synthesis and recommendations

All chemical sub-models discussed in this chapter are implemented at least in one CWF model. Several comparisons of the chemical schemes and also the modeling systems have been carried out and are documented in the literature. However, no one study covers all the schemes or sub-models discussed here, and both the objectives and the implementation of the intercomparisons differ greatly. Thus, it is not possible to rank the performance of the sub-models in relation to each other, based on the existing literature.

Table 5 provides a comprehensive overview of the intercomparisons between different chemical schemes, including some that were not part of this study. A common conclusion in several of the documented intercomparisons appears to be that most models are able to reproduce or predict the ozone concentrations fairly well, whereas they do not perform as well in simulating other compounds, such as  $\text{NO}_x$  and their reaction products (e.g., Kuhn et al., 1998; Gross and Stockwell, 2003; Jimenez et al., 2003; Vautard et al., 2007; Luecken et al., 2008). The skill of the models in simulating  $\text{PM}_{10}$  concentrations has also been poor or moderate (e.g., Vautard et al., 2007). A better understanding of the VOC oxidation mechanisms, especially because of their important role in secondary organic aerosol (SOA) formation (e.g., Kanakidou et al., 2005; Tunved et al., 2006) and the implementation of these processes in the CWF modeling systems also presents a formidable future challenge for the chemical scheme.

The relative importance of the different components of chemical schemes (e.g., inorganic, organic, and aqueous phase chemistry) depends on the scientific aim and the applications of the CWF modeling system. Clearly, besides the structure of the chemical sub-module, the amount of available computer resources is another limiting factor

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for the accuracy of the concentration predictions. Available computer power may set an upper level for the complexity of the chemical schemes that can be incorporated in the CWF modeling systems. The aim for any CWF model is therefore to find the chemical sub-model with the best balance between scientific accuracy and computational efficiency.

#### 4.4 Aerosols

The demands for more accurate and detailed aerosol-size distribution, microphysics and chemistry description capability in atmospheric models have increased dramatically during recent years. On the one hand, this is due to the fact that aerosols represent the largest uncertainty in global climate models when predicting radiative forcing; this has been stated, e.g., in the last Intergovernmental Panel on Climate Change (IPCC) report (Solomon et al., 2007). On the other hand, and more relevantly to this review, particle size, composition and morphology are crucial to estimate lung penetration of aerosols and their health effects. This important motivation has resulted in a development and refinement of aerosol modules that are used in CWF models.

Atmospheric particulates have numerous sources, ranging from primary emissions (such as dust or pollen) to complicated aerosol formation processes involving gas phase, liquid phase and surface reactions. This presents several challenges to CWF models, especially as only a limited number of aerosol process sub-models are generally available, and the state-of-the-art has not yet been established. As in the case of chemistry modules, there is no generally recognised single model that would be widely used by most of the CWF models.

Air-quality models also commonly include only a small fraction of the particulate matter components; this commonly leads to an underprediction of PM mass values. E.g., in most cases, natural pollen is missing, suspended dust may be missing or not accurately evaluated, sea salt and emissions from wild-land fires may be missing, and secondary organic compounds are in many cases poorly represented.

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The different aerosol description options can be classified by a) how the size distribution is represented and b) what kind of aerosol microphysics is included in the modelling system. We classify the aerosol process methods in the following according to the way they represent the size distribution. These can be grouped in three different categories: bulk schemes, modal schemes and sectional schemes. Some models have only one choice for the aerosol size distribution description, whereas others have several options.

One limitation to using detailed aerosol size distribution and composition descriptions arises from the lack of size- and composition-segregated emission data. The emission inventories are typically based on total mass only, and using a modal or sectional scheme requires assumptions about the emission size and chemical composition distributions.

The state-of-art at present consists of a size-resolved sectional representation for the aerosol size distribution with equilibrium chemistry partitioning packages for both inorganics and organics. In addition, all major microphysical processes (nucleation, coagulation, condensation, wet and dry deposition) are included, as well as schemes for biogenic and anthropogenic secondary organic aerosol (SOA) formation. Table 6 lists different characteristics of each of the various aerosol modules.

#### 4.4.1 Bulk schemes

In *bulk schemes*, typically the total mass of suspended particles (TSP) or the mass in a certain size interval, or several non-interacting intervals, is modelled. The intervals are typically one or some combination of  $PM_1$ ,  $PM_{2.5}$ ,  $PM_{10}$  and TSP. Such an approach is computationally efficient, but naturally has severe limitations, when size-dependent processes are important.

To estimate the health effects of the respirable particles better, the focus of both measurements and modelling has gradually moved from  $PM_{10}$  and TSP to  $PM_{2.5}$  and  $PM_1$ . Since the lung penetration function and the health effects are in a complicated manner dependent on both the size and chemical composition, bulk schemes will likely be

replaced gradually by the more accurate (but computationally more expensive) modal and sectional schemes.

#### 4.4.2 Modal schemes

In *modal schemes*, the aerosol size distribution is represented by a number of modes, the properties of which are modelled as functions of time and location. This typically involves a pre-described assumption (e.g., log-normal) of the functional form of the modes. This approach is computationally more expensive than bulk methods, but less resource-consuming than sectional methods. For this reason, such schemes have been quite common in regional and global models. The performance of modal schemes is limited, when new-particle formation is important.

#### 4.4.3 Sectional schemes

In *sectional schemes*, the continuous size distribution is replaced by a number of discrete bins (i.e., the size distribution is approximated by a histogram). The model has equations for the particle concentration (number or mass) and chemical composition that are solved for each bin. The sectional scheme is the most flexible and accurate one, but it is computationally the most expensive. With increasing computing power and memory, more CWF models are adopting sectional schemes as their choice for aerosol size distribution representation. A major challenge for CWF's using sectional aerosol representations is improving the quality and level of detail of the emission inventories to match the sophistication of the rest of the model.

#### 4.4.4 Aerosol microphysics

The main microphysical processes affecting the aerosol size distribution are nucleation, condensation/evaporation, coagulation and deposition. Nucleation, or the formation of new particles through a gas to particle phase change, has been observed to occur throughout the atmosphere (e.g., Kulmala et al., 2004) and is an important particle

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source, especially in the nucleation and Aitken mode size ranges. Clearly, particle growth by condensation does not change the number concentration, but alters particle size and the mass concentration. Atmospheric coagulation is typically a process between small nucleation or Aitken mode particles and larger accumulation-mode or coarse-mode particles. Coagulation does not change the mass concentration, but decreases the number concentration of particles.

In bulk schemes, typically only deposition is considered, without an accurate way to describe its dependence upon particle size. Condensation/evaporation is usually treated by assuming equilibrium between the gas and particle phases, by using a chemical equilibrium thermodynamics scheme, such as ISORROPIA, or the Equilibrium Simplified Aerosol Module (EQSAM). In sectional and modal schemes, all the above-mentioned microphysical processes can be adequately described, which is important especially, when detailed information is desired on the particle number concentration distribution or the chemical composition distribution as a function of size.

## 4.5 Deposition

Dry and wet deposition are processes that remove pollutants from the atmosphere. Not only are accurate schemes required for producing realistic concentrations of pollutants in the atmosphere, but deposited pollutants can affect soil and vegetation (e.g., acidification) and water bodies (e.g., eutrophication). The spatial distributions of wet and dry deposition are therefore commonly assessed in the various long-term environmental assessment programmes (e.g., EMEP). Uncertainties in modelling deposition, however, can limit accurate forecasts of ground-level pollutant concentrations. For example, sensitivity tests by Wesely and Hicks (2000) showed that daytime ozone concentration could increase by about 20%, when dry deposition is not acting.

References and brief characterizations of the dry and wet parameterization schemes used in the CWF models considered are summarized in Table 7.

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## 4.5.1 Dry deposition

Dry deposition is governed by the turbulent and molecular diffusion of pollutants in the atmosphere. The amount of deposition depends upon the characteristics of the surface, vegetation, and the characteristics of the depositing species (e.g., the solubility and chemical reactivity for gases and the size distribution and chemical composition for particles). Gravitational settling also needs to be accounted for for coarse particles. E.g., Seinfeld and Pandis (1998) and Sportisse (2007) provide a more comprehensive description of deposition.

Therefore, a successful dry deposition scheme should be capable of reproducing both the boundary-layer turbulent fluxes and the interaction between the pollutant and the surface. The choice of parameterization is conditioned by the meteorological model, which provides the surface-layer turbulence, by the surface and soil characteristics and by input data availability. For example, in regional models, bulk schemes for canopies (often called big-leaf schemes) are generally preferred to so-called multi-layer canopy models. The latter could be considered more suitable to describe deposition processes within tall canopies, but their use may be hindered by the lack of input data to describe the vertical structure of vegetation.

Dry deposition is commonly formulated in Eulerian models as a boundary condition at the ground surface for the vertical diffusion term of the pollutant transport equation. In this term, a species-dependent vertical concentration flux is the product of a deposition velocity  $V_d$  and the surface concentration. In state-of-the-art CWF models, the mathematical treatments of the dry deposition for gases and aerosols are usually based on the resistance analogy, where the inverse deposition velocity is the sum of three different resistances in series ( $V_d^{-1} = R_a + R_b + R_c$ ): the aerodynamic resistance  $R_a$ , due to turbulent diffusion, the quasi-laminar layer resistance  $R_b$ , due to molecular diffusion, and the canopy resistance  $R_c$ , due to the capture of pollutants by the surface (e.g., Wesely, 1989; Seinfeld and Pandis, 1998).

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Differences in modelling dry deposition among various CWF models arise from different ways to estimate the resistance terms, but also arise from the way the models are interfaced with the meteorological models. The aerodynamic and quasi-laminar resistances are a function of the atmospheric stability and friction velocity ( $u_*$ ), which depend on the coupling strategy chosen for each modelling system. Online coupled models and some offline coupled models use parameters (e.g., surface momentum flux) provided by the meteorological model, while other offline models prefer to re-estimate them through diagnostic parameterizations usually based on similarity theory. These different approaches can cause differences in the predicted deposition, even if we consider models implementing the exactly same parameterization.

The dry deposition schemes in the CWF models in this study are largely similar. The aerodynamic resistance  $R_a$  and the quasi-laminar sub-layer resistance  $R_b$  are parameterized in terms of the friction velocity, surface roughness and molecular diffusivity of species (Wesely and Hicks, 1977; Walcek et al., 1986; Hicks et al., 1987; Chang et al., 1987, 1990; Wesely, 1989). This approach is adopted by CAMx, CHIMERE, FARM, LOTOS-EUROS, MOCAGE, NAME, RCG, SILAM, THOR and EnviroHIRLAM.

Greater differences among the CWF models occur for the parameterization implemented for the surface resistance  $R_c$  (Table 7). Usually, the surface resistance is expressed as a set of parallel resistances associated with leaf stomata, leaf cuticles, lower canopy resistances (e.g., bark, stems), and surface soil and water. Over land,  $R_c$  can be expressed as the sum of foliar ( $R_{cf}$ ) and ground ( $R_{cg}$ ) resistances ( $1/R_c = 1/R_{cf} + 1/R_{cg}$ ), and foliar resistance is subdivided in stomatal ( $R_{st}$ ) and non-stomatal or cuticle ( $R_{cut}$ ) resistances ( $1/R_{cf} = 1/R_{st} + 1/R_{cut}$ ). Many different approaches have been developed for the calculation of stomatal resistance, varying from a simple function of solar radiation and temperature (Wesely, 1989), a big-leaf approach taking into account air temperature and humidity, together with leaf-area index and canopy wetness (Hicks et al., 1987), to a multilayer leaf-resistance model (Baldocchi et al., 1987).

For non-stomatal resistance, a constant value is often chosen, depending on season and land type (e.g., Wesely, 1989). Other models use meteorological variables such as  $u_*$  and canopy height as scaling parameters to characterize in-canopy aerodynamic resistance, and relative humidity to describe the cuticle resistance (Erisman et al., 1994). A more detailed parameterization for cuticles taking into account meteorological and season dependent vegetation parameters has been proposed by Zhang et al. (2003). The parameterizations implemented within each model are summarized in Table 7.

The dry deposition velocity of particles  $V_d$  can be written as  $V_d = V_s + (R_a + R_b + R_a R_b V_s)^{-1}$ , where  $V_s$  is the settling velocity. The previous formula is derived assuming that particle settling operates in parallel with the three resistances in series already introduced for gases. This approach is implemented in almost all the CWF models (Table 7).

Although the differences of these mathematical treatments may seem small, they can nevertheless result in substantial differences to the model predictions. For example, Sportisse (2007) showed that the implementation of a different mass-conserving formula, expressed as  $V_d = V_s(1 - \exp(-V_s(R_a + R_b)))^{-1}$  (Venkatram and Pleim, 1999), can reduce coarse-particle deposition velocities in low-wind conditions by up to 20%. Published comparisons of deposition velocities obtained by different models applied on the same areas showed uncertainties of  $\pm 30\%$  (Wesely and Hicks, 2000). Timin et al. (2007) performed a sensitivity analysis of CMAQ surface concentrations to the dry deposition scheme, showing that the simpler scheme available in CMAQ (based on Wesely, 1989) produces lower deposition velocities for all the species, and ozone 8 h average concentrations increased up to 10–20 ppb, with respect to the more up-to-date M3Dry scheme (Pleim et al., 2001). Dry deposition parameterization has been identified as one of the main causes of differences between their CMAQ and CAMx simulations.

In their summary of dry deposition, Wesely and Hicks (2000) found that resistance schemes are quite reliable in daytime conditions over flat terrain, but are less reliable

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for mountainous areas and during nighttime stable conditions. The reasons are that the parameterizations of aerodynamic resistance, usually based on surface layer similarity theory, do not provide an accurate evaluation of turbulent mixing during stable stratification and in complex terrain.

Additional uncertainties reside in the subgrid variation of surface and land use features, where horizontal advection effects are not considered in summing the contributions from different patches with different surface effects. For homogeneous atmospheric and surface conditions, improper definition of surface features, e.g., vegetation and soil moisture, can result in large differences between modeled and measured deposition. Zhang et al. (2003) showed that a detailed description of cuticles and soil resistances can improve the description of daily variation and maximum value of deposition velocity for wet canopies. In such conditions, stomatal uptake is not important, due to stomata blocking by waterdrops and to the presence of very weak solar radiation.

Petroff et al. (2008) recently compared performances of selected analytical and differential dry deposition models for aerosols versus measurements over grass and forest. Analytical models rely on parameterizations of different complexity, as those previously mentioned for the different resistances. Differential models solve the differential transport equations for the different chemical species within the canopy layer, and require as input vertical profiles of parameters describing vegetation features, as the leaf area density.

Differences in the deposition velocity of up to one order of magnitude have been obtained for fine particles (Petroff et al., 2008). Analytical models (Slinn, 1982; Zhang et al., 2001) displayed small variations in the deposition velocity, when applied to grass and forest. In contrast, differential models (Davidson et al., 1982; Wiman and Agren, 1985) exhibited large differences in deposition velocity, but showed a strong dependence on parameters describing canopy geometry and aerodynamics, such as the leaf area index, obstacle size, roughness length and displacement height, that can be difficult to properly determine for regional model applications.

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## 4.5.2 Wet deposition

Wet deposition refers to scavenging of contaminants and their transport to the earth surface by atmospheric hydrometeors and is usually subdivided into in-cloud scavenging (rainout) and below-cloud scavenging (washout). Although dry deposition is introduced in Eulerian numerical models as a lower boundary condition in flux form, wet deposition is described as a depletion term within transport-diffusion equation for pollutants concentration and can be parameterized by  $dC/dt = -\Lambda C$ , where  $C$  is the substance concentration and  $\Lambda$  is the scavenging coefficient ( $s^{-1}$ ). The scavenging coefficient is different from zero where precipitation occurs and in presence of condensation (clouds or fog). The existing computational schemes for the scavenging coefficient range from simple functions of rain rate and cloud-water content, to complex models describing the system of physical, microphysical and chemical processes that characterize the interaction of gases and aerosols with cloud condensate and precipitation (e.g., Seinfeld and Pandis, 1998; Sportisse, 2007).

Simple parameterizations can be considered that could potentially be sufficient to CWF models, especially for offline coupled models, which have no access to the full meteorological model microphysics. For a reliable short-term estimate of near-ground air-pollutant concentrations, below-cloud scavenging is expected to dominate, at least in areas characterized by relevant local and regional emissions, where short-range transport dominates over long-range contribution, such as, e.g., in continental and Mediterranean Europe. Neglecting in-cloud scavenging should underestimate the mass of deposited pollutant, but have only a weak effect on surface concentrations. Moreover, cloud-aerosol interactions can modify precipitation rate and its spacial distribution, and therefore indirectly influence near-surface scavenging. However, these phenomena can be described only by online coupled CWF's that can implement cloud-pollutant interactions and can take into account feedback effects of air pollution on meteorology.

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Wet deposition schemes vary much more than the dry deposition schemes for the operational CWF models in this article. For example, LOTOS-EUROS, MATCH, FARM and RCG use simple parameterizations of scavenging rates that are similar to those implemented in the EMEP Unified model (Simpson et al., 2003). These depend on Henry's law constant, rain rate and cloud water mixing ratio for gases, and on particle size, precipitation intensity and raindrop fall speed for aerosols. The possible release of scavenged gases and aerosols due to cloud- or rain-water evaporation is not taken into account by the latter parameterization. In contrast, NAME, SILAM and THOR use scavenging coefficients depending upon cloud type (convective vs. stratiform) and precipitation type (rain vs. snow). Other models, such as CHIMERE and EnviroHIRLAM, use more complex in-cloud and below-cloud scavenging parametrizations, whereas LOTOS-EUROS and RCG neglect in-cloud scavenging.

Even though rain has a polydisperse distribution of drop size and pollutant scavenging is dependent upon the fall velocity of the droplets, expressing the scavenging coefficients as a simple function of rain rate appears to be justified. However, it is dependent upon the properties of the pollutant (Mircea and Stefan, 1998; Andronache, 2003; Sportisse, 2007). The main uncertainty of this simplified approach, implemented in almost all the considered CWF models, is contained in the evaluation of rain intensity and its variability within the time interval, over which it is output from the NWP model. Although wet deposition seems weakly related to drop size, it is much more strongly dependent upon aerosol size. For example, Baklanov and Sørensen (2001) and Andronache (2003) showed that below-cloud scavenging was dependent upon aerosol size distribution, being important for very small ( $<0.01 \mu\text{m}$ ) and coarse ( $>2 \mu\text{m}$ ) particles. Therefore, boundary-layer aerosol-size distribution can be modified by precipitation, with quick removal of coarse particles. A proper description of aerosol size distribution within precipitation scavenging parameterizations is therefore required to estimate size-resolved PM concentrations.

Comparing the results from wet deposition schemes in different models is difficult because of the complexity of the CWF models (e.g., spatial and temporal differences

between forecasted cloud and precipitation, aerosol size and composition). Textor et al. (2007) compared results from 16 global models participating in the AeroCom project (Schulz et al., 2009) and found a large variability in the ability of models to handle wet deposition. They had difficulty in identifying the reasons for the main differences (e.g., the models did not provide the same indication about the type of rain; convective or stratiform precipitation) that was most efficient in removing aerosols from the atmosphere. Ultimately, a reliable evaluation of different parameterizations for wet deposition will only be obtained by implementing them within the same model, a task that remains yet to be done.

#### 4.6 Natural emissions

Emissions can be broadly classified into natural and anthropogenic ones. Natural emissions is a wide term that includes different compounds (e.g., NO<sub>x</sub>, SO<sub>2</sub>, NH<sub>3</sub>, PM, Non-Methane Volatile Organic Compounds (NMVOC's), CH<sub>4</sub> and CO) emitted from sources like vegetation, soils, animals, wetlands, sea salt, primary biological aerosol particles, wind blown dust, volcanoes, lightning, forest fires, etc. Anthropogenic emission inventories are not addressed in detail in this study, but some challenges in their development are discussed in Sect. 7.1.

Air pollutants from natural sources play a prominent role in the physics and chemistry of the atmosphere and also contribute to the ambient air concentrations of anthropogenic air pollutants (e.g., O<sub>3</sub>, PM, SOA; Seinfeld and Pandis, 2006). For example, the organic compounds released in the atmosphere by vegetation, collectively referred to as Biogenic Non-Methane Volatile Organic Compounds (BNMVOCs), contribute to the formation of O<sub>3</sub> (Curci et al., 2009; Wang et al., 2008; Bell and Ellis, 2004) and SOA (Kleindienst et al., 2007; Kanakidou et al., 2005). Curci et al. (2009) simulated an average 5% increase in summer daily ozone maxima over Europe due to BNMVOC's emissions with peaks over Portugal and the Mediterranean Region (+15%). BNMVOC's suppress the concentrations of the hydroxyl radical (OH), enhance the production of peroxy (HO<sub>2</sub> and RO<sub>2</sub>) radicals and generate organic nitrates that can sequester NO<sub>x</sub>

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and allow long-range transport of reactive N (Fehsenfeld et al., 1992).

The sea salt flux from the sea surface is an important factor in the formation of cloud condensation nuclei (CCN) in the marine boundary layer (MBL), impact sea surface-atmosphere exchange and heterogeneous chemistry, including the oxidation of SO<sub>2</sub> and NO<sub>2</sub> in the MBL (Foltescu et al., 2005; Pryor et al., 2001). In Europe, the contribution of mineral dust to PM<sub>10</sub> concentrations varies from 10% to more than 30% depending on location and season (Putaud et al., 2004) and, in the United States, the fraction of mineral dust found in PM<sub>2.5</sub> exceeds 10% in most areas and reaches 50% in dry areas (Vautard et al., 2005; Malm et al., 2004).

Volcanoes release considerable fluxes of gases and particles to the atmosphere, both during eruptions and by long-term noneruptive degassing. Water, carbon dioxide, and sulphur species represent by far the predominant component of volcanic gases. In Europe, significant volcanic emissions have been to date limited to Italy and Iceland. An extensive compilation of available, measured volcanic sulphur fluxes has been carried out for the Global Emissions Inventory Activity (GEIA) (Andres and Kasgnoc, 1998). The data set contains volcanic SO<sub>2</sub> emissions averaged over the twenty-five years from the early 1970's to 1997. It includes average SO<sub>2</sub> emissions from 49 continuously emitting volcanoes (four located in Europe: Etna, Stromboli, Vulcano and Kverkfjoll) and maximum SO<sub>2</sub> emissions from 25 sporadically emitting volcanoes (none located in Europe).

The gaseous and particulate natural emissions accounted for in the CWF systems, as well as their calculation methodologies, are presented in Table 8.

#### 4.6.1 Natural gaseous emissions

In most cases, the methodologies for the quantification of natural emissions require input data like emission potentials based on measurements, meteorological data and land use data (e.g. land cover, leaf area index (LAI)) derived from satellite observations. The estimated natural emissions are gridded data and have to be speciated according to chemical mechanisms used by the photochemical grid models. In European scale,

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there are some studies focusing on the estimation of natural emissions and on their impact on air quality (Simpson et al., 1999; NATAIR, 2007; Curci et al., 2009). However, the uncertainties with regard to natural emissions are still very large (larger than those of anthropogenic emissions).

5 Almost all CWF models use biogenic emissions (isoprene or/and monoterpenes or/and other volatile organic compounds (OVOCs) emissions from vegetation) in the forecast runs. Biogenic emissions are mostly calculated with the use of emission models (MEGAN, BEIS3, AUTH-NKUA model, BIOEMI model) and modules or in a few cases, they are taken from existing databases. The algorithms that are usually applied  
10 are those introduced by Guenther et al. (1993, 1994, 1995) according to which isoprene emissions are temperature and light dependent while monoterpenes and other VOC emissions are temperature dependent. Additional processes relevant with the emissions of biogenic compounds are described by some of the emission models like BEIS3 that provides species-specific biogenic emissions factors that are adjusted for  
15 the winter and LAI for each land use type to adjust the isoprene emissions for the effects of the Photosynthetically Active Radiation penetrating through the leaf canopy or the AUTH-NKUA model that accounts for the light dependency of monoterpenes emissions from some vegetation species.

20 MEGAN describes the variation of biogenic emissions as a function of numerous environmental variables and factors (except for temperature and light) like leaf area index (LAI), humidity, the wind conditions within the canopy environment, the leaf age and the soil moisture while it accounts also for the losses and productions in the canopy. Emissions from soils, mainly nitric oxide as a function of soil temperature, land use and fertilizer input, are used as input data to only some of the CWF  
25 models (ALADIN-CAMx, CAMx-AMWFG, FARM, MM5-CHIMERE, MOCAGE, RCG, SILAM, THOR, WRF/CHEM). Other gaseous natural emissions like those from volcanoes, oceans and animals are hardly accounted for in the air quality forecast models (only in CAMx-AMWFG, MOCAGE, SILAM and THOR). Lightning emissions of NO<sub>x</sub> from the Global Emissions Inventory Activity (GEIA) database are used in the opera-

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tional runs of THOR model.

#### 4.6.2 Natural particulate matter emissions

Some particulates occur naturally, originating from volcanoes, dust storms, forest and grassland fires, living vegetation, and sea spray. In this section, we focus on primary aerosol emissions, especially dust and sea salt particles, which constitute the largest contribution to total aerosol mass. Others are formed by way of the transformations of pollutants such as sulfur dioxide, nitrogen oxides and ammonia into sulfates, nitrates and ammonium, respectively (secondary aerosol). Many volatile organic compounds are converted to oxidized organic species with low volatility, thus becoming a component of ambient aerosol.

FARM and MM5-CHIMERE use the methods proposed by Vautard et al. (2005) and make use of a simplified bulk scheme for the calculation of mineral dust emissions (cf. Table 8). Vautard et al. (2005) also propose a simplified scheme to calculate the emissions which depend on turbulence near the ground because it is assumed that the resuspension of material which is available on the ground can explain remaining contributions of missing parts of the  $PM_{10}$  average load. The desert dusts emission fluxes mainly depend of wind velocity and on the surface features (Marticorena and Bergametti, 1995). The emission modules account for the effects of the soil size distribution, surface roughness and soil moisture. The dust module developed by the AM&WF (Atmospheric Modeling and Weather Forecasting Group, School of Physics, University of Athens, Athens, Greece) Group is used by SKIRON/Dust and CAMx-AMWFG. The current model version incorporates state-of-the-art parameterizations of all the major phases of the atmospheric dust lifecycle such as production, diffusion, advection, and removal, including as well the effects of the particle size distribution on aerosol dispersion and deposition. Different size bins can be considered with diameters ranging from 0.1–10  $\mu\text{m}$  following a log-normal distribution (Zender et al., 2003). During the model run, the prognostic atmospheric and hydrological conditions are used in order to calculate the effective rates of the injected dust concentration based on the

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viscous/turbulent mixing, shear-free convection diffusion and soil moisture. The RCG model uses the methods by Loosmore and Hunt (2000) and Claiborn (1998) to calculate the resuspension of dust. MOCAGE has been coupled with a module of dynamic source of dust emissions. According to Martet et al. (2009) it uses a size-resolved (bin) approach.

Sea spray droplets come in three varieties: film, jet, and spume. Film and jet droplets derive from one process: air bubbles bursting at the sea surface. When a bubble rises to the surface, its film-thin top eventually ruptures and ejects tens to hundreds of film droplets with radii ranging roughly from 0.5 to 5  $\mu\text{m}$ . After the bubble bursts, it collapses and in so doing shoots up a jet of water from its bottom. Because of velocity differences along this jet, it soon breaks up into a few jet droplets with radii typically from 3 to 50  $\mu\text{m}$ , depending on the size of the bubble. Spume droplets derive from another process: the wind tears them right off the wave crests. To estimate the sea salt emissions it is essential to know the rate at which spray droplets of any given size are produced at the sea surface (i.e., the sea-spray generation function) is essential. Spray droplets are the source of the local marine aerosol. LOTOS-EUROS, SILAM and MM5-CHIMERE quantify the bubble- and spume-production mechanisms using the approach of Monahan et al. (1986).

In SILAM, the aerosol-size distribution is extended to submicrometer particles according to Martensson et al. (2003). RCG and CAMx-AMWFG also simulate the processes of sea-salt aerosol generation, diffusive transport, transformation, and removal as a function of particle size (Gong et al., 1997). FARM and CAMx-AMWFG implemented the methods proposed by Zhang et al. (2005b), which present a straightforward method to correct sea-salt-emission particle-size distributions according to local relative humidity.

In comparison with the main anthropogenic emission sources, the released amount of pollen particles depends on numerous parameters that are related to meteorological conditions. The emission modules for pollen therefore should include treatments, e.g., for the effects of the accumulated heat sums, start and end dates of the pollinating sea-

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son, the mean climatological rate of release, the correction functions related to wind, temperature, humidity, and precipitation, and the diurnal cycle of the pollen production. Pollen emissions are used as input emission data only in SILAM and Enviro-HIRLAM forecast runs. For this reason, emission modules have been developed by FMI and DMI. The most difficult problems in pollen-dispersion are to evaluate the emission flux of grains and their time evolution. According to Sofiev et al. (2006a), SILAM used in the frame of trial forecasts during spring 2004 a “climatologic” emission term, which was based on the results of long-term mean observed birch flowering dates. The system is based on the European flowering start and duration maps from the International Phenological Garden Project (IPG, 2004). The maps were compiled by Rötzer and Chmielewski (2001) using multilinear regression analysis of phenological observations in Europe over 35 years (1961–1998).

Mahura et al. (2009) investigate the patterns of birch pollen counts over a diurnal cycle and propose a parameterization that is useful for inclusion into operational and research short- and long-term modeling with Enviro-HIRLAM for birch pollen atmospheric transport and deposition at different spatial scales. The evaluation of patterns of diurnal cycles on monthly and interannual bases has been done based on analysis of a 26 year time series of birch pollen counts from the Danish pollen measurement site in Copenhagen. The suggested parameterization, based on a simple trigonometric function, includes dependencies on the time of birch pollen maximum and minimum occurrence on a diurnal cycle, averaged concentration at the end of the previous day, and time shift.

Concerning the emissions from biomass burning and wild-land fires, THOR uses the emission dataset of the EU project REanalysis of the TROpospheric chemical composition over the past 40 years (RETRO). Sofiev et al. (2009) investigates the potential of two remotely sensed wild-land fire characteristics (4  $\mu\text{m}$  brightness temperature anomaly (TA) and fire radiative power (FRP)) for the needs of operational chemical transport modelling and short-term forecasting of atmospheric composition and air quality. The core of the methodology is based on empirical emission factors



that are used to convert the observed temperature anomalies and fire radiative powers into emission fluxes. In the paper a new generation fire assimilation system (FAS) is presented, which evaluates globally the emission fluxes of primary particulate matter originated from wild-land fires on a daily resolution. The predicted emissions in Europe are subsequently scaled to other pollutants using emission factors from the literature and submitted to the chemical transport model SILAM for diagnostic assessment and forecasting of the atmospheric composition.

#### 4.7 Horizontal and vertical grid spacing

In this article, we distinguish between grid spacing and resolution of the CWF models (Pielke, 1991, 2001; Laprise, 1992; Grasso, 2000a,b). Grid spacing can be simply defined as the distance between numerical grid points; however, resolution can in many cases be an ambiguous or poorly defined concept. Resolution commonly refers to the spatial or temporal scale, on which various phenomena can be resolved by the model or modelling system. However, for instance the minimum distance scale, on which phenomena can be resolved, may vary from two to ten times of the grid spacing. The resolution (or grid spacing) can also be different for the emission data, meteorological data, land use data, other input data, the computational grid of the model, the receptor grid of the model, and other data. It is therefore not always clear what is meant with the overall resolution of the modelling system, and how it has been validated for a specified phenomenon. Therefore, whenever possible we prefer to use the more precise term grid spacing.

A summary of the grid spacings and coordinate systems of the different models appear in Table 9. Clearly, CWF models can be implemented with various horizontal and vertical grid spacings, depending upon the atmospheric scales to be modeled. Computational time limitations of having forecasts appear in real-time during operational forecasts restrict the domain size and grid spacing. Modelling on the continental, regional, and background urban scales necessarily require different horizontal grid spacings. For example, a CWF model for forecasting regional or municipal air quality requires small

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horizontal grid spacing (e.g., of the order of from 1 to 20 km), but does not necessarily require model levels in the stratosphere. In contrast, continental-scale models typically have 10–50 km horizontal grid spacing and should in many applications include treatments at least for the entire troposphere and the lower stratosphere. Clearly, the selection of the appropriate grid spacing depends upon the details of the modelling system and the particular application.

Most of the models described in this paper use multiple grids that may have different horizontal grid spacings for the meteorological and air quality components (for the offline models). In that way, the CWF models may cover the continental and regional scale across Europe and, with the finer grids (sometimes nested), they may focus on a more detailed forecast of a specific region. For instance, the modelers used in 2010 coarse grids covering Europe with horizontal grid spacings in the range of 20 km (SILAM), 25 km (CAMx-AMWFG, RCG, SKIRON/Dust, EURAD-RIU), 30 km (ALADIN-CAMx, MM5-CAMx), 44 km (MATCH-HIRLAM) and 50 km (LOTOS-EUROS, MATCH-ECMWF, MM5-CHIMERE, MM5-CMAQ, MOCAGE, THOR, WRF-CHEM).

For the finer-grid forecast simulations, the variety of horizontal grid spacing in 2010 ranged from 2 km (MM5-CAMx for Athens area, MOCAGE over France at 2.5 km) to 27 km (MM5-CMAQ for the Iberian Peninsula) for the 3-D Eulerian models. Many models use 10–12 km horizontal grid spacing for their finer grids (MM5-CAMx for the Balkan region, MM5-CHIMERE for Portugal, MOCAGE for France and WRF/CMAQ) and 5 km (Enviro-HIRLAM, EURAD-RIU and SILAM for Northern Europe). The other applied horizontal grid spacing is 9.6 km for ALADIN-CAMx covering Austria, 12 km for FARM (Italian Peninsula), 25 km × 12 km for LOTOS-EUROS (covering the Netherlands) and 17 km for THOR.

Except for the grid spacing, another parameter that differs among models and applications is the selection of the coordinate system. Horizontal spatial coordinates may be expressed in polar coordinates on a sphere, Cartesian coordinates on a plane, or one of several projections of a sphere onto a plane. Curvilinear coordinates may be used in both polar and planar instances, where the model refers to a pseudo-longitude

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and latitude, that is then mapped to geographic longitude and latitude (following the curved surface of the earth).

Following the Cartesian map projections (fixed physical distance coordinates on a flat plane), a number of models included in this paper use the Lambert Conic Conformal coordinate system (ALADIN-CAMx, MM5-CAMx, MM5-CMAQ, WRF/CHEM and WRF-CMAQ) for the forecasting applications. Another Cartesian map projection is the Universal Transverse Mercator (FARM). A rotated longitude–latitude grid is used by Enviro-HIRLAM model, and a curvilinear geodetic latitude–longitude projection is used by CAMx-AMWFG and LOTOS-EUROS. In all geographic projections, the surface of the Earth is distorted since the Earth’s actual shape is irregular. Nevertheless, all projections produce similar results and most of the models allow the user to select the map projection among different options.

The models also have different vertical coordinate systems describing how the grid levels are separated in the vertical: height, terrain-following sigma, pressure, and step-mountain coordinates. LOTOS-EURO uses a dynamic mixing layer coordinate system with four layers (a surface layer of 25 m, mixing layer height, and two reservoir layers up to 3.5 or 5 km). RCG also uses a dynamic mixing layer coordinate system with surface level, 25 m surface layer, mixing layer and two reservoir layers up to 4 km. Uniformity appears on the selection of the surface layer, where most of the models use 20–50 m above the surface as the first model level. Also, most of the models are focused on the troposphere with the top layers located at 2.5–15 km, with three exceptions at 22 km (SKIRON/Dust), 500 hPa (~ 5.5 km, MM5-CHIMERE) and 1 hPa (~ 50 km, MOCAGE).

## 5 Sensitivity analysis and evaluation of CWF models

In order to develop and improve CWF models, different approaches can be employed to test their validity. In this section, we explore some of those approaches through sensitivity analysis (Sect. 5.1), individual model evaluation studies (Sect. 5.2), and multiple-models evaluation studies (Sect. 5.3); all of these are summarized in Sect. 5.4.

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Aiming to better comprehend the common evaluation procedures for operational CWF models, each individual model described here was overviewed regarding its evaluation practices. A short description of each individual model evaluation for the CWF's is presented in Table 10.

## 5.1 Sensitivity analysis

Sensitivity analysis is defined as the study of the variation in model output resulting from the variation in the model inputs. Sensitivity analysis quantifies the relative contributions of the input factors for the model output. This gives information on the input factors that are mainly responsible for the output uncertainties.

Sensitivity information from CWF models can be useful in various applications, such as the design of optimal pollution control strategies, inverse modelling, model parameter estimation, source apportionment and data assimilation. Uncertainty and sensitivity analysis are playing a crucial role to understand the relative importance of different processes in the atmosphere and to quantify the impact (either singular or with interactions) of uncertain inputs (e.g., data, parameterizations) in the results. The applications of the sensitivity analysis techniques include, for instance, the role of emissions, chemical kinetics, boundary conditions and parameterizations of vertical diffusion.

In recent years, an increasing number of CWF models have been reported to provide information on their sensitivity with respect to various input parameters. Sensitivity analysis attempts to apportion quantitatively the variation in the modeled concentrations to different sources of the variation. This is accomplished through either a statistical or deterministic approach. In the statistical approach, the model is executed several times, each time with slightly perturbed inputs and the sensitivity is estimated from the statistical properties of the multiple output variability. In the deterministic approach, the model output equations are differentiated with respect to its inputs and the sensitivity is calculated simultaneously with the concentration fields through an auxiliary set of equations.

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Deterministic sensitivity analysis techniques propagate the derivatives either forward or backward along the model trajectories. In the forward method, the uncertain inputs are perturbed and these perturbations are propagated forward through the modelling domain at future times, providing sensitivity information at all receptors with respect to a few uncertain parameters (*direct sensitivities*). Technically, this can be accomplished using either additional differential equations or by inserting additional lines of code in the model that calculate at each point the gradient of the output function. In the backward (adjoint) method, the perturbation is made at the receptor end and is propagated backward in time and space, providing sensitivity information about specific receptors with respect to all sources and parameters.

Implementation of *adjoint sensitivities* in CWF models is increasing, mainly because of their application in chemical data assimilation. For example, in 2010, the WRF-Chem adjoint has been under development, and will include both the adjoints of both the transport and chemistry schemes. As a starting point, the existing adjoint of the meteorological WRF model has been examined for compatibility with the current WRF-Chem version with the goal of developing an adjoint for WRF-Chem to treat initially chemical tracers and aerosols. The adjoint CWF models are reviewed in Table 13; for these models also deterministic adjoint sensitivity analysis modules can be implemented.

The direct and adjoint methods are included under the deterministic approach of sensitivity analysis. The statistical approach has limited applications in three-dimensional CWF models, due to its high computational requirements and its restrictions on the statistical distribution of uncertain inputs. Ensemble prediction appears to be a better framework to deal with those restrictions, as it can provide information both about the forecast uncertainty and the *ensemble sensitivity*, using a mixture of formal statistical treatments and an informal treatment on some parts of the modelling cascade.

## 5.2 Model evaluation

Before using a CWF model as an operational tool, one should ensure that the scientific evaluations, as well as all the other evaluation steps, have been critically performed. Clearly, the CWF models need to be properly evaluated also before their predictions can be used in any other context with confidence. It is therefore fundamental to assess whether the model is properly simulating the spatial and temporal features on the scales resolved by the model, and also to assess whether the physical and chemical processes are simulated correctly in the model, leading to proper model response to changes in meteorology and emissions.

The main goal of a forecast model evaluation exercise is to demonstrate that the model is making reasonable predictions, when compared with observations, taking into account the adequacy and correctness of the science represented in the model for the purposes, for which the model is applied (e.g., Britter et al., 1995). Evaluation exercises are usually based on the analysis of the systematic biases and errors in model outcomes, but should also indicate sensitivities and uncertainties in the atmospheric processes simulated within the model. The results of these exercises should lead to new directions in model development and improvement, as well as point to the need for additional measurements.

Several studies have discussed the evaluation of CWF models and the importance of improved characterization of model uncertainties (e.g., Hanna and Gifford, 1971; Fox, 1984; Demerjian, 1985; Borrego et al., 2008, Schlüenzen et al., 2010), and suggestions for model evaluation methods have been provided (e.g., Venkatram, 1979, 1988; Weil et al., 1992; Dabberdt et al., 2004). Within the scope of COST 728 activities, Schlüenzen and Sokhi (2008) and Schlüenzen et al. (2010) suggested a generic evaluation protocol that divides the evaluation of models into (i) general, (ii) scientific, (iii) benchmark testing and iv) operational. Of these four approaches to evaluation, the first three should be performed by the model developer and the last one by the model user. Clearly, model evaluations can be classified in several ways, one possibility is:

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(i) operational (ii) diagnostic, (iii) dynamic and iv) probabilistic.

In the first step, commonly referred to as operational evaluation, model predictions are compared to observed data and some statistical measures are computed to gauge overall model performance. This evaluation against data determines the degree to which a model does an accurate prediction of the real world from the perspective of the intended uses of the model. Schlunzen et al. (2010) present an overview of the most common statistical parameters used to indicate the ability of the model to predict the tendency of observed values, errors on the simulation of average and peak observed values, and the type of errors (systematic or unsystematic). According to Weil et al. (1992) and Hanna et al. (1993), in general, in the early 1990's there were three performance measures that were regularly applied in CWF model evaluation – the mean bias, the root mean square error, and the correlation. Currently, a more extensive collection of statistical measures is commonly used. In particular, operational evaluation should include a calculation of the statistical confidence levels.

In the next step (diagnostic and dynamic evaluation), the objective is to address whether the predicted concentrations stem from correct or incorrectly modelled processes, whether they be physical or chemical. This evaluation step determines whether the model implementation accurately represents the developer's conceptual description of the model and the solution to the model. These evaluation methods can cover a wide variety of evaluation studies that consider the physical, chemical, meteorological and emission processes.

Finally, model evaluation can include a third step, or probabilistic evaluation, which attempts to capture the uncertainty or level of confidence in model results for air quality forecasting applications. Many methods exist to estimate the uncertainty: ensemble runs, direct calculation of variances in predicted concentrations, Monte Carlo runs, and analytical error-propagation methods for simple-model algorithms. This probabilistic model evaluation should allow quantification of the confidence in model-predicted values and determination of how observed concentrations compare within an uncertainty range of model predictions. Sensitivity tests are one of the most common and tradi-

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tional ways to ascertain whether inputs have a notable influence on model performance issues. A structured intercomparison among models can also be a useful method to indicate whether a general consensus exists among the models or whether there are outliers.

5 Because all model systems described in this article are based on a NWP model and on a chemistry-transport model, a two-stage validation procedure (in which the weather forecast is independent of the chemistry model) is often the common model evaluation strategy. As a large experience with NWP verification already exists, a few general principles can be summarized in the following:

- 10 – No single verification statistic (e.g., false alarm ratio, probability of detection, root-mean-square error) is capable of presenting a complete picture of the verification statistics,
- Verifying higher-resolution forecasts will necessarily result in a relatively worse verification relative to lower-resolution forecasts using most of the statistical parameters (e.g., Roebber et al., 2004), and
- 15 – Statistical significance of errors should be evaluated and spatial fields should be tested for field significance (e.g., Livezey and Chen, 1983; Elmore et al., 2006).

The classification was defined according to the level of development, and five levels were identified ([http://pandora.meng.auth.gr/mds/long\\_help.php](http://pandora.meng.auth.gr/mds/long_help.php)), as follows:

- 20 1. High level of model evaluation and uncertainty analysis: this level of evaluation is hard to achieve because of either still pending work on evaluation, or minor limitations in the measurements available (quality, representativeness, coverage etc.), or both,
- 25 2. Diagnostic and dynamical model evaluation: extensive and good model evaluation has been performed, but still uncertainties because of major limitations in the measured data,

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3. Limited model evaluation: considerable uncertainties because of both lack of measurements and an inadequate evaluation procedure,
4. Only first attempts towards evaluation and
5. No evaluation at all.

### 5.3 Multi-model evaluation studies

Model evaluation studies also offer the chance to see the weaknesses in the models and thereby lead to efficient improvement. Although all the CWF models considered have been evaluated individually by comparison to observations (Table 10), multi-model evaluation projects can tackle some of the problems more effectively, and in many cases more cost-effectively.

Validation against field experiments includes e.g. ETEX (European Tracer EXperiment, <http://rem.jrc.ec.europa.eu/etex/>) and Kincaid (Atanassov, 2004) data. Past evaluation projects involving models in this article include: EuroDelta (<http://eurodelta.pangaea.de/>), CityDelta (Cuvelier et al., 2007, <http://aqm.jrc.ec.europa.eu/citydelta/>), ESCOMPTE (Expérience sur Site pour COntraindre les Modèles de Pollution atmosphérique et de Transport d'Emissions; <http://escomppte.mediasfrance.org>), ESQUIF (Etude et Simulation de la QUALité de l'air en Ile de France, a synthesis of the Air Pollution Over the Paris Region, Vautard et al., 2003), and the EU ENSEMBLE project (<http://ensembles-eu.metoffice.com/>). Three of these projects are described below: EuroDelta, CityDelta and ESCOMPTE. These three model intercomparison projects were selected, as they compare several CWF models, including many of those described in this article.

#### 5.3.1 EuroDelta

The EuroDelta experiment was designed to evaluate air-quality improvement at the European scale in response to regional emission reduction scenarios for 2020. Within

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the framework of EuroDelta, van Loon et al. (2007) studied the long-term ozone simulations from seven regional air-quality models: CHIMERE, DEHM, Unified EMEP model, LOTOS-EUROS, MATCH, RCG and TM5; the latter is global chemistry Transport Model, not included to this article. All models, except TM5, are regional-scale, limited-area models designed for short-term and long-term simulations of oxidant and aerosol formation. They intercompared the models and compared their output to ozone measurements. All modeling groups adapted the same annual emission inventory of ozone and O<sub>x</sub> to their model grid and model species.

Most of the models in EuroDelta realistically reproduced the observed ozone diurnal cycle, the daily averages, and the variability in the daily maxima. Except for TM5 and DEHM, daytime ozone concentrations were overestimated. LOTOS-EUROS and RCG had a more-pronounced diurnal cycle than observed, whereas TM5 had a less-pronounced diurnal cycle. CHIMERE had a large positive bias in ozone concentration, which probably resulted from a bias in the boundary conditions. The other models and the “ensemble model”, whose concentrations are the average of the concentrations from all seven models, accurately represented the diurnal cycle. In general, the daily maxima in ozone concentrations were better simulated than the daily averages, and summertime concentrations were better simulated than wintertime concentrations (van Loon et al., 2007).

### 5.3.2 CityDelta

The CityDelta project was designed to evaluate the air-quality response of several emission abatement scenarios for 2010 at the scale of the European continent, and specifically in cities. CityDelta (Cuvelier et al., 2007) proceeded in two stages. In the first stage, 15 modeling groups participated in the project, with more than 40 model configurations of various complexities. Participants were asked to perform a one-year control scenario simulation for PM and a 6-month simulation for ozone for six European cities (Berlin, Katowice, London, Milan, Paris and Prague). Since most of the additional costs of this project were not centrally funded, many groups offered several simulations

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on one or a few cities, sometimes all six. A second stage has been devoted particularly to the analysis of PM modeling, with a smaller number of modeling teams participating (Vautard et al., 2007; Thunis et al., 2007).

5 Within the second stage of CityDelta, Vautard et al. (2007) used the predictions of six models (CAMx, CHIMERE, EMEP, LOTOS, OFIS (not included in this article), and REM (RCG) (not included in this article)) to simulate a full year (1999) of ozone and PM<sub>10</sub>, encompassing a minimal model simulation domain of 300 km × 300 km around four cities: Berlin, Milan, Paris and Prague. Three models (CHIMERE, LOTOS, REM(RCG)) were used both at large-scale (typically 50 km) and small-scale grid spacing (5 km).

10 These models captured fairly well the mean, daily maxima and variability of ozone concentrations, as well as the time variability of the ozone response to emission scenarios for each city and the spatial variability between cities. However, the large-scale models overestimated the ozone concentration in the city centres. The PM<sub>10</sub> simulation skill was generally poor, and the large-scale models underestimated the mass of PM<sub>10</sub>. All models had difficulties in capturing the observed seasonal variations. The fine scale models show higher PM<sub>10</sub> and lower ozone concentrations in urban areas, which are closer to the observations than the corresponding values predicted by the larger-scale models.

### 5.3.3 ESCOMPTE

20 The European campaign ESCOMPTE documented four photochemical episodes, lasting 3–4 days each, near Marseilles in South-East France during June and July of 2001. These days corresponded to about 30% of the ozone pollution days (120 ppbv) in this region in 2001. The main objectives of the field campaign were to analyze and document several photochemical episodes in this area, as well as to create a detailed chemical and meteorological database for testing and evaluation of regional-scale CTM's. Aerosol measurements were also carried out during ESCOMPTE. The cooperative experimental project was open to all research groups. The objective of ESCOMPTE was not to rank modeling systems according to specific sta-

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tistical performance, but rather to provide a convenient and comprehensive benchmark to evaluate models or the performance of different versions of the models (<http://escompte.mediasfrance.org/exercice/HTML/overview.html>).

Coll et al. (2007) used the data from the ESCOMPTE campaign, focused on the simulation of two intense ozone episodes: those on 21–23 June 2001 (characterized by moderate synoptic wind) and 24–26 June 2001 (characterized by local land–sea breeze circulation). They used the predictions of two models, CAMx (ENVIRON, 2003) and CHIMERE (Vautard et al., 2005), having their own initial configurations, and then switching their meteorological fields and chemical boundary conditions. The domain was characterized by the presence of large urban and industrial centres along the coastline, and a dense road network. A statistical comparison of the model outputs was conducted over the whole set of model configurations.

The results of all the model configurations were examined in order to determine, how much the changes in dynamical and chemical input data affect the models outputs, trying to discriminate between the influence of internal and external configuration choices. One conclusion of Coll et al. (2007) was that ozone plumes are strongly influenced by the modelled representation of the wind circulation, even when using similar dynamical modules, based on the same types of parameterizations. Indeed, although ozone production rates along the day were mostly emission dependent, the structure of the ozone plume over the domain was completely driven by wind fields. The meteorological module is therefore a critical choice in modeling air quality in coastal areas (Coll et al., 2007).

## 6 User Operations

This section provides an overview of how the user interacts with the different models to produce the operational forecasts. Section 6.1 discusses the availability, documentation and user interfaces of the different models and the computer requirements, and lists the levels of documentation. Section 6.2 discusses how the output is dissem-

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inated. A summary of the availability, user communities, and documentation of the various CWF systems is presented in Table 11.

## 6.1 Model availability and documentation

The availability of CWF models, and more specifically their source code and documentation, may be described in terms of software availability, and their use may be categorized in a similar way. On this basis, many of the models are provided as free and open-source environmental software (Karatzas and Masouras, 2004), such as CAMx, CHIMERE, MM5, SILAM and WRF-Chem. In contrast, other models are not publicly available or are otherwise restricted in some way, such as ALADIN, EURAD, FARM, MATCH, MOCAGE, NAME, OPANA, SKIRON/Dust and THOR. There are also models that combine public and restricted source codes, such as CAMx-AMWFG, Enviro-HIRLAM and MM5-CHIMERE.

The terms of use for those models that are not freely available are not identical for all categories of users; research institutes are usually not charged for their use, although this may not be the case for commercial applications. In addition, model availability options may also exist, as in the case of free access being limited to institutes participating in a specific consortium, or in the case of a distinction between the operational version and the research version. Some models may have well-organized and regularly updated web sites, including documentation on model applications, validation and user communities. In contrast, others suffer from poor or partly incomplete documentation.

There is an on-line database for CWF models that provides various search facilities and a structured, homogenized way for model information provision, the Model Documentation System (MDS). This system has been available via the European Environment Agency for the last ten years (<http://pandora.meng.auth.gr/mds/mds.php>, Mousiopoulos et al., 2000). Another internet-based system of model properties is in the joint COST 728 and COST 732 Model Inventory, accessible at <http://www.cost728.org> (Schluenzen and Sokhi, 2008).

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Because CWF models are computationally intensive, they are not usually prepared as a software product ready to be installed and executed. To work on the application and use of a CWF model, various software tools may be used that commonly accompany the source code and are usually described in the model documentation. Few model packages have dedicated user interfaces that allow for the automatic installation, set-up and use of the model. Commonly, command-line scripts (usually shell scripts) and compilers are required to produce an operational executable. In addition, using CWF models requires software tools for the preprocessing (e.g., input data preparation, formatting, autofeeding), as well as post-processing (e.g., model visualization) of model output of data.

## 6.2 Users of CWF model results and information dissemination

CWF model users are usually scientists, who set-up and execute the model for operational or research uses and produce model results. However, CWF model results are of interest also for many other categories of users. The reason for that may be traced to the environmental regulatory and legal framework, and the resulting mandate for improved air-quality management.

In Europe, CWF has been regulated via a number of Directives that define the quantitative thresholds to be applied to address air-pollution problems. The latest update of this legal framework is related to the adoption of the “Clean Air for Europe” Directive 2008/50/EC, which states that “Member States shall ensure that timely information about actual or predicted exceedance of alert thresholds, and any information threshold is provided to the public”. On this basis, a set of CWF goals is defined, that include the geographical area of expected exceedance of an air-quality threshold, the expected changes in pollution (such as improvement, stabilization or deterioration), and the reasons for those changes.

Moreover, the same directive states that “it is necessary to adapt procedures for data provision, assessment and reporting of air quality to enable electronic means and the Internet to be used as the main tools to make information available”. This means that

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it is necessary to develop *operational* air-quality management and citizen notification systems that will make use of modern information and communication technologies and will allow for the *early forecasting* of air pollution levels (Karatzas, 2010). This means that environmental authorities are required to operate systems that will include operational CWF models, and would allow them to estimate the spatial and temporal occurrence of air pollution, in advance of any actual incidents, and thus notify citizens, as well as other interested parties.

The users of CWF model results may be defined with the aid of the air-quality information provision requirements of the 2008/50 EC Directive, as well as from common practice (e.g., Fedra and Witner, 2009; Slørdal et al., 2008; Karatzas and Nikolaou, 2009). These users include the following.

### 6.2.1 Industry and business activities

The main interest of these users is to forecast the impact of industrial emissions from installations such as power plants, oil company distilleries, etc. As these users are interested primarily in the results of CWF models, it is easier for them to commission these forecasts as a service rather than having to install and maintain the modeling system themselves.

An example of the use of CWF model results for this user category is the assessment of air quality in an industrial area, where the spatial scale may be in the order of tenths to hundreds of kilometers, and the temporal scale in the order of days, or years when it comes to producing forecasts for future scenarios. Thus, as an example, in the case of a multi-source industrial complex (various point sources – chimneys with various emission rates and emitting substances), the MM5-CMAQ air quality management system may be applied (San José et al., 2006, 2008a,b). Due to the computational demand of such problems, a computer cluster or a multi-processor machine are among the most appropriate hardware set-ups to be selected, where the models are prepared to be run in parallel, handling different emission scenarios.

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In the above mentioned applications, the service provider usually prepares the software for managing the simulations, the software required for the pre-processing of the input data and the post-processing of the results, as well as the necessary web-based interfaces for the client. Such systems provide, e.g., decision-making support for clients, who need to decide whether to switch off some emission sources, usually within the next 24 h, to avoid an air-quality episode.

## 6.2.2 The environment decision and policy makers

Those are the ones that are responsible for making decisions concerning air-quality abatement measures as well as for managing air-quality status and dealing with problems on a local to regional scale. An important category of users is city authorities. Clearly, the city authorities are interested in the capability of the modeling system to forecast all the parameters that are required by the relevant regulatory framework, and also on the accuracy and accountability of the information that is being produced. In both cases, information dissemination is usually based on the automatic (or semi-automatic) preparation of tables and graphs, providing estimates of concentrations, their spatial and temporal evolution, as well as scenario-based estimates of the emissions or meteorology.

Designing and predicting forecast-based scenarios is important for decision making, as it allows authorities to take preventive measures to avoid an air-quality episode or reduce the duration or spatial scale of a forecasted episode, in accordance to the mandates of the 2008/50/EC Directive. Originally, many city authorities had maintained and operated their own operational CWF modeling systems. However, due to the increased complexity of the latest versions of such systems and the capacity required in terms of experienced personnel and hardware, the tendency now is to hire such services from partners like institutes, universities or private companies that are active in this area, or to install the system locally and contract with consultants for services, upgrades, and maintenance.

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### 6.2.3 The CWF scientific community

This is a community with a strong interest in the science and the understanding of CWF phenomena and problems. This community requires detailed information, which is usually of little or no interest to the other user communities, and include model performance indicators, model improvements, and environmental decision-making analysis data. Nevertheless, in most cases, the detailed results of the operational CWF model calculations are not made available to anyone else outside the group that has developed and is maintaining the CWF modeling system.

### 6.2.4 The general public

These are the citizens, usually inhabitants of the area covered by the operational CWF models, as well as people living outside the specific area, who nevertheless are interested in the air-pollution levels, usually near the area where they live or work. For these users, CWF models are combined with air-quality information systems, that make use of complementary push-pull communication channels (Karatzas et al., 2005; Karatzas, 2007; Karatzas and Nikolaou, 2009; Zhu et al., 2009).

The dissemination of the air-quality information to the general public is usually in the form of air-quality indexes, graphical representations of air-pollution levels, text descriptions, and multimedia. The means of dissemination are quite variable, including mass media, Internet personalized SMS (short message system) messages, voice servers, and street panels. These characteristics have also resulted from the analysis of a set of air-quality information dissemination systems that was conducted under COST Action ES0602 (www.chemicalweather.eu; Kukkonen et al., 2009a). This COST Action inventoried the way that air-quality information was disseminated to the public by analyzing data from 93 air-quality information systems, originated from seven European countries (Karatzas and Kukkonen, 2009).

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The air-quality information systems that were screened were divided into two types:

1. Those that materialize air quality (AQ) information dissemination from observational data. In many of the systems analyzed, air-quality observations are provided to the public on the basis of hourly data. In some cases, this info is made available in near real time (with a time lag of 1–2 h), while in other cases this information is provided for the previous day, or up to the last period, for which data have been validated.
2. Those that disseminate AQ information based on operational CWF model forecasts. However, in many of the AQ Information systems investigated, no CWF models were applied. This suggests that the CWF modeling community needs to apply models, not only for regulatory purposes, but also for producing information for all three categories of users. In the cases where CWF models were applied, these were mostly three-dimensional models, although statistical models and computational-intelligence models were also employed. In some cases, human judgment is applied to estimate the quality of the atmospheric environment for those systems that have no CWF model support, whereas in some cases both human expertise and models are used.

### 6.3 Dissemination of forecasts on Internet

To investigate the basic characteristics of operational CWF modeling systems, an analysis was made based on the systems that are currently included in the European Open Access Chemical Weather Forecasting Portal, materialized in the frame of COST Action ES0602 (Balk et al., 2010; available at <http://www.chemicalweather.eu/Domains> and registered as a GEOSS service in 2010). This portal provides access to available CWF systems in Europe in a user-friendly graphical format. The portal currently includes about 20 operational CWF modeling systems from all over Europe, covering local to regional and continental scales of AQ. The basic characteristics of these systems are summarized in Table 12.

In all studied systems, users only had to make one or two selections to obtain the information (in terms of graphs or maps). Many systems do not archive forecasts, whereas others archived information for the last two days or two months, and others archived years of data.

5 The Internet is the most popular way to disseminate output from operational CWF models. For the models in the European Open Access CWF Portal, many provide output in the form of concentration fields, usually superimposed on maps of the area of interest.

## 7 Emerging areas and future challenges

10 The aim of this section is to highlight selected emerging scientific areas, as well as future challenges that would be expected to lead to improving the reliability of chemical weather forecasts. These topics include emission and chemistry uncertainties (Sect. 7.1), integration of NWP and ACT models (Sect. 7.2), boundary conditions (Sect. 7.3), assimilating chemical data into the models (Sect. 7.4), improved understanding and parameterization of physical processes (Sect. 7.5), evaluation of CWF  
15 models against data (Sect. 7.6) and generation of model ensembles (Sect. 7.7).

### 7.1 Emission inventories and modelling, and chemical modelling

The evaluation of emissions is one of the main sources of the uncertainties in the predictions of the CWF models. In this section, we address the research challenges  
20 both in terms of the pollutants and source categories, and in terms of how various emission inventories should be refined and harmonised.

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### 7.1.1 Research challenges of emission inventories of species and source categories

Improvement is required especially for the emission inventories of aerosols and organic species. Most of the regional emission inventories currently consider PM<sub>10</sub> and PM<sub>2.5</sub>; however, primary aerosol emissions need to be further specified in terms of the aerosol size distributions, chemical composition and source origins. In particular, particulate black carbon and organic carbon should be specified. Natural emissions of PM – for example, duststorms in arid or semi-arid areas, wild-land fires (e.g., Saarikoski et al., 2007; Sofiev et al., 2009; Saarnio et al., 2010) and sea-spray – are emerging areas of further research. In particular, information is scarce regarding the size distribution of particulate matter formed from natural dust sources and the temporal variability of dust emissions.

Substantial progress has recently been achieved in the representation of processes controlling biogenic VOC emissions (Monks et al., 2009). However, biogenic VOC inventories still need improved quantification by species type (e.g., isoprene) and increased number of species in inventories. Information on the emissions of residential and other small-scale combustion is scarce, although its influence on the exposure of the population may be substantial in some countries and regions (e.g., Karvosenoja et al., 2008, 2010; Denby et al., 2010).

Major uncertainties remain for emissions from transport, including emissions from shipping and aviation, and on the vehicular non-exhaust emissions. For example, not all emission inventories consider ship emissions, which can be important to air pollution in coastal areas (e.g., Jalkanen et al., 2009). Also, uncertainties remain in the modelling of emissions that are dependent upon meteorology, such as allergenic pollen (e.g., Sofiev et al., 2006b, 2011; Veriankaitė et al., 2010) and dust.

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## 7.1.2 Research challenges on harmonisation of emission inventories

The lack of harmonisation of emission inventories at European and national levels is one of the main obstacles to the quantitative comparison of the predictions of operational CWF systems. Currently, the horizontal grid spacing of the emission inventories can be reasonably accurate for regional CWF systems (e.g., the grid spacing for the pan-European domain is 6 km × 7 km in the emission inventory within the MEGAPOLI project). However, the temporal variability of emissions and the vertical distribution of the heights of the emission sources are not considered accurate in all cases, and these aspects of the emission inventories need to be improved.

Further work is also needed to improve the relationships between global, regional and local inventories, especially for developing countries and urban areas. Global emission inventories (e.g., EDGAR, Emission Database for Global Atmospheric Research; IPCC/IIASA and Intergovernmental Panel on Climate Change/International Institute of Applied System Analysis) result in major uncertainties for the total emissions of individual major cities. For example, non-methane hydrocarbon emissions for London as specified by the various available inventories differ by about 65%; for Moscow and Paris, they differ by almost a factor of three (Gurjar et al., 2008). Even for NO<sub>x</sub> emissions, the emissions for Paris differ about by a factor of 2.5 and for Moscow more than 60% (Gurjar et al., 2008).

The global emission inventories commonly underestimate the urban emissions in comparison with national and municipality databases, as is the case, e.g., for the London Atmospheric Emission Inventory database (LAEI, 2009). A quantitative analysis of such differences is therefore needed, and more accurate emission inventories are required on regional and city levels. The first step in this direction was taken within the European CityDelta project (Sect. 5.3.2; Cuvelier et al., 2007). Within the MEGAPOLI project, a new emission inventory has been developed for Europe and the world, with downscaling to urban areas at a horizontal grid spacing of down to 1 km (van der Gon et al., 2009).

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### 7.1.3 Research challenges on the temporal variation and satellite observations in emission modelling

Because CWF models typically use emission inputs with data every hour, emission models are used for characterization of daily, weekly, monthly and yearly cycles of sources or their categories. For anthropogenic sources, these models are usually static and simple. Typically, multiplicative coefficients are used to calculate proportions of the total annual emissions appropriate for a given month, weekday and hour. The next generation of dynamic anthropogenic emission models could take inspiration from energy consumption models, which take into account meteorological variables, especially ambient temperature, cloudiness and wind speed. For combustion, which is one of the key emission sectors, this parallel is obvious.

Satellite instruments (e.g., OMI, GOME-2, MODIS, MOPITT) provide new opportunities for verification and data-driven estimates of emissions. Burrows and Borrell (2009) provide an overview of different instruments. Standard approaching to analyzing satellite data often involve comparing long-term averages of satellite-retrieved columns with simulated columns based on a CWF model. This approach can also be used to validate emission inventories. Another approach is to estimate the long-term trends in emissions is the so-called analog approach where trends in observed columns are compared to trends based on inventories (e.g., Konovalov et al., 2008). Adjoint (i.e., inverse) dispersion modelling can also be used to evaluate the emissions, or the sensitivities of concentrations with respect to changes in emissions (e.g., Tanimoto et al., 2008; Kurokawa et al., 2009).

### 7.2 Improved integration of NWP and ACT models

Historically, air-pollution forecasting and NWP were developed separately and the corresponding communities had limited contact and cooperation. Although this situation could be tolerated in previous decades when NWP data was rarely available operationally for air-quality forecast models and the resolution of NWP models was too

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coarse for mesoscale air-pollution forecasting. However, this situation has changed during this century as modern NWP models approach or include mesoscale and city-scale resolution. This progress has been made possible due to advances in computing power, high-speed computing networks and the availability of land-use databases and remote-sensing data on a finer resolution.

As a result, the conventional concepts of air-pollution forecasting may need revision, as greater integration is required between NWP models and atmospheric chemical transport models. Several national meteorological services (e.g., Environment Canada, and the Danish and Finnish Meteorological Institutes) have suggested extending meteorological weather forecasting to environment forecasting that includes both NWP and CWF. Clearly, this concept would ideally also include biological forecasting, such as allergenic pollen species (Baklanov et al., 2010; Kukkonen et al., 2009a,b,c).

The on-line integration of NWP or other meteorological models with atmospheric chemical transport and aerosol models has several advantages. Such an integration provides the opportunity to use all three-dimensional meteorological fields in CTM's at each time step and to include feedbacks of air pollution (especially those due to aerosols) onto meteorological processes. Extensions into climate model include the feedbacks between air pollution and climate forcing, as well as the atmospheric chemical composition. Such a future direction of research could be viewed as part of a step towards Earth Modelling Systems, and could potentially lead to a new generation of models for NWP and CWF (Baklanov, 2010).

However, the on-line approach is not the best way for the model integration in all cases. For some tasks, such as for emergency preparedness, when NWP data are available, off-line coupling can provide results more quickly. Both off-line and on-line coupling of NWP models and CTM's are therefore useful. A future research area will therefore be to assess the interfaces of these two categories and to establish a basis for their harmonization and benchmarking.

The communication between off-line coupled meteorological and air-quality models is a problem of often underestimated importance. The multitude of modelling systems

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previously introduced gives rise to different approaches and methods implemented within interface modules. Tasks covered by interfaces are minimized in coupled systems. Other systems use interface modules that implement surface and boundary layer parameterisations to estimate dispersion parameters. Sometimes these latter choices are due to the need to rely on conventionally used meteorological products and to guarantee the robustness of air-quality modelling for practical applications.

In other cases, interfaces are used to enhance the resolution of local physiographic data and possibly to introduce advanced parameterisations (e.g., those for the urbanisation of models). Atmospheric physics parameterisations – and even default and upper- or lower-limit values assumed for some key parameters – can have effects on pollutant concentration fields in critical conditions (e.g., low wind-speed conditions, stable conditions). Moreover, interface modules may involve the evaluation of emissions of species that can be substantially influenced by meteorology, such as biogenic VOC, windblown dust and sea salt spray.

Improvements in CWF will also come from assimilating physical parameters that will lead to better estimates of clouds and mixing-layer heights. For example, the assimilation of satellite-derived skin temperatures can be used to better determine heat capacity and moisture fraction of grids, to fill gaps in diurnal energy budgets. This can result in improved model performance of short-term forecasts of temperatures, mixing heights, clouds, and photolysis rates (McNider et al., 2005; Arastoo et al., 2007). Recently established new COST Action ES1004: european framework for online integrated air quality and meteorology modelling (EuMetChem) will focus on further development of integrated CWF systems and on the new generation online integrated chemistry and meteorology models with two-way interactions between atmospheric chemistry (including gases and aerosols), clouds, radiation, boundary layer and other meteorological and climate processes.

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### 7.3 Boundary conditions and nesting of CWF models

An important aspect in the regional applications of CWF models is the type of initial and boundary conditions used by CWF models. The use of climatological averages is one of the common practices, but implementing boundary conditions obtained from global air-quality models is currently a significant challenge (Tang et al., 2007). This challenge consists in obtaining the required parameters (especially regarding the properties of particulate matter) from the global model computations within a sufficient temporal and spatial resolution. Another emerging research area is the development of optimal nesting techniques of CWF models from the global to city scale, using one- or two-way nesting techniques, with boundary conditions from larger-scale model domains to inner-domain model runs.

Chemical boundary conditions from global CWF systems are already provided operationally to some regional CWFs around the world. For example, within the MEGAPOLI project, the global forecasts are provided by the MATCH-MPIC (Max Planck Institute for Chemistry version) model. These provide boundary conditions for several operational European regional CWFs. The ECMWF global CWF model provides chemical boundary conditions for the regional-scale European CWF models in the GEMS project. The global CWF ensemble to be constructed in the MACC project will update the regional model ensemble provided within the GEMS project.

Although using boundary conditions from global models improves predictive skill in regional models by providing more realistic temporal and spatial variability, they also can transfer biases and errors. Further improvements are therefore needed in the observing systems that provide information on the three-dimensional pollutant distributions to improve our capability to predict pollution levels. Such improvements are needed, for example, to better quantify the influence of the Asian brown dust cloud on the US West Coast air quality (Huang et al., 2010).

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## 7.4 Data assimilation of chemical species

As there is only a limited amount of available near-real-time measurements of chemical concentrations, one of the challenges in CWF is how to insert that data into the models in order to obtain the best initial conditions (e.g., the initial spatial concentration distributions of the relevant chemical species) and to improve the quality of CWF. The way this data is inserted is called data assimilation. Powerful assimilation techniques may actually be more critical for achieving accurate forecasts than improvements in the model formulations, at least regarding the short-range forecasts (1–2 days) (e.g., Carmichael et al., 2008a). The implementation of the various chemical data assimilation methods in CWF models is therefore one of the crucial tasks in the improvement of regional CWF models.

The assimilation of meteorological data has traditionally been an essential part of weather forecasting. Different methods of data assimilation are used in NWP models: Newtonian nudging method, Optimum Interpolation (OI), regional four-dimensional data assimilation (FDDA), Kalman filter, the three-dimensional variational (3-D-VAR) and four-dimensional variational (4-D-VAR) data assimilation. In CWF, ensemble Kalman filters and 4-D-VAR are most commonly used. It is beyond the scope of this paper to provide a description of these methods. We confine ourselves to a few remarks relevant for data assimilation into CW models.

In both the 4-D-VAR and Kalman filter approaches, the difference between observed and model values is measured by a weighted sum of squares, where the weights are constructed from several covariance matrices. These matrices reflect uncertainties in both data and model, and at least some of them have very large dimensions. Ensemble methods circumvent the intractability of large covariance matrices by approximating them by an ensemble of model states (in the CWF case, these are usually states of the CWF model).

The ensemble Kalman filter advances each member of an ensemble one time step ahead. Then, a Kalman filter updating formula is applied, using observed data and

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covariance matrices approximated by low rank sample covariance matrices defined by the ensemble. The classical Kalman filter update formula is based on assumptions of an unbiased model and the error distribution being Gaussian. In real-life applications, nonlinearity of chemical reactions causes departures from Gaussianity, whereas deficiencies in the model and errors in the inputs contribute to the bias (one typical example is nightly values of ozone in some models). The departures from the Kalman filter assumptions are much larger in CWF models than in NWP models. These issues and other types of filters are studied in Hanea et al. (2007).

A substantial difference between data assimilation in NWP models and CWF models is due to different type of model equations. In CWF models, stiff differential equations with forcing terms from meteorological and emission inputs make the model quickly converge from any reasonable initial conditions to a stable solution. Thus, in offline CWF models, improvement of initial conditions by means of data assimilation brings only a limited improvement in the forecast. The same issue causes loss of spread in ensembles generated by perturbations of initial conditions. The sample covariance matrices generated by the ensemble become ill-conditioned and covariance inflation or similar methods have to be used to avoid divergence of ensemble filters (Constantinescu et al., 2007; Eben et al., 2005).

Another challenge in data assimilation into CWF models is the complexity of the problem (the number of chemical species varies in the models from tens to hundreds). A key issue is choosing which chemical species to optimize in order to provide the best results of the target forecast species. In variational methods, one may select a receptor location and investigate which variables or parameters are responsible for changes and errors of the model at the receptor. These methods (called adjoint sensitivity analysis or receptor-oriented approach; Carmichael et al., 2008a) may be used for selection of state variables for data assimilation. Also, short-lived species and radicals are usually not subject to optimization.

The difficulties mentioned above are the main causes why the number of applications of data assimilation in the area of CWF has grown only slowly during the last

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decade. Operational forecasting with incorporated data assimilation is occurring for the EURAD model and for RCG (only ozone maxima), and research-based studies have also been performed for LOTOS-EUROS, MATCH, RCG and SILAM. Most of the operational CWF models are routinely initialized using concentrations of species obtained from the forecasts of the previous day, with no regard to the observations. In order to make data assimilation more beneficial for the forecast, other parameters than initial conditions should be optimized, too. Emission rates are the first candidate for optimization, but photolysis rates and deposition rates also may come into consideration (Hanea et al., 2004). However, stability and validity (from the point of view of chemistry or emission modelling) of such corrected parameters has to be checked in order to avoid artifacts.

Instead of optimizing initial conditions and other parameters for the operational forecasts, data assimilation methods can be applied. A fast-growing research area is inverse modeling of emissions using adjoint methods and 4-D-VAR. Although it is being used mainly in global modelling for monitoring atmospheric constituents (e.g., Kopacz et al., 2010), its benefit to the forecast has also been demonstrated. For example, this path has been followed by Elbern et al. (2000, 2007) for the EURAD model. In the US, the adjoints of the global model GEOS-Chem (Henze et al., 2007) and mesoscale models STEM (Sandu et al., 2005) and CMAQ (Hakami et al., 2007) have been developed. Adjoint modelling methods have been briefly reviewed in Table 13.

Research on both inverse modelling and data assimilation has been boosted by the availability of satellite-retrieved measurements (e.g., Chai et al., 2009). Global spatial coverage, better representativeness of the measured area and gradually improving resolution are the main virtues of these data, whereas censoring by clouds, relatively poor time resolution (e.g. two times daily over one spot) and inaccuracies of the retrieval process are the main drawbacks. Satellite instruments can also provide information that is largely complementary to that obtained from in-situ measurements. An overview of European research on remote-sensing of tropospheric constituents is the ACCENT-TROPOSAT-2 report (Burrows and Borrel, 2009). We confine ourselves here to some

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general remarks related to CWF.

The satellite-based data, which enter a data assimilation system, are most commonly integrated over the whole atmospheric column, although vertical profiles are also provided in some cases (e.g., the IASI instrument). Tropospheric columns are derived from total columns; one then has to address the generally poorer sensitivity of satellite observations to concentrations in the lower troposphere. Cloud cover has to be estimated, as well as other meteorological variables. For example, air-mass factor (the ratio between the retrieved slant column and the atmospheric vertical column) is needed for knowing the absorption of the light path through the atmosphere. As a result, satellite columns are a result of a complicated retrieval process leading from the observed spectra to a vertical column density. The uncertainty of the retrieval process therefore needs to be quantified for successful data assimilation.

At some stage, a data assimilation routine may be used, having as its first guess the vertical profile of a global CW model. For example, a global CWF model TM (<http://www.knmi.nl/~velthove/tm.html>) is used in retrieving NO<sub>2</sub> column from the OMI instrument in the near-real-time service TEMIS (Tropospheric Emission Monitoring Internet Service, [www.temis.nl](http://www.temis.nl)) of the European Space Agency.

## 7.5 Improved understanding and parameterization of physical processes

The improvements required for the understanding and parameterization of subgrid-scale physical processes for CWF include at least two emerging areas. The first area is the accuracy of meteorological parameters (e.g., atmospheric boundary layer structure, velocity, temperature, turbulence, humidity, cloud water, precipitation) within NWP models or in meteorological pre-processors. The second area is the description of the interactions of chemical species in the atmosphere (clouds, radiation, removal processes, chemical reactions, aerosol formation and dynamics, etc.) within CWF models themselves.

Areas of necessary NWP model improvement include the overall treatment of complex terrain and rough surfaces (e.g., for urban areas), turbulence closure and

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mesoscale convection. The description of complex terrain and mesoscale circulations can be of crucial importance in CWF models, as discussed by, e.g., Millan et al. (1996), Gangoiti et al. (2001), Dayan and Levy (2002) and Dayan and Lamb (2005). Amongst the most challenging cases for CWFs to predict are episodes of high pollutant concentrations, which commonly occur with low winds and stable stratification, possibly in complex terrain, that cause shallow boundary layers with suppressed turbulent mixing (e.g., Kukkonen et al., 2005a,b). These situations create problems for current methods and models to realistically reproduce meteorological input fields. A gap has thus emerged between modern understanding of boundary layer physics and the limited applicability of boundary layer schemes in operational CWF models.

As most of the pollutants are dispersed within the boundary layer, the mechanisms controlling concentrations substantially depend on the turbulence and the boundary layer height. The temporal and spatial variations of the boundary layer height and the entrainment processes at the top of the boundary layer lead to the infiltration of pollutants from the boundary layer to the free troposphere and, vice versa, to the intrusion of some chemical compounds (e.g., ozone) from the upper-atmospheric layers down to the surface. Physical processes controlling the boundary layer height and the turbulent entrainment are therefore of crucial importance for CWFs. Some of the important physical processes at the top of the boundary layer (e.g., Zilitinkevich et al., 2007) are still insufficiently understood, such as turbulent entrainment in rapidly deepening convective boundary layers and non-steady interactions between the stable boundary layers and the free flow.

Most of the operational CWF models use simplified wet deposition schemes based on two-dimensional surface precipitation intensity data; however, online integrated models (e.g., Enviro-HIRLAM) are allowed to realise more comprehensive schemes using fully three-dimensional real-time cloud characteristics. However, one of the challenges in this emerging area is to improve the quality of the simulation of cloud processes and precipitation forecasts within NWP models.

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Improving computational power makes it possible to reduce the model resolution towards smaller scales. As the physical parameterization is dependent on the resolution of a prediction model, some adjustments of parameterizations have to be made when the resolution is increased.

Piriou et al. (2007) presented an approach in which the grid-scale budget equations of parameterization used separate microphysics and transport terms. This separation is used both as a way to introduce into the parameterization a more explicit causal link between all involved processes and as a vehicle for an easier representation of the memory of convective cells. Piriou et al. (2007) argued that future results could be improved by using more complex microphysics (e.g., prognostic liquid, ice, rain, snow, etc.), getting closer to that of a cloud-resolving model, and relaxing the small-area assumption. According to Piriou et al. (2007), the microphysics and transport advective scheme equations can manage all types of convection.

In the future, a possible perspective will be to unify the convection parameterization exercise, using a single equation set at grid-scale and a single microphysical package. As an example, Gerard (2007) has introduced microphysics and transport advective scheme equations into a scheme using more complex prognostic microphysics, area fraction, and vertical velocity with encouraging results. Gerard (2007) developed a package that aims at solving efficiently the problem of combining resolved and sub-grid condensation at all resolutions, in particular in the range between 10 km and 2 km, where deep convection is partly resolved and partly subgrid.

Knowledge of the emissions of relevant organic species and their atmospheric chemistry limits the understanding of secondary organic aerosols, which are of importance for both air quality and climate change (e.g., Monks et al., 2009). Correspondingly, the models for the aerosol formation and dynamics need to be implemented into CWF models, and the chemical mechanisms used in CWF models should be substantially improved to be able to simulate sufficiently accurately such processes.

Combined models have already been developed for dispersion modelling and aerosol processes, including the size distributions and chemical speciation (e.g., Vi-

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gnati et al., 2004; Gross and Baklanov, 2004; Pohjola et al., 2007; Hussein et al., 2007; Medina et al., 2007; Dusek et al., 2006; Langmann et al., 2008). The aerosol processes include the growth and nucleation processes, and the transport and deposition pathways of the aerosols. Furthermore, as the aerosol dynamics models (this term is used here as a synonym to aerosol process models) are important tools to investigate both the direct and the indirect effects on climate, aerosol–radiation–cloud interactions are important processes that need to be treated in the models (Ramanathan et al., 2001; Rosenfeld et al., 2008; Levin and Cotton, 2009). Several of these processes require direct coupling of the meteorological and air quality models.

These processes need to be included to achieve a comprehensive representation of the atmosphere. State-of-the-art aerosol modules include a sectional representation of the size and chemical composition distribution functions, as well as aerosol microphysical processes. However, the available emission databases do not currently provide sufficient details for executing such combined dispersion and aerosol process models over extensive regions. This means that estimates of the sectional emissions that are needed as input for the detailed models have to be mostly based on indirect information.

## 7.6 Better evaluation of CWF models with data

The evaluation of models by comparison with measured data has also to advance the model performance, rather than solely characterize whether a simulation is successful or not (e.g., Gilliland et al., 2008). The comparisons should use as broad and diverse set of measured data as possible. Currently the evaluation of chemical weather models is mainly based on the comparison of measured and simulated concentration levels at the ground level, and in some cases on satellite data. Clearly, the data comparison only based on one vertical level does not assure a proper simulation of the state of the atmosphere. Whenever available, especially vertical profiles of air pollutants should be included in the evaluation procedure.

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Moreover, the performance of models is usually evaluated only for a limited number of pollutants or PM measures, such as  $\text{NO}_x$ ,  $\text{O}_3$  and  $\text{PM}_{10}$ , which are the ones measured routinely at most monitoring networks. An ideal comparison would be based on the analysis of a sufficiently large number of pollutants, for the selected period of time (or periods) and location (or locations). Clearly, monitoring supersites (or their networks) are useful for this kind of evaluation and could potentially allow evaluating the model capabilities to simulate various physical-chemical processes.

Regarding the evaluation of operational CWF models, a special concern is the availability of near real time (NRT) meteorological and air quality data. Efforts to deliver NRT data (centralised in a common and accessible data base) have been made within the GEMS project, which fits into the current WMO (World Meteorological Organization) activities. However, there is still substantial amount of work to be done in this area; fast mechanisms need to be developed, implemented and tested to access the data and to evaluate the CWF models.

Currently, the evaluation of models regarding particulate matter (PM) commonly uses mostly the measurements of  $\text{PM}_{10}$  and, only to a smaller extent,  $\text{PM}_{2.5}$ , and size- and chemically-resolved PM data. However, the evaluation of models in Europe should in the future focus on  $\text{PM}_{2.5}$  (or  $\text{PM}_{1}$ ) instead of  $\text{PM}_{10}$ , as it is more relevant from a health perspective. Due to the new European legislation,  $\text{PM}_{2.5}$  monitoring data will be extensively measured in the European Union, and the new monitoring network needs to be evaluated.

Furthermore, the understanding and evaluation of the chemical components of particulate matter is needed to make sure that the model predictions are right for the right reasons, and to close the gap between modeled and measured concentrations of PM. For instance, the evaluation of only the total  $\text{PM}_{10}$  concentration may not reveal serious shortcomings in a model with respect to the treatments of the PM components. Moreover, size-resolved PM data are crucial in order to reduce uncertainties in our understanding of the modelling of the emissions, dispersion and transformation of PM. Aerosol chemistry and process modules are needed to evaluate the aerosol compo-

nents; the model evaluation does not in that case need to restrict to only PM<sub>10</sub> and PM<sub>2.5</sub>.

Clearly, measurements routinely carried out at air pollution networks can only be used for model evaluation in case of a limited set of chemical components and measures. Species of interest for model comparison are not necessarily measured (e.g., peroxyacetyl nitrate (PAN), aldehydes, actinic flux, turbulent flux, other particulate matter measures except for PM masses), and the measurement locations are not always representative of the regional background air (e.g., the station could be located downwind of an urban area). In addition, the vertical profiles of concentrations are typically not measured.

More emphasis should also be given to the systematic evaluation of the spatial representativeness of the monitored and simulated data. Clearly, when comparing model predictions to measured data we compare one spatially and temporally averaged value (a predicted one) to another one (the measured one). However, in general the averaging or representativeness space and time scales are not the same.

The model validation against observed data requires statistical analysis that should give information about the ability of the model to predict the observed values and type of errors (systematic or unsystematic). Generally the statistical analysis contains a computation of a set of parameters and measures. It is possible to define various subsets of such statistical parameters that can fairly well represent the various aspects of the performance of the model, e.g., the correlation coefficient, the fractional bias and the root and normalized mean square errors. However, these statistical quality indicators should be accompanied by other methods, for instance, time series and scatter plots could be an important complement to the referred parameters. Clearly, parameters that reflect the capability to simulate concentration peaks should also be taken into consideration in chemical weather forecasting.

Clearly, besides the comparison of model results to data, several other steps should be considered to ensure model quality. These include model sensitivity tests, model intercomparisons and uncertainty analysis (e.g., Borrego et al., 2008). In terms of model

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intercomparison, several international model exercises have been and are currently ongoing within the MEGAPOLI and MACC projects, CityDelta and EURODELTA, various COST Actions, AQMEII (Air Quality Model Evaluation International Initiatives) and FAIRMODE (Forum for AIR quality MODElling). Such inter-comparison exercises are useful to identify the strengths and weaknesses of models, and to show the strategies to improve their performance.

## 7.7 Model ensembles

Ensemble forecasting has been a key area of traditional meteorology during the last decades. From the experience of operational meteorology, two major sources of forecast errors can be distinguished. The first source resides in the uncertainties of the initial conditions, as a result of the limited number and inaccuracies of available observations. The second source is the imperfectness of the models, resulting from limitations in the descriptions of physical processes, the finite spatio-temporal resolution of numerical models and the inability to explicitly resolve and simulate processes beyond the selected grid-scale. As a consequence of these two sources of forecast errors, weather forecasts deteriorate as the forecasting period increases.

In addition to the accuracy of the initial conditions and the limitations of the numerical model, the forecast skill also depends on instabilities of the flow itself, as was already identified in the early works of Lorenz (1963, 1965). Simmons et al. (1995) note the difficulty to assess a-priori whether a forecast would be skillfull or unskillfull, using only a deterministic approach to weather prediction. Clearly, presentation of the history of ensemble prediction is beyond the scope of this paper. However, two important benchmarks need to be mentioned in the implementation of operational ensemble prediction systems, at both ECMWF and NCEP (e.g. Palmer et al., 1993; Molteni et al., 1996; Tracton and Kalnay, 1993). These systems were focused on the perturbation of the initial conditions, following indications on the relative importance of the uncertainties in initial conditions compared to deficiencies in the model (e.g., Downton and Bell, 1988; Richardson, 1998). Ensemble forecasting continues to be an area of active research,

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concerning, e.g., the design and composition of the ensembles (e.g., Kalney, 2002).

In the field of chemical weather, ensemble forecasting is still an emerging area (e.g., Potempski et al., 2008). There are currently numerous well-validated CWFIS's in Europe that are used both for research and operational applications in direct support of decision making. However, any of these single modelling approaches bears inherent uncertainties, both originated from its formulation, the parameterization used and from the input data used (meteorology, emissions, chemical rate constants, etc.). It is therefore desirable to enrich the information provided by the individual deterministic models with probabilistic information, e.g., the range of uncertainties, taking stock of the existing diversity of different modelling systems in Europe (e.g., Kukkonen et al., 2009c). The three key objectives of ensemble forecasting as identified by, e.g., Kalney (2002), are to (i) improve the forecast by ensemble averaging, (ii) to provide an indication of the reliability of the forecast, and (iii) to provide a quantitative basis for probabilistic forecasting.

Compared to traditional weather forecasting using model ensembles, chemical weather ensemble prediction has a much shorter historical record. Early studies comprise works in the field of air quality forecasting (Delle Monache and Stull, 2003) and dispersion modelling (Galmarini et al., 2004b,c). Like in meteorology, these studies have investigated both techniques based on the perturbation of single modelling systems (Mallet and Sportisse, 2006) and on a collection of results from different modelling systems (van Loon et al., 2007; Vautard et al., 2008). Unlike in meteorology, however, air quality is not primarily determined by initial conditions but rather is the result of a range of processes (such as, e.g., emissions, transport, deposition, chemistry) that all provide tendencies that have similar orders of magnitude. This state of affairs requires one to develop approaches that are more complex than the well-established techniques used in numerical weather prediction (e.g., Pinder et al., 2009).

The forecasts obtained by processing the ensemble of models (for instance, taking the median of all values in each grid-point) can, in many cases, perform better than any single model. Riccio et al. (2007) have proposed a theoretical basis in the case of dis-

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5 person, providing some justification to the relatively better performance of the median  
of models. The current operations in the GEMS and MACC projects have used a more  
elaborate ensemble technique, based upon the differential weighting of the individual  
models, according to their skill monitored over the last few days. However, a long-term  
improvement in chemical weather forecast performances is based on the improvement  
of individual models and their representation of dynamical, physical and chemical  
processes. The elaboration of sophisticated hybridizing ensemble methods merely aims at  
achieving the best from what is currently available. The spread of predictions in a col-  
lection of models can also be used as a measure of the model uncertainty (Vautard  
10 et al., 2006).

## 8 Conclusions

What do we see in the future for CWF models? To summarize this paper, we focus  
on two challenge areas: the large number of chemical species and processes, and  
communicating uncertainty.

15 First, although a relatively new field, CW forecasting is developing quickly, touching  
upon research, development, and operational forecasting. An analogy with weather  
forecasting can be useful to demonstrate the challenges ahead. Although CTM's can  
be coupled to NWP models either off-line or on-line at present, a scientific perspective  
of CWF would argue for an eventual migration from off-line modeling (where the CTM is  
run after the NWP model run is completed) to on-line modeling, allowing coupling and  
integration of the physical and the chemical components of CWFIS's. Such a future  
is not hard to imagine, given similar trends of Earth system modelling, for example.  
Specifically, better and more complete representations of physical and chemical pro-  
cesses and interactions in the models are needed. When compared to weather fore-  
casting, CW forecasting has still a long way to go. Despite the nearly 50-year lead that  
25 NWP has over CWF (e.g., Harper et al., 2007), CWF models have other challenges  
that inhibit as rapid a progress.

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A key challenge appears to rather be the dimensionality and complexity of the problem itself. For example, the traditional set of prognostic state variables in weather forecasting (e.g., temperature, wind, precipitation) expands to hundreds of prognostic variables because of the extensive number of chemical species involved. In particular, resolving, simulating, and parameterizing processes is no longer limited to relatively well-known physical processes, but is compounded by a huge amount of both chemical and physical processes (e.g., interactions between species, emission, deposition, radiation). This simple fact has important ramifications for predictability, data assimilation, and ensemble prediction, where scientific and technological progress in CW is slower than in traditional meteorology. Importantly, progress is also inhibited by the lack of or insufficient monitoring of many relevant species and the lack of well-established monitoring data-exchange mechanisms, although several projects and initiatives are working to address these issues.

Second, as is evident from this review article, numerous well-validated operational CWFIS's operate in Europe, addressing the needs of a large spectrum of users from governmental organizations to the individual citizen (e.g., Schluenzen and Sokhi, 2008; Karatzas and Kukkonen, 2009; Baklanov et al., 2010; Balk et al., 2010). How is the output from CWF models assessed and interpreted for the end users? Moreover, how do we interact with those users to provide the needed services? Through initiatives such as the GMES Atmospheric Service and its implementation projects GEMS, PROMOTE, MACC and PASODOBLE (Promote Air Quality Services integrating Observations – Development Of Basic Localised Information for Europe) and the various relevant COST actions, such as COST 728 and COST ES0602, scattered modelling initiatives and efforts – which are often national or regional in scale – can be integrated. This also offers the possibility to move from deterministic forecasts of chemical weather to ensemble chemical weather prediction systems.

With the ability to assess and explore ensemble prediction systems comes the challenge in communicating probabilistic chemical weather forecasts. Again, many lessons can be learned from the weather forecasting community, who are actively facing such

concerns with weather forecasts, in general (e.g., Board on Atmospheric Sciences and Climate, 2006; Novak et al., 2008; Morss et al., 2008), and the communication of hurricane tracks, in particular (e.g., Broad et al., 2007). Although some user communities of weather information (e.g., industrial, agricultural, hydrological) are comfortable dealing with probabilistic forecasts, many air-quality users are relatively new to this concept. Thus, much can be gained through a closer dialogue with relevant user communities (e.g., the so-called “end-to-end-to-end” approach described by Morss et al. (2005), and this communication can spawn future research opportunities.

Successful CWFIS services will also need to aggregate and integrate information and deliver it in a way that is comprehensible, user-friendly, timely, and reliable, and international activities such as the World Meteorological Organisation Global Atmospheric Watch, Urban Research Meteorology and Environment (GURME) project can assist in these efforts. As a first step, the European chemical weather forecasting portal by the COST ES0602 action (Balk et al., 2010) attempts to integrate existing chemical weather forecast and information solutions offered by numerous institutions within Europe. This portal provides a direct gateway to the individual resources and is intended to complement and support other European initiatives such as the GMES Atmospheric Services.

### Frequently used abbreviations and acronyms in this article

ABL	Atmospheric Boundary layer
ALADIN	Aire Limitée Adaptation Dynamique Initialisation
ALADIN-CAMx	Comprehensive Air quality Model with extensions based on ALADIN-Austria forecast data
BEIS3	Biogenic Emission Inventory System
CAC	tropospheric Chemistry Aerosol Cloud transport model
CAMx	Comprehensive Air quality Model with extensions

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CAMx-AMWFG	Comprehensive Air Quality Model with Extensions – The Atmospheric Modeling and Weather Forecasting Group
CWF	chemical weather forecasting
CWFIS	chemical weather forecasting and information system
CTM	chemistry-transport models
DMAT	Dispersion Model for Atmospheric Transport
DMI	Danmarks Meteorologiske Institut
ECMWF	the European Centre of Medium-Range Weather Forecasts
EEA/MDS	European Environment Agency/Model Documentation System
EMEP	European Monitoring and Evaluation Programme
Enviro-HIRLAM	Environment-High Resolution Limited Area Model
EURAD	European Air Pollution and Dispersion Model
FARM	Flexible Air quality Regional Model
GEMS	Global and regional Earth-system (Atmosphere) Monitoring using Satellite and in-situ data
GME	Global Model of DWD (DWD – German Weather Service)
GMES	Global Monitoring for Environment and Security
HIRLAM	High Resolution Limited Area Model
IFS	Integrated Forecast System (ECMWF)
LAI	Leaf Area Index
LOTOS-EUROS	LONG Term Ozone Simulation – EUROpean Operational Smog model
MACC	Monitoring Atmospheric Composition and Climate
MATCH	Multi-scale Atmospheric Transport and Chemistry Model
MEGAPOLI	Megacities: Emissions, urban, regional and Global Atmospheric POLLution and climate effects, and Integrated tools for assessment and mitigation
MM5	Fifth Generation PSU/NCAR Mesoscale Model

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MM5-CAMx	Fifth Generation PSU/NCAR Mesoscale Model – Comprehensive Air quality Model with extensions
MM5-CHIMERE	Fifth Generation PSU/NCAR Mesoscale Model – CHIMERE
MM5-CMAQ	Fifth Generation PSU/NCAR Mesoscale Model – Community Multiscale Air Quality Model
MOCAGE	Modèle de Chimie Atmosphérique à Grande Echelle
NAME	Numerical Atmospheric-dispersion Modelling Environment
NCAR	National Center for Atmospheric Research
NCEP	National Centres for Environmental Prediction
NRT	Near-Real Time
NWP	numerical weather prediction
OPANA	Operatina I version of Atmospheric mesoscale Numerical pollution model for urban and regional Areas
PBL	Planetary Boundary Layer
PM	Particulate Matter
PROMOTE	PROtocol MOiNitoring for the GMES Service Element
RACM	Regional Atmospheric Chemistry Mechanism
RADM	Regional Acid Deposition Model
RCG	REM3-CALGRID – Regional Eulerian Model – California Grid Model
SILAM	Air Quality and Emergency Modelling System
THOR	an integrated air pollution forecast and scenario management system
TNO	the Netherlands Organisation for Applied Scientific Research
VOC	volatile organic compounds
WRF/CHEM	The Weather Research and Forecast model coupled with Chemistry

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*Acknowledgements.* We acknowledge the funding of COST ES0602, COST 728, and EU TRANSPHORM. The research leading to these results has received funding from the European Union's Seventh Framework Programme FP/2007-2011 within the project MEGAPOLI, grant agreement n° 212520. David Schultz is partially funded by Vaisala Oyj. We thank the following people for their contributions to this manuscript: Paul Agnew, Mark Lawrence, Gregory Carmichael, Dimitros Melas, Arjo Segers, William Skamarock, Lucy Davis and Christos Zerefos.

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**Table 1.** Selected main characteristics of the 18 chemical weather forecasting (CWF) models considered in this study.

Model name	Coupling	Country and institution using it	Dispersion model	NWP model	Type	Horizontal grid spacing	Vertical grid spacing	Basic reference
ALADIN-CAMx	Offline	ZAMG, Austria, Marcus Hirtl	CAMx	ALADIN-Austria	3-D Eulerian	~ 28.8 km for the mother grid and 9.7 km for the inner modeling domain	Grid spacing from 30 m to 2500 m in Troposphere	<a href="http://www.cnrm.meteo.fr/aladin/">http://www.cnrm.meteo.fr/aladin/</a> ; <a href="http://www.camx.com">http://www.camx.com</a>
CAMx-AMWFG	Offline	National and Kapodistrian University of Athens, Greece, George Kallos, Marina Astitha	CAMx	SKIRON/Dust	3-D Eulerian	0.24 × 0.24* (~ 24 km)	22 layers up to 8 km	<a href="http://forecast.uoa.gr/index.php">http://forecast.uoa.gr/index.php</a> ; <a href="http://www.camx.com">http://www.camx.com</a>
ENVIRO-HIRLAM	Online	DMI, Denmark, International HIRLAM team, Alexander Baklanov	Enviro	HIRLAM	3-D Eulerian	Europe: 15–45 km; Nest grids: 1.4–5 km	40 layers, grid spacing from 30 m to 500 m	<a href="http://hirlam.org">http://hirlam.org</a> ; <a href="https://hirlam.org/trac/wiki">https://hirlam.org/trac/wiki</a>
EURAD-RIU	Offline	RIU, Cologne, Germany Hermann Jakobs, Hendrik Elbern, Michael Memmesheimer	EURAD	MM5	3-D Eulerian	Europe: 125 km; Central Europe: 25 km, German States: 5 km	23 layers from 40 m to 2000 m at top (100 hPa)	<a href="http://www.eurad.uni-koeln.de">http://www.eurad.uni-koeln.de</a>
FARM	Offline	ARIANET s.r.l. Italy, Giuseppe Calori, Camillo Silibello	FARM	RAMS	3-D Eulerian	Grid size 1 km–50 km; 50 to 100 cells in each dimension	Grid spacing from 10 m to 1000 m, domain size from 3 km to 10 km	<a href="http://www.aria-net.it/index_eng.php">http://www.aria-net.it/index_eng.php</a> ; <a href="http://www.minni.org/htm.farm2/Introduzione.htm">http://www.minni.org/htm.farm2/Introduzione.htm</a>
LOTOS-EUROS	Offline	TNO/RIVM/PBL/KN, The Netherlands, P.J.H. Buitjes, M. Schaap, R.M.A. Timmermans	LOTOS-EUROS	ECMWF	3-D Eulerian	~ 25 km, zooming to 12 km or 6 km	4 layers, domain size from 25 m to 3.5 km	<a href="http://www.lotos-euros.nl/">http://www.lotos-euros.nl/</a>
MATCH	Offline	SMHI, Sweden, Lennart Robertson, Thomas Klein	MATCH	ECMWF, HIRLAM	3-D Eulerian	From ~ 50 km down to 0.5 km	Usually depending on met. model. At present for HIRLAM: domain high ~ 8 km, lowest level at ~ 30 m	<a href="http://www.smhi.se/sgn0106/it/FoU/en/index.html">http://www.smhi.se/sgn0106/it/FoU/en/index.html</a> ; Robertson et al. (1999), Langner et al. (2005)
MM5-CAMx	Offline	National and Kapodistrian University of Athens Aristotle University of Thessaloniki, Greece Zerefos Christos, Melas Dimitrios	CAMx	MM5	3-D Eulerian	Mother grid: Europe (30 km) Nest grids: Balkan Peninsula (10 km) and Athens (2 km)	CAMx: 15 vertical layers, layer height 20 m, top at 7 km. MM5: 29 vertical sigma-levels, top at 100 mbar	<a href="http://www.mmm.ucar.edu/mm5">http://www.mmm.ucar.edu/mm5</a> ; <a href="http://www.camx.com">http://www.camx.com</a> ; <a href="http://lap.phys.auth.gr/gems.asp">http://lap.phys.auth.gr/gems.asp</a>
MM5-CHIMERE	Offline	Mesoscale Prediction Group in the Mesoscale and Microscale Meteorology Division, NCAR, Greece, Lia Fragkou (Model user)	CHIMERE	MM5	3-D Eulerian	MM5: 1 km–90 km CHIMERE: 1 km–100 km over domains 50 km–5000 km	CHIMERE: grid spacing from 10 m to 3000 m, domain size from 10 m to 5 km	<a href="http://www.mmm.ucar.edu/mm5">http://www.mmm.ucar.edu/mm5</a> ; <a href="http://www.lmd.polytechnique.fr/chimere">http://www.lmd.polytechnique.fr/chimere</a>
MM5/WRF-CMAQ	Offline	MM5-PSU/NCAR, Run operationally by the ESMG at Computer Science School of the Technical University of Madrid (UPM), Spain, Roberto San Jose WRF-NCAR/NCEP run routinely at the Centre for Atmospheric and Instrumentation Research (CAIR), University of Hertfordshire, UK, Ranjeet Sokhi	CMAQ	MM5/WRF	3-D Eulerian	Up to 1 km spatial resolution. For the European domain: 30–50 km/15–45 km	MM5/WRF: 29/26 vertical layers. CMAQ: 17–26 vertical layers	<a href="http://www.mmm.ucar.edu/mm5">http://www.mmm.ucar.edu/mm5</a> ; <a href="http://www.mmm.ucar.edu/wrf/users/">http://www.mmm.ucar.edu/wrf/users/</a> ; <a href="http://www.cmaq-model.org">http://www.cmaq-model.org</a>

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Model name	Coupling	Country and institution using it	Dispersion model	NWP model	Type	Horizontal grid spacing	Vertical grid spacing	Basic reference
MOCAGE	Offline	Météo-France, Direction de la Production and Centre National de Recherches Météorologiques, France, Vincent-Henri Peuch (project leader)	MOCAGE	ARPEGE, ALADIN, ECMWF	3-D Eulerian	Up to 4 nested domains (two-ways). 2009 operational version covers the globe at 2° resolution, Europe and Mediterranean area at 0.5° and France at 0.1°	60 vertical layers from the surface to 0.2 hPa	Dufour et al. (2004); <a href="http://www.preva.ir.org">http://www.preva.ir.org</a>
NAME	Offline	Atmospheric Dispersion Group, UK Paul Agnew	NAME	Met Office Unified Model	3-D Lagrangian	NAME: no intrinsic grid. The Met Office Unified: globally at 40 km resolution and in a European limited area configuration at 12 km	Continuously variable	<a href="http://www.metoffice.gov.uk/research/modelling-systems/dispersion-model">http://www.metoffice.gov.uk/research/modelling-systems/dispersion-model</a>
OPANA	Offline	Environmental Software and Modelling Group, Computer Science School, Technical University of Madrid, LHTEE, AUT, NCAR/Pen, Spain, Roberto San Jose	OPANA	MEMO	3-D Eulerian	0.001–10 km, domain dimensions: 10–500 km	Cell height: 1–500 m (varying with height), total height: up to 10 km	<a href="http://atmosfera.lma.fi.upm.es/equal/show_Long.htm">http://atmosfera.lma.fi.upm.es/equal/show_Long.htm</a> ; <a href="http://artico.lma.fi.upm.es">http://artico.lma.fi.upm.es</a>
RCG	Offline	FU-Berlin, Institute for Meteorology Germany, Rainer Stern, Eberhard Reimer, Andreas Kerschbaumer	REM-CALGRID	GME	3-D Eulerian	~ 1–25 km	5 layers, surface layer of 25 m, 2 layers above surface layer and mixing height and 2 reservoir layers	<a href="http://www.trumf.de; Stern (2003)">http://www.trumf.de; Stern (2003)</a>
SILAM	Offline	Finnish Meteorological Institute, Finland, Mikhail Sofiev	SILAM	ECMWF, HIRLAM, WRF, AROME, ...	3-D Lagrangian, 3-D Eulerian	5 km for Lagrangian and 1 km (untested: 0.5 km) for Eulerian	Allows free selection of output vertical layers in several vertical types	<a href="http://silam.fmi.fi/">http://silam.fmi.fi/</a>
SKIRON/Dust	Online	National and Kapodistrian University of Athens, Greece, George Kallos	SKIRON	Eta	3-D Eulerian	0.24 × 0.24 (~ 24 km)	38 vertical levels from the surface up to 22 km	<a href="http://forecast.uoa.gr/dustinfo.php">http://forecast.uoa.gr/dustinfo.php</a> , Kallos et al. (2006), Spyrou et al. (2010)
THOR	Offline	National Environmental Research Institute, Denmark, Jorgen Brandt	DEHM (UPM, OSPM)	Eta	3-D Eulerian (DEHM) 3-D Lagrangian (UPM)	DEHM mother domain: 150 × 150 km DEHM first nest: 50 km × 50 km DEHM second nest: 16.67 × 16.67 km UBM: 1 km × 1 km OSPM: 0.001 km	DEHM: 20 layers up to ~ 15 km, lowest model layer 50 m	<a href="http://thor.dmu.dk; http://www2.dmu.dk/atmosphericenvironment/thor/index.htm">http://thor.dmu.dk; http://www2.dmu.dk/atmosphericenvironment/thor/index.htm</a>
WRF/CHEM	Online	NOAA 2008, Currently under research application in the ESMG-Computer Science School – Technical University of Madrid (UPM), Spain, Roberto San Jose	CHEM	WRF	3-D Eulerian	European domain: 90 km Nest grid: Germany (30 km)	23 layers from 35 m (approx.) to at top 100 hPa	<a href="http://cpm.acd.ucar.edu/Models/WRF-Chem; http://ruc.noaa.gov/wrf/WG11/">http://cpm.acd.ucar.edu/Models/WRF-Chem; http://ruc.noaa.gov/wrf/WG11/</a>

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**Table 2.** Selected main characteristics of the numerical weather prediction models considered.

Model name	Hydrostatic/nonhydrostatic	Vertical coordinate	Reference	Cloud microphysics	Convective parameterization scheme	PBL scheme	Global or Limited-area model
ALADIN	Hydrostatic	Pressure or Sigma–pressure hybrid	<a href="http://www.cnrm.meteo.fr/aladin/">http://www.cnrm.meteo.fr/aladin/</a>	Kessler (1969)	Bougeault (1985)	First order turbulence closure (Louis, 1979; Louis et al., 1982)	Limited-area
ECMWFIFS	Nonhydrostatic	Hybrid	<a href="http://www.ecmwf.int/research/ifsdocs/">http://www.ecmwf.int/research/ifsdocs/</a>	Tiedke (1993)	Modified Tiedke (1989) scheme (Nordeng 1994)	Modified Louis et al. (1982) <i>K</i> -theory scheme (Beljaars and Viterbo 1999)	Global
Eta	Nonhydrostatic	Eta	Mesinger et al. (1988), Janjic (1990, 1994)	Ferrier et al. (2002)	Betts–Miller–Janic and Kain–Fritsch	Mellor–Yamada 2.5-order	Limited-area
GME	Hydrostatic	Sigma–pressure hybrid	Majewski et al. (2002)	Kessler-type scheme (Doms and Schättler, 1997)	Tiedtke (1989)	2nd order, Mellor and Yamada (1974)	Global
HIRLAM	Hydrostatic/nonhydrostatic	Sigma–pressure hybrid	<a href="http://hirlam.org">http://hirlam.org</a>	STRACO (Soft Transition Condensation)	STRACO (modified Kuo scheme), Rasch and Kristjánsson (1998), Kain–Fritsch	Cuxart Bougeault Lacarrere, order 1.5 TKE scheme	Limited-area
MEMO	Nonhydrostatic	Sigma	Kunz and Moussiopoulos (1995), Moussiopoulos et al. (1997)	No moist processes	No moist processes	<i>K</i> -theory	Limited-area
MM5	Nonhydrostatic	Sigma	Dudhia (1993), Grell et al. (1995)	Various possible schemes	Various possible schemes	Various possible schemes	Limited-area
Unified Model	Nonhydrostatic	Height	Cullen et al. (1997), Davies et al. (2005)	Wilson and Ballard extended by Forbes	Gregory and Rowntree (1990)	Lock et al. (2000)	Limited-area or global
WRF	Nonhydrostatic	Sigma or sigma–pressure hybrid	Janic et al. (2001), Janic (2003), Skamarock et al. (2005)	Various possible schemes	Various possible schemes	Level 2.5 Mellor and Yamada Janic, or non local YSU scheme	Limited-area

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**Table 3.** Brief characterizations of the main physical and chemical components of the CWF models.

Model name	Advection and convection	Diffusion	Dry deposition	Wet deposition	Chemistry package	Aerosol package
ALADIN-CAMx	Eulerian continuity equation closed by <i>K</i> -theory equations in flux form	Horizontal diffusion: Smagorinsky approach. Vertical diffusion: Louis (1979) approach (uses the Richardson number and the mixing length)	Physical: Separate resistance models for gases and aerosols. Numerical: deposition velocity as surface boundary condition for vertical diffusion	Physical: Separate scavenging models for gases and aerosols. Numerical: Uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size	SAPRC-99: 73 species, 211 reactions	Not described
CAMx-AMWFG	Eulerian continuity equation closed by <i>K</i> -theory	Horizontal diffusion based on Smagorinsky approach. Vertical diffusion coefficients supplied via input file (from the meteorological model)	Separate resistance models for gases and aerosols. Numerical: Deposition velocity as surface boundary condition for vertical diffusion	Separate scavenging models for gases and aerosols. Numerical: Uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size	Carbon Bond (CB-IV)	RADM aqueous chemistry scheme, ISORROPIA gas/aerosol partitioning scheme, SOAP scheme for SOA formation, both Coarse/Fine scheme and Multi sectional approach. Options for two variable (coarse/fine) bulk scheme and fixed sectional scheme (sections by user choice) with all microphysics. 16 aerosol chemical species. (Sulfate, Nitrate, Ammonium, Water, Anthropogenic SOA, Biogenic SOA, Polymerized anthropogenic SOA, Polymerized biogenic SOA, Sodium, Chloride, Primary Organic Aerosol, Primary Elemental Carbon, Fine Other Primary, Fine Crustal, Coarse Other Primary, Coarse Crustal)
Enviro-HIRLAM	Several possibilities: globally and locally-conservative schemes for advection (Bott, 1989; Kaas, 2008). STRACO convection and Tiedtke mass-flux schemes to convect aerosols and gases. Eulerian continuity equation closed by <i>K</i> -theory	Vertical diffusion by native TKE-1 scheme (Cuxart, 2000). Horizontal diffusion by the native extra scalar system. Improved parameterisation for urban boundary layer and mixing height	Separate resistance models for gases and aerosols. Three regimes gravitation settling parameterisations for different size aerosols	Separate 3-D scavenging models for gases and aerosols, and for rain-out and wash-out with particle size-dependent parameterisations (Baklanov and Sørensen, 2001)	Four mechanisms for gas-phase chemistry can be used: NWP-Chem (default scheme), RADM2, RACM and an extended version (includes isoprene and DMS chemistry) of CBMZ	Aerosol module comprises thermodynamic equilibrium model NWP-Chem-Liquid and an aerosol dynamics model (Korsholm et al., 2008). 4 aerosol modules: modal CAC (default, Gross and Baklanov, 2004) and MADE (Ackermann et al., 1998), and sectional MOSAIC (Zaveri et al., 2007) and SALSA (on test phase, Kokkola et al., 2008)
EURAD-RIU	fourth order Bott scheme (Bott, 1989)	Vertical mixing based on scaling regimes (Holtslag et al., 1990)	Deposition velocity based on landuse type and season. Revised parameterization by Zhang et al. (2003)	Gas-phase: Henrys law equilibria for all prognostic species. Aerosol phase (Binkovski, 1999): The accumulation mode particles form cloud condensation nuclei and are 100% absorbed into the cloud water. The Attkin mode forms interstitial aerosol which is scavenged by cloud droplets. The wet removal of aerosol is proportional to the wet removal of sulfate	RADM2 (Stockwell et al., 1990), RACM (Stockwell et al., 1997), Euro-RADM (Stockwell and Klej, 1994) – The Euro-RADM chemical mechanism was developed to model European atmospheric chemistry. It is based upon the Regional Acid Deposition Model mechanism, version 2 (RADM2)	The aerosol dynamics model MADE (Ackermann et al., 1998), SORGAM (Schell et al., 2001)

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Table 3. Continued.

Model name	Advection and convection	Diffusion	Dry deposition	Wet deposition	Chemistry package	Aerosol package
FARM	Horizontal: Blackman cubic polynomials (Yamartino, 1993). Vertical: hybrid semi-implicit Crank-Nicolson/fully implicit scheme (Yamartino et al., 1992)	Horizontal diffusion based on Smagorinsky approach or stability dependent parameterizations. Different vertical diffusion parameterizations based on ABL-scaling. $K_x$ and $K_z$ evaluated by SURFPRO pre-processor	Deposition velocity (from SURFPRO pre-processor) depending on land type, season, surface meteorology, surface wetness, by means of a big leaf resistance model after Walcek et al. (1986) and Wesely (1989)	Precipitation scavenging based on EMEP (2003)	Two mechanisms implemented through KPP chemical pre-processor (Sandu et al., 1995): an updated version of the chemical mechanism implemented in the EMEP Lagrangian Acid Deposition Model (Hov et al., 1989) including the treatment of Persistent Organic Pollutants (POPs) and mercury and SAPRC-99 (Carter, 2000). Photolysis reaction rates estimated either using simple look-up tables or an on-line version of the Tropospheric Ultraviolet-Visible Model (TUV, Madronich, 1987). Cloud effects on actinic flux considered	CMAQ aer3 module to include aerosol processes: modal scheme with three modes and all microphysics. ISORROPIA and SORGAM models to include aerosol thermodynamics/ partitioning respectively for inorganic and organic species
LOTOS-EUROS	Advection following Walcek (2000). No explicit convection, vertical grid follows pbl from meteorology	Vertical turbulent mixing formulation uses $K$ -diffusion	Resistance approach	Scavenging rates depending on Henry's law constants for gases and following Scott (1978) for particles	Updated CBM-4 with Carter's 1-product isoprene scheme: homo- and heterogenous conversion of $\text{NO}_2$ to $\text{HNO}_3$ , 28 species and 66 reactions, including 12 photolytic reactions	Bulk scheme with possibility for several size ranges. ISORROPIA, MARS or EQSAM options for calculating equilibrium between gas and particle phase sulfate, nitrate, ammonium, water
MATCH	Modeled using a Bott-type advection scheme (Bott, 1989). Up to fourth order schemes are implemented in the horizontal and up to second order in the vertical	Parameterized using three primary parameters: the surface friction velocity, the surface sensible heat flux and the boundary layer height	Modelled using a resistance approach. Deposition schemes with different degrees of sophistication are available	Assumed to be proportional to the precipitation intensity using species-specific scavenging coefficients. For particles, several different schemes are available	Extended EMEP MSC-W model chemistry (Simpson et al., 1993). Aqueous-phase oxidation is implemented following Berge (1993). The formation of ammonium sulfate and -nitrate is modelled following Hov et al. (1994). 110 thermal, 28 photochemical, 2 aqueous-phase, 5 aerosol reactions and 4 gas-phase aqueous-phase and aerosol equilibria between 60 chemical components	Bulk scheme with several non-interacting size ranges. Equilibrium between particle and gas phase

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**Table 3.** Continued.

Model name	Advection and convection	Diffusion	Dry deposition	Wet deposition	Chemistry package	Aerosol package
MM5-CAMx	MM5: Vertical advection of moisture and temperature are resolved by applying linear interpolation methods. Convection in cumulus clouds is parameterized with the Kain–Fritsch 2 parameterization. CAMx: Eulerian continuity equation closed by <i>K</i> -theory	MM5: MRF Planetary Boundary Layer (PBL) scheme. CAMx: Horizontal diffusion based on Smagorinsky approach. Vertical diffusion coefficients supplied via input file (from the meteorological model)	CAMx: Physical: Separate resistance models for gases and aerosols. Numerical: Deposition velocity as surface boundary condition for vertical diffusion	Separate scavenging models for gases and aerosols. Numerical: Uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size	CAMx: Carbon Bond (CB-IV)	RADM aqueous chemistry algorithm, ISORROPIA inorganic aerosol thermodynamics/partitioning, SOAP scheme for SOA formation. Options for two variable (coarse/fine) bulk scheme and fixed sectional scheme (sections by user choice) with all microphysics. 16 aerosol chemical species (sulfate, nitrate, ammonium, water, anthropogenic SOA, biogenic SOA, polymerized anthropogenic SOA, polymerized biogenic SOA, sodium, chloride, primary organic aerosol, primary elemental carbon, fine other primary, fine crustal, coarse other primary, coarse crustal)
MM5-CHIMERE	MM5: Based on a finite difference formulation of the time-dependent Navier-Stokes equations. CHIMERE: 3 advection schemes: The Parabolic Piecewise Method, the Godunov scheme and the simple upwind first-order scheme	MM5: Bulk PBL, high resolution Blackadar PBL, Burk, Thompson PBL, Eta PBL, MRF PBL, Gayno-Seaman PBL, Pleim-Chang PBL. CHIMERE: Vertical turbulent mixing takes place only in the boundary-layer. The formulation uses <i>K</i> -diffusion, without counter-gradient term	CHIMERE: Considered for model gas species and is parameterized as a downward flux out of the lowest model layer. The deposition velocity is described through a resistance analogy (Wesely 1989)	MM5: Nonconvective precipitation scheme, warm rain, simple ice, mixed-phase, Goddard microphysics, Reisner graupel, Schultz microphysics. CHIMERE: follows the scheme proposed by Loosmore (2004)	CHIMERE: Offers the option to include different gas phase chemical mechanisms. MELCHIOR1 (Latuati, 1997): more than 300 reactions of 80 gaseous species. The hydrocarbon degradation is fairly similar to the EMEP gas phase mechanism. MELCHIOR2: 44 species and about 120 reactions is derived from MELCHIOR (Derognat, 2003), following the concept of chemical operators (Carter, 1990)	Sectional with 6 size bins (each bin internally mixed). All microphysical processes included. 7 species (primary particle material, nitrate, sulfate, ammonium, biogenic secondary organic aerosol (SOA), anthropogenic SOA and water)
MM5/WRF-CMAQ	Several possibilities. Normally Global-mass conserving scheme. Vertical diffusion is mainly done with the Asymmetric Convective model (ACM2) for MM5 and the Yonsei University (YSU) PBL parameterization for WRF	PBL scheme and diffusion (MRF PBL); surface scheme: Noah Land Surface Scheme and Monin Obukhov surface layer scheme	Physical: Separate resistance models for gases and aerosols. Numerical: Deposition velocity as surface boundary condition for vertical diffusion	Physical: Separate scavenging models for gases and aerosols. Numerical: Uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size	CB04 and CB05; Also RADM chemistry. It includes cloud and aerosol chemistry	Modal scheme with three modes and all microphysics. Aerosol species: elemental and organic carbon, dust, and other species not further specified. Secondary species considered are sulfate, nitrate, ammonium, water, and secondary organics from precursors of anthropogenic and biogenic origin. Possibilities to run the aerosol MADRID scheme

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**Table 3.** Continued.

Model name	Advection and convection	Diffusion	Dry deposition	Wet deposition	Chemistry package	Aerosol package
MOCAPE	Advection is based upon the semi-lagrangian scheme of (Williamson and Rash, 1989) with global mass conservation imposed, while convection is parameterised using (Bechtold et al., 2001). See details and evaluation in (Josse et al., 2004)	$K$ -diffusion approach, based upon (Louis, 1979)	Resistance approach: for gases, it is based upon (Wesely, 1989) with refinements for stomatal resistance (Michou et al., 2004); for aerosol, the approach is described in (Nho-Kim et al., 2004)	For scavenging by large-scale precipitation and below convective cloud, the parameterisation is based upon (Giorgi and Chameides, 1986), with a special treatment for snow flakes. For scavenging within convective clouds, it is done within the convective parameterisation as described in (Mari et al., 2000)	Several options are available. In the operational version, the scheme is a merge from the schemes RACM (Stockwell et al., 1997) and REPROBUS (Lefevre et al., 1994), thus offering a comprehensive representation of both tropospheric and stratospheric chemistry. The scheme comprises 118 species for a total of over 300 homogeneous and heterogeneous chemistry reactions	Aerosol is described using a bulk approach with size bins (typically 5 to 20 bins per species). Evaluation is currently available for black carbon (Nho-Kim et al., 2005), dust (Martet et al., 2009) and sulfate (Ménégoz et al., 2009)
NAME	NAME does not have its own convection scheme. It obtains advection ascheme from the UK Met. Office's numerical weather prediction model, the Unified Model (Cullen, 1993)	Modelled using random walk techniques. Parameterised profiles of turbulence parameters such as velocity variances and Lagrangian time scales are employed. Normally a Gaussian scheme is used. However for convective conditions a skewed turbulence scheme is available	Uses a resistance analogy approach and sedimentation of heavy particles is also included	Based on parameterised scavenging coefficients and differs according to precipitation type (convective, dynamic)	Based on the scheme for the STOCHEM model. 40 advected tracers + 18 non-advected 140 reactions + 23 photolytic reactions 16 emitted species	A mass based scheme incorporating sulphate, nitrate, ammonium, and secondary organic aerosols. Additional scheme exist for sea salt (2 size bias) and mineral dust (6 size bias)
OPANA	Piecewise parabolic method (PPM) which is a monotonic scheme with geometric non-linear adjustments to the parabolic concentration distributions	Two convective boundary layer schemes: Blackadar and ACM. Local diffusion, vertically continuous integration, smooth transition from stable to convective and faster matrix solver. Updated eddy diffusion scheme	Chemical gases: Wesely (1989). Aerosol chemistry: Binkowski and Shankar (1995) approach. These schemes are based on the resistance approach which assumes a canopy, aerodynamical and bulk resistance	Physical: Separate scavenging models for gases and aerosols. Numerical: Uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size	The CBM-IV chemical mechanism in short and long modes are included in the system. The RADM model and the SAPRC-99 chemical scheme are also included. These schemes simulate the chemical reactions in the atmosphere for organic and also inorganic reactions	Modal scheme with three modes and all microphysics. Aerosol species: elemental and organic carbon, dust, and other species not further specified. Secondary species considered are sulfate, nitrate, ammonium, water, and secondary organics from precursors of anthropogenic and biogenic origin. Possibilities to run the aerosol MADRID scheme
RCG	Walcek (2000). The number of steps within the advection scheme is chosen such that the Courant restriction is fulfilled	Vertical turbulent mixing formulation uses $K$ -diffusion. Stable and convective boundary layer diffusion coefficients based on PBL scaling regimes. In addition: mixing by use of time and space dependent coordinate based on mixing height	Resistance approach (Erisman et al., 1994). Gases: function of species dependent Henry constant and precipitation rate. Particles: Below-cloud simple scavenging coefficient approach with identical coefficients for all particles	Gases: function of species dependent Henry constant and precipitation rate. Particles: Below-cloud simple scavenging coefficient approach with identical coefficients for all particles	Gas phase: updated CBM-4 with Carter's 1-product isophere scheme: homo- and heterogeneous conversion of $\text{NO}_2$ to $\text{HNO}_3$ , aqueous phase conversion of $\text{SO}_2$ to $\text{H}_2\text{SO}_4$ through oxidation by $\text{H}_2\text{O}_2$ and $\text{O}_3$ , equilibrium concentration for $\text{SO}_2$ , $\text{H}_2\text{O}_2$ and $\text{O}_3$ from Henry constants	ISORROPIA. Bulk equilibrium scheme. species: mineral coarse between $2.5\ \mu\text{m}$ and $10\ \mu\text{m}$ , primary aerosol smaller than $2.5\ \mu\text{m}$ , primary elemental carbon, primary organic carbon, secondary organic aerosols, sulfate, nitrate, ammonium, sea-salt

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Table 3. Continued.

Model name	Advection and convection	Diffusion	Dry deposition	Wet deposition	Chemistry package	Aerosol package
SILAM	Lagrangian kernel uses the iterative advection of Eerola (1990). Eulerian kernel is built on the basis of Galperin (2000)	Lagrangian: assumes the well-mixed ABL and fixed random-walk parameters in the free troposphere. Exchange between the ABL and troposphere takes place due to variation of the ABL height. Eulerian: follows the $K$ -closure with approach of Gernikovich et al. (2004) and Sofiev et al. (2010a) for $K_z$ evaluation	Varies for different chemical schemes but generally is based on resistive analogy with certain simplifications or extensions. Aerosols: both gravitational and diffusional paths are considered with the sedimentation treated via Stokes terminal velocity	Follows the scavenging coefficient approach, distinguishing between the in- and sub-cloud, as well as rain-, snow-types of scavenging	1. Acid basic transformations 2. CB-4 3. Sox module 4. Radioactive decay of up to ~500 nuclides 5. Toxic species 6. Aerosols 7. Natural birch pollen 8. Sea salt 9. Passive tracer	Two schemes: bulk and ADB (Aerosol Dynamics Basic – research mode only). Both schemes use the user-defined set of bins. Bulk scheme allows treatment of any chemically inert aerosol. ADB scheme distinguishes between SIA, sea salt, dust, primary PM – in soluble and insoluble phases
SKIRON/Dust	Horizontal: The Eta/NCEP model scheme for advection of a passive substance (Janjic, 1997). Vertical: The scheme of Van Leer (1977)	A 2nd order diffusion scheme is used for lateral diffusion by utilizing the Smagorinsky-type horizontal diffusion coefficient modified by the presence of the model turbulent kinetic energy term (Janjic, 1990)	Surface deposition of particles occurs via diffusion, impaction, and/or gravitational settling using the resistance approach of Slinn and Slinn (1980)	Wet deposition of particles occur above and below the clouds as described by Seinfeld and Pandis (1996)	No chemistry	Bulk scheme for dust
THOR	Time integration for the advection term is performed with a predictor-corrector scheme with several correctors (Zlatev, 1995)	$K$ -theory, constant $K$ in horizontal, and vertical $K_z$ based on Monin-Obukhov similarity theory for the surface layer, extended to the whole mixing layer	DEHM: velocities of the species are based on the resistance method	DEHM: parameterised by a simple scavenging ratio formulation with different in-cloud and below-cloud scavenging	A chemical scheme similar to the EMEP scheme with 60 species and 120 chemical reactions is included in the model	DEHM: Bulk scheme. Three of the species are primary particulates ( $PM_{2.5}$ , $PM_{10}$ , TSP). Furthermore sea salt is implemented in the model
WRF/CHEM	Several possibilities. Normally Global-mass conserving scheme. Vertical diffusion is mainly done with the Yonsei University PBL parameterization	PBL scheme with the Yonsei University parameterization	Physical: separate resistance models for gases and aerosols. Numerical: deposition velocity as surface boundary condition for vertical diffusion	Physical: separate scavenging models for gases and aerosols. Numerical: uptake as a function of rainfall rate, cloud water content, gas solubility and diffusivity, PM size	CB05, CBMZ and RADM chemical schemes	Option for sectional (MOSAIC, 8 bins) and modal (MADE) aerosol models



**Table 4.** Selected main characteristics of the chemical submodels that are included in the CWF models. ND = no data found.

Chemical sub-model	Dispersion models	Chemical species	Photolysis rates	Aqueous-phase	References
CBM-IV (CB-IV)	CAMx CMAQ LOTOS-EUROS OPANA RCG	33 compounds 81 reactions	12 reactions. For most of the species the clear sky photolysis rates are calculated according to the Roeths flux algorithm	ND	Gery et al. (1989)
MELCHIOR	CHIMERE	Extended mechanism: 80 compounds 320 reactions (26 inorganic) Reduced mechanism: 44 compounds 133 reactions (26 inorganic)	22 photolysis reactions Photolysis rates calculated under clear sky conditions as a function of height and attenuated by cloudiness	Aqueous oxidation of SO <sub>2</sub> by O <sub>3</sub> , H <sub>2</sub> O <sub>2</sub> , NO <sub>3</sub> and O <sub>2</sub> catalyzed by metal ions	<a href="http://www.lmd.polytechnique.fr/chimere">http://www.lmd.polytechnique.fr/chimere</a> Schmidt et al. (2001)
ISORROPIA	CAMx CHIMERE CMAQ LOTOS-EUROS RCG	22 species 17 equilibrium reactions	ND	ND	Nenes et al. (1998a,b) New version: <a href="http://nenes.eas.gatech.edu/ISORROPIA/">http://nenes.eas.gatech.edu/ISORROPIA/</a> Fountoukis and Nenes (2007)
NWP-Chem	Enviro-HIRLAM	17 (28) advected species 27 (32) gas-phase reactions	4 photolysis reactions	Simplified liquid-phase equilibrium mechanism NWP-Chem-Liquid with 13 reactions	Korsholm et al. (2008)
RADM2 (RADM)	CAMx CHEM CMAQ Enviro-HIRLAM EURAD OPANA WRF/CHEM	63 compounds 156 reactions (38 inorganic)	21 photolysis reactions The photolysis module uses a radiative transfer model. This module calculates photolysis frequencies that considers changes in the radiation with height and changes in air composition such as O <sub>3</sub> ; aerosols and water vapor		Stockwell et al. (1990)
RACM	Enviro-HIRLAM EURAD MOCAGE	77 compounds 214 reactions	23 photolysis reactions, procedure the same as in RADM2	ND	Stockwell et al. (1997)
SAPRC-99	Aladin-CAMx CMAQ FARM OPANA	80 compounds 214 reactions (48 inorganic) 16 radicals	24 photolysis reactions Rate constants must be calculated from their corresponding absorption cross sections and quantum yields given the spectrum and intensity of the sunlight or other light source in the simulation	ND	SAPRC-99: <a href="http://www.engr.ucr.edu/~carter/SAPRC99.htm">http://www.engr.ucr.edu/~carter/SAPRC99.htm</a>  SAPRC-07: <a href="http://www.engr.ucr.edu/~carter/SAPRC">http://www.engr.ucr.edu/~carter/SAPRC</a>
UNI-OZONE	EMEP MATCH(EMEP- MSC-W)	71 compounds 123 reactions (22 inorganic) 24 radicals (Ozone concentrations from 2-D global model scaled by observed total ozone columns)	22 photolysis reactions J-values calculated over clear sky conditions and for two predefined clouds	Aqueous oxidation of SO <sub>2</sub> by O <sub>3</sub> , H <sub>2</sub> O <sub>2</sub> and O <sub>2</sub> catalyzed by metal ions	<a href="http://www.emep.int/OpenSource/index.html">http://www.emep.int/OpenSource/index.html</a> Simpson et al. (2003)

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**Table 5.** Comparison studies of the various chemical sub-models.

References	CBM-IV (CB-IV)	ISORROPIA	MELCHIOR	RADM2 (RADM)	SAPRC- 99	UNI- OZONE (EMEP)	Other not discussed chemical submodules
Anderson-Sköld and Simpson (1999)						X	X
Ansari and Pandis (1999a,b)		X					X
Cuvelier et al. (2007)	X	X	X		X	X	X
Dodge (2000)	X			X	X		X
Faraji et al. (2008)	X				X		
Gross and Stockwell (2003)				X		X	
Jimenez et al. (2003)	X			X	X	X	X
Kuhn et al. (1998)	X			X		X	X
Luecken et al. (2008)	X				X		X
Sarwar et al. (2008)	X						X
Tilmes et al. (2002)	X			X		(X)	X
van Loon et al. (2007)	X	X	X			X	X
Vautard et al. (2007)	X	X	X		X	X	X
Yu et al. (2005)		X					X

N.B. EMEP refers to older versions of the EMEP model chemistry.

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**Table 6.** The treatments for aerosols in the CWF models: size distribution, chemical composition and aerosol microphysics.

Model	Size distribution representation			Sea salt	Dust	Elem. C	Chemical components in particle phase					Water	Biog. SOA	Anthr. SOA	Aerosol microphysics			
	Bulk	Modal	Sectional				Org. C	Sulfate	Nitrate	Ammonium	Nucl.				Cond.	Coag.	Dep.	
ALADIN-CAMx	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	
CAMx-AMWFG	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	
Enviro-HIRLAM		X		X	X			X						X	X	X	X	
FARM		X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	
LOTOS-EUROS	X			X	X	X	X	X	X	X	X	X					X	
MATCH	X			X	X	X	X	X	X	X	X						X	
MM5-CAMx	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	
MM5-CHIMERE			X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	
MM5-CMAQ		X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	
NAME	X			X	X	X	X	X	X	X	X	X	X				X	
OPANA		X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	
RCG	X			X	X	X	X	X	X	X	X	X	X				X	
SILAM	X		X	X	X	X	X	X	X	X	X			X	X	X	X	
SKIRON/Dust	X				X												X	
THOR	X			X													X	
WRF/CHEM		X(MADE)	X(MOSAIC)	X	X	X	X	X	X	X	X	X	X	X	X	X	X	

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**Table 7.** References or brief characterizations of the treatments for dry and wet deposition in the CWF models.

Model name	Canopy Resistance	Aerosol settling velocity and deposition	In-cloud scavenging	Below-cloud scavenging
CAMx	Wesely (1989)	Slinn and Slinn (1980)	Different scavenging coefficients for gases and aerosols following Seinfeld and Pandis (1998); precipitating water, snow and ice considered	Different scavenging coefficients for gases and aerosols following Seinfeld and Pandis (1998); precipitating water, snow and ice considered
Enviro-HIRLAM	Wesely (1989) and Binkowski (1999)	Näslund and Thaning (1991)	Scavenging coefficients for gases following Seinfeld and Pandis (1998); in-cloud scavenging of aerosols dependent on the aerosol radius and rain rate (Baklanov and Sørensen, 2001)	Scavenging coefficients for gases following Seinfeld and Pandis (1998); below-cloud scavenging of aerosols dependent on the aerosol radius and rain rate (Baklanov and Sørensen, 2001)
EURAD-RIU	Walcek et al. (1986)	Size dependent resistance model and gravitational settling depending on the three aerosol lognormal modes	Different scavenging coefficients based on Henry's law equilibria for each specie; aerosol mode dependent scavenging (Binkowski, 1999)	Different scavenging coefficients based on Henry's law equilibria for each specie; aerosol mode dependent scavenging (Binkowski, 1999)
FARM	Wesely (1989)	Seinfeld and Pandis (1998); Binkowski and Shankar (1995)	Gas scavenging as in EMEP Unified model (Simpson et al., 2003)	Gas scavenging as in EMEP Unified model (Simpson et al., 2003); aerosols following Scott (1978)
LOTOS-EUROS	Erisman et al. (1994)	Erisman and Draaijers (1995)	Neglected at start of paper writing, now via scavenging coefficients	Gases: scavenging rates depending on Henry's law constant and precipitation intensity (Simpson et al., 2003); aerosols following Scott (1978)
MATCH	Erisman et al. (1994) Bartnicki et al. (2001)	Seinfeld and Pandis (1998)	Ozone, H <sub>2</sub> O <sub>2</sub> and SO <sub>2</sub> in-cloud scavenging is calculated by assuming Henry's law equilibrium in the clouds; for sulfate particles, in-cloud scavenging is assumed to be 100% effective	For sulfate particles Berge (1993); neglected for ozone, H <sub>2</sub> O <sub>2</sub> and SO <sub>2</sub> ; for other species proportional to the precipitation intensity and a species-specific scavenging coefficient
CHIMERE	Erisman et al. (1994)	Seinfeld and Pandis (1998); Zhang et al. (2001); Giorgi (1986); Peters and Eiden (1992)	Dissolution of gases in cloud droplets (Seinfeld and Pandis, 1998); aerosol nucleation (Tsyro, 2002; Guelle et al., 1998)	Dissolution of gases in precipitating drops (Mircea and Stefan, 1998); scavenging by raining drops (Loosmore and Cederwall, 2004)
CMAQ	RADM (Wesely, 1989); M3Dry (Pleim et al., 2001)	Binkowski and Shankar (1995)	Wet deposition algorithms taken from RADM (Chang et al., 1987); wet deposition of chemical species depending on precipitation rate and cloud water concentration (Roselle and Binkowski, 1999); accumulation and coarse mode aerosols completely absorbed by cloud and rain water, Aitken mode aerosols slowly absorbed into cloud and rain water	Wet deposition algorithms taken from RADM (Chang et al., 1987); wet deposition of chemical species depending on precipitation rate and cloud water concentration (Roselle and Binkowski, 1999); accumulation and coarse mode aerosols completely absorbed by cloud and rain water, Aitken mode aerosols slowly absorbed into cloud and rain water
MOCAGE	ISBA (Interface Soil Biosphere Atmosphere) scheme (Michou et al., 2004)	Nho-Kim et al. (2004)	Convective (Mari et al., 2000) and stratiform precipitation (Giorgi and Chameides, 1986)	Giorgi and Chameides (1986)
NAME	Resistance analogy incorporating canopy resistance	Resistance analogy; particles removed by sedimentation and impaction with the surface	Rain and snow scavenging coefficients for large-scale and convective precipitation (Maryon et al., 1996)	Rain and snow scavenging coefficients for large-scale and convective precipitation (Maryon et al., 1996)

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Table 7. Continued.

Model name	Canopy Resistance	Aerosol settling velocity and deposition	In-cloud scavenging	Below-cloud scavenging
OPANA	Wesely (1989)	Binkowski and Shankar (1995)	wet deposition algorithms taken from RADM (Chang et al., 1987); wet deposition of chemical species depending on precipitation rate and cloud water concentration (Roselle and Binkowski, 1999); accumulation and coarse mode aerosols completely absorbed by cloud and rain water, Aitken mode aerosols slowly absorbed into cloud and rain water	Wet deposition algorithms taken from RADM (Chang et al., 1987); wet deposition of chemical species depending on precipitation rate and cloud water concentration (Roselle and Binkowski, 1999); accumulation and coarse mode aerosols completely absorbed by cloud and rain water, Aitken mode aerosols slowly absorbed into cloud and rain water
RCG	Erisman et al. (1994)	From Stoke's law (Pleim et al., 1984)	neglected	Species dependent scavenging coefficients for gases from Henry constant and precipitation rate (Seinfeld and Pandis, 1998); scavenging coefficient identical coefficients for all particles
SILAM	Hicks et al. (1987); Lindfors et al. (1991)	From Stoke's law	Water and snow scavenging from large-scale and convective precipitation (Smith and Clark, 1989; Jylhä, 1991)	Water and snow scavenging from large-scale and convective precipitation (Smith and Clark, 1989; Jylhä, 1991)
SKIRON/ Dust	–	Slinn and Slinn (1980), Kumar et al. (1996)	Constant scavenging coefficient (Seinfeld and Pandis, 1998)	Constant scavenging coefficient (Seinfeld and Pandis, 1998)
THOR	Wesely and Hicks (1977)	Gravitational settling velocity given by Stokes equation (Hanna et al., 1991)	Rain and snow scavenging coefficients for large-scale and convective precipitation (Maryon et al., 1996)	Rain and snow scavenging coefficients for large-scale and convective precipitation (Maryon et al., 1996)
WRF/ CHEM	Wesely (1989) and Erisman et al. (1994)	Slinn and Slinn (1980), Pleim et al. (1984)	In-cloud wet removal of aerosol particles involves removal of the cloud-borne aerosol particles collected by rain, graupel and snow, using the same first-order rate that cloud water is converted to precipitation. For trace gases, the same removal rate is applied to the fraction of each gas that is dissolved in cloud water	Below-cloud wet removal of aerosol particles by impaction scavenging via convective brownian diffusion and gravitational or inertial capture. Irreversible uptake of $\text{H}_2\text{SO}_4$ , $\text{HNO}_3$ , $\text{HCl}$ , $\text{NH}_3$ and simultaneous reactive uptake of $\text{SO}_2$ , $\text{H}_2\text{O}_2$ . (Easter, 2004)

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**Table 8a.** The gaseous natural emissions accounted for in the CWF models, as well as their calculation methodologies.

Model name	Vegetation		Soil		Volcanoes		Oceans		Animals (wild and domestic)	
	Component	Method	Component	Method	Component	Method	Component	Method	Component	Method
ALADIN-CAMx	Isoprene, 2-Methyl-3-buten-2-ol, Methanol, Ethene, Propene, Ethanol, Acetone, Hexanal, Hexenol, Hexenylacetate, Formaldehyde, Acetaldehyde, Butene, Ethane, Formic acid, Acetic acid, Butenone, other reactive VOCs and Monoterpenes	SMOKE emission model (Houyoux and Vukovich, 1999) using the Biogenic Emissions Inventory System (BEIS3) ( <a href="http://www.epa.gov/asmdner/biogen.html">http://www.epa.gov/asmdner/biogen.html</a> ); Guenther et al. (1994, 2000)	Nitric oxide, Carbon monoxide	SMOKE emission model (Houyoux and Vukovich, 1999) using the BEIS3 mechanism ( <a href="http://www.epa.gov/asmdner/biogen.html">http://www.epa.gov/asmdner/biogen.html</a> ); Guenther et al. (2000)	Not included	Not included	Not included	Not included	Not included	Not included
CAMx-AMWFG	Isoprene	Global Emissions Inventory Activity (GEIA) database ( <a href="http://www.geiacenter.org">www.geiacenter.org</a> )	Ammonia	Global Emissions Inventory Activity (GEIA) database ( <a href="http://www.geiacenter.org">www.geiacenter.org</a> )	Sulphur dioxide	Global Emissions Inventory Activity (GEIA) database ( <a href="http://www.geiacenter.org">www.geiacenter.org</a> ). Continuously erupting volcanoes	Ammonia	Global Emissions Inventory Activity (GEIA) database ( <a href="http://www.geiacenter.org">www.geiacenter.org</a> )	Ammonia	Global Emissions Inventory Activity (GEIA) database ( <a href="http://www.geiacenter.org">www.geiacenter.org</a> )
ENVIRO-HIRLAM	ND	ND	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
FARM	Isoprene, Monoterpenes	Guenther et al. (1993, 1995)	Nitric oxide	Williams et al. (1992)	Not included	Not included	Not included	Not included	Not included	Not included
LOTOS-EUROS	Isoprene, Monoterpenes	Guenther et al. (1993, 1995)	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
MATCH	Isoprene	Simpson et al. (1995) (E-94 methodology); Guenther et al. (1993)	Not included	Not included	Sulphur dioxide, sulphate	EMEP expert emission inventory ( <a href="http://www.emep.int/">http://www.emep.int/</a> )	Not included	Not included	Ammonia	EMEP expert emission inventory ( <a href="http://www.emep.int/">http://www.emep.int/</a> )
MM5-CAMx	Isoprene, Monoterpenes, other VOCs	Emission model developed by the Aristotle University of Thessaloniki and the National and Kapodistrian University of Athens (Poupkou et al., 2010; Symeonidis et al., 2008; Guenther et al., 1995)	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
MM5-CHIMERE	Isoprene, <i>A</i> -pinene, <i>B</i> -pinene, Limonene, Ocimene	MEGAN emission model (Guenther et al., 2006)	Nitric oxide	Stohl et al. (1996)	Not included	Not included	Not included	Not included	Not included	Not included
MM5-CMAQ	Isoprene, Monoterpenes	BIOEMI emission model developed by the Technical University of Madrid (Guenther et al., 1993, 1995; Schoenemeyer et al., 1997; Steinbrecher, 1997)	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
MOCAGE	Isoprene, Monoterpenes, other VOCs	Guenther et al. (1993, 1995)	Nitrogen oxides, Carbon monoxide	Emmons and Lamarque (NCAR), personal communication (2006)	Sulphur dioxide	Andres and Kasgnoc (1998)	Carbon monoxide, Methane	Emmons and Lamarque (NCAR), personal communication (2006)	Not included	Not included
NAME	No natural emissions									

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**Table 8a.** Continued.

Model name	Vegetation		Gaseous emissions				Volcanoes		Oceans		Animals (wild and domestic)	
	Component	Method	Component	Method	Component	Method	Component	Method	Component	Method	Component	Method
OPANA	Isoprene, Monoterpenes	BIOEMI emission model developed by the Technical University of Madrid (Guenther et al., 1995; Schoenemeyer et al., 1997; Steinbrecher, 1997)	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
RCG	Isoprene, Monoterpenes, other VOCs	Simpson et al. (1995) (E-94 methodology); Guenther et al. (1993); CORINAIR (CORE Inventory of AIR emissions) emission handbook	Nitric oxide	Simpson et al. (1995)	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
SILAM	Isoprene, Monoterpenes	Guenther et al. (1993, 1995)	Ammonia	EMEP/GEMS/GEIA/RETRO emission inventories	Sulphur oxides	EMEP/GEMS/GEIA/RETRO emission inventories	Not included	Not included	Ammonia	EMEP/GEMS/GEIA/RETRO emission inventories	Not included	Not included
SKIRON/ Dust	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included
THOR	Isoprene	Global Emissions Inventory Activity (GEIA) database (www.geiacenter.org)	Nitrogen oxides	Global Emissions Inventory Activity (GEIA) database (www.geiacenter.org)	Not included	Not included	Not included	Not included	Ammonia	Global Emissions Inventory Activity (GEIA) database (www.geiacenter.org)	Not included	Not included
WRF/CHEM	Isoprene, Monoterpenes, other VOCs	Biogenic emission module based on Guenther et al. (1993, 1994), Hahn et al. (1994), Simpson et al. (1995), Schoenemeyer et al. (1997) OR the Biogenic Emissions Inventory System (BEIS3) (Vukovich and Pierce, 2002)	Nitric oxide	Simpson et al. (1995)	Not included	Not included	Not included	Not included	Not included	Not included	Not included	Not included



**Table 8b.** The particulate emissions accounted for in the CWF models, as well as their calculation methodologies.

Model name	Particulate emissions		
	Dust Methodology	Sea salt Methodology	Pollen Methodology
ALADIN-CAMx	Not included	Not included	Not included
CAMx-AMWFG	Desert dust fluxes from the SKIRON/Dust modelling system	Module developed by the AM&WF Group at the National and Kapodistrian University of Athens (de Leeuw et al., 2000; Gong et al., 2002; Gong, 2003; Zhang et al., 2005; Shankar et al., 2005; Astitha and Kallos, 2009)	Not included
ENVIRO-HIRLAM	Not included	Not included	Birch pollen emission module developed by the Danish Meteorological Institute and the Finnish Meteorological Institute (Mahura et al., 2009)
FARM	Vautard et al. (2005)	Zhang et al. (2005b)	Not included
LOTOS-EUROS	Not included	Monahan et al. (1986); TNO (2005)	Not included
MATCH	Only anthropogenic: Andersson et al. (2009)	Foltescu et al. (2005)	Not included
MMS-CAMx	Not included	Not included	Not included
MMS-CHIMERE	Vautard et al. (2005), Marticorena and Bergametti (1995), Menut et al. (2007)	Monahan et al. (1986)	Not included
MMS-CMAQ	Not included	Not included	Not included
MOCAGE	Martet et al. (2009)	Gong et al. (1997)	Not included
NAME	No natural emissions		
OPANA	Not included	Not included	Not included
RCG	Loosmore and Hunt (2000), Claiborn et al. (1998)	Gong et al. (1997)	Not included
SILAM	Not included	Module developed in the Finnish Meteorological Institute based on Monahan et al. (1986) and Martensson et al. (2003)	Modules developed in the Finnish Meteorological Institute for birch and grass pollen (Sofiev et al., 2006b)
SKIRON/Dust	Dust module developed by the AM&WF Group at the National and Kapodistrian University of Athens (Marticorena and Bergametti, 1995; Nickovic et al., 2001; Zender et al., 2003; Pérez et al., 2006)	Not included	Not included
THOR	Not included	Not included	Not included
WRF/CHEM	Not included	Not included	Not included



**Table 9.** Details on the grid spacings and coordinate systems of the different CWF models.

Model name	Coupling	Type/Coordinate system	Horizontal grid spacing	Vertical grid spacing
ALADIN-CAMx	Offline	3-D Eulerian Lambert Conformal Arakawa C grid	28.9 km for the mother grid (Central Europe) 9.63 km for the inner modeling domain (Austria and surroundings)	15 vertical layers (30 m to 2.5 km). The highest grid spacing (about 30 m) is achieved in the lowest 5 levels (up to about 350 m)
CAMx-AMWFG	Offline	3-D Eulerian Curvilinear geodetic latitude/longitude Arakawa C grid	0.24° × 0.24° (~ 24 km) The area covered is the Mediterranean region, Europe (up to 55° N), North and Central Africa, Turkey and part of the Arabian Peninsula	22 layers up to 8 km with variable spacing First layer from the ground at 50 m
ENVIRO-HIRLAM	Online	3-D Eulerian rotated latitude-longitude Arakawa C grid	5 km (pollen forecast)	Hybrid terrain-following sigma and pressure coordinate system 40 layers, grid spacing from 30 m to 500 m
EURAD-RIU	Offline	3-D Eulerian	Europe: 125 km; Central Europe: 25 km, German States: 5 km	23 layers from 40 m to 2000 m at top (100 hPa)
FARM	Offline	3-D Eulerian UTM (Universal Transverse Mercator); polar stereographic; latitude/longitude; mercator	12 km (Italian Peninsula)	Terrain following coordinates with variable vertical spacing up to 10 km
LOTOS-EUROS	Offline	3-D Eulerian Normal latitude-longitude	0.5° × 0.25° (Europe) (~ 25 × 25 km) 0.25° × 0.125° (Netherlands) (~ 12 × 12 km) 0.125° × 0.0625° (Netherlands) (~ 6 × 6 km)	Dynamic mixing layer approach 4 layers (surface layer of 25 m, mixing height layer and 2 reservoir layers up to 3.5 or optionally 5 km)
MATCH	Offline	3-D Eulerian	44 km (MATCH-HIRLAM) (Europe) 0.5° (~ 50 km) (MATCH-ECMWF) (Europe)	Usually depending on met. model. At present for HIRLAM: domain height ~ 8 km, lowest level at ~ 60 m
MMS-CAMx	Offline	3-D Eulerian Lambert conformal	30 km for Europe (mother grid) 10 km for the Balkan Peninsula and 2 km for Athens (nested grids)	CAMx: 15 vertical layers, 1st layer height 20 m, top at 7 km. MMS: 29 vertical sigma-levels, top at 100 mbar
MMS-CHIMERE	Offline	3-D Eulerian	50 km (Western Europe) 10 km (Portugal)	In the vertical there are 8 layers up to 500 hPa with the surface layer located at 50 m
MMS-CMAQ	Offline	3-D Eulerian Lambert conformal	50 km (Europe) 27 km (Iberian Peninsula)	15 layers up to 100 hPa
MOCAGE	Offline	3-D Eulerian	PREVAIR: 2° (~ 200 km) (global); 0.5° (~ 50 km) (Europe and Mediterranean area); 0.1° (~ 10 km) (France) GEMS, MACC: 2° (global); 0.2° (Europe) Currently testing: 0.025° (France)	Hybrid (sigma, P) coordinate system with currently 60 levels from the surface up to 1 or 0.1 hPa (7–8 levels in the PBL with a first layer of 20 to 40 m)
NAME	Offline	3-D Lagrangian	No intrinsic grid. The Met Office Unified: globally at 40 km resolution and in a European limited area configuration at 12 km	Continuously variable
OPANA	Offline	3-D Eulerian UTM	5 km (coarse grid, Madrid) 1 km (nested grid, Madrid)	Terrain following coordinates with 15 layers up to 6 km. Surface layer at 20 m
RCG	Offline	3-D Eulerian	25 km	5 layers, surface layer of 25 m, 2 layers above surface layer and mixing height and 2 reservoir layers
SILAM	Offline	3-D Lagrangian, 3-D Eulerian	0.2° × 0.2° (~ 20 km) (Europe) 5 km (Northern Europe)	Multi-vertical approach with the meteorology-resolving grid corresponding to the tropospheric part of the IFS vertical: hybrid levels. The chemical transformations and vertical fluxes are computed on the basis of thick staggered layers
SKIRON/Dust	Online	3-D Eulerian Polar stereographic Arakawa E-grid	0.24 × 0.24° (~ 24 km) 2 grids: one for the Mediterranean Region and Europe and one extended to the North Atlantic Region	Eta step-mountain vertical coordinate system with 38 vertical levels from the surface up to 22 km
THOR	Offline	3-D Eulerian (DEHM) 3-D Lagrangian (UBM)	DEHM mother domain: 150 × 150 km (hemispheric) DEHM first nest: 50 km × 50 km (Europe) DEHM second nest: 16.67 × 16.67 km UBM: 1 km × 1 km (urban) OSPM: 0.001 km (street pollution)	DEHM: 20 layers up to ~15 km, lowest model layer 50 m
WRF/CHEM	Online	3-D Eulerian Lambert conformal	50 km (Europe)	The vertical structure has 12 layers in sigma coordinates with the top pressure at 100 hPa
WRF/CMAQ	Offline	3-D Eulerian Lambert Conformal Arakawa C	12 km	Terrain-following hydrostatic pressure coordinates. 22 layers extending from the surface to 100 hPa are interpolated from the 60 WRF layers

**Table 10.** A summary description of the evaluation of each CWF model. The evaluation levels have been defined in the text.

Model name	How model was evaluated	Evaluation level	References (up to 4)	Quantities evaluated
ALADIN-CAMx	Citydelta project: Aimed to explore the changes in urban air quality predicted by different chemistry-transport dispersion models in response to changes in urban emissions. Model provided good performances for ozone (both on average and for extreme values). Acceptable results have been obtained for PM <sub>10</sub> yearly means. ESCOMPTE project: The Model has highlighted quite good performance for both ozone and NO <sub>2</sub>	Level 2	- Hirtl et al. (2007) - Baumann-Stanzer et al. (2005) - Vautard et al. (2007)	O <sub>3</sub> , O <sub>x</sub> , PM <sub>10</sub> , NO <sub>2</sub>
CAMx-AMWFG	The evaluation of the model performance on the known gas and aerosol species has been included in several publications worldwide. The model intercomparison has been done against in-situ measurements for the species concentration and against AERONET data for the dust optical depth used for the calculation of the photolysis rates	Level 2	- Astitha et al. (2006) - Astitha et al. (2007b) - Astitha and Kallos (2008) - Astitha et al. (2010)	The evaluation of the model performance on the known gas and aerosol species like ozone, NO <sub>x</sub> , sulfates, nitrates etc
Enviro-HIRLAM	Validation against field experiments of ETEX and MEGAPOLI, and Chernobyl measurements. Meteorology and air quality forecasts validated against Paris surface observation network for specific episodes. Model intercomparison: Participant in EU MEGAPOLI project. Needs further verification over long-term periods	Level 2	- Chenevez et al. (2004) - Korsholm et al. (2009) - Korsholm (2009) - Mahura et al. (2008)	Transport and scavenging processes have been evaluated using ETEX and Chernobyl observations; meteorology (with feedbacks), surface O <sub>3</sub> , NO <sub>x</sub> , SO <sub>2</sub> , PM using Paris monitoring and MEGAPOLI campaign data
EURAD-RIU	GEMS: Evaluation against measurements and other air quality forecast models. Participation of the COST 728 model intercomparison for the winter 2003 case	Level 2	- Hass et al. (1997) - Jakobs et al. (2002) - Schlünzen and Fock (2008)	O <sub>3</sub> , PM <sub>10</sub> , NO <sub>2</sub> ,
FARM	On single model components and against monitoring data in real applications. Long-term model intercomparison exercise over Po Valley (Northern Italy), carried out by Regional Environmental Protection Agencies. Ongoing long-term model intercomparison exercise over Po Valley (Northern Italy), carried out by Regional Environmental Protection Agencies	Level 2	- Silibello et al. (2008) - Schlünzen and Fock (2008)  - Calori et al. (2008) - Gariazzo et al. (2007)	O <sub>3</sub> , NO <sub>2</sub> , NO <sub>x</sub> , PM <sub>10</sub>
LOTOS-EUROS	Validation with groundbased measurements. EURODELTA: A regional scale model intercomparison to analyse the responses of different CTMs to emission changes/scenarios	Level 2	- Schaap et al. (2008)	O <sub>3</sub> , NO <sub>2</sub> , NO, NH <sub>3</sub> , SO <sub>4</sub> , SO <sub>2</sub> and NH <sub>4</sub> . Secondary organic aerosols, sea salt, and heavy metal concentrations
MATCH	Eurodelta: Evaluation of seven regional air quality models and their ensemble for Europe and Mics Asia – Model intercomparison study for Southern and Eastern Asia, Phase 1 and 2	Level 2	- Carmichael et al. (2002) - Carmichael et al. (2008b)	Evaluated reference dataset: chemistry and transport including SO <sub>2</sub> , NO <sub>2</sub> , NO <sub>x</sub> , NH <sub>3</sub> , HNO <sub>3</sub> , O <sub>3</sub> , CO, CF <sub>6</sub> , <sup>137</sup> Cs, seasalt, (CF <sub>6</sub> during the ETEX-experiment and <sup>137</sup> Cs for the Tjernobyl accident). Model intercomparison: including SO <sub>2</sub> , NO, NO <sub>2</sub> , NO <sub>x</sub> , NH <sub>3</sub> , HNO <sub>3</sub> , O <sub>3</sub> , HCHO

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**Table 10.** Continued.

Model name	How model was evaluated	Evaluation level	References (up to 4)	Quantities evaluated
MM5-CAMx	Within the European project GEMs, the air quality forecast has been operationally evaluated against surface measurements in Europe (rural stations of EMEP, urban stations of AIRBASE in Athens, Greece) and compared with the forecasts from other models (e.g. CHIMERE, EMEP, EURAD etc.) and the European ensemble forecast. Tropospheric columns of NO <sub>2</sub> and O <sub>3</sub> have been compared with satellite data. There has been also upper air evaluation with WOUDC sites measurements	Level 3	<ul style="list-style-type: none"> <li>- Huijnen et al. (2010)</li> <li>- Kioutsioukis et al. (2009)</li> <li>- Kioutsioukis et al. (2010)</li> <li>- Poupkou et al. (2008)</li> <li>- Poupkou et al. (2006)</li> </ul>	Ozone, nitrogen dioxide, sulphur dioxide, carbon monoxide and particulate matter (PM <sub>10</sub> )
MM5-CHIMERE	MM5: Evaluated in many model intercomparison studies, particularly compared to RAMS. CHIMERE: Analysis evaluation was performed through studies published in more than 30 peer reviewed papers. For the forecast, the evaluation of the model is updated daily on the PREVAIR web site with correlations scores compared to hourly surface measurements. Model intercomparison: City-Delta, Euro-Delta, Esquif, escompte. Numerous projects, described on the CHIMERE web site	Level 2	<ul style="list-style-type: none"> <li>- Hara et al. (2005)</li> <li>- O'Neil et al. (2005)</li> <li>- Menut et al. (2005)</li> <li>- Vautard et al. (2007)</li> </ul>	Dispersion simulations of O <sub>3</sub> , O <sub>x</sub> , PM <sub>10</sub>
MM5/WRF-CMAQ	The model is used for several experiments and compared the results with the observational data. Results show correlation coefficients between 0.5 to 0.9 for Ozone concentrations for one year hourly concentrations (8760 data)	Level 2	<ul style="list-style-type: none"> <li>- Meng et al. (2007)</li> <li>- Vijayaraghavan et al. (2007)</li> <li>- San Jose et al. (2007)</li> <li>- Appel et al. (2009)</li> </ul>	Analysis of the amount of air pollutant concentrations due to the industrial plant emissions. Evaluation of the potential impact of an incinerator. Modeling the transport and transformation of mercury. Performance of the model system is compared with the existing measurements of a total of 22 PCB congeners and the 17 most toxic PCDD/F congeners
MOCAGE	Meteorological forcings from MOCAGE are provided by numerical weather prediction suites at Météo-France (ARPEGE, ALADIN) and ECMWF (IFS), with operational skill score verifications. MOCAGE has been evaluated against observations in the context of a range of field campaigns and international exercises (ESQUIF, ESCOMPTE, City-Delta, ICARTT-ITOP,...), with over 40 publications in the international refereed literature. Evaluation range from the global scale (including the stratosphere) to the regional/local scale for gases and primary aerosol species. Continuous operational skill score monitoring for regulatory species is performed at Météo-France and INERIS in the context of PREVAIR (Rouil et al., 2009)	Level 2	<ul style="list-style-type: none"> <li>- Josse et al. (2004)</li> <li>- Dufour et al. (2004)</li> <li>- Bousserrez et al. (2007)</li> <li>- Ménégoz et al. (2009)</li> </ul>	Transport and scavenging processes have been evaluated using ETEX and Rn/Pb observations; surface O <sub>3</sub> , NO <sub>x</sub> , SO <sub>2</sub> , HNO <sub>3</sub> , PAN using routine surface observation and campaign data; deposition of ozone using ESCOMPTE data; global tropospheric and stratospheric distributions of Ozone, CO, NO <sub>2</sub> , N <sub>2</sub> O using a range of satellite data products; aerosol was evaluated using surface PM observations, Lidar and AERONET data, as well as campaign data

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Table 10. Continued.

Model name	How model was evaluated	Evaluation level	References (up to 4)	Quantities evaluated
NAME	Validation against field experiments including ETEX, and Kincaid. Air quality forecasts validated against UK surface obs network. Model intercomparison: Participant in EU ENSEMBLE project	Level 2	- Webster and Thomson (2002) - Ryall and Maryon (1998) - Simmonds et al. (1996)	Plume rise scheme is validated against Kincaid data set. NAME model predictions are compared against ETEX. Model has been validated against observations of a number of trace gases. Intercomparisons amongst European models used to simulate foot and mouth disease spread
OPANA	Evaluated at the end of EMMA project (CGXIII, 1996–98). The system has been tested again many data during the last 10 years. Model intercomparison: The model has been tested and compared with observational data in every air quality impact assessment (calibration phase) and in every real-time air quality forecasting system developed for urban and/or industrial areas since the system is calibrated with one year air quality monitoring data in the subjected area and surroundings	Level 2	- San José et al. (2005)	O <sub>3</sub> , NO <sub>2</sub> , CO, SO <sub>2</sub> , PM <sub>10</sub> , PM <sub>2.5</sub> , Cadmium, Arsenic, Nickel, Lead and Benzo(a)pyrene
RCG	PM <sub>10</sub> -measurements done in and around the Greater Berlin Area have been used to validate RCG on different scales. EuroDelta model intercomparison for Europe. EUROTRAC – GLOREAM: The focus is primarily on model performance for aerosol components in conjunction with the EMEP observational data that has been extended using Dutch and German special observation sites	Level 2	- Beekmann et al. (2007) - van Loon et al. (2004) - Hass et al. (2003)	PM <sub>10</sub> (EC, OC, inorganic aerosols, metals), sulphate, nitrate, ammonium, elemental carbon, wind-blown-dust events
SILAM	Regular emergency-type evaluations whenever possible. Operational validation of the air quality forecasts using present-week observations over Finland. European-scale re-analysis for 2000–2003. Emergency-type model intercomparisons within EU-ENSEMBLE and follow-up projects, NKS-MetNet network, etc. Air quality intercomparison projects are on-going within the scope of COST-728, EU-GEMS, and ESA-PROMOTE	Emergency applications: Level 1. Others: Level 2– Level 3	- Sofiev et al. (2006c) - Galmarini et al. (2004a) - Huijnen et al. (2010)	Air quality forecasts. Individual model units were compared against analytical solutions, chemical scheme tested as a box model, etc.
SKIRON/Dust	Validation and evaluation of the model SKIRON/ Dust have been performed from AM&WFG during several projects (SKIRON, MEDUSE and ADIOS). Also, the modeling system has been used by other Universities and Institutes world-wide. Model intercomparison has been performed against measurements and observations	Level 2	- Astitha et al. (2007a) - Kallos et al. (2009) - Kallos et al. (2007)	Intercomparison against in-situ measurements of dust and PM concentration, remote measurements of aerosol optical depth from satellites or radars

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**Table 10.** Continued.

Model name	How model was evaluated	Evaluation level	References (up to 4)	Quantities evaluated
THOR	EuroDelta experiment: Long-term ozone simulations from seven regional air quality models were intercompared and compared to ozone measurements. Validation and comparison for two cities in Denmark with Urban Backround Model, BUM, and Operational Street Pollution Model, OSPM, included to THOR system	Level 2	- Brandt et al. (2001)	Performance of the air pollution models BUM and OSP for NO <sub>x</sub> , O <sub>3</sub> , NO, NO <sub>2</sub>
WRF/CHEM	WRF/Chem-MADRID has been evaluated with Satellite and Surface Measurements	Level 2	- Zhang et al. (2005a)	The simulated concentrations of gas and aerosol species (e.g., O <sub>3</sub> , SO <sub>2</sub> , NO <sub>x</sub> , and PM <sub>2.5</sub> ) and aerosol optical properties (e.g., aerosol optical depth, single scattering albedo, aerosol direct radiative) are being compared against available observational data

**Table 11.** A summary of the availability, user communities, and documentation of the various CWF systems.

Model name	User interface availability	User community	Documentation status	Availability
ALADIN-CAMx	Mainly Linux shell scripts and Fortran90 (fortran) code	Researchers for regulatory applications. Combination of ALADIN-Austria and CAMx is only implemented at ZAMG	Level 1: CAMx ( <a href="http://www.camx.com">www.camx.com</a> ), physical description of model, code administration, installation guide, evaluation. Level 1: ALADIN ( <a href="http://www.cnrm.meteo.fr/aladin">www.cnrm.meteo.fr/aladin</a> ), physical description of the model, variable settings	Not a public domain programme. Information on the conditions for obtaining the model can be provided by the contact person. CAMx is open source software: <a href="http://www.camx.com">www.camx.com</a>
CAMx-AMWFG	Linux shell scripts, Intel Fortran using OpenMP, NCAR graphics	The model can be used properly by a highly skilled person	Level 1: Complete documentations available, ranging from the scientific description down to users manuals with details on the machine code	CAMx-AMWFG (with the new features) availability should be discussed with the contact person. CAMx is open source code available from <a href="http://www.camx.com">www.camx.com</a>
Enviro-HIRLAM	Shell scripts and FORTRAN code. METGRAF graphics	Enviro-HIRLAM is baseline system for the international HIRLAM chemical branch. The model can be used properly by a highly skilled person	Model formulation, practical lectures notes and web-description. Level 2, English. <a href="https://hirlam.org/trac/wiki">https://hirlam.org/trac/wiki</a>	For users of the HIRLAM chemical branch. Enviro-HIRLAM is an open community model, source code is available from <a href="http://hirlam.org">hirlam.org</a> upon agreement
EURAD-RIU	Linux shell scripts, Portland Fortran compiler using OpenMP or MPI, NCAR Graphics	The EURAD research group at RIU	Model description and user manual	Not a public domain model system. Availability possible within common projects
FARM	Post-processor for statistical analysis of modelled fields and data extraction as well as interface with visualization tools (AVISU, Savi3-D, GRADS, Vis3D)	Italian national and local environmental authorities, research institutes. Users of FARM should have a sufficient background in atmospheric sciences and experience in the use of complex numerical models	Model formulation and user manual. Level 1-2, English	Available to selected users
LOTOS-EUROS	Configuration file including description, shell scripts to compile and start	Scientists within national and international projects. Forecasts provided to the public	Yearly reports with description of physics and parameterisation. Technical documentation for daily usage	Limited to institutes participating in model consortium. Information on the conditions for obtaining the model can be provided by the contact person
MATCH	Shell scripts and Fortran code, requiring technical expertise. More user-friendly frontends with less configuration options exist for specific applications	Scientists within national and international projects. Environmental agencies and decision makers (access mostly through tailored interfaces). Forecasts provided to the public	Level 2: Rather good scientific documentation and less complete user's manuals. Automatically generated html-documentation included in model installation. General information also available on the web-page	The model is not a public domain programme. Information on the conditions for obtaining the model can be provided by the contact person
MMS-CAMx	Linux shell scripts, Intel Fortran using OpenMP, PAVE and GRADS visualization tools	Research groups, environmental agencies, private companies. The modelling system can be applied by skilled users	Complete documentation (scientific description, user's guide, software) available at: MMS: <a href="http://www.mmm.ucar.edu/mms/">http://www.mmm.ucar.edu/mms/</a> ; and CAMx: <a href="http://www.camx.com">http://www.camx.com</a>	The MMS-CAMx system used for air quality forecast in Europe, in the Balkans and in Athens is not public available. The availability of the system can be discussed with the contact persons. Both MMS and CAMx are public available models
MMS-CHIMERE	CHIMERE: Fortran program called CHIM2FIG for automatic generation of maps, vertical cross-section, time-series using GMT free software. The exachim tool using Grads free software	CHIMERE users mailing list: <a href="mailto:chimere-users@lmd.polytechnique.fr">chimere-users@lmd.polytechnique.fr</a> Website: <a href="http://suler.lmd.polytechnique.fr/chimere">http://suler.lmd.polytechnique.fr/chimere</a> Questions: <a href="mailto:chimere@lmd.polytechnique.fr">chimere@lmd.polytechnique.fr</a>	MMS: Journal publications, workshop preprints, NCAR technical notes and manuals are available from the NCAR MMS Community Model Homepage. CHIMERE: Complete documentations available, ranging from the scientific description down to users manuals	MMS: The model is a public domain programme. The source code and utility programmes can be downloaded from the NCAR MMS Community Model Homepage: <a href="http://www.mmm.ucar.edu/mms/3/wh/rev3.html">http://www.mmm.ucar.edu/mms/3/wh/rev3.html</a> CHIMERE: Online free access to the code under the General Public License
MMS/WRF-CMAQ	Shell and Tcl shell scripts. IDV and PAVE visualization tools. Interfaces developed to convert output original files (NETCDF) to Ferret format	Research groups, environmental agencies, private companies. The modelling system can be applied by skilled users. Operational air quality forecasting systems for cities and industrial plants. Used for air quality impact studies for new power plants, incinerators and oil companies	All documentation can be found in <a href="http://www.cmascenter.org/">http://www.cmascenter.org/</a> . MMS was originally developed by NCAR/PSU in US and the development of WRF is a collaborative partnership among the NCAR, NCEP, FSL, AFWA, the Naval Research Laboratory, University of Oklahoma, and FAA. CMAQ was originally developed by US EPA	MMS/WRF-CMAQ is in the public domain. Scripts developed ad-hoc for running the systems and for specific customized applications have to be developed on demand. Please contact Director ESMG or CAIR, University of Hertfordshire for details
MOCAGE	UNIX/Linux shells or PreP/PS/Olive interfaces to run the model. Output is available in NetCDF (CF) or/and LFI or GRIB. Tools (fortran code, shell script in UNIX/LINUX or PYTHON) are available for graphical production with GMT, FERRET and IDL	Météo-France research centre, Météo-France operational departments (environment and health division, forecasters in support of accidental crises), research labs (Laboratoire d'Aérodynamique, CERFACS), PREVAIR users (local air quality agency, ministry for environment...), National Met Services (AEMET Spain, DMN Morocco, NMA Roumania, KMA Korea)	In addition to peer-reviewed international literature, model documentation (scientific, user) is currently composed of several documents. Harmonization of these and further developments are on-going. Detailed information on demand	The code is not in the public domain, but it is available free of charge for research purposes under a specific scientific applications agreement. For operational and/or commercial application of the code or outputs, a negotiation is needed with Météo-France (contact us)
NAME	Simple text file	UK Met Office Universities, UK government and defence organisations	Level 2/level 3 documentation. Adequate user manual. Significant validation of model against experimental data	The model can be made available to research and commercial users via negotiation with the Met Office
OPANA	Friendly user interface which can be easily customised to user specifications	City Council, Environmental Administrations or Regional Authorities, industry, etc	Model is having an on-line help and on-line manual	Conditions to have a licence of OPANA framework can be provided by the contact person
RCG	Input ascii-file must be compiled	Governmental or local authorities, scientists within national and international projects	Reports and publications. Documentation available on demand	NO INFO

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**Table 11.** Continued.

Model name	User interface availability	User community	Documentation status	Availability
SILAM	Available for emergency tasks (restricted access via SILAM Web portal)	Operational dept. of Finnish Met. Inst. (Emergency preparedness, Operational air quality forecasts), Finnish Radiation Protection Authority (Emergency preparedness), Research purposes: Finnish Met. Inst., and other Research groups	Level 1 documentation for the operational version is available from the Web site ( <a href="http://silam.fmi.fi/">http://silam.fmi.fi/</a> )	The model is public. Well-tested operational version v.3.6.5 is available from the Web site. Research version of the model is available on request
SKIRON/Dust	Linux shell scripts, Intel Fortran using MPI parallel processing, NCAR graphics	The model can be used properly by a highly skilled person	Level 2	Information on the availability can be provided by the contact person
THOR	Linux shells, Pathscale, portland and Intel Fortran, UNIRAS graphics, vis5d, IDV, NCL	Research groups. The modelling system can be applied by skilled users	Peer review papers and some documentations available	Not a public domain model system. Availability possible within common projects
WRF/CHEM	Shell and Tcl shell scripts. IDV and PAVE visualization tools. Interfaces developed to convert output original files (NETCDF) to Ferret format	WRF/CHEM is used as a research tool by ESMG-UPM. Recently applied for internal tests in operational air quality forecasting systems. Applied in several COST 728 projects	No info	WRF/CHEM is in the public domain. Scripts developed ad-hoc for running the systems and for specific customized applications have to be developed on demand. Please contact Director ESMG for details

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**Table 12.** Dissemination of CWF system predictions in the Internet. The results correspond to characteristic properties for European regional scale CWF systems (Balk et al., 2010).

Operational CWF modeling system characteristic	Parameters and explanation
Forecasting period	The time frame of the forecasting, ranging from 24 h to 3 days in advance
Pollutants forecasted	Two to seven pollutants were addressed, and include PM <sub>2.5</sub> , PM <sub>10</sub> , NO, NO <sub>2</sub> , NH <sub>3</sub> , O <sub>3</sub> , SO <sub>2</sub> , CO, benzene, and radon
Information type provided	Varies on a case-by-case basis, and includes daily mean, daily maxima, hourly values, hourly averages, hourly maxima, 8 h running average (for Ozone), and Air Quality Index
Information presentation	In the majority of cases, the information is presented with the aid of two-dimensional pseudo-color concentration contours. Some times are available as animations or spot maps. Images are GIF formatted, and in a few cases are available also as PNG files, or via a Java Applet
Additional information	Some systems also provided information on the road and railroad network, wind speed, cloud coverage, temperature, mixing layer, animated trajectories, wet deposition, and time series graphs for selected locations. Animations of various days were also available for some parameters ion some systems
Web site technology and user interface	In the majority of cases, this was covered with HTML and AJAX. Although in many cases, the solution adopted was HTML and PHP, or the applications used HTML and Java, HTML, AJAX and Java, HTML, or PHP and AJAX

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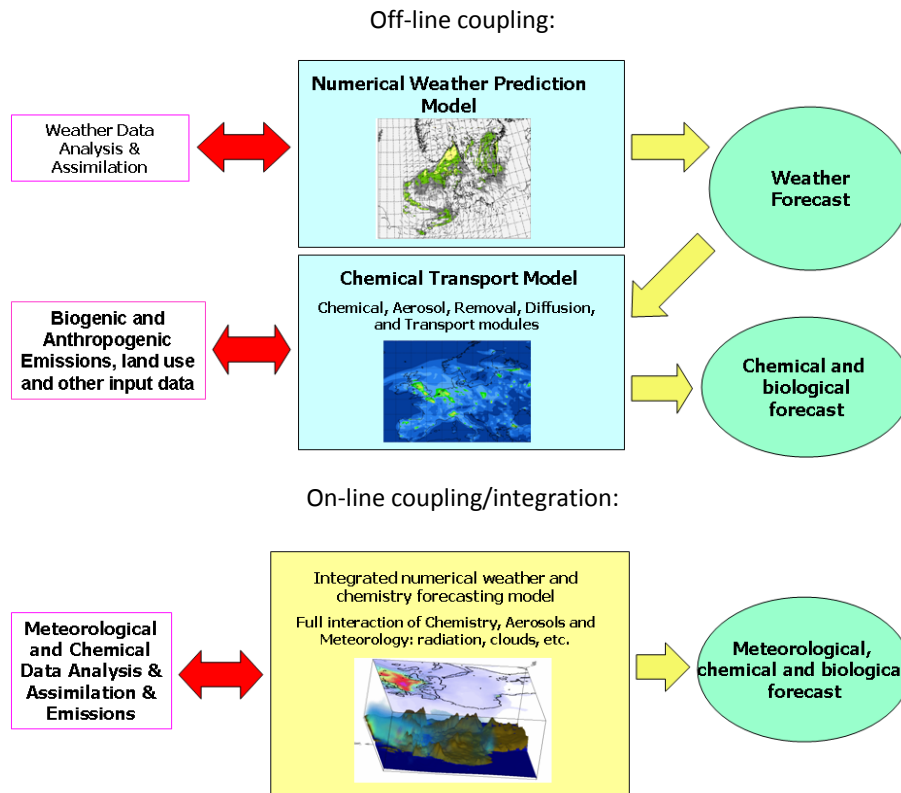


**Table 13.** The CWF models that include adjoint modelling, and the classification of the method and references.

Model	Method	References
CAMx	Direct Decoupled Method, Tangent Linear Model	Dunker et al. (2002), Kioutsioukis et al. (2005)
CHIMERE	Adjoint Model	Vautard et al. (2000), Menut (2003)
CMAQ	Adjoint Model	Hakami et al. (2007)
EURAD-RIU	Adjoint model	Elbern et al. (2000)
HIRLAM	Adjoint Model	Gustafsson and Huang (1996)
MOCAGE	Adjoint Model (transport) + Tangent Linear (chemistry)	Geer et al. (2006), Barret et al. (2008)
SILAM	Adjoint Model	Sofiev et al. (2006c)

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**Fig. 1.** Schematic diagram of the off-line and on-line coupled NWP and CTM modelling approaches for CWF.

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